Monograph Series on
Nonlinear Science and Complexity
EDITORS: A.C.J. LUO AND G. ZASLAVSKY

Volume 7

Quantum Mechanics of Non-Hamiltonian and Dissipative Systems

VASILY E. TARASOV

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MONOGRAPH SERIES ON NONLINEAR SCIENCE AND COMPLEXITY

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Elsevier
Radarweg 29, PO Box 211, 1000 AE Amsterdam, The Netherlands
The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, UK

First edition 2008

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Library of Congress Cataloging-in-Publication Data
A catalog record for this book is available from the Library of Congress

British Library Cataloguing in Publication Data
A catalogue record for this book is available from the British Library

ISBN: 978-0-444-53091-2
ISSN: 1574-6917

For information on all Elsevier publications
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Printed and bound in The Netherlands

06 07 08 09 10 10 9 8 7 6 5 4 3 2 1

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Preface

This book is the expanded version of lectures on quantum mechanics, which author read for students of the graduate level and which have been published in Russian. The main attention is given to the consecutive and consistent description of foundations of modern quantum mechanics. Difference of the suggested book from others is consistent use of the functional analysis and operator algebras. To read the text, preliminary knowledge of these sections of mathematics is not required. All the necessary information, which is beyond usual courses of the mathematical analysis and linear algebra, is included.

To describe the theory, we use the fact that quantum and classical mechanics are connected not only by limiting transition, but also realized by identical mathematical structures. A common basis to formulate the theory is an assumption that classical and quantum mechanics are different representations of the same totality of mathematical structures, i.e., the so-called Dirac correspondence principle. For construction of quantum theory, we consider mathematical concepts that are the general for Hamiltonian and non-Hamiltonian systems. Quantum dynamics is described by the one-parameter semi-groups and the differential equations on operator spaces and algebras. The Lie–Jordan algebraic structure, Liouville space and superoperators are used. It allows not only to consistently formulate the evolution of quantum systems, but also to consider the dynamics of a wide class of quantum systems, such as the open, non-Hamiltonian, dissipative, and nonlinear systems. Hamiltonian systems in pure states are considered as special cases of quantum dynamical systems.

The closed, isolated and Hamiltonian systems are idealizations that are not observable and therefore do not exist in the real world. As a rule, any system is always embedded in some environment and therefore it is never really closed or isolated. Frequently, the relevant environment is in principle unobservable or is unknown. This would render the theory of non-Hamiltonian and dissipative quantum systems to a fundamental generalization of quantum mechanics. The quantum theory of Hamiltonian systems, unitary evolution, and pure states should be considered as special cases of the generalized approach.

Usually the quantum mechanics is considered as generalization of classical mechanics. In this book the quantum mechanics is formulated as a generalization of modern nonlinear dynamics of dissipative and non-Hamiltonian systems. The quantization of equations of motion for dissipative and non-Hamiltonian classical systems is formulated in this book. This quantization procedure allows one to derive quantum analogs of equations with regular and strange attractors. The regular

attractors are considered as stationary states of non-Hamiltonian and dissipative quantum systems. In the book, the quantum analogs of the classical systems with strange attractors, such as Lorenz and Rössler systems, are suggested. In the text, the main attention is devoted to non-Hamiltonian and dissipative systems that have the wide possibility to demonstrate the complexity, chaos and self-organization.

The text is self-contained and can be used without introductory courses in quantum mechanics and modern mathematics. All the necessary information, which is beyond undergraduate courses of the mathematics, is presented in the book. Therefore this book can be used in the courses for graduate students. In the book the modern structure of the quantum theory and new fundamental results of last years are described. Some of these results are not considered in monographs and text books. Therefore the book is supposed to be useful for physicists and mathematicians who are interested in the modern quantum theory, nonlinear dynamics, quantization and chaos.

The book consists of two interconnected parts. The first part is devoted to the quantum kinematics that defines the properties of quantum observable, states and expectation values. In the second part, we consider the quantum dynamics that describes the time evolution of the observables and states.

Quantum mechanics has its mathematical language. It consists of the operator algebras, functional analysis, theory of one-parameter semi-groups and operator differential equations. Although we can have some sort of understanding of quantum mechanics without knowing its mathematical language, the precise and deep meaning of the physical notions cannot be obtained without using operator algebras, functional analysis, etc. Many theorems of operator algebra and functional analysis, etc. are easy to understand and use, although their proofs may be quite technical and time-consuming to present. Therefore we explain the meaning and significance of the theorems and ask reader to use them without proof.

The author is greatly indebted to Professor George M. Zaslavsky for his invaluable suggestions and comments. Thanks are expressed also to Edward E. Boos, Vyacheslav A. Ilin, Victor I. Savrin, Igor V. Volovich, colleagues of THEP division, and my family for their help and invaluable support during the work on the book. Finally, the author wishes to express his appreciation to Elsevier for the publication of this book.

Vasily E. Tarasov
Moscow
September 2007

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A Very Few Preliminaries

To motivate the introduction of the basic concepts of the theory of non-Hamiltonian and dissipative systems, we begin with some definitions.

1. Potential and conservative systems

Suppose that a classical system, whose position is determined by a vector $\mathbf{x}$ in a region $\mathcal{M}$ of n-dimensional phase-space $\mathbb{R}^n$, moves in a field $\mathbf{F}(\mathbf{x})$. The motion of the system is described by the equation

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}(\mathbf{x}). \tag{1}$$

Let us give the basic definitions regarding this system.

(1) If the vector field $\mathbf{F}(\mathbf{x})$ satisfies the condition

$$curl\, \mathbf{F}(\mathbf{x}) = 0$$

for all $\mathbf{x} \in \mathcal{M}$, then the system is called *potential*, or *locally potential*. The field $\mathbf{F}(\mathbf{x})$ is called irrotational.

(2) If there is a unique single-valued function $H = H(\mathbf{x})$ for all $x \in \mathcal{M}$ such that

$$\mathbf{F}(\mathbf{x}) = grad\, H(\mathbf{x}),$$

then the system is *gradient*, or *globally potential*.

The globally potential system is locally potential. The converse statement does not hold in general. It is well known that a locally potential system with the field $\mathbf{F} = (-y/r^2)\mathbf{e}_1 + (x/r^2)\mathbf{e}_2$, where $r^2 = x^2 + y^2$ in the region $\mathcal{M} = \{(x, y) \in \mathbb{R}^2\colon (x, y) \neq (0, 0)\}$ is not globally potential.

(3) If there are $\mathbf{x} \in \mathcal{M} \subset \mathbb{R}^n$ such that

$$curl\, \mathbf{F}(\mathbf{x}) \neq 0,$$

then the system is called *nonpotential*.

(4) If we have the condition

$$div\, \mathbf{F}(\mathbf{x}) = 0$$

for all $\mathbf{x} \in \mathcal{M}$, then the system is called *nondissipative*. The vector field $\mathbf{F}(\mathbf{x})$ is called solenoidal.

2. Hamiltonian and non-Hamiltonian classical systems

Let $\mathcal{M}$ be a symplectic manifold and let $\mathbf{x} = (q, p)$.

(1) The locally potential system on $\mathcal{M}$ is called *locally Hamiltonian*.
(2) The globally potential system on $\mathcal{M}$ is called *globally Hamiltonian*.
(3) The nonpotential system on $\mathcal{M}$ is called *non-Hamiltonian*.
(4) If $div\,\mathbf{F}(\mathbf{x}) \neq 0$ for some $\mathbf{x} \in \mathcal{M}$, then the system is called *generalized dissipative*.

3. Examples of non-Hamiltonian systems

Suppose that a classical system, whose position and momentum are described by vectors $q = (q_1, \ldots, q_n)$ and $p = (p_1, \ldots, p_n)$, moves in the force field $F(q, p) = (F_1, \ldots, F_n)$. The motion of the system is defined by the equations

$$\frac{dq_k}{dt} = \frac{\partial H(q, p)}{\partial p_k}, \qquad \frac{dp_k}{dt} = -\frac{\partial H(q, p)}{\partial q_k} + F_k(q, p). \tag{2}$$

The Hamiltonian function $H(q, p) = p^2/2m + U(q)$ gives the Newton's equations

$$\frac{d^2q_k}{dt^2} = -\frac{\partial U(q)}{\partial q_k} + F_k(q, mv),$$

where $v = dq/dt$. If the conditions

$$\frac{\partial F_k(q, p)}{\partial p_l} = 0, \qquad \frac{\partial F_k(q, p)}{\partial q_l} - \frac{\partial F_l(q, p)}{\partial q_l} = 0 \tag{3}$$

hold for all q, p, then equations (2) describe a classical Hamiltonian system. If these conditions are not satisfied, then (2) is a non-Hamiltonian system. If

$$\Omega(q, p) = \sum_{k=1}^{n} \frac{\partial F_k(q, p)}{\partial p_k} \neq 0,$$

then we have a generalized dissipative system. For example, the force field

$$F_k(q, p) = \sum_{l=1}^{n} a_{kl} p_l + \sum_{l,s=1}^{n} b_{kls} p_l p_s \tag{4}$$

describes non-Hamiltonian system.

Suppose that $H(q, p) = p^2/2m$ and $F_k(q, p)$ is defined by (4). Using the variables $x = p_1$, $y = p_2$, $z = p_3$, we can obtain the well-known Lorenz and Rössler systems in the space of $(x, y, z) \in \mathbb{R}^3$. The field

$$F_1 = -\sigma x + \sigma y, \qquad F_2 = rx - y - xz, \qquad F_3 = -bz + xy,$$

gives the Lorenz equations [100]. All $\sigma, r, b > 0$, but usually $\sigma = 10$, $b = 8/3$ and r is varied. This system exhibits chaotic behavior for $r = 28$. The field

$$F_1 = -y - z, \qquad F_2 = x + ay, \qquad F_3 = b + cz - zx$$

defines the Rössler system [128]. Rössler studied the chaotic attractor with $a = 0.2$, $b = 0.2$, and $c = 5.7$. These Lorenz and Rössler systems defined by equations (2) and (4) are non-Hamiltonian and dissipative. The systems demonstrate a chaotic behavior for some values of parameters.

4. Non-Hamiltonian and dissipative classical systems

Let $A = A(\mathbf{x})$ be a smooth function on $\mathcal{M}$. Equation (1) gives

$$\frac{d}{dt}A = (\mathbf{F}, \mathit{grad}\, A), \tag{5}$$

where the brackets is a scalar product. We can define the operator $\mathcal{L} = (\mathbf{F}, \nabla_{\mathbf{x}})$, where $\nabla_{\mathbf{x}}$ is the nabla operator.

(1) For globally Hamiltonian systems, $\mathcal{L}$ is an inner derivation operator, i.e., there is $H \in \mathcal{M}$ such that

$$\mathcal{L} = \{H, \cdot\}, \tag{6}$$

where $\{\ ,\ \}$ is a Poisson bracket, and H is a unique single-valued function on $\mathcal{M}$.

(2) A locally Hamiltonian system is characterized by the conditions

$$Z_{\mathcal{L}}(A, B) = \mathcal{L}(AB) - (\mathcal{L}A)B - A(\mathcal{L}B) = 0, \tag{7}$$

$$J_{\mathcal{L}}(A, B) = \mathcal{L}\big(\{A, B\}\big) - \{\mathcal{L}A, B\} - \{A, \mathcal{L}B\} = 0 \tag{8}$$

for all real-valued smooth functions $A = A(\mathbf{x})$ and $B = B(\mathbf{x})$ on $\mathcal{M}$. Equations (7) and (8) can be used as a definition of locally Hamiltonian systems.

These equations mean that $\mathcal{L}$ is a derivation operator. In general, the derivation operator is not inner. For example, every derivation $\mathcal{L}$ of polynomial A in real variables q, p can be presented in the form

$$\mathcal{L}A = \{H, A\} + b\left(A - ap\frac{\partial A}{\partial p} - (1 - a)q\frac{\partial A}{\partial q}\right),$$

where a, b are numbers. Thus every derivation of polynomial is a sum of an inner derivation $\{H, A\}$ and an explicitly determined outer derivation. (However this decomposition is not unique.) As a result, locally Hamiltonian system is not equivalent to globally Hamiltonian.

(3) For non-Hamiltonian systems, there exist functions $A(\mathbf{x})$ and $B(\mathbf{x})$ and points $\mathbf{x}$, such that equations (6) and (7) are not satisfied. We can use this property as a definition of classical non-Hamiltonian systems.

(4) A generalized dissipative classical system is characterized by the condition

$$\Omega(q, p) = -\sum_{k=1}^{m} J_{\mathcal{L}}(q_k, p_k) \neq 0.$$

The function $\Omega(q, p)$ is a phase space compressibility. It is not hard to see that the generalized dissipative system is non-Hamiltonian. The converse statement does not hold in general.

5. Non-Hamiltonian and dissipative quantum systems

Let us consider a quantum system, whose coordinates and momenta are determined by operators Q_k and P_k, $k = 1, \ldots, n$. The motion of the system is described by the operator differential equation

$$\frac{d}{dt}A(t) = \mathcal{L}A(t) \tag{9}$$

under a variety of conditions and assumptions. In each example the operator $A = A(0)$ corresponds to an observable, or state, of the quantum system and will be represented by an element of some suitable operator space, or algebra, $\mathcal{M}$. The map $t \in \mathbb{R} \to A(t) \in \mathcal{M}$ describes the motion of A, and $\mathcal{L}$ is a superoperator on $\mathcal{M}$, which generates the infinitesimal change of A. In other words, a superoperator $\mathcal{L}$ is a rule that assigns to each operator A exactly one operator $\mathcal{L}(A)$. The dynamics is given by solution of the operator differential equation.

Let us give the basic definitions regarding the quantum system described by (9).

(1) For *globally Hamiltonian quantum systems*, $\mathcal{L}$ is an inner derivation operator, i.e., there is $H \in \mathcal{M}$ such that

$$\mathcal{L}(A) = \frac{1}{i\hbar}[H, A],$$

for all $A \in \mathcal{M}$, where $[\ ,\ ]$ is a commutator on $\mathcal{M}$.

(2) A *locally Hamiltonian quantum system* is characterized by the conditions

$$\begin{aligned} Z_{\mathcal{L}}(A, B) &= \mathcal{L}(AB) - (\mathcal{L}A)B - A(\mathcal{L}B) = 0, \\ J_{\mathcal{L}}[A, B] &= \mathcal{L}\big([A, B]\big) - [\mathcal{L}A, B] - [A, \mathcal{L}B] = 0, \end{aligned} \tag{10}$$

where A, B are self-adjoint operators. These equations mean that $\mathcal{L}$ is a derivation superoperator.

(3) For *non-Hamiltonian quantum systems*, there exist operators A and B such that conditions (10) are not satisfied.

(4) A *generalized dissipative quantum system* is characterized by

$$\Omega(Q, P) = -\frac{1}{i\hbar}\sum_{k=1}^{n} J_{\mathcal{L}}[Q_k, P_k] \neq 0.$$

Then, generalized dissipative systems are non-Hamiltonian.

6. Quantization of non-Hamiltonian and dissipative systems

Suppose that a classical system is described by the equation

$$\frac{d}{dt}A_t(q,\,p) = \mathcal{L}[q,\,p,\,\partial_q,\,\partial_p]A_t(q,\,p) \tag{11}$$

under a variety of conditions and assumptions. In each instance the real-valued function A_0 corresponds to an observable, or state, of the classical system. If the conditions (7) and (8) are not valid for $\mathcal{L} = \mathcal{L}[q,\,p,\,\partial_q,\,\partial_p]$, then the classical system is non-Hamiltonian.

Quantization is usually understood as a procedure, where any classical observable, i.e., a real-valued function $A(q,\,p)$, is associated with a relevant quantum observable, i.e., a self-adjoint operator $A(Q,\,P)$.

Let us define the operators L_A^- and L_A^+ acting on classical observables by the formulas

$$L_A^- B(q,\,p) = \big\{A(q,\,p),\,B(q,\,p)\big\}, \qquad L_A^+ B(q,\,p) = A(q,\,p)B(q,\,p).$$

From these definitions, we get

$$L_{q^k}^+ A(q,\,p) = q^k A(q,\,p), \qquad L_{p^k}^+ A(q,\,p) = p^k A(q,\,p), \tag{12}$$

and

$$L_{q^k}^- A(q,\,p) = \frac{\partial A(q,\,p)}{\partial p^k}, \qquad L_{p^k}^- A(q,\,p) = -\frac{\partial A(q,\,p)}{\partial q^k}. \tag{13}$$

Then the operator $\mathcal{L}[q,\,p,\,\partial_q,\,\partial_p]$, will be presented by

$$\mathcal{L}[q,\,p,\,\partial_q,\,\partial_p] = \mathcal{L}\big[L_q^+,\,L_p^+,\,-L_p^-,\,L_q^-\big].$$

Using the operators L_A^+ and L_A^-, which act on quantum observables and defined by

$$L_A^-\hat{B} = \frac{1}{i\hbar}\big(\hat{A}\hat{B} - \hat{B}\hat{A}\big), \qquad L_A^+\hat{B} = \frac{1}{2}\big(\hat{A}\hat{B} + \hat{B}\hat{A}\big),$$

the Weyl quantization π_W is defined by

$$\pi_W\big(L_{q^k}^+ A\big) = L_{Q^k}^+\hat{A}, \qquad \pi_W\big(L_{q^k}^- A\big) = L_{Q^k}^-\hat{A},$$
$$\pi_W\big(L_{p^k}^+ A\big) = L_{P^k}^+\hat{A}, \qquad \pi_W\big(L_{p^k}^- A\big) = L_{P^k}^-\hat{A}$$

for any $\hat{A} = A(Q,\,P) = \pi_W(A(q,\,p))$, where $Q_k = \pi_W(q_k)$, and $P_k = \pi_W(p_k)$.

Since these relations are valid for any $\hat{A} = \pi_W(A)$, we can define the quantization of operators $L^{\pm}_{q^k}$ and $L^{\pm}_{p^k}$ by the equations

$$\pi_W\big(L^+_{q^k}\big) = L^+_{Q^k}, \qquad \pi_W\big(L^-_{q^k}\big) = L^{\pm}_{Q^k},$$
$$\pi_W\big(L^+_{p^k}\big) = L^+_{P^k}, \qquad \pi_W\big(L^-_{p^k}\big) = L^-_{P^k}.$$

These relations define the Weyl quantization of the operator $\mathcal{L}[q, p, \partial_q, \partial_p]$.

The Weyl quantization π_W for the classical system (11) is defined by the formula

$$\pi_W\big(\mathcal{L}[q, p, \partial_q, \partial_p]\big) = \mathcal{L}\big[L^+_Q, L^+_P, -L^-_P, L^-_Q\big].$$

Note that the commutation relations for the operators $L^{\pm}_{q^k}$, $L^{\pm}_{p^k}$ and $L^{\pm}_{Q^k}$, $L^{\pm}_{P^k}$ coincide. Then the ordering of $L^{\pm}_{P^k}$ and $L^{\pm}_{Q^k}$ in the superoperator $\mathcal{L}[L^+_Q, L^+_P, -L^-_P, L^-_Q]$ is uniquely determined by ordering in $\mathcal{L}[L^+_q, L^+_p, -L^-_p, L^-_q]$.

As a result, the quantization of (11) gives the operator equation

$$\frac{d}{dt}A_t(Q, P) = \mathcal{L}\big[L^+_Q, L^+_P, -L^-_P, L^-_Q\big]A_t(Q, P).$$

If the classical system (11) is non-Hamiltonian, then the quantum system are also non-Hamiltonian.

We may also say that the quantization is realized by the replacement

$$q^k \longrightarrow L^+_{Q_k}, \qquad p^k \longrightarrow L^+_{P_k},$$
$$\frac{\partial}{\partial p^k} \longrightarrow L^-_{P_k}, \qquad \frac{\partial}{\partial q^k} \longrightarrow -L^-_{Q_k}.$$

We illustrate this technique with a simple example. The equations of motion

$$\frac{dp}{dt} = \frac{p}{m}, \qquad \frac{dq}{dt} = -\frac{m\omega^2}{2}q - \gamma p$$

describe a damped harmonic oscillator. For $A(q, p)$, we have

$$\frac{d}{dt}A_t(q, p) = \frac{p}{m}\partial_q A_t(q, p) + \left(-\frac{m\omega^2}{2}q - \gamma p\right)\partial_p A_t(q, p).$$

The quantization gives

$$\frac{d}{dt}A_t(Q, P) = -\frac{1}{m}L^+_P L^-_P A_t(Q, P) + \left(-\frac{m\omega^2}{2}L^+_Q - \gamma L^+_P\right)L^-_Q A_t(Q, P),$$

where $\hat{A}_t = A(Q, P) = \pi_W(A(q, p))$ is a quantum observable. As a result, we obtain

$$\frac{d}{dt}\hat{A}_t = \frac{i}{2m\hbar}\big[P^2 + m^2\omega^2 Q^2, \hat{A}_t\big] + \frac{i\gamma}{2\hbar}\big(P\big[Q, \hat{A}_t\big] + \big[Q, \hat{A}_t\big]P\big).$$

This is the equation for quantum damped oscillator. The Weyl quantization of classical dissipative Lorenz-type system can also be realized [162,163].

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PART I

QUANTUM KINEMATICS

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Chapter 1

Quantum Kinematics of Bounded Observables

1.1. Observables and states

Physical theories consist essentially of two interconnected structures, a kinematical structure describing the instantaneous states and observables of a system, and a dynamical structure describing the time evolution of these states and observables. In the quantum mechanics observables and states are represented by operators on a Hilbert space.

(a) The *observables* of a quantum system are described by the self-adjoint linear operators on some separable Hilbert space.
(b) The *states* of the quantum system are identified with the positive self-adjoint linear operator with unit trace.

As a result, to formulate quantum kinematics, the mathematical language of operator algebras must be used. Before we start to study the mathematical structures that are considered on sets of quantum observables and states, we should describe a Hilbert space $\mathcal{H}$ and operators on $\mathcal{H}$.

1.2. Pre-Hilbert and Hilbert spaces

A Hilbert space generalizes the notion of the Euclidean space $\mathbb{R}^n$ with a scalar product. In a Hilbert space, the elements are abstractions of usual vectors, whose nature is unimportant (they may be, for example, sequences or functions).

DEFINITION. A *linear space* (or *vector space*) over $\mathbb{C}$ is a set $\mathcal{H}$, together with two following operations:

(1) An addition of elements of $\mathcal{H}$ such that
   (a) $x + y = y + x$ for all $x, y \in \mathcal{H}$.
   (b) $(x + y) + z = x + (y + z)$ for all $x, y, z \in \mathcal{H}$.
   (c) $0 + x = x + 0 = x$ for all $x \in \mathcal{H}$.
(2) A multiplication of each element of $\mathcal{M}$ by a complex number such that

(a) $a(bx) = (ab)x$ for all $x \in \mathcal{H}$, and $a, b \in \mathbb{C}$.
(b) $(a + b)x = ax + bx$ for all $x \in \mathcal{H}$, and $a, b \in \mathbb{C}$.
(c) $a(x + y) = ax + ay$ for all $x, y \in \mathcal{H}$, and $a \in \mathbb{C}$.
(d) $1x = x$ and $0x = 0$ for all $x \in \mathcal{H}$.

The most familiar linear spaces over $\mathbb{R}$ are two and three-dimensional Euclidean spaces. In physics, the mathematical notions have physical interpretations. For example, the elements of the linear space $\mathcal{H}$ can be mathematical images of pure states.

DEFINITION. A *scalar product* in a linear space $\mathcal{H}$ is a complex-valued numerical function (x, y) of arguments $x, y \in \mathcal{H}$ satisfying the axioms:

(1) $(x + y, z) = (x, z) + (y, z)$ for all $x, y, z \in \mathcal{H}$.
(2) $(x, ay) = a(x, y)$ and $(ax, y) = a^*(x, y)$ for all $x, y \in \mathcal{H}$, $a \in \mathbb{C}$, where $*$ denotes complex conjugation.
(3) $(x, y) = (y, x)^*$ for all $x, y \in \mathcal{H}$.
(4) $(x, x) > 0$ for $x \neq 0$, and $(x, x) = 0$ if and only if $x = 0$.

A scalar product is also called an inner product. Scalar products allow the rigorous definition of intuitive notions such as the angle between vectors and orthogonality of vectors in linear spaces of all dimensions. A linear space, together with a scalar product is called the pre-Hilbert space.

DEFINITION. A *pre-Hilbert space* is a set $\mathcal{H}$, such that the following conditions are satisfied:

(1) $\mathcal{H}$ is a linear space.
(2) A scalar product exists to each pairs of elements x, y of $\mathcal{H}$.

A pre-Hilbert space is also called an inner product space.

DEFINITION. Suppose $\mathcal{H}$ is a linear space and x is in $\mathcal{H}$. A *seminorm* of $x \in \mathcal{H}$ is a nonnegative real number $\|x\|_{\mathcal{H}}$, such that the following conditions are satisfied:

(1) $\|x + y\|_{\mathcal{H}} \leqslant \|x\|_{\mathcal{H}} + \|y\|_{\mathcal{H}}$ for all $x, y \in \mathcal{H}$ (triangle inequality).
(2) $\|ax\|_{\mathcal{H}} = |a|\|x\|_{\mathcal{H}}$ for all $x \in \mathcal{H}$, and $a \in \mathbb{C}$ (homogeneity).
(3) $\|x\|_{\mathcal{H}} \geqslant 0$ for all $x \in \mathcal{H}$ (nonnegativity).

A *norm* of $x \in \mathcal{H}$ is a seminorm $\|x\|_{\mathcal{H}}$ such that $\|x\|_{\mathcal{H}} = 0$ if and only if $x = 0$.

A norm generalizes the notion of the length of vector. Each norm can be considered as a function that assigns a positive number to a non-zero element of a linear space. A seminorm is allowed to assign zero value to some non-zero elements. A linear space with a norm is called a normed linear space.

DEFINITION. A *normed space* is a linear space $\mathcal{H}$ over $\mathbb{C}$, if there is a norm for each element of $\mathcal{H}$.

A seminormed space is a pair $<\mathcal{H}, \| \|_{\mathcal{H}}>$, where $\mathcal{H}$ is a linear space, and $\| \|_{\mathcal{H}}$ is a seminorm on $\mathcal{H}$. A normed space is a linear space $\mathcal{H}$, together with a norm $\| \|_{\mathcal{H}}$. In general, a given space $\mathcal{H}$ can be made into a normed space in different ways by using different norms. We can denote the normed space by $<\mathcal{H}, \| \|_{\mathcal{H}}>$.

We will often need a notion of distance (called a metric) between elements of the set. It is reasonable to define a notion of metric that has the most important properties of ordinary distance in $\mathbb{R}^n$.

DEFINITION. A *metric space* is a set $\mathcal{H}$, together with a real-valued function $d(\ ,\ )$ on $\mathcal{H} \times \mathcal{H}$, such that the following conditions are satisfied:

(1) $d(x, y) \geqslant 0$ for all $x, y \in \mathcal{H}$ (nonnegativity condition).
(2) $d(x, y) = 0$, if and only if $x = y$.
(3) $d(x, y) = d(y, x)$ for all $x, y \in \mathcal{H}$ (symmetry condition).
(4) $d(x, z) \leqslant d(x, y) + d(y, z)$ for all $x, y, z \in \mathcal{H}$ (triangle inequality).

The function $d(\ ,\ )$ is called the *metric* on $\mathcal{H}$.

We denote by $\mathcal{H}_1 \times \mathcal{H}_2$ the set of all ordered pairs of elements x, y, where $x \in \mathcal{H}_1$ and $y \in \mathcal{H}_2$. The set $\mathcal{H}_1 \times \mathcal{H}_2$ will be called the *direct product* of $\mathcal{H}_1$ and $\mathcal{H}_2$.

Any normed space is a metric space with the metric

$$d(x, y) = \|x - y\|_{\mathcal{H}}.$$

A pre-Hilbert space $\mathcal{H}$ is a normed linear space with the norm

$$\|x\|_{\mathcal{H}} = \sqrt{(x, x)}.$$

Then, the pre-Hilbert space $\mathcal{H}$ is a metric space with the metric

$$d(x, y) = \sqrt{(x - y, x - y)}.$$

The metric and norm allow us to define a topology, i.e., a certain convergence of infinite sequences of space elements. Convergence describes limiting behavior, particularly of an infinite sequence toward some limit.

DEFINITION. A sequence $\{x_k\colon\ k \in \mathbb{N}\}$ of elements in a normed space $\mathcal{H}$ is said to be *convergent* to an element $x \in \mathcal{H}$ if

$$\lim_{k \to \infty} \|x_k - x\|_{\mathcal{H}} = 0. \tag{1}$$

The element x is called the *limit point*.

DEFINITION. A *fundamental sequence* (or *Cauchy sequence*) is a sequence of elements x_k of a normed space $\mathcal{H}$ if

$$\lim_{k,l\to\infty} \|x_k - x_l\|_{\mathcal{H}} = 0. \tag{2}$$

Using the triangle inequality, it is easy to see that a convergent sequence $\{x_k\}$ in $\mathcal{H}$ satisfies condition (2). As a result, we have the following theorem.

THEOREM. *Let $\mathcal{H}$ be a normed space and let $\{x_k\}$ be a sequence of elements in $\mathcal{H}$. If $\{x_k\}$ converges to an element $x \in \mathcal{H}$, then $\{x_k\}$ is a fundamental sequence.*

Although every convergent sequence is a fundamental sequence, the converse statement need not be true. In general, a fundamental sequence of a normed space $\mathcal{H}$ is not convergent to an element of $\mathcal{H}$. We now define a space such that the converse statement is true. A normed linear space is said to be complete if and only if all Cauchy sequences are convergent.

DEFINITION. A *complete space* is a normed space in which all fundamental sequences convergent, and its limit points belong to this space.

For example, $\mathbb{R}$ is complete, but $\mathbb{Q}$ is not. Here $\mathbb{Q}$ is a linear space of all rational numbers with the usual norm $\|x\| = |x|$. A complete normed space is called the Banach space.

DEFINITION. A *Banach space* is a normed space $\mathcal{H}$, such that each fundamental sequence $\{x_k\} \in \mathcal{H}$ converges to an element of $\mathcal{H}$, i.e., if we have (2) for all $\{x_k\colon k \in \mathbb{N}\} \subset \mathcal{H}$, then there exists $x \in \mathcal{H}$, such that (1) holds.

A complete pre-Hilbert space is a Hilbert space.

DEFINITION. A *Hilbert space* is a set $\mathcal{H}$ such that the following requirements are satisfied:

(1) $\mathcal{H}$ is a linear space.
(2) A scalar product exists to each pairs of elements x, y of $\mathcal{H}$.
(3) $\mathcal{H}$ is a Banach space.

A Hilbert space $\mathcal{H}$ is a Banach space with the norm $\|x\|_{\mathcal{H}} = \sqrt{(x,x)_{\mathcal{H}}}$. In general, the norm does not arise from a scalar product, so Banach spaces are not necessarily Hilbert spaces and will not have all of the same geometrical properties.

PARALLELOGRAM THEOREM. *A Banach space $\mathcal{H}$ is a Hilbert space if and only if the norm $\| \ \|_{\mathcal{H}}$ of $\mathcal{H}$ satisfies the parallelogram identity*

$$\|x+y\|_{\mathcal{H}}^2 + \|x-y\|_{\mathcal{H}}^2 = 2\|x\|_{\mathcal{H}}^2 + 2\|y\|_{\mathcal{H}}^2 \tag{3}$$

for all $x, y \in \mathcal{H}$.

If the parallelogram identity is satisfied for all elements of a Banach space $\mathcal{H}$, then it is possible to define a scalar product by the norm $\| \ \|_{\mathcal{H}}$. The associated scalar product, which makes $\mathcal{H}$ into a Hilbert space, is given by the polarization identity:

$$(x, y) = \frac{1}{4}\sum_{s=0}^{3} i^s \left\|x + i^s y\right\|_{\mathcal{H}}^2. \tag{4}$$

This function (x, y) satisfies the axioms of scalar product if and only if requirement (3) holds.

The scalar product makes it possible to introduce into $\mathcal{H}$ the concept of the orthogonality. The elements x and y of a Hilbert space $\mathcal{H}$ are called orthogonal if $(x, y) = 0$. If the elements x and y are orthogonal, then the equality

$$\|x+y\|_{\mathcal{H}}^2 = \|x\|_{\mathcal{H}}^2 + \|y\|_{\mathcal{H}}^2$$

is easily verified. This is the Pythagorean theorem.

Hilbert spaces arise in quantum mechanics as some function and sequence spaces. The following are examples of some Hilbert spaces.

(1) *Euclidean space*. The simplest example of a Hilbert space is the finite-dimensional linear space $\mathbb{C}^n$ (or $\mathbb{R}^n$) with the scalar product

$$(x, y) = \sum_{k=1}^{n} x_k^* y_k.$$

(2) *Sequence space*. Consider the infinite-dimensional space l_2, whose elements are sequences of complex numbers x_k such that

$$\sum_{k=1}^{\infty} |x_k|^2 < \infty.$$

We introduce a scalar product of the elements $\{x_k\}$ and $\{y_k\}$ of this space by the equation

$$\big(\{x_k\}, \{y_k\}\big) = \sum_{k=1}^{\infty} x_k^* y_k.$$

(3) *Lebesgue space*. Consider the space $L^2[a, b]$ of square-integrable complex-valued functions $\Psi(x)$ on the closed interval $[a, b]$. If $\Psi(x) \in L^2[a, b]$, then

$$\int_a^b \left|\Psi(x)\right|^2 dx < \infty.$$

The scalar product in this space is defined by

$$(\Psi_1, \Psi_2) = \int_a^b dx\, \Psi_1^*(x)\Psi_2(x).$$

1.3. Separable Hilbert space

In this section, we extend the idea of "basis" from finite-dimensional linear spaces to Hilbert spaces. In quantum mechanics, we would like to use a Hilbert space, in which every element has an expansion over the countable basis.

Two elements, x and y, in a Hilbert space $\mathcal{H}$ are said to be orthogonal if $(x, y) = 0$. These elements is called orthonormal if $(x, x) = (y, y) = 1$ and $(x, y) = 0$.

DEFINITION. A *orthonormal system* in a Hilbert space $\mathcal{H}$ is a set of elements $e_a \in \mathcal{H}$, $a \in R$, such that the following conditions are satisfied:

(1) $(e_a, e_a) = 1$ for all $a \in R$.
(2) $(e_a, e_b) = 0$ for $a \neq b$.

Here, R is a set of indices. In general, this set is not countable.

Let $\mathcal{H}$ be a linear space over $\mathbb{C}$. The elements in a subset $S = \{e_a\colon\ a \in R\}$ of $\mathcal{H}$ *generate* the whole $\mathcal{H}$ if for every $x \in \mathcal{H}$, we have

$$x = \sum_{a \in R} x_a e_a \tag{5}$$

for some $x_a \in \mathbb{C}$. In this case, the element x is a linear combination of e_a and $\mathcal{H}$ is a linear span. The elements in the subset $S = \{e_a\colon\ a \in R\}$ of $\mathcal{H}$ are *linearly independent* if $\sum_{a \in R} x_a e_a = 0$ implies that all $x_a = 0$. If $\mathcal{H}$ is a linear space, the elements in a subset $S = \{e_a\colon\ a \in R\}$ of $\mathcal{H}$ form a *basis* if they generate $\mathcal{H}$ and e_a are linearly independent.

DEFINITION. A *complete orthonormal system* in a Hilbert space $\mathcal{H}$ is an orthonormal system $\{e_a\} \in \mathcal{H}$, $a \in R$, such that $(e_a, x) = 0$ for all $a \in R$ implies $x = 0$.

A *orthonormal basis* is a complete orthonormal system $\{e_a\colon\ a \in R\}$ in $\mathcal{H}$, such that each element $x \in \mathcal{H}$ can be presented as a unique linear combination of e_a by (5), where $x_a = (e_a, x)$.

The equality in (5) means that the sum on the right-hand side converges to x in $\mathcal{H}$. Every basis is a complete system. However, a complete system may not be a basis for the space.

In study of complete systems $\{e_k\}$ it is very important question whether a given system forms a basis of a separable space, i.e., whether any element x of the space can be presented by (5), and in only one way. Here x_k are numbers and the series converges in the norm of the space. Although bases have been constructed for all the basic separable Banach spaces, the question whether there exists a basis for an arbitrary separable Banach space happens to be complicated. A negative answer has been obtained by P. Enflo. In 1972 he constructed a reflexive separable Banach space having no basis.

Each Hilbert space has an orthonormal basis. In general, this basis is not a countable set. In quantum theory, it is important to have a countable basis.

DEFINITION. Let $\mathcal{H}$ be a Hilbert space. If there exists a countable complete system in $\mathcal{H}$, then the space $\mathcal{H}$ is called *separable*.

A Hilbert space is separable if and only if it has a countable orthonormal basis.

THEOREM. *If $\mathcal{H}$ is a separable Hilbert space, then each complete orthonormal system $\{e_k\}$ in $\mathcal{H}$ is a basis. Any element x of $\mathcal{H}$ can be represented in the form*

$$x = \sum_{k=1}^{\infty} x_k e_k, \quad x_k = (e_k, x), \tag{6}$$

and

$$\|x\|_{\mathcal{H}}^2 = \sum_{k=1}^{\infty} |x_k|^2 = \sum_{k=1}^{\infty} \big|(e_k, x)\big|^2 \leqslant \infty. \tag{7}$$

Equation (7) is called the *Parseval's identity*. The coefficients $x_k = (e_k, x) \in \mathbb{C}$ are often called the *Fourier coefficients* of x with respect to the basis e_k, and this representation of $x \in \mathcal{H}$ is called the *Fourier series*.

Inequality (7) gives that any infinite-dimensional separable Hilbert space is isomorphic to a space l_2. Two spaces are isomorphic if the spaces are identical except for the names of the elements and operations, i.e., if the spaces are structurally the same.

If $\mathcal{H}$ is a separable Hilbert space, then a complete orthonormal system is a basis. As a result, we have the following important property of separable Hilbert spaces:

There exists an isomorphism between separable Hilbert spaces. The isomorphism is a one-to-one correspondence that preserves the linear space operations and the scalar product. In the finite-dimensional case, we have the following statement.

THEOREM. *Each finite-dimensional* (*n-dimensional*) *separable Hilbert space over* $\mathbb{C}$ *is isomorphic to* $\mathbb{C}^n$.

Let us give the basic theorem regarding infinite-dimensional spaces.

THEOREM. *Any two infinite-dimensional separable Hilbert spaces are isomorphic to each other.*

Thus any two separable Hilbert spaces are isomorphic to (in one-to-one correspondence that preserves the linear space operation and the scalar product) the space l_2, and, consequently isomorphic to each other. If $\{x_k\colon\ k \in \mathbb{N}\}$ is arbitrary sequence of numbers x_k such that $\sum_{k=1}^{\infty} |x_k|^2 < \infty$, then the series $\sum_{k=1}^{\infty} x_k e_k$ converges in $\mathcal{H}$. If we denote the sum by x, then taking the scalar product of x with e_k, we shall have $x_k = (x, e_k)$. Hence there is a one-to-one correspondence between of sequences of numbers x_k the series of whose squared moduli converges, i.e., the space l_2, and the elements of the Hilbert space $\mathcal{H}$.

In particular the space $L_2[a, b]$ whose elements are square-integrable functions is a Hilbert space isomorphic to the space l_2. The space $L_2[a, b]$ is a complete space. It is obviously also separable. As a result, the space $L_2[a, b]$ and l_2 are isomorphic to each other and may be identified. These spaces can be considered as different realizations of an abstract infinite-dimensional separable Hilbert space $\mathcal{H}$. The isomorphism of $L^2[-\pi, \pi]$ and l_2 can be presented by the Fourier transform:

$$x_k = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} \Psi(x) e^{ikx}\, dx,$$

where $\Psi(x) \in L^2[-\pi, \pi]$, and $\{x_k\} \in l_2$.

1.4. Definition and examples of operators

A function can be presented as a "black box" that generates a number at the output in response to an number at the input.

DEFINITION. Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be linear spaces. We say that an *operator* A with values in $\mathcal{H}_2$ is defined on a set $D(A) \subset \mathcal{H}_1$ if to every element $x \in \mathcal{H}_1$ there corresponds an element $y = Ax \in \mathcal{H}_2$. The set $D(A)$ is called the *domain* of

the operator. The set of all elements y of $\mathcal{H}_2$, representable in the form $y = Ax$, $x \in D(A)$, is called the *range* of the operator and is denoted by $R(A)$.

For example, an operator may be pictured as a "black box" that generates a function at the output in response to a function at the input; it is said that an operator applied to a function generates a new function. The operator squaring: $A\Psi(x) = \Psi(x)^2$ is an example of an operator on the space $L^2[0, 1]$. The entire space $L^2[0, 1]$ serve as the domain of this operator. The set of all non-negative functions of $L^2[0, 1]$ is its range.

DEFINITION. A *linear operator* is a map A from a linear space $\mathcal{H}_1$ into a linear space $\mathcal{H}_2$, such that $A(ax + by) = aAx + bAy$ for all $x, y \in D(A) \subset \mathcal{H}_1$ and $a, b \in \mathbb{C}$.

The operator of differentiation, $A\Psi(x) = d\Psi(x)/dx$, is an example of a linear operator. The operator squaring is not linear.

As emphasized in the definition, an operator is not simply a formal operating rule. Two operators, which act in the same way, must be considered as different if they are not defined on the same subspace of a Hilbert space. A typical example for this situation is given by a physical problem on a compact or semi-infinite interval. In this case, the domain of operators includes some boundary conditions whose choice depends on the experimental device. In general, two non equivalent devices for the measurement of a given observable lead to different experimental results. Therefore it is important to consider as different two operators that act in the same way, but admit different domains of definition. Thus, strictly speaking, a Hilbert space operator is a triple $<D(A), A, R(A)>$ consisting of a rule of operation on the Hilbert space, together with the Hilbert space subsets $D(A)$ and $R(A)$.

DEFINITION. Suppose $\mathcal{H}_1$ and $\mathcal{H}_2$ are Hilbert spaces. A linear operator A from $\mathcal{H}_1$ into $\mathcal{H}_2$ is called *bounded*, if there exists a real number $C > 0$ such that $\|Ax\|_{\mathcal{H}_2} \leqslant C\|x\|_{\mathcal{H}_1}$ for all $\in \mathcal{H}_1$.

If A is bounded, then $\|Ax\|_{\mathcal{H}_2}/\|x\|_{\mathcal{H}_1} \leqslant C$ for all $x \in \mathcal{H}_1$. The smallest of the numbers C in this inequality is called the norm of the operator A.

DEFINITION. A *norm of operator* A is a non-negative number $\|A\|$ that is defined by the equation

$$\|A\| = \sup_{\|x\|_{\mathcal{H}_1}=1} \|Ax\|_{\mathcal{H}_2} = \sup_{x\neq 0} \frac{\|Ax\|_{\mathcal{H}_2}}{\|x\|_{\mathcal{H}_1}}.$$

That is, $\|A\|$ is a least upper bound of the Hilbert space norm $\|Ax\|_{\mathcal{H}_2}$ when $\|x\|_{\mathcal{H}_1} = 1$. If C is equal to infinity then the operator A is called *unbounded*. The operator norm represents the greatest possible absolute value for the observable.

DEFINITION. A *continuous operator* is a linear operator A, such that

$$\lim_{k\to\infty} \|x_k - x\|_{\mathcal{H}_1} = 0 \quad \text{implies} \quad \lim_{k\to\infty} \|Ax_k - Ax\|_{\mathcal{H}_2} = 0$$

for all $x \in D(A)$ and $x_k \in D(A)$.

STATEMENT. *Let A be a linear operator from $\mathcal{H}_1$ into $\mathcal{H}_2$. Then A is a continuous operator if and only if A is bounded.*

As a result, the use of the adjective "continuous" is an equivalent for "bounded".

The following are examples of some linear operators.

(1) We say that I is a unit operator if $Ix = x$ for all $x \in \mathcal{H}$.
(2) We say that A^{-1} is an inverse operator of A if $A^{-1}A = AA^{-1} = I$.
(3) We say that A^* is an adjoint operator if $(A^*x, y) = (x, Ay)$ for all $x, y \in \mathcal{H}$.
(4) A is a self-adjoint operator if $(Ax, y) = (x, Ay)$ for all $x, y \in \mathcal{H}$ or $A^* = A$.
(5) A is a unitary operator if $(Ax, Ay) = (x, y)$ for all $x, y \in \mathcal{H}$.
(6) A is a projection operator if $A^2 = A$ and $A^* = A$.
(7) A is a nonnegative operator if $A^* = A$, and $(x, Ax) \geqslant 0$ for all $x \in \mathcal{H}$.
(8) A is a positive operator if $A^* = A$ and $(x, Ax) > 0$ for all $x \neq 0$.

1.5. Quantum kinematical postulates

Let us give the basic postulates regarding observables, states and expectation values. These postulates relate the main physical concepts with some mathematical notions.

POSTULATE *(Observable).* An observable of a quantum system is described by a linear self-adjoint operator on a complex separable Hilbert space.

Note that to identify an observable one must give the domain on which its operator acts. This domain is a subset of a separable Hilbert space.

DEFINITION. Let A be a linear bounded operator A on a separable Hilbert space $\mathcal{H}$. A *trace* of A is a complex number $Tr[A]$ such that

$$Tr[A] = \sum_{k=1}^{\infty} <e_k, Ae_k>, \tag{8}$$

where $\{e_k\}$ is an orthonormal basis of $\mathcal{H}$.

If the sum (8) is absolutely convergent and is independent of the choice of the orthonormal basis, then the following properties of Tr are satisfied:

(1) $Tr[aA + bB] = a\,Tr[A] + b\,Tr[B]$.
(2) If $0 \leqslant A \leqslant B$, then $Tr[A] \leqslant Tr[B]$.
(3) $Tr[A^*] = (Tr[A])^*$.
(4) $Tr[AB] = Tr[BA]$, $Tr[ABC] = Tr[BCA] = Tr[CAB]$.

POSTULATE *(State).* A state of the quantum system is described by a nonnegative self-adjoint linear operator ρ of unit trace, i.e., $\rho \geqslant 0$, $\rho^* = \rho$, $Tr[\rho] = 1$.

A set of all states is decomposed into two disjoint subsets of pure and mixed states. A *pure state* is described by a density operator ρ that satisfies the idempotent condition $\rho^2 = \rho$. If ρ describes a pure spate, then ρ is a projection operator, i.e., $\rho^* = \rho$ and $\rho^2 = \rho$. Note that to each element Ψ of a Hilbert space $\mathcal{H}$ such that $\|\Psi\|_{\mathcal{H}} = 1$ there corresponds a pure state $\rho_\Psi = P_\Psi$, where P_Ψ is the projection on the one-dimensional subspace. Note that Ψ is determined by $\rho = P_\Psi$ only up to a phase. Note that $\rho^2 = \rho$ if and only if the entropy $S = -<\ln\rho>$ is equal to zero, $S = 0$.

POSTULATE *(Expectation value).* An expectation value of an observable A on a state ρ is a real value $<A>$ defined by the equation $<A> = Tr[\rho A]$.

The following are properties of expectation values:

(1) $<aA + bB> = a<A> + b<B>$ for all observables A, B and $a, b \in \mathbb{C}$.
(2) $<A>$ is real number if A is a self-adjoint operator.
(3) $<A^*A>$ is nonnegative.
(4) $<I> = 1$, and $<0> = 0$.

1.6. Dual Hilbert space

Let $\mathcal{H}$ be a Hilbert space. We say that a functional Y with values in $\mathbb{C}$ is defined on $\mathcal{H}$ if to every element $x \in \mathcal{H}$ there corresponds a complex number $Y(x) \in \mathbb{C}$.

For example, a functional may be pictured as a "black box" that generates a number at the output in response to an operator at the input, i.e., a concrete number is obtained in response to a concrete operator.

DEFINITION. A *linear functional* on a Hilbert $\mathcal{H}$ is a linear operator Y from $\mathcal{H}$ into $\mathbb{C}$.

If Y is an operator that maps a Hilbert space $\mathcal{H}$ into the space of complex numbers $\mathbb{C}$, then Y is a functional. A functional is an operator Y such that $R(Y) \subset \mathbb{C}$.

DEFINITION. A linear functional Y is *bounded*, if there is a positive constant C such that $|Y(x)| \leqslant C\|x\|_{\mathcal{H}}$ for all $x \in \mathcal{H}$.

A norm of Y is a nonnegative number $\|Y\|$ that is defined by the equation

$$\|Y\| = \sup_{\|x\|=1} \big|Y(x)\big| = \sup_{x\neq 0} \frac{|Y(x)|}{\|x\|_{\mathcal{H}}}.$$

A linear functional is continuous if

$$\lim_{k\to\infty} \|x_k - x\|_{\mathcal{H}} = 0 \quad \text{implies} \quad \lim_{k\to\infty} \big|Y(x_k) - Y(x)\big| = 0.$$

A linear functional is continuous if and only if it is bounded.

We shall denote the linear space of all bounded linear functionals on $\mathcal{H}$ by $\mathcal{H}^*$. For any $x \in \mathcal{H}$ and $Y \in \mathcal{H}^*$, we shall denote by $Y(x)$ the value of the functional at the element x.

DEFINITION. Let $\mathcal{H}$ be a Hilbert space. A *dual space* of $\mathcal{H}$ is a linear space $\mathcal{H}^*$ of all continuous linear functionals on $\mathcal{H}$.

Each element y of a Hilbert space $\mathcal{H}$ determines a continuous linear functional $Y \in \mathcal{H}^*$ by the equation

$$Y(x) = (y, x).$$

Conversely, every continuous linear functional is representable in the form of the scalar product with some element y. This is the Riesz–Fréchet theorem.

RIESZ–FRÉCHET THEOREM. *For each bounded linear functional $Y \in \mathcal{H}^*$, there exists a unique element $y \in \mathcal{H}$, such that $Y(x) = (y, x)$ for all $x \in \mathcal{H}$. Moreover, $\|Y\| = \|y\|_{\mathcal{H}}$.*

The Riesz–Fréchet theorem establishes the general form of a continuous linear functional on $\mathcal{H}$. Every continuous linear functional on $\mathcal{H}$ has the form $Y(x) = (y, x)$, where y is a fixed element of the space $\mathcal{H}$. Conversely, if $y \in \mathcal{H}$, then $Y(x) = (y, x)$ is a bounded linear functional on $\mathcal{H}$.

As a result, there exists an isomorphism between a Hilbert space $\mathcal{H}$ and its dual space $\mathcal{H}^* : x \in \mathcal{H} \to (x, \ ) \in \mathcal{H}^*$. By the Riesz–Fréchet theorem, the dual space $\mathcal{H}^*$ of a Hilbert space $\mathcal{H}$ is isomorphic to $\mathcal{H}$, i.e., $\mathcal{H}^* = \mathcal{H}$. The spaces $\mathcal{H}^*$ and $\mathcal{H}$ are identical except for the names of the elements and operations, such that $\mathcal{H}^*$ and $\mathcal{H}$ are structurally the same.

THEOREM OF ISOMORPHISM BETWEEN $\mathcal{H}^*$ AND $\mathcal{H}$. *For each element y of a Hilbert space $\mathcal{H}$ there exists a unique element Y of $\mathcal{H}^*$, such that $Y(x) = (y, x)$ for all $x \in \mathcal{H}$. Conversely, for each element Y of $\mathcal{H}^*$ there exists a unique element y of $\mathcal{H}$, such that $Y(x) = (y, x)$ for all $x \in \mathcal{H}$. Thus the spaces $\mathcal{H}^*$ and $\mathcal{H}$ are isomorphic.*

Therefore, the element x can be considered not only as an element of $\mathcal{H}$, but also as an element of the dual space $\mathcal{H}^*$.

1.7. Dirac's notations

Suppose $\mathcal{H}$ be a Hilbert space. By the fundamental Riesz–Fréchet theorem, the element x can be considered not only as an element of $\mathcal{H}$, but also as an element of the dual space $\mathcal{H}^*$ of linear continuous functionals on $\mathcal{H}$. Denote x, treated as an element of $\mathcal{H}$, by $|x>$. This element is called the *ket-vector*. We shall denote x, treated as an element of $\mathcal{H}^*$, by $<x|$. The elements $<x|$ are called the *bra-vectors*. Then $|x> \to <x|$ is a one-to-one linear map of $\mathcal{H}$ onto $\mathcal{H}^*$. The symbol for scalar product $<y|x>$ is the graphic junction of the symbols $<y|$ and $|x>$:

$$<y|x> = <y||x> = \big(|y>, |x>\big) = (y, x).$$

Note, that the scalar product in a Hilbert space $\mathcal{H}$ satisfies the condition

$$<y|x>^* = <x|y>,$$

where $|y>, |x> \in \mathcal{H}$. Here we can use $(|x>)^* = <x|$ and $(<x|)^* = |x>$. The scalar product (x, y) will be denoted by $<x|y>$. This notation is widely used.

The main convenience of this Dirac's notation [46] is the possibility of simple representation of operators in terms on an outer product. We shall denote by $\hat{P}(x, y) = |x><y|$ the operator which maps an element $|z>$ of $\mathcal{H}$ into the element $|x><y|z>$:

$$\hat{P}(x, y)|z> = |x><y||z> = |x><y|z>.$$

Thus the action of $\hat{P}(x, y) = |x><y|$ on $|z>$ is described by a simple graphic junction of the symbols. Operators of this form map onto the one-dimensional subspace $\mathcal{H}_x = \{|x>z\colon z \in \mathbb{C}\}$, and will be called the ket-bra operators. Note that

$$\hat{P}(x, y)^* = \big(|x><y|\big)^* = |y><x| = \hat{P}(y, x).$$

If $|x>$ is a ket-vector with the norm $\|x\|_{\mathcal{H}} = \sqrt{<x|x>} = 1$, then the operator $P(x) = \hat{P}(x, x)$ is a projection on $|x>$, i.e.,

$$P^*(x) = P(x), \qquad P^2(x) = P(x).$$

DEFINITION. A *ket-bra operator* is an operator $\hat{P}(x, y) = |x><y|$ that assigns to each element $|z>$ of $\mathcal{H}$ exactly one element $|x>a(y, z)$, where $a(y, z) = <y|z>$.

Finite linear combinations of ket-bra operators describe operators of finite rank. If A is a linear operator whose domain $D(A)$ and range $R(A)$ both lie in the same Hilbert space $\mathcal{H}$, and $\dim R(A) < \infty$, then A is a finite-rank operator. The rank of A is $\dim R(A)$.

1.8. Matrix representation of operator

Each complete orthonormal system of ket-vectors $|e_k>$ in a separable Hilbert space $\mathcal{H}$ is a basis for $\mathcal{H}$. Using equation (6), any ket-vector $|x>$ of the space $\mathcal{H}$ can be represented in the form

$$|x> = \sum_{k=1}^{\infty} |e_k> x_k, \tag{9}$$

where $x_k = <e_k|x>$. The ket-bra operators

$$P_k = \hat{P}(e_k, e_k) = |e_k><e_k| \tag{10}$$

are *projection operators*, such that $P_k^* = P_k$ and $P_k P_l = P_k \delta_{kl}$. Each P_k maps onto the one-dimensional subspace $\mathcal{H}_k = \{|e_k> a,\ a \in \mathbb{C}\}$, $\dim \mathcal{H}_k = 1$.

We can consider the sum $\sum_{k=1}^{N} P_k$ for infinite-dimensional case ($N \to \infty$). The question of convergences arises since an infinite sum is used. The operator norm (uniform) convergence is not relevant here since $\| P_k \| = <e_k|e_k> = 1$ for all $k \in \mathbb{N}$.

We distinguish three types of convergences of a sequence $\{A_k\}$ of bounded linear operators defined everywhere in a Hilbert space $\mathcal{H}$.

DEFINITION. A sequence of operators $\{A_k\colon\ k \in \mathbb{N}\}$ *converges uniformly* to the operator A, if

$$\lim_{k \to \infty} \| A_k - A \| = 0.$$

Thus, a uniform convergence is a convergence with respect to the operator norm.

DEFINITION. A sequence of operators A_k *converges strongly* to the operator A, if

$$\lim_{k \to \infty} \| A_k x - A x \|_{\mathcal{H}} = 0$$

for all $x \in \mathcal{H}$. The sequence $\{A_k\}$ *converges weakly* to the operator A, if

$$\lim_{k\to\infty} <y|A_k x - Ax> = 0$$

for all $x, y \in \mathcal{H}$.

Using Cauchy–Schwarz inequality, it is not hard to see that the strong limit is stronger than the weak limit, i.e., if a sequence of operators converges strongly, then it also converges weakly. Since $\|Ax\|_{\mathcal{H}} \leqslant \|A\|\|x\|_{\mathcal{H}}$, it is evident that the uniform limit is stronger that the strong limit, i.e., if a sequence of operators converges uniformly, then it also converges strongly.

Suppose $\{|e_k>\}$ is an orthonormal system in a separable Hilbert space $\mathcal{H}$. For any $|x> \in \mathcal{H}$ the series

$$|x_N> = \sum_{k=1}^{N} |e_k><e_k|x> = \sum_{k=1}^{N} P_k|x>$$

converges to $|x>$. Hence, the operator P_N converges strongly ($N \to \infty$). As a result, for each orthonormal basis $\{|e_k>\}$ in $\mathcal{H}$, we have

$$\sum_{k=1}^{\infty} |e_k><e_k| = I, \qquad \sum_{k=1}^{\infty} P_k = I. \tag{11}$$

These equations are symbolic form of relation (9), expressing the completeness of the orthonormal system $\{|e_k>\}$. Let A be a bounded linear operator on a separable Hilbert space $\mathcal{H}$. Using (11) and $A = IAI$, we obtain the following theorem.

STATEMENT. *Each bounded linear operator A on a separable Hilbert space $\mathcal{H}$ can be represented in the form*

$$A = \sum_{k,l=1}^{\infty} |e_k><e_k|A|e_l><e_l| = \sum_{k,l=1}^{\infty} A_{kl} P_{kl}, \tag{12}$$

where $P_{kl} = \hat{P}(e_k, e_l) = |e_k><e_l|$ are ket-bra operators, and $\{|e_k>\}$ is an orthonormal basis for $\mathcal{H}$. The numbers $A_{kl} = <e_k|A|e_l> = <e_k|Ae_l>$ are called the matrix elements of the operator A.

This is the *matrix representation* of A. This theorem gives the decomposition of a bounded operator into the linear combination of ket-bra operators. As a result, the operators P_{kl} can be considered as an operator basis. If $\mathcal{B}(\mathcal{H})$ is a linear space of all bounded operators on $\mathcal{H}$, then P_{kl} form a basis for $\mathcal{B}(\mathcal{H})$.

A linear operator can be considered to act on a ket-vector to change it, usually changing both its magnitude and its direction. An eigenvector of a given

linear operator is a ket-vector which is simply multiplied by a constant called the eigenvalue. The direction of the eigenvector is either unchanged (for positive eigenvalues) or reversed (for negative eigenvalues). Let A be a linear operator A on a Hilbert space $\mathcal{H}$. An eigenvalue problem for A is a determination of nonzero elements $|x>$ of $\mathcal{H}$ and complex numbers z, such that the following equation is satisfied: $A|x> = |x>z$. Then the nonzero element $|x>$ is called the *eigenvector* of A. The number $z \in \mathbb{C}$ is called the *eigenvalues* of A.

THEOREM. *If A is a self-adjoint bounded operator, then its eigenvalues z_k are real, and eigenvectors corresponding to distinct eigenvalues are orthogonal.*

As a result, we can define the orthonormal basis $\{|e_k>\}$, such that $A|e_k> = |e_k>z_k$ and $<e_k|e_l> = \delta_{kl}$.

STATEMENT. *For every bounded self-adjoint operator A on a separable Hilbert space $\mathcal{H}$ there exists an orthonormal basis $|e_k>$ such that $|e_k>$ are eigenvectors of A.*

Suppose A is a bounded self-adjoint operator. Using $A|e_k> = |e_k>z_k$, it is not hard to prove that the matrix $A_{kl} = <e_k|A|e_l>$ has diagonal form $A_{kl} = z_l\delta_{kl}$. Using (12), we obtain

$$A = \sum_{k=0}^{\infty} z_k|e_k><e_k| = \sum_{k=1}^{\infty} z_k P_k. \tag{13}$$

As a result, we have the following statement.

STATEMENT. *Each bounded self-adjoint operator A on a separable Hilbert space $\mathcal{H}$ can be represented by* (13)*, where P_k are the projections* (10) *on $\mathcal{H}_k = \{|e_k>a\colon\ a \in \mathbb{C}\} \subset \mathcal{H}$.*

Note that the expectation value of the bounded observable A on the pure state $\rho = P_k = |e_k><e_k|$ is the eigenvalue z_k.

Chapter 2

Quantum Kinematics of Unbounded Observables

2.1. Deficiencies of Hilbert spaces

A Hilbert space $\mathcal{H}$ can be an infinite-dimensional space. The Hilbert space $\mathcal{H}$ is infinite-dimensional in the following sense. It is complete with respect to a particular convergence of infinite sequences. Physical measurements cannot tell us anything about infinite sequences, but can give us information about arbitrary large but finite sequences. Therefore, physics cannot give us sufficient information to describe how to take the limit to infinity, i.e., how to choose the topology. Therefore the topology can be chosen from convenience. A physical reason to use only a Hilbert space convergence do not exist. In quantum mechanics, it is accepted to use a Hilbert space, instead of any another Banach space. Any physical proof of this choice, except of convenience, does not exist.

The quantum observables are identified with the self-adjoint linear operators acting on some Hilbert space. The simplest self-adjoint differential operator $P = -i\hbar d/dq$ (the momentum operator), which is defined for absolutely continuous functions in $\mathcal{H} = L^2(\mathbb{R})$, whose derivatives are square-integrable, has no eigenvector in $L^2(\mathbb{R})$. An eigenvector of the operator $P = -i\hbar d/dq$ is the function $\exp(i/\hbar)qp$. This eigenvector does not belong to $L^2(\mathbb{R})$, since $\| \exp(i/\hbar)qp\|^2_{\mathcal{H}} = 1$ is not integrable over the whole $\mathbb{R}$.

In general, the self-adjoint operators (even if they are bounded) have not only discrete, but also a continuous set of eigenvalues. However, only the eigenvectors of the discrete set of eigenvalues belong to a Hilbert space. In the general case, we deal with eigenvectors which cannot be described by the elements of the Hilbert space. In general, the scalar product is not defined for these eigenvectors, which cannot be normalized. A natural way out of this difficulty is the introduction of a rigged Hilbert space.

2.2. Spaces of test functions

Fréchet space

Let us give the basic definitions regarding test functions and distributions.

DEFINITION. A *countably-normed space* is a linear space $\mathcal{H}$, together with a countable system of norms (or seminorms) $\| \ \|_m$, $m \in \mathbb{N}$, such that the following conditions are satisfied:

(1) The inequalities $\|x\|_1 \leqslant \|x\|_2 \leqslant \cdots \leqslant \|x\|_m \leqslant \cdots$ holds for all $x \in \mathcal{H}$.
(2) Each sequence $\{x_k\} \in \mathcal{H}$ converges to an element x of $\mathcal{H}$ for all $m > 0$.

A pseudometric is a generalization of a metric, which does not satisfy the condition that requires $d(x, y) = 0$ only when $x = y$. If $\{\| \ \|_m \colon m \in \mathbb{N}\}$ is a countable system of seminorms, then

$$d(x, y) = \sum_{m=1}^{\infty} \frac{1}{2^m} \frac{\|x - y\|_m}{1 + \|x - y\|_m}$$

is a pseudometric. The complete countably-normed space is called the Fréchet space.

DEFINITION. A *Fréchet space* is a countably-normed space $\mathcal{H}$ that is complete with respect to the metrics $d_m(x, y) = \|x - y\|_m$ for all integer $m > 0$.

For example, the linear space $C^\infty[0, 1]$ of all infinitely differentiable functions $\Psi : [0, 1] \to \mathbb{R}$ is a Fréchet space with respect to the seminorms

$$\|\Psi\|_m = \sup\big\{\big|\Psi^{(m)}(x)\big| \colon x \in [0, 1]\big\},$$

where $m \geqslant 0$. Here, $\Psi^{(m)}$ denotes the mth derivative of $\Psi(x)$, and $\Psi^{(0)} = \Psi$. Note that each Banach space is a Fréchet space.

A smooth function is an infinitely differentiable function that has derivatives of all finite orders. A function is called C^0, if it is a continuous function. A function is called C^k for $k \geqslant 1$ if it can be differentiated k-times, leaving a continuous kth derivative. The smooth functions are those that lie in the space C^k for all k, they are often referred to as C^∞ functions. For example, the exponential function is evidently smooth because the derivative of the exponential function is the exponential function itself. Note the inclusion $C^{k+1}(\mathbb{R}^n) \subset C^k(\mathbb{R}^n)$. If the kth derivative of Ψ is continuous for all k, then Ψ is said to be C^∞.

Let M be an open subset of $\mathbb{R}^n$, and let $\mathcal{E}(M) = C^\infty(M)$ be a space of infinitely differentiable functions on M. Then $\mathcal{E}(M)$ is a Fréchet space with respect to the

seminorms:

$$\big\|\Psi(x)\big\|_m = \sum_{|k|\leqslant m} \sup_{x\in M} \big|\partial_x^k \Psi(x)\big| < \infty,$$

where k is a multi-index, i.e., $k = (k_1, \ldots, k_n)$, k_i is an integer nonnegative numbers, and

$$\partial_x^k = \frac{\partial^{|k|}}{\partial x_1^{k_1} \cdots \partial x_n^{k_n}}, \quad |k| = \sum_{i=1}^{n} k_i = k_1 + \cdots + k_n.$$

The test function space $\mathcal{D}(M)$

Functions which vanish outside a certain finite region of the space are called *functions of compact support*. The closure of the set of all points such that $\Psi(x) \neq 0$ is called *support* of the function $\Psi(x)$.

Let M be a finite domain (i.e., a bounded connected open set) in $\mathbb{R}^n$. We shall denote by $\mathcal{D}(M)$ the set of infinitely smooth or $C^\infty(\mathbb{R}^n)$ functions (i.e., functions with continuous partial derivatives of all orders) which vanish outside the domain M.

The space $\mathcal{D}(M) \subset C^\infty(M)$ of infinite differentiable functions on a compact set $M \subset \mathbb{R}^n$ is called the space of compactly supported functions. A function $\Psi : \mathbb{R}^n \to \mathbb{R}$ is said to have compact support if there exists a compact subset M of $\mathbb{R}^n$ such that $\Psi(x) = 0$ for all $x \in (\mathbb{R}^n - M)$. The function with compact support is identically zero except on some closed, bounded set.

DEFINITION. A *space of finitary functions*, or *space of compactly supported functions*, is a linear space $\mathcal{D}(M)$ of infinitely differentiable functions $\Psi(x) \in C^\infty(M)$ on a compact subspace $M \subset \mathbb{R}^n$, such that $\Psi(x) = 0$ outside of M, i.e.,

$$\mathcal{D}(M) := \Big\{\Psi(x)\colon\ \big\|\Psi(x)\big\|_k = \sup_{x\in M} \big|\partial_x^k \Psi(x)\big| < \infty\ \forall k, l\Big\}.$$

The function $\Psi(x)$, such that $\Psi(x) = \exp -a^2/(a^2 - |x|^2)$ for $|x| < |a|$, and $\Psi(x) = 0$ for $|x| \geqslant |a|$ is a compactly supported function.

It is easy to see that $\mathcal{D}(M) \subset C^\infty(M)$. Spaces of infinitely differentiable functions defined on compact sets are typical examples of Fréchet spaces.

STATEMENT. *The space $\mathcal{D}(M)$ of finitary functions is a Fréchet space with respect to the seminorms*

$$\|\Psi\|_m = \max_{|k|\leqslant m} \big\|\Psi(x)\big\|_k = \max_{|k|\leqslant m} \sup_{x\in M} \big|\partial_x^k \Psi(x)\big|. \tag{1}$$

The test function space $\mathcal{J}(\mathbb{R}^n)$

The space $\mathcal{J}(\mathbb{R}^n)$ consists of the infinitely differentiable functions $\Psi(x)$ that, together with all their derivatives, decrease faster than any power of $|x|^{-1}$, i.e., $\Psi(x) \in \mathcal{J}(\mathbb{R}^n)$ if for any fixed k, l there exists a constant C_{kl} such that

$$\left|x^k \partial^l \Psi(x)\right| < C_{kl}.$$

If $\mathcal{D}(\mathbb{R}^n)$ is a set of smooth functions of compact support on $\mathbb{R}^n$, then this set is a subset of $\mathcal{J}(\mathbb{R}^n)$.

DEFINITION. A *space of rapidly-decreasing functions*, or *Schwarz space*, is a linear space $\mathcal{J}(\mathbb{R}^n)$ of infinitely differentiable functions $\Psi(x) \in C^\infty(\mathbb{R}^n)$, which decrease together with its derivatives at $x \to \infty$ is faster than any power of $|x|^{-1}$.

$$\mathcal{J}\left(\mathbb{R}^n\right) := \left\{\Psi(x)\colon\ \|\Psi\|_{kl} = \sup_{x\in\mathbb{R}^n} \left|x^k \partial_x^l \Psi(x)\right| < \infty \text{ for all } k, l\right\}.$$

Here $x^k = x_1^{k_1} \cdots x_n^{k_n}$, and

$$\partial_x^l = \frac{\partial^{|l|}}{\partial x_1^{l_1} \cdots \partial x_n^{l_n}}, \quad |l| = \sum_{i=1}^n l_i,\ |x| = \sqrt{\sum_{i=1}^n x_i^2}.$$

The following are examples of some rapidly-decreasing functions.

(1) If k is a multi-index, and a is a positive real number, then $\Psi(x) = x^k \exp\{-ax^2\}$ is in $\mathcal{J}(\mathbb{R})$.
(2) Any smooth function Ψ with compact support on $\mathbb{R}^n$ is in $\mathcal{J}(\mathbb{R}^n)$.

It is easy to see that a space of finitary functions is a subspace of a Schwarz space $\mathcal{D}(\mathbb{R}^n) \subset \mathcal{J}(\mathbb{R}^n)$. Let $L^p(\mathbb{R}^n)$ be a space of p-integrable functions on $\mathbb{R}^n$. Note that $\mathcal{J}(\mathbb{R}^n) \subset L^p(\mathbb{R}^n)$ for $p \geqslant 1$.

One can introduce the structure of a countably normed space on the space $\mathcal{J}(\mathbb{R}^n)$ by setting

$$\left\|\Psi(x)\right\|_m = \sum_{|k|\leqslant m} \sum_{|l|\leqslant m} \left\|\Psi(x)\right\|_{kl} < \infty. \tag{2}$$

STATEMENT. *The Schwarz space* $\mathcal{J}(\mathbb{R}^n)$ *is a Fréchet space with respect to the seminorms* (2).

The spaces $C^\infty(M)$, $\mathcal{D}(M)$ and $\mathcal{J}(M)$ are usually used as spaces of test functions. A generalized function (or distribution) is a bounded linear functional on some space of test functions.

2.3. Spaces of generalized functions

Generalized functions (also known as distributions) are objects that generalize functions and probability distributions. They extend the concept of derivative to all integrable functions, and are used to formulate generalized solutions of differential equations. These notions are very important in quantum mechanics. Generalized functions were introduced by S. Sobolev in 1935. Then the theory of these functions was developed by L. Schwartz.

The basic idea is to identify generalized functions with linear functionals on a space of well-behaved functions (test functions). An operator on a set of generalized functions can be understood by mapping distributions to the test function. For example, if $Y(x) : \mathbb{R}^n \to \mathbb{R}$ is a locally integrable function, and $\Psi(x) : \mathbb{R}^n \to \mathbb{R}$ is a smooth function with compact support, then we set

$$<Y, \Psi> = \int\limits_{\mathbb{R}^n} Y(x)\Psi(x)\,dx. \tag{3}$$

This is a real-valued functional that linearly and continuously depends on $\Psi(x)$. One can therefore consider the function $Y(x)$ as a continuous linear functional on the space of all test functions Ψ. Probability distributions can thus also be considered as continuous linear functionals on the space of test functions. This notion of (continuous linear) functional on the space of test functions is therefore used as the definition of distribution. Such distributions may be multiplied by numbers and can be added together, so they form a linear space. In general, it is not possible to define a multiplication for distributions, but distributions may be multiplied with infinitely differentiable functions. Note that several constructions of algebras of generalized functions have been proposed. These are intended to solve the problem of multiplication of distributions. The most widely used approach to construct such associative differential algebras is based on Colombeau algebra [37].

To define the derivative of a distribution, we consider the integration by parts:

$$\int\limits_{\mathbb{R}^n} \partial_k Y(x)\Psi(x)\,dx = -\int\limits_{\mathbb{R}^n} Y(x)\partial_k\Psi(x)\,dx,$$

where $\partial_k\Psi(x) = \partial\Psi(x)/\partial x_k$. Note that $\Psi(x)$ is zero outside of a bounded set and that therefore no boundary values have to be taken into account. Then if Y is a distribution, we can define its derivative $\partial_k Y$ by

$$<\partial_k Y, \Psi> = -<Y, \partial_k\Psi>.$$

Each distribution becomes infinitely differentiable and the usual properties of derivatives hold.

Suppose M is a finite domain (i.e., a bounded connected open set) in $\mathbb{R}^n$. Let $\mathcal{E}^*(M)$ be a set of all continuous linear functionals on $\mathcal{E}(M) = C^\infty(M)$. Then $\mathcal{E}^*(M)$ is a dual space of $\mathcal{E}(M)$. The value of a functional Y on an element Ψ is denoted by

$$Y(\Psi) = <Y, \Psi>.$$

A continuity of $Y \in \mathcal{E}^*(M)$ means that if $\Psi_k \to \Psi$ in $\mathcal{E}(M)$, then $<Y, \Psi_k> \to <Y, \Psi>$ in $\mathcal{E}^*(M)$. This convergence can be defined in terms of seminorms. If $|<Y, \Psi>| \leqslant C\|\Psi\|_m$ for all $\Psi \in \mathcal{E}(M)$ and some constants C, m, then Y is a bounded functional.

DEFINITION. A *generalized function*, or *distribution*, is a bounded linear functional on $\mathcal{J}(\mathbb{R}^n)$. A *space of generalized functions*, or *space of distributions*, is a linear space $\mathcal{J}^*(\mathbb{R}^n)$ dual of $\mathcal{J}(\mathbb{R}^n)$.

Each function $Y(x) \in \mathcal{J}(\mathbb{R}^n)$ defines a functional $Y \in \mathcal{J}^*(\mathbb{R}^n)$ by equation (3). Using $\mathcal{D}(\mathbb{R}^n) \subset \mathcal{J}(\mathbb{R}^n)$, we obtain $\mathcal{J}^*(\mathbb{R}^n) \subset \mathcal{D}^*(\mathbb{R}^n)$.

The following are some properties of generalized functions.

(1) Differentiation of a distribution Y can be defined by the equation

$$<\partial^k Y, \Psi> = (-1)^{|k|}<Y, \partial^k \Psi>.$$

(2) Multiplication of a distribution $Y \in \mathcal{D}^*(M)$ by a smooth function $a(x) \in C^\infty(M)$ is defined by

$$<aY, \Psi> = <Y, a\Psi>,$$

where $\Psi \in \mathcal{D}(M)$. We would like to describe the class of smooth functions $a(x)$ such that $a(x)Y(x) \in \mathcal{J}^*(\mathbb{R}^n)$ if $Y(x) \in \mathcal{J}^*(\mathbb{R}^n)$. Then it is necessary and sufficient that function $a(x)$ is a multiplicator in $\mathcal{J}(\mathbb{R}^n)$. This multiplication by $a(x)$ is a continuous linear operator on $\mathcal{J}(\mathbb{R}^n)$ if $|\partial^k a(x)| \leqslant C_k(1 + |x|)^{N_k}$, where k is a multi-index, and C_k, N_k are constants.

(3) Let A be a linear differential operators on $M \subset \mathbb{R}^n$ of the form

$$A = \sum_{|k| \leqslant m} a_k(x) D^k, \quad D^k = D_1^{k_1} D_2^{k_2} \cdots D_n^{k_n}, \; D_j = -i\partial/\partial x_j, \tag{4}$$

where k is a multi-index, $k = (k_1, \ldots, k_n)$, k_j is integer nonnegative numbers, $|k| = k_1 + \cdots + k_n$, and $a_k(x) \in C^\infty(M)$.

The linear differential operator A on $\mathcal{D}^*(M)$ and $\mathcal{J}^*(\mathbb{R}^n)$ is defined by the equation

$$<AY, \Psi> = <Y, A^t \Psi>,$$

where $\Psi \in \mathcal{D}(M)$, or $\Psi \in \mathcal{J}(\mathbb{R}^n)$, and

$$A^t\Psi(x) = \sum_{|k|\leqslant m} (-1)^{|k|} D^k\big(a_k(x)\Psi(x)\big).$$

(4) Let $\mathcal{F}$ be a Fourier transform operator. If $\Psi(x) \in \mathcal{J}(\mathbb{R}^n)$, then

$$\tilde{\Psi}(p) = (\mathcal{F}\Psi)(p) = \frac{1}{(2\pi)^{n/2}} <\Psi(x), e^{-ixp}> = \frac{1}{(2\pi)^{n/2}} \int e^{-ixp}\Psi(x)\,dx, \tag{5}$$

where $xp = x_1p_1 + \cdots + x_np_n$. The operator $\mathcal{F}$ is a map from $\mathcal{J}(\mathbb{R}^n)$ into itself. It is not hard to prove that $\mathcal{F}^t = \mathcal{F}$, i.e.,

$$<\mathcal{F}\Psi, \Phi> = <\Psi, \mathcal{F}\Phi>,$$

where $\Psi, \Phi \in \mathcal{J}(\mathbb{R}^n)$. This equation allows us to define $\mathcal{F}$ as a map from $\mathcal{J}^*(\mathbb{R}^n)$ into itself. The Fourier transform of a generalized function $\Psi \in \mathcal{E}^*(\mathbb{R}^n)$ can be defined by formula (5).

(5) It is easy to verify the equation

$$\mathcal{F}\big(D^k\Psi\big)(p) = p^k(\mathcal{F}\Psi)(p) \tag{6}$$

for $\Psi \in \mathcal{J}(\mathbb{R}^n)$. Equation (6) is also valid for $\Psi \in \mathcal{J}^*(\mathbb{R}^n)$. This formula means that $\mathcal{F}$ maps an operator of differentiation D^k into an operator of multiplication by p^k.

2.4. Rigged Hilbert space

Hilbert and rigged Hilbert spaces

In quantum mechanics a Hilbert space $\mathcal{H}$ usually arises as the result of the completion with respect to the norm defined by the scalar product of some space $\mathcal{B}$ of sufficiently well-behaved functions (test functions). For example, $\mathcal{B} = \mathcal{J}(\mathbb{R}^n)$ or $\mathcal{D}(\mathbb{R}^n)$. The space $\mathcal{B}$ is usually considered as a Banach space, i.e., as a normed linear space that is complete with respect to the norm $\| \ \|_{\mathcal{B}}$.

Let $\mathcal{B} \subset \mathcal{H}$ be a space, which is complete with respect to convergence in $\mathcal{B}$. One can show that the space $\mathcal{B}$ cannot be complete with respect to convergence in the norm $\|x\|_{\mathcal{H}} = \sqrt{(x, x)}$. We can find a sequence $\{x_k\}$ in $\mathcal{B}$ such that $\{x_k\}$ is fundamental, but it does not converge to an element of $\mathcal{B}$. However, $\mathcal{B}$ can always be completed with respect to the new topology defined by the norm $\|x\|_{\mathcal{H}} = \sqrt{(x, x)}$ to form a Hilbert space $\mathcal{H}$, which is uniquely defined up to isomorphism. By the fundamental Riesz–Fréchet theorem, the space $\mathcal{H}^*$ of all linear functionals on $\mathcal{H}$ is isomorphic to $\mathcal{H}$ itself. On the other hand, functionals in $\mathcal{H}^*$ are also

continuous linear functionals on $\mathcal{B} \subset \mathcal{H}$ because of the continuity of the scalar product in the topology of $\mathcal{B}$. The space $\mathcal{B}^*$ of all linear functionals on $\mathcal{B}$ is bigger. It includes the Hilbert space $\mathcal{H}^* = \mathcal{H}$. A system of three embedded spaces $\mathcal{B} \subset \mathcal{H} = \mathcal{H}^* \subset \mathcal{B}^*$ with the described properties is called the rigged Hilbert space.

Often when one deals with a Hilbert space $\mathcal{H}$ one forgets about the space $\mathcal{B}$ from which $\mathcal{H}$ was obtained by completion and hence also about the natural extension $\mathcal{B}^*$ of $\mathcal{H}$. Nevertheless, it is precisely the simultaneous consideration of the triplet of spaces $\mathcal{B}$, $\mathcal{H} = \mathcal{H}^*$, and $\mathcal{B}^*$ gives a natural basis for the quantum mechanics.

DEFINITION. A *rigged Hilbert space* is the ordered triplet

$$\mathcal{B} \subset \mathcal{H} = \mathcal{H}^* \subset \mathcal{B}^*,$$

where $\mathcal{H}$ is a Hilbert space, $\mathcal{B}$ is a Banach space, and $\mathcal{B}^*$ is dual of $\mathcal{B}$.

The term "rigged Hilbert space" is also used to describe the dual pair $(\mathcal{B}, \mathcal{B}^*)$ generated from a Hilbert space $\mathcal{H}$. The term "Gelfand triplet" is sometimes used instead of the term "rigged Hilbert space".

In general, the self-adjoint operators have discrete, and continuum spectrum of eigenvalues. However, only eigenvectors of a discrete spectrum belong to a Hilbert space $\mathcal{H}$. If the rigged Hilbert space is used, then the eigenvectors of a continuum spectrum can be refer to the extension $\mathcal{B}^*$ of the Hilbert space $\mathcal{H} = \mathcal{H}^*$.

Example of a rigged Hilbert space is the following triple of spaces:

$$\mathcal{J}\big(\mathbb{R}^n\big) \subset L^2\big(\mathbb{R}^n\big) \subset \mathcal{J}^*\big(\mathbb{R}^n\big).$$

This triplet consists of the Banach space $\mathcal{J}(\mathbb{R}^n)$ of test functions, the Hilbert space $L^2(\mathbb{R}^n)$ of square integrable functions, and the Banach space $\mathcal{J}^*(\mathbb{R}^n)$ of the linear functionals on $\mathcal{J}(\mathbb{R}^n)$.

A rigged Hilbert space can be considered as a pair of spaces $(\mathcal{B}, \mathcal{B}^*)$ that can be generated from a separable Hilbert space $\mathcal{H}$ using a sequence of norms (or semi-norms). The space $\mathcal{B}$ is characterized as a Banach (or Fréchet) space. In distribution theory, the space $\mathcal{B}$ is characterized as a test-function space, where a test-function is considered as a well-behaved function (being continuous, n-times differentiable, having a bounded domain or at least decreasing exponentially beyond some finite range, etc). $\mathcal{B}^*$ is a space of generalized functions, and it is the dual of $\mathcal{B}$, meaning that it corresponds to the complete space of continuous linear functionals on $\mathcal{B}$. Because the elements of $\mathcal{B}$ are well-behaved, $\mathcal{B}^*$ may contain elements that are not so well-behaved functions (such as Dirac's delta-function).

The space $\mathcal{B}$ can be considered as the anti-dual of $\mathcal{B}^*$, meaning that it is the complete set of continuous anti-linear functionals on $\mathcal{B}^*$. It is anti-linear rather than linear because multiplication by a scalar $a \in \mathbb{C}$ is defined in terms of the scalar complex conjugation $<x|y> = <y|x>^*$, $<ay|x> = a^*<y|x>$.

Note that $\mathcal{B}$ and $\mathcal{B}^*$ are not Hilbert spaces. In these spaces lack a scalar product that induces a metric with respect to which the spaces are complete. However for each space there is a topology with respect to which the space is complete. Nevertheless, each of them is closely related to the Hilbert space $\mathcal{H}$ from which they are generated. $\mathcal{B}$ is densely embedded in $\mathcal{H} = \mathcal{H}^*$, which in turn is densely embedded in $\mathcal{B}^*$, i.e., $\mathcal{B} \subset \mathcal{H} = \mathcal{H}^* \subset \mathcal{B}^*$.

The Hilbert space can be equipped by different approaches, which depend on type of Banach subspace $\mathcal{B}$ of $\mathcal{H}$. Usually, the space $\mathcal{B}$ should remains invariant under action of the complete set of commutative observables.

Operators and rigged Hilbert space

The dual pair $(\mathcal{B}, \mathcal{B}^*)$ allows to represent important operators of quantum mechanics that are problematic in a separable Hilbert space. For example, the unbounded operators that correspond to the position and momentum have no eigenvectors in a separable Hilbert space. Moreover, they are only defined on a dense subset of the elements of the space and this leads to domain problems. In a rigged Hilbert space, the operators corresponding to position and momentum can have a complete set of eigenfunctionals (i.e., generalized eigenfunctions). The key result is known as the Gelfand–Maurin theorem.

THEOREM *(Gelfand–Maurin). If A is a symmetric linear operator defined on the space $\mathcal{B}$ and it admits a self-adjoint extension to the Hilbert space $\mathcal{H}$, then A has a complete system of eigenfunctionals belonging to the dual space $\mathcal{B}^*$.*

As a result, A can be extended by duality to $\mathcal{B}^*$, its extension A^* is continuous on $\mathcal{B}^*$. The operator A^* satisfies a completeness relation, which meaning that it can be decomposed in terms of its eigenfunctionals and their associated eigenvalues.

The duality formula for extending A to $\mathcal{B}^*$ is

$$<A^*Y|\Psi> = <Y|A\Psi>$$

for all $\Psi \in \mathcal{B}$ and for all $Y \in \mathcal{B}^*$. The completeness relation says that for all $|\Psi_1> \in \mathcal{B}$ and $<Y| \in \mathcal{B}^*$, we have

$$<Y|A\Psi> = \int_{\sigma(A)} z<Y|z><z|\Psi> \, d\mu(z) = \int_{\sigma(A)} zY(z)^*\Psi(z) \, d\mu(z),$$

where $\sigma(A)$ is the set of all generalized eigenvalues of A^*. Here, $\sigma(A)$ is the set of all scalars z for which there is $< z| \in \mathcal{B}^*$ such that

$$<A^*z|\Psi> = z<z|\Psi>$$

for all $|\Psi> \in \mathcal{B}$.

Note that the rigging can result in different sets of generalized eigenvalues being associated with an operator. For example, the set of (generalized) eigenvalues for the momentum operator (in one dimension) corresponds to the real line, if the space of test functions is the space $\mathcal{J}(\mathbb{R})$ of rapidly-decreasing functions. Its associated set of eigenvalues is the complex plane, if the space of test functions is the space $\mathcal{D}(\mathbb{R})$ of infinitely differentiable functions with compact support. If complex eigenvalues are not desired, then $\mathcal{J}(\mathbb{R})$ would be a more suitable choice than $\mathcal{D}(\mathbb{R})$. Of course, it is impossible for a self-adjoint operator to have complex eigenvalues in a Hilbert space $\mathcal{H}$.

2.5. Linear operators on a rigged Hilbert space

Let A be a linear operator whose domain $D(A)$ and range $R(A)$ both lie in the same Hilbert space $\mathcal{H}$. The operator A is called bounded if the norm

$$\|Ax\|_{\mathcal{H}} = \sqrt{<Ax|Ax>}$$

is bounded for $x \in D(A)$ and $\|x\|_{\mathcal{H}} = 1$. The upper bound of $\|Ax\|_{\mathcal{H}}$ when x in the intersection of the domain $D(A)$ with the unit sphere $\{x\colon \|x\|_{\mathcal{H}} = 1\}$ is called the norm of A and is denoted by $\|A\|$. If this upper bound is infinite, A is said to be *unbounded*. Any bounded operators A with domain $D(A) \subset \mathcal{H}$ can be extended to the whole Hilbert space, remaining linearity and boundedness on all of $\mathcal{H}$ with the same norm. For unbounded operators this is not possible.

In study of unbounded operators the graph of an operator plays an important role. We denote by $\mathcal{H} \times \mathcal{H}$ the set of all ordered pairs $\{x, y\}$, where $x, y \in \mathcal{H}$. Then $\mathcal{H} \times \mathcal{H}$ will be called the direct product. Let us define the concept of the graph of an operator A.

DEFINITION. Let A be a linear operator with domain $D(A) \subset \mathcal{H}$. A *graph* of A is a set of all pairs $\{x, Ax\}$, where $x \in D(A)$.

The graph of A, denoted by $G(A)$, is a subset of $\mathcal{H} \times \mathcal{H}$. If $\mathcal{H}$ is a Hilbert space, then it is not hard to prove that $G(A)$ is a Hilbert space with the scalar product

$$<\{x_1, y_1\}|\{x_2, y_2\}> = <x_1|x_2> + <y_1|y_2>.$$

The operator is said to be closed if its graph is a closed subset of $\mathcal{H} \times \mathcal{H}$. A closed operator defined on the whole space $\mathcal{H}$ is bounded. We shall be dealing, as a rule, with unbounded closed operators, or at least with operator which have closures. These operators cannot be defined on the whole space $\mathcal{H}$. We shall always assume that the domain $D(A)$ of a unbounded closed operator is dense in $\mathcal{H}$.

DEFINITION. The operator B is called *extension* of A if the graph of A is contained in the graph of B, i.e., $G(A) \subset G(B)$.

If $D(A) \subset D(B)$ and $A|x> = B|x>$ for all $x \in D(A)$, then B is an extension of A.

Hilbert space is a very important concept in quantum mechanics since the fundamental notion of self-adjoint operator is defined in terms of a scalar product. It is only the framework of a Hilbert space that one can define a self-adjoint operator, corresponding to a quantum observable. By the Riesz–Fréchet theorem, each continuous functional Y on a Hilbert space can be presented in the form $Y(x) = <y|x>$ for some fixed $y \in \mathcal{H}$ and all $x \in \mathcal{H}$.

In general, *we can consider a functional Y on a Banach space $\mathcal{B}$ as a generalization of scalar product*. We use for the functional $Y(x)$ the symbol

$$<Y|x> = Y(x).$$

Consider a functional $Y_A(x) = <y|Ax>$, where $x \in D(A)$ and $y \in \mathcal{H}$. If $<y|Ax>$ is bounded for some y in $\mathcal{H}$ and for all $x \in D(A)$, where C is a positive number, then, according to the Riesz–Fréchet theorem, there exists $y_A \in \mathcal{H}$ such that the form of linear functional $Y_A(x) = <y|Ax>$ on $\mathcal{H}$ is $Y_A(x) = <y_A|x>$. If the domain $D(A)$ is dense in $\mathcal{H}$, then the element y_A is uniquely determined by the element y. We define the operator A^*, called *adjoint* (or dual) of A, by the equation $A^*y = y_A$. If A is bounded ($D(A) = \mathcal{H}$), then $C = \|A\|\|y\|_{\mathcal{H}}$ and the dual operator A^* is defined on all of $\mathcal{H}$. An operator A is called *symmetric* if $D(A) \subset D(A^*)$, and $<Ay|x> = <y|Ax>$ for all $x, y \in \mathcal{H}$. If $D(A^*) = D(A)$, then A is called *self-adjoint*.

We illustrate these notions with the following example.

(a) Suppose $\mathcal{H} = L_2([0, 1])$ is the Hilbert space of square-integrable functions on the interval $[0, 1]$. Let D be a set of all absolutely continuous functions $\Psi(q)$ on $[0, 1]$ whose derivatives belong to $\mathcal{H}$, such that $\Psi(0) = \Psi(1)$. The operator $P = -i\hbar\partial_q$ with domain $D(P) = D$ is a self-adjoint operator.

(b) Let D_0 be a subset of D consisting of $\Psi(q) \in D$ such that $\Psi(0) = \Psi(1) = 0$. The operator $P = -i\hbar\partial_q$ with domain D_0 is not a self-adjoint operator, but A is symmetric. Since $D_0 \subset D$, the self-adjoint operator P with the domain D is a self-adjoint extension of the symmetric operator with the domain D_0.

(c) The symmetric operator $A = Q^3P + PQ^3$ with $D(A) = \mathcal{H} = L_2(\mathbb{R})$, where $Q = q$ and $P = -i\hbar\partial_q$, does not admit any self-adjoint extension in $\mathcal{H}$.

In general, self-adjoint operators have not just a discrete but also a continuous spectrum of eigenvalues. Only the eigenvectors of the discrete spectrum belong to the Hilbert space $\mathcal{H}$. If we use a rigged Hilbert space, then it is possible to formulate the theory in physical terms, treating the eigenvectors of the continuous spectrum as elements of the extension $\mathcal{B}^*$ of the Hilbert space $\mathcal{H}$.

We can illustrate this situation by a simple example. Consider the rigged Hilbert space $\mathcal{J}(\mathbb{R}) \subset L^2(\mathbb{R}) \subset \mathcal{J}^*(\mathbb{R})$. The simplest self-adjoint differential operator $P = -i\hbar\partial_q$ (the momentum operator), which is defined for absolutely continuous functions in $\mathcal{H} = L^2(\mathbb{R})$, whose derivatives are square-integrable, has no eigenvector in $L^2(\mathbb{R})$. An eigenvector of the operator $P = -i\hbar\partial_q$, corresponding to the real eigenvalue p, is the function $\exp\{(i/\hbar)qp\}$. This function does not belong to $L^2(\mathbb{R})$, since $\| \exp(i/\hbar)qp\|^2_{\mathcal{H}} = 1$ is not integrable over the whole $\mathbb{R}$. Thus statement on the existence and completeness of a set of eigenvectors of a self-adjoint operator does not apply even to such simple observable as momentum P. At the same time it is obvious that the functions $\exp\{(i/\hbar)qp\}$ belong to the space $\mathcal{J}^*(\mathbb{R})$ of linear functionals, and it can be proved that they form a complete set of functionals in that space. Note that every functional in $\mathcal{J}^*(\mathbb{R})$ and every function in $\mathcal{H} = L^2(\mathbb{R})$ can be expanded in a Fourier integral over the functions $\exp\{(i/\hbar)qp\}$. In the space $\mathcal{H} = L^2(\mathbb{R})$ this expansion converges. As a result, the momentum operator P has a complete set of eigenfunctions in the rigged Hilbert space $(\mathcal{J}(\mathbb{R}), L^2(\mathbb{R}), \mathcal{J}^*(\mathbb{R}))$. The operator P is not continuous with respect to the scalar product in $L^2(\mathbb{R})$. At the same time, the operator P is continuous in the topology of $\mathcal{J}(\mathbb{R})$ and it maps this space into itself. All these properties are satisfied for a wide class of operators in the rigged Hilbert spaces.

The situation, which we have for the operator $P = -i\hbar\partial_q$ in the rigged Hilbert space $(\mathcal{J}(\mathbb{R}), L^2(\mathbb{R}), \mathcal{J}^*(\mathbb{R}))$, holds for any rigged Hilbert space.

DEFINITION. Let A be a linear operator which maps a Banach space $\mathcal{B}$ into itself. A *generalized eigenvector* of A is a linear functional $Y \in \mathcal{B}^*$ such that for all $x \in \mathcal{B}$ the equation $Y(Ax) = zY(x)$ holds.

DEFINITION. An operator A, which maps a Banach space $\mathcal{B}$ into itself, is called a *self-adjoint operator on the rigged Hilbert space* $(\mathcal{B}, \mathcal{H}, \mathcal{B}^*)$, if the following conditions are satisfied:

(1) $<Ay|x> = <y|Ax>$ for all elements x, $y \in D(A)$.
(2) From the equation $<y|Ax> = <y_A|x>$ holds for all $x \in D(A)$ and fixed y, $y_A \in \mathcal{H}$, it follows that $y \in D(A)$ and hence $Ay = y_A$.

Each self-adjoint operator A on the space $(\mathcal{B}, \mathcal{H}, \mathcal{B}^*)$ can be continued to the whole space $\mathcal{B}^*$ by the equation $<Ay|x> = <y|Ax>$, where $x \in \mathcal{B}$ and $y \in \mathcal{B}^*$. Let us give the basic theorem regarding the existence of a complete set of generalized eigenvectors for every self-adjoint operator.

THEOREM. *A self-adjoint operator on a rigged Hilbert space has a complete set of generalized eigenvectors corresponding to real eigenvalues.*

For every continuous linear operator A on $\mathcal{B}$ one can define an adjoint operator A^* on $\mathcal{B}^*$ by

$$<A^*Y|x> = <Y|Ax>,$$

i.e., $A^*Y(x) = Y(Ax)$. One can prove that A^* is a linear continuous operator on $\mathcal{B}^*$. This is the extension of an adjoint operator A^* of A on the Hilbert space $\mathcal{H}$ such that $<A^*y|x> = <y|Ax>$ for all $x \in \mathcal{H}$. In general, $D(A^*) \neq \mathcal{H}$. For a symmetric operator A on $\mathcal{B}$ which has a unique self-adjoint extension $A_{\mathcal{H}} = A^*_{\mathcal{H}}$ to $\mathcal{H}$, we have the following triplet of operators

$$A \subset A_{\mathcal{H}} = A^*_{\mathcal{H}} \subset A^*$$

on the triplet of spaces $\mathcal{B} \subset \mathcal{H} = \mathcal{H}^* \subset \mathcal{B}^*$.

A functional Y on $\mathcal{B}$ is a generalized eigenvector of the operator A on $\mathcal{B}$ with eigenvalue z, if

$$<A^*Y|x> = <Y|Ax> = z<Y|x> \tag{7}$$

for all $x \in \mathcal{B}$. Then $A^*Y(x) = Y(Ax) = zY(x)$. The generalized eigenvector Y is also denoted by $|Y> = |z>$. Equation (7) can be written in the form $A^*|z> = |z>z$ that is often presented as $A|z> = |z>z$.

Rigged Hilbert space and embedding operator

Let $\mathcal{H}$ be a Hilbert space. Suppose $\mathcal{B} \subset \mathcal{H}$ is a Banach space with norm $\| \ \|_{\mathcal{B}}$. Denote by J the *embedding operator* $J : \mathcal{B} \to \mathcal{H}$. The operator J will be assumed to be bounded. Then there exists a positive constant C, such that $\|x\|_{\mathcal{H}} \leqslant C\|x\|_{\mathcal{B}}$ for all $x \in \mathcal{B}$.

We introduce the space $\mathcal{B}^*$ of continuous linear functionals on $\mathcal{B}$. The value of a functional Y on a vector $x \in \mathcal{B}$ will be also expressed as $<Y|x>$. If $Y \in \mathcal{B}^*$, then

$$<Y|ax_1 + bx_1> = a<Y|x_1> + b<Y|x_2>$$

for all $x_1, x_2 \in \mathcal{B}$ and $a, b \in \mathbb{C}$, and $|<Y|x>| \leqslant C\|x\|_{\mathcal{B}}$ for some $C > 0$. We can define addition and multiplication by a number in $\mathcal{B}^*$ by setting

$$<aY_1 + bY_2|x> = a^*<Y_1|x> + b^*<Y_2|x>$$

for all $Y_1, Y_2 \in \mathcal{B}^*$ and $x \in \mathcal{B}$.

There exists a natural linear map $J^* : \mathcal{H} = \mathcal{H}^* \to \mathcal{B}^*$, which to each element $y \in \mathcal{H}$ assigns a functional $J^*y \in \mathcal{B}^*$ defined by the formula

$$<J^*y|x> = <y|Jx> = <y|x>$$

for all $x \in \mathcal{B} \subset \mathcal{H}$.

We can define the norm in $\mathcal{B}^*$ by the formula

$$\|Y\|_{\mathcal{B}^*} = \sup\bigl\{|<Y|x>|:\ \|x\|_{\mathcal{B}} = 1,\ x \in \mathcal{B}\bigr\}.$$

It is not hard to prove that J^* is a continuous linear operator from $\mathcal{H} = \mathcal{H}^*$ into $\mathcal{B}^*$.

As a result, we have the triple of spaces $\mathcal{B} \subset \mathcal{H} \subset \mathcal{B}^*$, where $\mathcal{H}$ is a Hilbert space, $\mathcal{B}$ is a Banach space densely embedded in $\mathcal{H}$ and $\mathcal{B}^*$ is the space of continuous linear functionals on $\mathcal{B}$. To each $Y \in \mathcal{B}^*$ and $x \in \mathcal{B}$, there exists the value $<Y|x> = Y(x)$ of Y at x. This value is an extension of the scalar product in $\mathcal{H}$, that is, if $Y \in \mathcal{H}^* \subset \mathcal{B}^*$, then the scalar product $<Y|x>$ in $\mathcal{H}$ equals to the value of the functional Y at x.

We define

$$<x|Y> = <Y|x>^* = \bigl(Y(x)\bigr)^*.$$

Then $<x|Y>$ is the complex conjugate of $Y(x) = <Y|x>$. This definition is a generalization of the property $<x|y> = <y|x>^*$ of the scalar product in $\mathcal{H}$.

THEOREM *(Banach). Let $\mathcal{B}$ be a Banach space, and $\mathcal{B}^*$ its dual space. A linear functional $\tilde{X}$ on $\mathcal{B}^*$ is of the form*

$$\tilde{X}(Y) = <Y|x>$$

with a certain $x \in \mathcal{B}$ and $Y \in \mathcal{B}^*$, if and only if $\tilde{X}$ is continuous in the weak topology of $\mathcal{B}^*$.

One can now consider anti-linear continuous functional $\tilde{X}$ on $\mathcal{B}^*$ and denote the space of all $\tilde{X}$ by $\mathcal{B}^{**}$. For a wide class of Banach spaces $\mathcal{B}$ (called reflexive) there is a natural one-to-one correspondence between a $x \in \mathcal{B}$ and $\tilde{X} \in \mathcal{B}^{**}$ given by

$$\tilde{X}(Y) = \bigl(Y(x)\bigr)^* = <Y|x>^*.$$

Then $<Y|x>^*$ is a generalization of $<x|y> = <y|x>^*$, and we can consider the functional $\tilde{X}$ at the element $Y \in \mathcal{B}^*$ as a generalization of the scalar product. Therefore we use notation $<x|Y>$ for $Y(x)^*$, i.e., $<x|Y> = Y(x)^*$.

2.6. Coordinate representation

Let Q be a coordinate operator, and let P be a momentum operator. If $\Psi(q) \in L^2(\mathbb{R})$ is a smooth function, then these operators can be represented by the equations

$$Q\Psi(q) = q\Psi(q), \qquad P\Psi(q) = -i\hbar\frac{d}{dq}\Psi(q). \tag{8}$$

The operator $P = -i\hbar d/dq$ has no eigenfunctions in $L^2(\mathbb{R})$. The eigenfunctions

$$<q|p> = (2\pi\hbar)^{-1/2} \exp\{(i/\hbar)qp\} \tag{9}$$

does not belong to the space $L^2(\mathbb{R})$, since $\| \exp\{(i/\hbar)qp\}\|^2_{\mathcal{H}} = 1$. At the same time it is obvious that (9) belong to the space $\mathcal{J}^*(\mathbb{R})$ of linear functionals, and it can be proved that they form a complete set of functionals in that space. Every functional in $\mathcal{J}^*(\mathbb{R})$ and every function in $\mathcal{H} = L^2(\mathbb{R})$, can be expanded in a Fourier integral over the functions (9). In the space $\mathcal{H} = L^2(\mathbb{R})$ this expansion converges in norm.

If $\Psi(q) \in \mathcal{J}(\mathbb{R})$, then

$$\int dq \left| Q^k \left(i P^l \right) \Psi(q) \right| < \infty$$

for all $k, l \in \mathbb{N}$, and then the operators Q and P are maps from $\mathcal{J}(\mathbb{R})$ into itself.

For Ψ_1 and Ψ_2 in $\mathcal{J}(\mathbb{R}) \subset L^2(\mathbb{R})$, we define the scalar product

$$<\Psi_1|\Psi_2> = \int dq\, \Psi_1^*(q)\Psi_2(q).$$

As a result, we can consider $\mathcal{J}(\mathbb{R}) \subset L^2(\mathbb{R}) \subset \mathcal{J}^*(\mathbb{R})$ as a rigged Hilbert space that gives the coordinate representation.

Eigenvectors of operators Q and P

Let $|q>$ and $|p>$ be eigenvectors of the operators Q and P:

$$Q|q> = |q>q, \qquad P|p> = |p>p. \tag{10}$$

These vectors are orthonormal

$$<q|q'> = \delta(q - q'), \qquad <p|p'> = \delta(p - p'),$$

and the following completeness condition are satisfied

$$\int |q>dq<q| = I, \qquad \int |p>dp<p| = I. \tag{11}$$

Relations (11) are compact forms of the equations

$$<\Psi_1|\Psi_2> = \int <\Psi_1|q>dq<q|\Psi_2> = \int <\Psi_1|p>dp<p|\Psi_2>.$$

Here $<q|\Psi>$ and $<p|\Psi>$ are representations of $|\Psi> \in \mathcal{H}$ by the square-integrable functions

$$<q|\Psi> = \Psi(q), \qquad <p|\Psi> = \Psi(p),$$

where $<\Psi|q> = \Psi^*(q)$ and $<\Psi|p> = \Psi^*(p)$. The function $\Psi(q) \in L^2(\mathbb{R})$ is a coordinate representation of $|\Psi>$, and $\Psi(p) \in L^2(\mathbb{R})$ is a momentum representation of $|\Psi>$, where $L^2(\mathbb{R})$ is a representation of the Hilbert space $\mathcal{H}$. The Hilbert space $\mathcal{H}_q = L^2(\mathbb{R})$ of all $\Psi(q) \in L^2(\mathbb{R})$ is called the coordinate representation of a Hilbert space $\mathcal{H}$. The space $\mathcal{H}_p = L^2(\mathbb{R})$ of all $\Psi(p) \in L^2(\mathbb{R})$ is a momentum representation of $\mathcal{H}$.

Let A be a linear operator on $\mathcal{H}$. Then

$$(A\Psi)(q) = <q|A\Psi>, \qquad (A\Psi)(p) = <p|A\Psi>.$$

In particular, the operators Q and P give

$$(Q\Psi)(q) = <q|Q\Psi> = <q|Q|\Psi> = q<q|\Psi> = q\Psi(q),$$
$$(P\Psi)(p) = <p|P\Psi> = <p|P|\Psi> = p<p|\Psi> = p\Psi(p).$$

As a result, the operator Q is represented by the multiplication operator on $\mathcal{H}_q$, and P is represented by the multiplication operator on $\mathcal{H}_p$. Moreover, we have equations (8). Then P is a differential operator on $\mathcal{H}_q$.

Multiplication of (10) by $<q'|$ gives

$$q'<q'|q> = q<q'|q>, \qquad -i\hbar\frac{d}{dq'}<q'|p> = p<q'|p>.$$

These equations have the solutions

$$<q'|q> = \delta(q'-q), \qquad <q'|p> = \frac{1}{(2\pi\hbar)^{1/2}}e^{\frac{i}{\hbar}q'p},$$

where $\delta(q'-q)$ is a Dirac delta-function. Then $<q'|q>$ is a generalized eigenfunction of the operator Q. The function $<q'|p>$ is an eigenfunction of P. These eigenfunctions are not square-integrable.

Unitary equivalence of representations

There is a map that transforms the coordinate representation into momentum. It can be realized by the Fourier integral operator $\mathcal{F}$ on $L^2(\mathbb{R}^n)$. The *Fourier operator* $\mathcal{F}$ is defined by the relation

$$\Psi(p) = \mathcal{F}\big[\Psi(q)\big] = \frac{1}{(2\pi\hbar)^{n/2}}\int e^{-\frac{i}{\hbar}qp}\Psi(q)\,dq.$$

The Fourier operator $\mathcal{F}$ is unitary since

$$<\Psi|\Psi> = \int |\Psi(q)|^2\,dq = \int |\Psi(p)|^2\,dp = <\mathcal{F}\Psi|\mathcal{F}\Psi>.$$

This is the Parseval's equality. The Fourier transform is a map of a test function $\Psi(q) \in \mathcal{J}(\mathbb{R}^n)$ into a test function $\Psi(p) \in \mathcal{J}(\mathbb{R}^n)$. This transformation is realized by the functions

$$<q|p> = \frac{1}{(2\pi\hbar)^{n/2}} \exp \frac{i}{\hbar} qp, \qquad <p|q> = \frac{1}{(2\pi\hbar)^{n/2}} \exp -\frac{i}{\hbar} qp.$$

Note, that $<q'|q> = \delta(q' - q)$ can be presented as

$$<q'|q> = \int <q'|p> dp <p|q> = \frac{1}{(2\pi\hbar)^n} \int dp \exp \frac{i}{\hbar}(q' - q)p.$$

As a result, the coordinate and momentum representations are unitary equivalent to each other. These representations are also called the *kinematical Schrödinger representations*.

2.7. *X*-representation

If $\mathcal{H}$ is a separable Hilbert space, then there is a countable basis $|k> = |e_k> \in \mathcal{H}$, where $k \in \mathbb{N}$, such that

$$<k|l> = \delta_{kl}, \qquad \sum_{k=1}^{\infty} |k><k| = I.$$

In the general case, we can consider a complete basis $|x> = |e_x>$, where $x \in \mathbb{R}$ is a continuous index. The ket-vectors $|x> = |e_x>$ form a basis, if the following conditions are satisfied:

$$<x|y> = \delta(x - y), \qquad \int |x> dx <x| = I.$$

The second equation means that

$$\int <\Psi_1|x><x|\Psi_2> dx = <\Psi_1|\Psi_2>$$

for all $|\Psi> \in \mathcal{H}$. The ket-vectors $|x>$ does not belong to a Hilbert space. However, any linear combination of $|x>$ of the form

$$|\Psi> = \int |x> \Psi(x)\, dx, \tag{12}$$

where $\Psi(x) \in L^2(\mathbb{R})$ has a finite norm $\|\Psi\|^2_{\mathcal{H}} = <\Psi|\Psi> < \infty$, and $|\Psi>$ belongs to a Hilbert space $\mathcal{H}$. A set of all linear combinations (12) forms a subspace $\mathcal{H}_x$ of the Hilbert space $\mathcal{H}$. The subspace $\mathcal{H}_x$ is generated by the ket-vector $|x>$.

In quantum mechanics, we postulate that for the set $\mathcal{M}$ of observables there is a set of commuting observables $X_1, \ldots, X_n$ in $\mathcal{M}$, which have a set of (generalized)

eigenvectors $|x> = |x_1, \ldots, x_n>$:

$$X_k|x_1, \ldots, x_n> = |x_1, \ldots, x_n> x_k,$$

such that every element $|\Psi>$ in $\mathcal{H}$ can be represented as

$$|\Psi> = \int |x_1, \ldots, x_n><x_1, \ldots, x_n|\Psi> dx_1 \ldots dx_n,$$

where $\Psi(x_1, \ldots, x_n) = <x_1, \ldots, x_n|\Psi> \in L^2(\mathbb{R}^n)$. As a result, the ket-vectors $|x_1, \ldots, x_n>$ are considered as eigenvectors of operator $X_1, \ldots, X_n$. An orthonormal and complete system of such ket-vectors $|x_1, \ldots, x_n>$ defines a *X-representation*. For example, the coordinate (q) representation is a X-representation.

Let A be a linear operator on a Hilbert space $\mathcal{H} = L^2(M)$. Then A is called a Hilbert–Schmidt operator if there exists a function $a(x, y) = <x|A|y> \in L^2(M \times M)$, such that A is expressed via $a(x, y)$ in the form

$$\begin{aligned}(A\Psi)(x) = <x|A\Psi> &= \int <x|A|y><y|\Psi> dy \\ &= \int a(x, y)\Psi(y)\, dy. \end{aligned} \tag{13}$$

The function $a(x, y) = <x|A|y>$ is called the *kernel* of the operator A. In general, it is possible to express a broad class of operators A in the form (13), but with the more general (distribution) kernels. As a result, the kernel $a(x, y) = <x|A|y>$ is a generalized function (distribution) on $M \times M$. For example, the operator Q has the kernel $<q'|Q|q> = <q'|q>q = q\delta(q' - q)$.

Suppose $|x> = |e_x>$ is a complete orthonormal system. Let $\hat{P}(x, y) = |x><y|$ be a ket-bra operator. The following properties are satisfied.

(1) Multiplication is defined by $\hat{P}(x, y)\hat{P}(z, s) = <y|z>\hat{P}(x, s)$. If $|x>$ is an orthonormal system, then $<y|z> = \delta(y - z)$. Moreover, we have

$$\int dy \hat{P}(x, y)\hat{P}(y, z) = \hat{P}(x, z).$$

(2) The trace of $\hat{P}(x, y)$ is $Tr[\hat{P}(y, x)] = <x|y>$.
(3) If $[\hat{P}(x, y)]^*$ is an adjoint operator of $\hat{P}(x, y)$, then $[\hat{P}(x, y)]^* = \hat{P}(y, x)$. The operator $P(x) = \hat{P}(x, x)$ is self-adjoint.
(4) The operator $P(x) = \hat{P}(x, x)$ is a projection, i.e., $[P(x)]^2 = \hat{P}(x)$, and $[P(x)]^* = P(x)$.
(5) For each projection operator $P(x)$, we can define the ket-bra operator $\hat{P}(x, y)$ by the polarization procedure.

Then an operator A can be uniquely represented in the form

$$A = \int dx\, dy\, a(x, y)\hat{P}(x, y),$$

where $a(x, y) = <x|A|y>$ is the kernel of the operator A. The kernel of A can be presented as

$$a(x, y) = <x|A|y> = Tr\big[\hat{P}(y, x)A\big].$$

Note that any bounded self-adjoint operator A on a Hilbert space $\mathcal{H}$ can be represented as a multiplication operator on $L^2(M)$ such that $(A\Psi)(x) = a(x)\Psi(x)$, where $a(x)$ is a bounded real-valued measurable function on M.

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Chapter 3

Mathematical Structures in Quantum Kinematics

3.1. Mathematical structures

Mathematics as a hierarchy of mathematical structures

A mathematical structure is obtained by taking a set of objects and equipping this set with a structure by defining relations between these objects. The common character of the different structures is that they can be applied to sets of objects whose nature has not been specified.

To define a structure, one takes as given one or several relations, into which these elements enter. Then one postulates that the given relation, or relations, satisfy certain conditions, which are explicitly stated and which are the axioms of the structure under consideration. The logical consequences are deduced without any hypothesis about the nature of the elements.

Modern mathematics distinguishes three basic kinds of structures.

(a) *Algebraic structures* in which the relations are "laws of composition", for example, relations between three elements determining the third uniquely in terms of the other two.
(b) *Order structures*, in which the relations are order relations, as, for example, the real number structure, in which the order relation is $\leqslant$.
(c) *Topological structures*, which give an abstract mathematical formulation of the intuitive concepts of neighbourhood, limit and continuity.

These mathematical structures are also called the mother-structures.

There are also multiple structures, which arise when two or more of basis king of structures (mother-structures) are combined organically by one or more axioms which set up a connection between them.

The great problem is the relation between the empirical world and mathematical world. That there is a connection between physical phenomena and mathematical structures, seems to be fully confirmed by the discoveries of quantum physics.

The mother-structures

(1) The relations which form the starting point for the definition of a structure can be of very different characters. The relation that used in the group structure is called a "law of composition", i.e., a relation between three elements which determines the third uniquely as a function of the first two. When the relations which enters the definition of a structure are "laws of composition", the corresponding structure is called an *algebraic structure*. For example, a ring structure is defined by two laws of composition with suitable axioms: the addition and multiplication define a ring structure on the set of these numbers.

(2) Another important type is furnished by the *structures defined by an order relation*. This is a relation between two elements x, y which is expressed most frequently in the form "x is less than or equal to y", and which is represented in general by xRy. It is not at all supposed here that it determines one of the two elements x, y uniquely as a function of the other. The axioms to which it is subjected are following: (a) for every x we have xRx; (b) from the relations xRy and yRx follows $x = y$; (c) the relations xRy and yRz have as a consequence xRz. An obvious example of a set with a structure of this kind is the set of real numbers, when the symbol R is replaced by the symbol $\leqslant$. Note that we have not included among the axioms the following property: for every pair of elements x and y either xRy or yRx. In other words, the case in which x and y are incomparable is not excluded. It is easy to give examples of very important order structure, in which such a phenomenon appears. This is what happens when X and Y denote parts of the same set and the relation XRY is interpreted to mean "X is contained in Y". Also if $f(x)$ and $g(x)$ are real-valued functions defined on an interval $a \leqslant x \leqslant b$, while $f(x)Rg(x)$ is interpreted to mean $f(x) \leqslant g(x)$ for all x.

(3) We want to say a few words about a third large type of structures—topological structures (or topologies). They define a mathematical formulation of the intuitive concepts of neighborhood, limit and continuity. For example, a continuous function is a function $y = f(x)$ for which small changes in the input x result in small changes in the output y. In calculus, a function $f(x)$ in a single variable x is said to be continuous at point x_0 if $\lim_{x \to x_0} f(x) = f(x_0)$.

The multiple and particular structures

In mathematics, the organizing principle is the concept of a hierarchy of mathematical structures, going from the simple to the complex, from the general to the particular [29].

(1) At the center of the mathematics are founded the great types of structures that are called the mother-structures. Mathematics distinguishes three basic kinds of structures: algebraic, ordering, and topology. Each structure has its own set of

general theorems. These are available once the underlying type of structures is recognized in any situation.

(2) Beyond this center, appear the structures which can be called the multiple structures. They involve two or more of great mother-structure combined organically by one or more axioms. Thus, one has topological algebra. This is a theory of structures in which occur at the same time, one or more laws of composition and a topology, connected by the condition that the algebraic operations be continuous (for the topology under consideration) functions of the elements on which they operate. The combination of order structure and algebraic structure gives the theory of integration and the spectral theory of operators.

(3) Beyond the multiple structures there are the particular theories. In these theories the elements of the sets under consideration, which, in the general structures have remained entirely indeterminate, obtain a more definitely characterized individuality. But they have no longer their former autonomy. They have become crossroads, where several more general mathematical structures meet and react upon one another.

(4) It should be noted the theory of categories and functors that deals with mathematical structures and relationships between them. Categories now appear in most branches of mathematics and have been a unifying notion. Instead of focusing merely on the individual objects (spaces, rings, algebras) possessing a given structure, category theory emphasizes the morphisms (the structure-preserving mappings) between these objects. By studying these morphisms, we are able to learn more about the structure of the objects. The study of morphisms then provides a tool for studying general properties of mathematical structures. The notion of a category is an axiomatic formulation of this idea of relating mathematical structures to the structure-preserving maps between them. Functors are structure-preserving maps between categories. The theory of categories and functors is not widely used in physics. As an example of the functor, we can point out the quantization as a structure-preserving map between classical and quantum theories [16,92].

3.2. Order structures

If M is a set, then its square $M \times M$ is defined as the set of all pairs (x, y), where $x, y \in M$. Let R be an arbitrary subset of $M \times M$. In the following way R defines a binary relation on M: If $x, y \in M$, then we say that the element x has the relation to the element y, and we express this by xRy if and only if the pair belongs to the subset R. In other words, the notations xRy and $(x, y) \in R$ are equivalent.

An important type of binary relation is that of the *equivalence relations*, that is, binary relations having the properties of reflexivity, transitivity and symmetry. To denote equivalence relations, we shall use the symbol $x \sim y$, and $x \equiv y$, or $x = y(\mathrm{mod}\, R)$.

DEFINITIONS. An *equivalence relation* on a set M is a binary relation R given on M such that the following properties are satisfied:

(1) Reflexivity: xRx for all $x \in M$.
(2) Transitivity: If xRy and yRz, then xRz.
(3) Symmetry: If xRy, then yRx.

Another important type of binary relation is constituted by the *relation of partial order*, that is, binary relations having the properties of reflexivity, transitivity and antisymmetry. A set M on which a partial order is given is called partially ordered. To denote partial order, we shall use the symbol $\leqslant$.

DEFINITIONS. A *relation of partial order* on a set M is a binary relation R given on M such that the following conditions are satisfied:

(1) Reflexivity: xRx for all $x \in M$.
(2) Transitivity: If xRy and yRz, then xRz.
(3) Antisymmetry: If xRy and yRx, then $x = y$.

If $x, y \in M$ and $x \leqslant y$, then depending on the circumstances, we say that x is less than or equal to y, x is contained in y, x precedes y. If $x \leqslant y$ and $x \neq y$, we write $x < y$. The binary relation $<$, of course, is not reflexive. We shall denote by $\geqslant$ the relation that is inverse to the relation $\leqslant$, i.e., $x \geqslant y$ if and only if $x \leqslant y$.

Let M be a set on which a partial order is given. The elements x and y of this set are called *comparable* if $x \leqslant y$ or $y \leqslant x$. It is by no means true that *any* two elements of M must necessarily be comparable—this is precisely the reason why we speak of a "partial" order. A partially ordered set in which any two elements are comparable is called an *ordered set*, or linearly ordered set, or chain.

On a set of observables, it is possible to consider a structure of partially ordered set. Suppose $(\rho|A) = Tr[\rho A]$. We say that $A \leqslant B$ whenever $(\rho|A) \leqslant (\rho|B)$ for all ρ. In particular, we write $A \geqslant 0$ if and only if $(\rho|A) \geqslant 0$ for all ρ. The relation $\leqslant$ defined above is a partial ordering relation on the set of observables.

3.3. Topological structures

Topological structures are mathematical structures that give the formalization of intuitive concepts such as neighborhood, continuity, compactness, connectedness.

A system T of subsets of a set M defines a *topology* on M if T contains the following:

(1) the empty set and the set M itself,
(2) the union of every one of its subsystems,
(3) the intersection of every one of its finite subsystems.

The sets in T are called the *open sets* of the topological space (M, T). We shall often omit T and refer to M as a topological space.

A topology can be defined in terms of set operations. A *topological space* is a set M, together with a collection T of subsets of M satisfying the following conditions:

(1) The empty set and M are in T.
(2) The intersection of any collection of sets in T is also in T.
(3) The union of any pair of sets in T is also in T.

Under this definition, the sets in the topology T are the *closed sets*, and their complements in M are the open sets.

A *neighbourhood* of the element A of M is a set containing an open set which contains A. An element A of M is a *limit point* of a subset M_0 of M if every neighbourhood of A contains at least one element $B \in M_0$ different from A. A set M_0 of a topological space M is *closed* if it contains all its limit points. If $M_0 \subset M$, the intersection of all closed subsets of M which contain M_0 is called the *closure* of M_0.

Suppose M is a topological space, and A, B are in M. We say that A and B can be *separated by neighbourhoods* if there exists a neighbourhood U_A of A and a neighbourhood U_B of B such that U_A and U_B are disjoint $U_A \cap U_B = \emptyset$. M is a separated space if any two distinct points of M can be separated by neighborhoods.

A topological space (M, T) is said to be T_2 or *separated space*, if for every pair of distinct points $A, B \in M$, there exist disjoint open sets $U_A, U_B \in T$ such that $A \in U_A$ and $B \in U_B$. A separated space is also called the *Hausdorff space*.

Almost all spaces used in quantum theory are Hausdorff. For example, the real numbers form a Hausdorff space. More generally, all metric spaces are Hausdorff.

There are many ways of defining a topology on $\mathbb{R}$, the set of real numbers. The standard topology on $\mathbb{R}$ is generated by the open intervals. The open intervals form a base or basis for the topology, meaning that every open set is a union of basic open sets.

For each metric we can give a metric topology, in which the basic open sets are open balls defined by the metric. This is the standard topology on any normed linear space. On a finite-dimensional linear space this topology is the same for all norms. Many sets of operators are endowed with topologies that are defined by specifying when a particular sequence of functions converges to the zero function. In fact, many topological spaces of quantum kinematics have the Hausdorff condition explicitly stated in their definitions.

A set M is called the *metric space* if there is defined a real-valued function d with domain $M \times M$ such that

(a) $d(A, B) \geqslant 0$ for all $A, B \in M$.
(b) $d(A, B) = 0$ if and only if $A = B$.

(c) $d(A, B) = d(B, A)$ for all $A, B \in M$.
(d) $d(A, B) \leqslant d(A, C) + d(C, B)$ for all $A, B, C \in M$.

The function d is called the metric.

For each element $A \in M$ of a metric space M and each positive number ε, we associate the set

$$U_\varepsilon(A) = \{B\colon\ d(A, B) < \varepsilon\}, \tag{1}$$

and call it the open sphere with center A and radius ε. The totality of such open sets satisfies the axioms of open sets in the definition of the topological space. Hence a metric space M is a topological space.

A set of all neighborhoods (1) forms a base $\mathcal{B} = \{U_\varepsilon(A)\colon\ A \in M,\ \varepsilon \in \mathbb{R}_+\}$ for the topology. This topology is called the *metric topology*.

In normed space M with the norm $\|\cdot\|$, it is possible to define a topology. The set of all neighborhoods $U_\varepsilon(A) = \{B\colon\ \|A - B\| < \varepsilon\}$ forms a base $\mathcal{B} = \{U_\varepsilon(A)\colon\ A \in M,\ \varepsilon \in \mathbb{R}_+\}$ of the topology on set M. This topology is called the *norm topology*.

A *seminorm* on a linear space $\mathcal{H}$ over $\mathbb{R}$ is a mapping $p : \mathcal{H} \to \mathbb{R}$, such that the following conditions are satisfied:

(1) Triangle inequality (subadditivity): $p(A + B) \leqslant p(A) + p(B)$.
(2) Positive scale property: $p(aA) = |a|p(A)$ $(a \in \mathbb{R})$.

A seminorm $p(x)$ satisfies $p(0) = 0$, and $p(A) \geqslant 0$ for all A. A norm is a seminorm with the additional property $p(A) = 0$ implies $A = 0$. In general, there exists $A \neq 0$ such that $p(A) = 0$.

The set of all neighborhoods $U_\varepsilon(A) = \{B\colon\ p(A - B) < \varepsilon\}$ forms the base $\mathcal{B} = \{U_\varepsilon(A)\colon\ A \in M,\ \varepsilon \in \mathbb{R}_+\}$. This is the *seminorm topology*.

If p is a seminorm that is not a norm, then there exists $A \neq 0$ such that $p(A) = 0$. All such elements A are in every neighborhood of 0. Hence these points are not separated from 0 and the seminorm p does not define a Hausdorff topology.

3.4. Algebraic structures

Maps

The general idea of assigning to each element of some set an element from the same set or possibly from different set will arise so often in algebraic structures that we give a separate definition for this concept.

DEFINITIONS. A *mapping f from a set M into a set N* is a rule that assigns to each element A of M exactly one element B of N. We say that *f maps A into B*, and that *f maps M into N*.

The classic notation to denote that f maps A into B is $f(A) = B$. The element B is the *image of A under* f. The fact that f maps M into N will be symbolically expressed by $f : M \to N$.

We remark that for $f : M \to N$, the set M is the *domain of* f, the set N is the *codomain of* f, and the set $\mathrm{Im}(f) = f(M) = \{f(A)\colon\ A \in M\}$ is the *image of M under* f.

DEFINITIONS. A mapping from a set M into a set N is *one-to-one* if each element of N has at most one element of M mapped into it.

A mapping from a set M into a set N is *onto* N if each element of N has at least one element of M mapped into it.

To show that f is one to one, you show that $f(A) = f(B)$ implies $A = B$. To show that f is onto N, you show that for each $B \in N$, there exists $A \in M$ such that $f(A) = B$. In the Bourbaki's terminology, a one-to-one map is an *injection*, an onto map is a *surjection*, and a map that is both one to one and onto is a *bijection*.

The following are examples of some mappings from $\mathbb{R}$ into $\mathbb{R}$.

(1) $x \iff x^3$ is a bijection.
(2) $x \iff \exp(x)$ is one-to-one, but not onto.
(3) $x \iff x^3 + x^2$ is onto, but not one-to-one.
(4) $x \iff \sin(x)$ is neither onto, nor one-to-one.

Algebraic structure

An algebraic structure consists of one or more sets closed under one or more operations, satisfying some axioms. An algebraic structure can be considered as the collection of all possible models of a given set of axioms. More concretely, an algebraic structure is any particular model of some set of axioms. This definition of an algebraic structure should not be taken as restrictive. Anything that satisfies the axioms defining a structure is an example of this structure, regardless of how many other axioms are used. For example, all groups are also semi-groups and loops.

The Cartesian product of set M is the set of all ordered n-tuples $\{A_1, A_2, \ldots, A_n\}$, where $A_k \in M$. The Cartesian product is denoted by M^n.

DEFINITION. A *n-ary operation* on set M is a mapping $g : M^n \to M$ that assigns to each ordered system of n elements $A_1, A_2, \ldots, A_n$ of the set M exactly one element $g(A_1, A_2, \ldots, A_n) \in M$.

A n-ary operation is also called the interior composition law.

DEFINITION. An *exterior composition law* for a set M is a mapping g from a set $N \times M$ into M. The set N is called the set of operators.

Algebraic structures are determined by given interior and exterior laws of compositions on a set.

DEFINITION. An *algebraic structure* on a set M is defined by the following conditions.

(1) There are interior (n-ary) laws of compositions on the set M.
(2) There are exterior laws of compositions for M and the sets of operators.
(3) There are axioms for interior and exterior composition laws.

Algebraic operation

In its simplest meaning, an operation combines two values to produce a third. Examples include addition, subtraction, multiplication and division. Such operations are often called binary operations. Other operations can involve a single value, for example negation (changing the sign of a number), inversion (dividing one by the number) and taking a square or square root. These are called unary operations.

Operations can involve mathematical objects other than numbers.

(1) The logical values true and false can be combined using logic operations, such as and, or, not.
(2) Vectors can be added and subtracted.
(3) Operations on sets include the binary operations union and intersection, and the unary operation of complementation.
(4) Operations on functions include pointwise multiplication, composition and convolution.

Operations may not be defined for every possible value. For example, in the real numbers one cannot divide by zero or take square roots of negative numbers. The values for which an operation is defined form a set called its *domain*. The set, which contains the produced values, is called the *codomain*, but the set of actual values attained by the operation is its *range*. For example, in the real numbers, the squaring operation only produces nonnegative numbers. The codomain is the set of real numbers but the range is the nonnegative numbers.

Operations can involve dissimilar objects. For example, a vector can be multiplied by a scalar to form another vector, and the scalar product of two vectors gives a scalar.

DEFINITION. An *operation* g is a map from $M_1 \times \cdots \times M_n$ into N. The sets M_k, where $k = 1, \ldots, n$, are called the domains of the operation, the set N is

called the codomain. The fixed nonnegative integer n (the number of arguments) is called the *arity of the operation*.

Thus a unary operation has arity one, and a binary operation has arity two. An operation of arity zero, called the nullary operation, is simply an element of the codomain N. The operation of arity n is called the n-ary operation.

The case of a nullary operation, means that in M a certain element is fixed that does not depend on the choice of any elements in M. Thus, in choosing the unit element of a group, we are making use of a nullary operation.

A unary operation is an operation that assigns to every element $A \in M$ a uniquely determined element $g(A) \in M$, i.e., it is a single-valued mapping of M into itself. For example, squaring is a unary operation on the real numbers. Another unary operation is the factorial, $n!$. A unary operation g on the set M is a function $g : M \to M$.

A *binary operation* (composition law) on a set M is a map g from $M \times M$ into M that assigns to each ordered pair of elements $A, B \in M$ some element $g(A, B)$ of the set. That g takes values in the same set M that provides its arguments is the property of closure. The word *ordered* in this definition is very important. It allows the possibility that the element assigned to the pair A, B may be different from the element assigned to the pair B, A. Note, that we were careful not to say that to each ordered pair of elements is assigned *another* or a *third element*, for we wish to permit cases such as occur in addition of numbers $0 + A = A$, and multiplication of numbers $1 \cdot A = A$. Typical examples of binary operations are the addition and multiplication of numbers and matrices as well as composition of functions.

Commutativity and associativity

DEFINITION. A binary operation g on a set M is said to be *commutative* if $g(A, B) = g(B, A)$ for all $A, B \in M$. Otherwise, the operation is noncommutative.

The well-known examples of commutative binary operations are addition and multiplication of real numbers. For example, multiplication of real numbers is commutative since $AB = BA$ for all $A, B \in \mathbb{R}$. On the other hand, division of real numbers is noncommutative, since $A/B = B/A$, if and only if A and B are identical.

DEFINITION. A binary operation $g(A, B)$ on a set M is said to be *anticommutative* if $g(A, B) = -g(B, A)$ for all $A, B \in M$.

The most well-known example of anticommutative binary operation is subtraction of real numbers, i.e., $g(A, B) = A - B = -(B - A) = -g(B, A)$.

DEFINITION. A binary operation g on a set M is said to be *noncommutative*, if there exists A and B in M such that $[A, B] = g(A, B) - g(B, A) \neq 0$. The element $[A, B]$ of M is called the *commutator* of A and B with respect to the binary operation g.

Examples of the noncommutative binary operations are subtraction $g(A, B) = A - B$, division $g(A, B) = A/B$, exponentiation $g(A, B) = A^B$. In general, we have

$$A - B \neq B - A, \qquad A/B \neq B/A, \qquad A^B \neq B^A,$$

where A and B are real numbers. Examples of the noncommutative operations are also function composition and matrix multiplication.

The commutator can be considered as a new binary operation $g_c(A, B) = [A, B]$ on the set M, which is anticommutative. As a result, the set M with noncommutative binary operation g can be presented as a set with the anticommutative operation $[A, B]$.

DEFINITION. A binary operation g on a set M is said to be *associative*, if it satisfies the associative law: $g(g(A, B), C) = g(A, g(B, C))$ for all $A, B, C \in M$. For multiplicative operation, $(AB)C = A(BC)$ for all $A, B, C \in M$.

The following are examples of some associative operations.

(1) Addition and multiplication of real numbers are associative.
(2) Addition and multiplication of complex numbers and quaternions are associative. Addition of octonions is also associative, but multiplication of octonions is nonassociative.
(3) Matrix multiplication is associative. Because linear transformations can be represented by matrices, one can conclude that linear transformations compose associatively.

DEFINITION. A binary operation g on a set M is said to be *nonassociative* if $(A, B, C) = g(g(A, B), C) - g(A, g(B, C)) \neq 0$ for some $A, B, C \in M$.

Here, (A, B, C) is called the *associator* of elements A, B and C with respect to binary operation g. The associator can be considered as a new ternary operation on the set M.

Subtraction, division and exponentiation are well-known examples of nonassociative operations:

(1) Subtraction of real numbers A, B, C is nonassociative: $(A - B) - B \neq A - (B - C)$.

(2) Division of real numbers A, B, C is nonassociative: $(A/B)/C \neq A/(B/C)$, where $B \neq 0$ and $C \neq 0$.
(3) Exponentiation of real numbers A, B, C is nonassociative $g(g(A, B), C) \neq g(A, g(B, C))$, where $g(A, B) = A^B$.

3.5. Examples of algebraic structures

In its widest sense, a binary operation is a rule that assigns one element of M to certain ordered pair of elements of a given set M. A binary algebraic operation will be understood, as a rule, in a narrower sense: the operation must be defined for every ordered pair of elements and must be unique. Every set in which an algebraic operation of this type is given is called a groupoid. This is still rather too wide a concept. The concept of a semi-group, which has application in quantum dynamics, is somewhat narrower.

A.1. Groupoid. A groupoid is a set M, together with a binary internal operation g. Many books have another axiom for a groupoid, namely that M is closed under the operation g, that is $g(A, B) \in M$ for all $A, B \in M$. For us, this is a consequence of our definition of a binary operation on M.

Note that a groupoid is not just a set M. Rather, a groupoid $<M, g>$ is made up of two objects, the set M and the binary operation g on M. There are two ingredients involved. Denoting the groupoid by the single set symbol M is logically incorrect. Nevertheless, as you get into the theory, the logical extensions of the notation become hard to read. We emphasize that when you are speaking of a specific algebraic structure on M, you must make it clear what the algebraic operations on M are to be. A set could have a family of binary operations defined on it, all giving different algebraic structures.

A.2. Semi-group. A semi-group is an associative groupoid. A semi-group is a groupoid, in which the associative law holds: for arbitrary elements A, B, and C, $(AB)C = A(BC)$. A semi-group in which any two elements A, B satisfy the commutative law $AB = BA$ is called commutative, or abelian.

A.3. Unital groupoid. A groupoid with unity (or unital groupoid) is a set M, together with a binary internal operation g and a nullary operation e. The operation e assigns to each element of M the unity I such that $g(I, A) = g(A, I) = A$.

A.4. Monoid. A monoid is a unital semi-group. A monoid is a set M, together with a binary operation $g : M \times M \to M$, such that the following axioms are satisfied:

(1) The binary operation g is associative: $g(g(A, B), C) = g(A, g(B, C))$ for all A, B, C in M.
(2) There exists an element I in M such that $g(A, I) = g(I, A) = A$ for all A in M. This element I is an *identity element* for g on M.

An *inverse element* of $A \in M$ is an element $B \in M$ such that $g(A, B) = g(B, A) = I$. It is clear, that A is inverse of B if and only if B is inverse of A.

A.5. Group. A group is a set M, together with three internal algebraic operations g, e, and g' on M, such that the following axioms are satisfied:

(1) The binary operation g is associative, i.e., $g(g(A, B), C) = g(A, g(B, C))$ for all $A, B, C \in M$.
(2) The nullary operation e that assigns to each element $A \in M$ an element $e(A) = I \in M$, such that $g(e(A), A) = g(A, e(A)) = A$ for all $A \in M$. The element $e(A) = I$ is an identity element for g on M.
(3) The unary operation g' that assigns to each element $A \in M$ exactly one element $g'(A)$ of M called the inverse of A with respect to g, such that $g(g'(A), A) = g(A, g'(A)) = I$ for all $A \in M$. The element $g'(A)$ is an inverse of A with respect to g.

Using the notation $g(A, A) = AB$, $e(A) = I$, $g'(A) = A^{-1}$, we have the conditions

$$(AB)C = A(BC), \qquad IA = AI = A, \qquad A^{-1}A = AA^{-1} = I.$$

A group M is *abelian* if its binary operation g is commutative.

A.6. Quasigroup. A quasigroup is a groupoid in which the equations

$$AX = B, \qquad YA = B$$

are uniquely solvable for arbitrary elements A and B.

Let $B\backslash A$ be a solution of the equation $AX = B$, and let B/A be a solution of the equation $YA = B$. Then we can consider two binary operations that are called the left and right divisions. A quasigroup is a set M, together with three binary internal operations: the multiplication AB, the right division $B\backslash A$, and the left division B/A, such that

$$A(B\backslash A) = B, \quad (AB)\backslash A = B, \quad (B/A)A = B, \quad (BA)/A = B.$$

A.7. Loop. A loop is a quasigroup M with identity element I. A unital quasigroup is called a loop. For each A in M, there exist elements $I\backslash A$ and I/A. In general, these elements are not inverse of A.

A.8. Loop with reversibility. A loop with reversibility is a loop M such that the elements $I\backslash A$ and I/A are inverse of A, i.e.,

$$(BA)(I\backslash A) = B, \qquad (I/A)(AB) = B$$

for all $A, B \in M$.

Substitution of $B = I\backslash A$ into the equation $(I/A)(AB) = B$ gives $I\backslash A = I/A$ for all A of M. As a result, each element of a loop with reversibility has the inverse

element

$$A^{-1} = I\backslash A = I/A,$$

such that $A^{-1}A = AA^{-1} = I$. Then a loop M is a loop with reversibility if and only if there exists an element A^{-1} in M such that $A^{-1}(AB) = (BA)A^{-1} = I$ for all $A, B \in M$. A group is a loop M with reversibility such that the binary operation g is associative.

A.9. Valya loop. A Valya loop, is a loop with reversibility, such that its commutant (a set of elements $(AB)(BA)^{-1}$) is an associative subloop, i.e., the set $\{(AB)(BA)^{-1}\colon A, B \in M\}$ is a group.

Algebraic structures with two binary operations

B.1. Ringoid. A ringoid is a set M, together with two binary operations, addition and multiplication, with multiplication distributing over addition.

B.2. Ring. A ring is a set M in which two binary algebraic operations are given: addition and multiplication. Under the operation of addition, it must be a commutative group, and multiplication must be connected with addition by the distributive laws.

A ring $(M, +, \cdot)$ is a set M, together with two internal binary operations $+$ and $\cdot$, such that the following conditions are satisfied:

(1) $(M, +)$ is a commutative (abelian) group.
(2) $(M, \cdot)$ is a groupoid.
(3) These operations are connected by the distributive laws:

$$(A + B) \cdot C = A \cdot C + B \cdot C, \qquad C \cdot (A + B) = C \cdot A + C \cdot B$$

for all $A, B, C \in M$.

A ring is a commutative group with respect to the operation of addition, and it is a groupoid with respect to the operation of multiplication. The multiplication is, in general, not subjected to any restrictions. That is, under the operation of multiplication the ring is only a groupoid—the multiplicative groupoid of M. If the multiplication in the ring is associative, then we speak of an associative ring. In general, the ring is nonassociative. If $(M, \cdot)$ is a semi-group, then the ring is associative.

As an example of an associative, but not commutative ring, we mention the ring of square matrices of order $n \geqslant 2$ with real elements, under the usual operations of addition and multiplication of matrices. Finally, we give one example of a nonassociative ring. This is the ring of vectors of three-dimensional Euclidean space under the usual operations of addition and of vector multiplication. It is easy to verify that this multiplication is neither associative nor commutative.

B.3. Field. A field is a ring $(M, +, \cdot)$, such that the multiplicative groupoid $(M, \cdot)$ is a commutative group. A field is a commutative division ring. For example, $\mathbb{R}$ and $\mathbb{C}$ are fields. We use only fields of real and complex numbers. Note that quaternions form a division ring, which is not a field.

Algebraic structures with exterior compositions law

C.1. Module. Let M be an additively written commutative group and R an associative ring. M is called a left R-module, or a commutative group with operator ring, if for arbitrary $a, b \in R$ and $A, B \in M$ the equations

$$(a+b)A = aA + bA, \quad a(A+B) = aA + aB, \quad (ab)A = a(bA) \tag{2}$$

hold.

Note that multiplication for a module is not a binary operation on one set. It is a rule that associates an element aA of M with each ordered pair (a, A) consisting of an element a of R and A of M. This can be viewed as an operation mapping $R \times M$ into M.

If the ring R has a unit element I_R, then we shall consider only R-modules for which I_R is the identity operator. In other words, to the operator I_R there corresponds the identity map from M into itself, such that $I_R A = A$ for all $A \in M$. Left R-modules with this property are called unitary.

A set M is a right S-module, if for arbitrary $a, b \in S$ and $A, B \in M$ the equations

$$A(a+b) = Aa + Ab, \quad (A+B)a = Aa + Ba, \quad A(ab) = (Aa)b$$

hold. If S is a ring with unity I_S and $AI_S = A$, then M is a unitary right S-module.

A left R-module consists of a commutative group M, together with an operation of *external multiplication* of each element of M by each element of a ring R on the left such that for all $a, b \in R$ and $A, B \in M$, equations (2) are satisfied. The external operation is also called the left multiplication by a.

A left R-module M can be considered as an algebra, such that the following operations are defined:

(1) A binary operation of addition on a commutative group M.
(2) Infinite number of unary operations L_a of left multiplications by $a \in R$ such that $L_a(A) = aA$ and

$$L_a(A+B) = L_a A + L_a B, \quad L_{a+b}A = L_a A + L_b A,$$
$$L_{ab}A = L_a(L_b A)$$

for all $a, b \in R$ and $A, B \in M$.

If A is an element in an arbitrary ring R, then the mapping L_A, such that $L_A B = AB$ where $B \in R$, is called the left multiplication. The additive subgroup of R can therefore be considered as an operator group with R itself as operator domain. Then the ring R is a R-module. Right multiplications are defined similarly.

A R-module M is *cyclic* if there exists $A \in M$ such that $M = \{aA\colon\ a \in R\}$. Thus a cyclic R-module is generated by a single element.

C.2. Bimodule. A bimodule is a commutative group M, such that the following axioms are satisfied:

(a) M is a left R-module.
(b) M is a right S-module.
(c) $(aA)c = a(Ac)$ for all $a \in R$, $c \in S$ and $A \in M$.

C.3. Linear space. We shall consider R-modules in the case where the associative ring R is a field. Every unitary module over an associative field R is called a linear space (or vector space) over this field.

Let F be a field. A linear space over F consists of a commutative group M under addition, together with an operation of multiplication of each element of M by each element of F on the left, such that for all $a, b \in F$ and $A, B \in M$ the following conditions are satisfied:

$$aA \in M, \quad (a+b)A = aA + bA, \quad a(A+B) = aA + aB,$$
$$(ab)A = a(bA), \quad IA = A.$$

The elements of M are vectors and the elements of F are scalars. We shall consider the linear spaces over the fields $\mathbb{R}$ and $\mathbb{C}$.

Note that a module is a generalization of a linear space notion. Instead of numerical fields or fields of other nature of elements, the module allows us to consider an arbitrary properties of multiplication.

A subset X consisting of elements E_k (k ranges over an index set) is a *basis* of a linear space M over a field R if and only if every non-zero element A of M has a unique expression

$$A = \sum_{e_k \in X} a_k E_k, \tag{3}$$

where $E_k \in X$, and a_k are non-zero elements of R.

C.4. Linear algebra. A ring M that has a field R as ring of operators is called a linear algebra over R. The additive group of every algebra M over a (commutative) field R is a linear space over this field as follows immediately from definition of an algebra.

A linear algebra consists of a linear space M over a field F, together with a binary operation of multiplication on the set M, such that for all $a, b \in F$ and

$A, B, C \in M$, the following conditions are satisfied:

$$(aA)B = a(AB) = A(aB), \quad (a+b)A = aA + bA,$$
$$A(B+C) = AB + AC.$$

To define a linear algebra, we use a linear space, where the commutative group $(M, +)$ is replaced by a ring $(M, +, \cdot)$.

In the additive linear space of an algebra M over R let us choose a basis X, consisting of elements E_k (k ranges over an index set). Every element A of M has unique expression (3) where a_k are non-zero elements of R. The addition of elements of M and their multiplication by an element b of R reduce to the addition of corresponding coefficients and the multiplication by b. If $E_i, E_j \in X$, then the product $E_i E_j$, being an element of M, also has an expression in terms of the basis X,

$$E_i E_j = \sum_k c_{ij}^k E_k.$$

The system of elements c_{ij}^k of the field R completely determines the multiplication in the algebra M.

Clearly, the algebra defined by c_{ij}^k will in general be neither associative nor commutative, if the choice of the numbers c_{ij}^k is not subjected to additional restrictions.

Important rings and algebras

Let us consider a linear algebra consists of a linear space M over a field F, together with a binary operation g of multiplication on the set M. We shall speaking of an algebra M.

D.1. An *associative algebra* is a linear algebra M such that the multiplicative bilinear operation g satisfies the condition

$$(A, B, C) = g\big(g(A, B), C\big) - g\big(A, g(B, C)\big) = 0$$

for all A, B, C of M. The operation (A, B, C) is called the *associator*.

D.2. A *Lie algebra* is a linear algebra M over some field F such that the multiplicative binary operation g satisfies the following axioms:

(1) The skew-symmetry condition $g(A, B) = -g(B, A)$ for all $A, B \in M$.
(2) The Jacobi identity

$$J(A, B, C) = g\big(g(A, B), C\big) + g\big(g(B, C), A\big) + g\big(g(C, A), B\big) = 0$$

for all $A, B, C \in M$.
(3) The bilinear condition $g(aA + bB, C) = ag(A, C) + bg(B, C)$ for all $A, B, C \in M$ and $a, b \in F$.

The operation $J(A, B, C)$ is called the *Jacobian*.

There is the following fundamental relationship between the associative and Lie algebras.

(a) The replacement of the operation of multiplication AB in an associative algebra M by the operation of commutation $[A, B] = AB - BA$, makes it into a Lie algebra $M^{(-)}$. If M is an algebra over a commutative field F, then $M^{(-)}$ is also an algebra over the same field.
(b) For every Lie algebra L over an arbitrary commutative field F there exists an associative M over the same field such that L can be isomorphically embedded in the algebra $M^{(-)}$. This is the Poincaré–Birkhoff–Witt theorem.

D.3. A *Jordan algebra* is a linear algebra M over some field F such that the multiplicative binary operation g satisfies the following axioms:

(1) The symmetry condition $g(A, B) = g(B, A)$ for all $A, B \in M$.
(2) The Jordan identity

$$I(A, B) = g\big(g\big(g(A, A), B\big), A\big) - g\big(g(A, A), g(B, A)\big) = 0$$

for all $A, B, C \in M$.
(3) The bilinear condition $g(aA + bB, C) = ag(A, C) + bg(B, C)$ for all $A, B, C \in M$ and $a, b \in F$.

The operation $I(A, B, C)$ is called the *Jordanian*.

There is the following relationship between the associative and Jordan algebras. The replacement of the operation of multiplication AB in an associative algebra M by the operation $[A, B]_+ = (1/2)(AB + BA)$, makes it into a Jordan algebra $M^{(+)}$. If M is an algebra over a commutative field F, then $M^{(+)}$ is also an algebra over the same field. The algebra $M^{(+)}$ is called the special algebra. The Jordan algebras that are not special are called exceptional. In contrast to the theory of Lie algebras, in which the Poincaré–Birkhoff–Witt theorem states that every Lie algebra is isomorphic to a subalgebra of $M^{(-)}$ for some M, exceptional Jordan algebras exist.

D.4. Alternative algebras are algebras in which all the subalgebras generated by two elements are associative. An *alternative algebra* is a linear algebra M such that the multiplicative bilinear operation g satisfies the following conditions

$$g\big(g(A, A), B\big) = g\big(A, g(A, B)\big), \quad g\big(B, g(A, A)\big) = g\big(g(B, A), A\big)$$

for all A and B in the algebra.

The theory of exceptional Jordan algebras is based on the theory of alternative algebras.

D.5. A *Maltsev algebra* (or Malcev algebra) is a linear algebra M over some field F, such that the multiplicative binary operation g satisfies the following axioms:

(1) The skew-symmetry condition $g(A, B) = -g(B, A)$ for all $A, B \in M$.
(2) The Maltsev identity $J(A, B, g(A, C)) = g(J(A, B, C), A)$ for all $A, B, C \in M$.
(3) The bilinear condition $g(aA + bB, C) = ag(A, C) + bg(B, C)$ for all $A, B, C \in M$ and $a, b \in F$.

Each Lie algebra is a Maltsev algebra. On the other hand, any two elements of Maltsev algebra generate a Lie subalgebra.

There is the following relationship between the alternative and Maltsev algebras. The replacement of the operation of multiplication AB in an alternative algebra M by the operation $[A, B]_+ = (1/2)(AB + BA)$, makes it into a special Jordan algebra $M^{(+)}$. The replacement of the operation of multiplication AB in an alternative algebra M by the operation $[A, B] = AB - BA$, makes it into a Malcev algebra $M^{(-)}$. The algebra $M^{(-)}$ is not a Lie algebra, it is a Maltsev algebra.

D.6. A *commutant-associative algebra* is a linear algebra M such that the multiplicative bilinear operation g satisfies the condition

$$\big([A_1, A_2], [A_3, A_4], [A_5, A_6]\big) = 0$$

for all $A_k \in M$, where $k = 1, 2, \ldots, 6$. Here $[A, B] = AB - BA$.

We say that M is a commutant-associative algebra if the commutant of this algebra is an associative subalgebra. A commutant of M is a subalgebra of M generated by all commutators $[A, B]$, where $A, B \in M$.

D.7. A *Valya algebra* (or Valentina algebra) is a linear algebra M over some field F such that the multiplicative binary operation g satisfies the following axioms:

(1) The skew-symmetry condition $g(A, B) = -g(B, A)$ for all $A, B \in M$.
(2) The Valya identity $J(g(A_1, A_2), g(A_3, A_4), g(A_5, A_6)) = 0$ for all $A_k \in M$, where $k = 1, 2, \ldots, 6$.
(3) The bilinear condition $g(aA + bB, C) = ag(A, C) + bg(B, C)$ for all $A, B, C \in M$ and $a, b \in F$.

We say that M is a Valya algebra if the commutant of this algebra is a Lie subalgebra. Each Lie algebra is a Valya algebra.

There is the following relationship between the commutant-associative and Valentina algebras. If M is a commutant-associative algebra, then $M^{(-)}$ is a Valya algebra.

Multiple algebraic structures

Algebraic structures can also be defined on sets with added nonalgebraic structure, such as a topology or an order structure. The added structure must be compatible,

in some sense, with the algebraic structure. For example, a *linear topological space* is a set M such that M is a linear space over F and at the same time a topological space, where the two maps $M \times M \to M$: $A, B \to AB$ and $F \times M \to M$: $a, A \to aA$ are both continuous.

Homomorphism of algebraic structure

A set $\mathcal{M}$, together with a single binary operation on $\mathcal{M}$, is called a groupoid. Let us give more mathematically precise the idea that two groupoids $\mathcal{M}_1$ and $\mathcal{M}_2$, are structurally the same or isomorphic. Clearly that $\mathcal{M}_1$ and $\mathcal{M}_2$ are isomorphic if the groupoids are identical except for the names of the elements and operations.

(a) To each element $A_1 \in \mathcal{M}_1$ is assigned its counterpart $A_2 \in \mathcal{M}_2$.
(b) Two different elements A_1 and B_1 in $\mathcal{M}_1$ should have two different counterparts $A_2 = f(A_1)$ and $B_2 = f(B_1)$, that is, the map f must be one-to-one.
(c) Every element of $\mathcal{M}_2$ must be counterpart of some element of $\mathcal{M}_1$, that is, f must be onto $\mathcal{M}_2$.
(d) If the groupoid are to be structurally the same and if we denote the groupoid operation of $\mathcal{M}_1$ by g_1 and that of $\mathcal{M}_2$ by g_2, then the counterpart of $g_1(A, B)$ should be $g_2(A_2, B_2)$, or $f(g_1(A_1, B_1))$ should be $g_2(A_2, B_2)$:

$$f\big(g_1(A_1, B_1)\big) = g_2\big(f(A_1), f(B_1)\big). \tag{4}$$

Usually we drop the notations g_1 and g_2 for the operations and use multiplicative notations.

Requirement (b) express the mathematical statement that f is a monomorphism. A homomorphism f of $\mathcal{M}_1$ into $\mathcal{M}_2$ that is a one-to-one map is a monomorphism. Requirement (c) is a statement that f is an epimorphism. A homomorphism f of $\mathcal{M}_1$ into $\mathcal{M}_2$ is an epimorphism if it is onto $\mathcal{M}_2$.

Then an isomorphism of a groupoid $\mathcal{M}_1$ with a groupoid $\mathcal{M}_2$ is a one-to-one function f mapping $\mathcal{M}_1$ onto $\mathcal{M}_2$ such that for all A_1 and B_1 in $\mathcal{M}_1$, equation (4) holds. The groupoids $\mathcal{M}_1$ and $\mathcal{M}_2$ are then isomorphic. An isomorphism of a groupoid onto itself is an automorphism of the groupoid.

An isomorphism of a groupoid $\mathcal{M}_1$ with a groupoid $\mathcal{M}_2$ was defined as a one-to-one map f of $\mathcal{M}_1$ onto $\mathcal{M}_2$ such that we have (4) for all A and B in $\mathcal{M}_1$. If we drop the condition that f be one-to-one and onto, just retaining (4), the map f is then a homomorphism. This requirement is the only one that distinguishes a homomorphism from just any map of $\mathcal{M}_1$ into $\mathcal{M}_2$. It asserts that f is a structure-relating map. The algebraic structure of $\mathcal{M}_1$ is completely determined by the binary operation on $\mathcal{M}_1$, and that of $\mathcal{M}_2$ is completely determined by the operation on $\mathcal{M}_2$. The homomorphism condition thus relates the structure of $\mathcal{M}_1$ to that of $\mathcal{M}_2$. A homomorphism of $\mathcal{M}$ into itself is an endomorphism of $\mathcal{M}$.

3.6. Mathematical structures in kinematics

Kinematical structures

The common property of the different mathematical structures is that they can be applied to sets of elements whose physical nature has not been specified. In physics, the great problem is a relation between the real physical objects and mathematical structures.

A physical theory is a rule that assigns to each real physical object exactly one abstract model that is called the physical system. Each abstract model consists of a mathematical model, which is a collection of mathematical structures, and a physical interpretation of these mathematical structures.

A physical system is not equivalent to a real object. The given object can be described by different physical systems, and a physical system can describe various objects.

Physical theories consist essentially of two elements, a kinematical structure describing the initial states and observables of the system, and a dynamical structure describing the change of these states and observables with time.

POSTULATE *(Physical system).* To each physical system we associate the ordered pair $(\mathcal{K}, \mathcal{D})$ consists of the following physical structures:

(1) The kinematical structure $\mathcal{K}$ on a kinematical set K.
(2) The dynamical structure $\mathcal{D}$ on a dynamical set D.

The ordered pair $(\mathcal{K}, \mathcal{D})$ is sometimes called the mathematical model of given physical system.

A kinematical structure is determined by postulates that define mathematical structures on sets of observables, states, and expectation values.

To each physical system we can associate the triple (M, S, B) formed by the set M of all its observables, the set S of all its states, and the set B of all its expectation values. There exists a mapping $(M, S) \to \mathbb{R}$ which associates with each pair (A, ρ) in (M, S) a real number $(\rho|A)$ in B. The number is interpreted as the expectation value of the observable A when the system is in the state ρ.

POSTULATE *(Kinematical structure).* A kinematical structure $\mathcal{K}$ consists of the following sets and structures.

(1) A kinematical set K is a triple (M, S, B) of the following sets:
  (1.1) A set M, whose elements are interpreted as the observables.
  (1.2) A set S, whose elements are interpreted as the states.
  (1.3) A set B, whose elements are interpreted as the results of measurements (the expectation values). There exists a mapping $(.|.)$ that associates with each pair (ρ, A) of (S, M) an expectation value $(\rho|A)$ in B.

(2) Mathematical structures $(\mathcal{M}, \mathcal{S}, \mathcal{B})$ on the kinematical set $K = (M, S, B)$.

The elements $\rho \in S$ can be considered as mappings $(\rho|.)$ from M into B. Therefore S can be presented as a set M^* of maps on M.

A kinematical structure $\mathcal{K}$ is determined by definition of a kinematical set (M, S, B) and mathematical structures. The following are examples of some basic kinematical structures.

(1) M can be equipped with the following mathematical structures: M is a partially ordered set, M is a linear space; M can be Lie, Jordan and Lie–Jordan algebras; M is a universal enveloping (universal associative) algebra; M can be metric, normalized, Banach, Hilbert, Liouville spaces; M can be B^*-algebra, C^*-algebra or W^*-algebra.
(2) S can be equipped with the following mathematical structures: S is a dual Hilbert space; S is a convex set; S is a positive cone; S is a cone Banach space.
(3) B can be equipped with the following mathematical structures: B is a Borel space, i.e., B is a σ-algebra of subsets; B is a linear space; B is a probability space; B is a field of real numbers.

Kinematical postulates

The observables of a quantum system are identified with the self-adjoint linear operators on some Hilbert space. Suppose $(\rho|A) = Tr[\rho A]$.

(1) The set of observables M can be equipped with a structure of partially ordered set. We say that $A \leqslant B$ whenever $(\rho|A) \leqslant (\rho|B)$ for all ρ in S. In particular, we write $A \geqslant 0$ if and only if $(\rho|A) \geqslant 0$ for all $\rho \in S$. The relation $\leqslant$ defined above is a partial ordering relation on M, in particular $A \leqslant B$ and $A \geqslant B$ imply $A = B$.

POSTULATE *(Order structure).* The inequality $A \leqslant B$ between any two elements A and B of M holds if and only if $(\rho|A) \leqslant (\rho|B)$ for all states $\rho \in S$. In particular, $A \leqslant B$ and $B \leqslant A$ implies $A = B$.

The fact that M can be equipped with a structure of partially ordered set play an important role in quantum kinematics. This postulate has the following consequence. The set of states S is such that $(\rho|A) = (\rho|B)$, or $<A> = <B>$, for all $\rho \in S$ implies $A = B$. Hence the postulate assumes that there are enough states in S so that we can distinguish between two observables by measuring their expectation values. In other words, we identify two observables whose expectation values coincide on all states. For any pair of observables A and B in M, we have $A = B$ if and only if $(\rho|A) = (\rho|B)$ for all $\rho \in S$.

(2) The set of observables M can be equipped with an algebraic structure.

POSTULATE *(Algebraic structure).*

(1) For any pair of observables A and B in M there exists an element $(A + B)$ in M, such that $(\rho|A + B) = (\rho|A) + (\rho|B)$ for all $\rho \in S$.
(2) For any observable A in M and any real number $a \in \mathbb{R}$ there exists an element aA in M such that $(\rho|aA) = a(\rho|A)$ for all $\rho \in S$.
(3) There exists in M two elements 0 and I such that $(\rho|0) = 0$, $(\rho|I) = 1$ for all $\rho \in S$.

By virtue of the postulate of order structure, we have that 0, I, aA, and $(A+B)$ are uniquely defined. For the same reason, we conclude that the sum is distributive with respect to the multiplication by real numbers and is both commutative and associative. We then see that this postulate equipped M with the algebraic structure of a real linear space.

(3) The set of observables M can be equipped with a natural topological structure. For this purpose, we define the nonnegative number

$$\|A\|_\rho = \sup_{\rho \in S} \big|(\rho|A)\big| \tag{5}$$

for all A in M. It follows immediately from this definition that $\|A\|_\rho$ is a norm for M, and $|(\rho|A)| \leqslant \|A\|_\rho$ for all (A, ρ) in (M, S).

In an intuitive physical meaning, the norm represents a greatest possible absolute value for the observable. The norm allows us to define a topological structure on M, which is called the *natural weak topology*. Neighbourhoods of an element $A \in M$ in this topology are the sets $U_\varepsilon(A) = \{B \in M\colon \|B - A\|_\rho < \varepsilon\}$. The space M of observables can be considered as a complete space in the natural weak topology. As a result, the set of observables has a Banach space structure with respect to natural norm.

POSTULATE *(Topological structure).*

(1) The norm (5) for all $A \in M$ is finite.
(2) M is a metric space with the metric $d(A, B) = \|A - B\|_\rho$.
(3) M is a Banach space.
(4) S is identified with the set of all positive bounded linear functionals $\omega_\rho = (\rho|\ )$ on M, such that $\omega_\rho(I) = (\rho|I) = 1$.

As a result, M is equipped with the structure of a real Banach space relative to the natural norm $\|\ \|_\rho$, and S is the set of all positive bounded linear functionals on M.

More information in the kinematical postulates and mathematical structures see, for instance, the books [25,26,51].

Chapter 4

Spaces of Quantum Observables

4.1. Space of bounded operators

The quantum observables are identified with the self-adjoint linear operators acting on some separable Hilbert space. Let us define some mathematical structures on a set of observables.

If $\mathcal{H}$ is a linear space, the set of all operators on $\mathcal{H}$ is a linear space if we define addition of operators and multiplication of operators by scalars in the natural way, namely,

$$(A + B)x = Ax + Bx, \qquad (aA)x = a(Ax)$$

for all $x \in \mathcal{H}$, and $a \in \mathbb{C}$. We shall denote the linear space of all linear operators on $\mathcal{H}$ by $L(\mathcal{H})$.

DEFINITION. Let $L(\mathcal{H})$ be a set of all linear operators from a linear space $\mathcal{H}$ into itself. A *linear operator space* consists of a set $L(\mathcal{H})$, together with an addition of operators and a multiplication of operators by scalars.

If $\mathcal{H}$ is a normed linear space, a linear operator A on $\mathcal{H}$ is bounded on $\mathcal{H}$ if

$$\sup\bigl\{\|Ax\|_{\mathcal{H}}\colon\ x \in \mathcal{H},\ \|x\|_{\mathcal{H}} = 1\bigr\} < \infty.$$

This means that A transforms norm bounded sets of $\mathcal{H}$ into the norm bounded sets.

DEFINITION. The operator A is called *bounded* if $\|Ax\|_{\mathcal{H}} \leqslant c\|x\|_{\mathcal{H}}$ for some constant c and all $x \in \mathcal{H}$. The least value of c, equal to

$$\|A\| = \sup_{x \neq 0} \frac{\|Ax\|_{\mathcal{H}}}{\|x\|_{\mathcal{H}}} = \sup_{\|x\|_{\mathcal{H}}=1} \|Ax\|_{\mathcal{H}} \tag{1}$$

is called the *norm* of the operator A.

For example, if A is a linear operator on $C[0, 1]$ and

$$(A\Psi)(x) = \int_0^x dy\, \Psi(y),$$

then A is bounded. The inverse operator

$$\left(A^{-1}\Psi\right)(x) = \frac{d}{dx}\Psi(x)$$

is defined on a set of all continuously differentiable functions such that $\Psi(0) = 0$. The operator A^{-1} is not bounded.

The norm represents the greatest possible absolute value for the observable. We shall denote the space of all bounded linear operators on $\mathcal{H}$ by $\mathcal{B}(\mathcal{H})$.

STATEMENT. *If $\mathcal{H}$ is a normed linear space, then $\mathcal{B}(\mathcal{H})$ is a normed linear space.*

Suppose that A_n and A in $\mathcal{B}(\mathcal{H})$ such that

$$\lim_{n\to\infty} \|A_n - A\| = 0.$$

This is equivalent to the statement that $\|A_n x - Ax\|_{\mathcal{H}} \to 0$ uniformly for all x such that $\|x\|_{\mathcal{H}} = 1$. For this reason the topology for $\mathcal{B}(\mathcal{H})$ defined by the norm (1) is called the *uniform topology* for $\mathcal{B}(\mathcal{H})$.

STATEMENT. *If $\mathcal{H}$ is a Banach space, then $\mathcal{B}(\mathcal{H})$ is a Banach operator space.*

As a result, the set of all bounded linear operators on a separable Hilbert space $\mathcal{H}$ is a Banach operator space. Then bounded observables form a Banach space.

DEFINITION. Let A be a linear operator on a topological space $\mathcal{H}$. Then A is called *continuous* at $x \in \mathcal{H}$ if to every neighbourhood U_y of $y = Ax$ there corresponds a neighbourhood V_x of x such that $\{Az\colon z \in V_x\} \subset U_y$. The operator A is said to be continuous if it is continuous at every element x of its domain $D(A) = \mathcal{H}$.

The use of the adjective "bounded" as an equivalent for "continuous" is explained by the following statement. A continuous linear operator on a normed linear space $\mathcal{H}$ is a bounded operator on $\mathcal{H}$, since, for such an operator A, the norm $\|Ax\|_{\mathcal{H}}$ is bounded when x ranges over the unit sphere $\{x \in \mathcal{H}\colon \|x\|_{\mathcal{H}} \leqslant 1\}$ of $\mathcal{H}$. As a result, $\mathcal{B}(\mathcal{H})$ is a space of continuous operators.

4.2. Space of finite-rank operators

Let $\mathcal{H}$ be a separable Hilbert space. By the Riesz–Fréchet theorem, any element $x \in \mathcal{H}$ can be considered not only as an element of $\mathcal{H}$, but also as an element of the dual space $\mathcal{H}^*$ of the linear continuous functionals on $\mathcal{H}$. We denote x, treated as an element of $\mathcal{H}$, by $|x>$, and treated as an element of $\mathcal{H}^*$, by $<x|$. The main convenience of this Dirac's notation is the possibility of simple representation of operators in terms of an outer product. We shall denote by $|x><y|$ the operator which maps element $|z>$ of $\mathcal{H}$ into the element $|x>a(y, z)$, where $a(y, z) = <y|z>$. Operator of the form $|x><y|$ is called the ket-bra operator.

DEFINITION. A *ket-bra operator* is an operator $\hat{P}(x, y) = |x><y|$ that assigns to each element $|z>$ of $\mathcal{H}$ exactly one element $|x>a(y, z)$, where $a(y, z) = <y|z>$, i.e.,

$$\hat{P}(x, y)|z> = |x><y|z>.$$

This operator is a map from $\mathcal{H}$ onto the one-dimensional subspace $\mathcal{H}_x = \{a|x>,\ a \in \mathbb{C}\}$. If A is a ket-bra operator whose domain $D(A)$ and range $R(A)$ both lie in the same Hilbert space $\mathcal{H}$, then $D(A) = \mathcal{H}$, $\dim R(A) = 1$.

If $|x>$ is a unit vector of $\mathcal{H}$, $\|x\|_{\mathcal{H}} = \sqrt{<x|x>} = 1$, then the operator $P(x) = \hat{P}(x, x)$ is a projection onto the ket-vector $|x>$, i.e., $P^*(x) = P(x)$, $P^2(x) = P(x)$. Finite linear combinations of ket-bra operators describe operators of finite rank.

DEFINITION. A *finite-rank operator* is a linear operator A that can be presented as a finite sum of ket-bra operators:

$$A = \sum_{k=1}^{N} |x_k><y_k| = \sum_{k=1}^{N} \hat{P}(x_k, y_k),$$

where $|x_k>, |y_k> \in \mathcal{H}$. The rank of A is N. A finite-rank operator is also called finite-dimensional.

Let A be a linear operator whose domain $D(A)$ and range $R(A)$ both lie in $\mathcal{H}$. If A is a finite-rank operator, then $D(A)$ is $\mathcal{H}$ and $R(A)$ is a finite-dimensional subspace of $\mathcal{H}$. A finite-rank operator is a map from a Hilbert space $\mathcal{H}$ into a finite-dimensional subspace of $\mathcal{H}$.

THEOREM. *If A is a linear operator whose domain $D(A)$ and range $R(A)$ both lie in the same Hilbert space $\mathcal{H}$, and* $\dim R(A) < \infty$, *then A is a finite-rank operator. The rank of A is* $\dim R(A)$.

We agree to call the sum of the eigenvalues of a linear operator A in n-dimensional linear space the *spectral trace* and the sum of the diagonal elements of the matrix of the operator A the *matrix trace*. Let us give the important theorem regarding finite-rank operators.

THEOREM. *If A is a finite-rank operator, then its matrix trace coincides with its spectral trace*:

$$\sum_{k=1}^{\infty} <e_k|A|e_k> = \sum_{k=1}^{n} z_k,$$

where $|e_k>$ is an arbitrary orthonormal basis for $\mathcal{H}$ and z_k are eigenvalues of the operator A.

A finite-rank operator is bounded. A set of all finite-rank operators on $\mathcal{H}$ is a normed linear space. We shall denote this space by $\mathcal{K}(\mathcal{H})$.

We shall proceed by completing the space of all finite-rank operators with respect to corresponding norms:

(1) The completion of $\mathcal{K}(\mathcal{H})$ with respect to the operator norm $\| \ \|$ is the space $\mathcal{K}_{comp}(\mathcal{H})$ of compact (completely continuous) operators.
(2) The completion of $\mathcal{K}(\mathcal{H})$ with respect to the norm $\| \ \|_1$ is the space $\mathcal{K}^1(\mathcal{H})$ of trace-class (nuclear) operators.
(3) The completion of $\mathcal{K}(\mathcal{H})$ with respect to $\| \ \|_2$ is the space $\mathcal{K}^2(\mathcal{H})$ of Hilbert–Schmidt operators.

4.3. Space of compact operators

Let $\mathcal{H}$ be a topological space. A system of sets V_k, $k \in \mathbb{N}$, is called a covering of $\mathcal{H}$ if $\mathcal{H}$ is contained as a subset of the union $\bigcup_{k\in\mathbb{N}} V_k$. A subset $\mathcal{H}_0$ of $\mathcal{H}$ is called *compact* if every system of open sets of $\mathcal{H}$ which covers $\mathcal{H}_0$ contains a finite subsystem also covering $\mathcal{H}_0$. A subset of $\mathcal{H}$ is called *relatively compact* if its closure is compact.

DEFINITION. Let A be a linear operator on a normed linear space $\mathcal{H}$. We say that A is a *compact operator* if, for each bounded subset $\mathcal{H}_s$ of $\mathcal{H}$, the set $\{Ax\colon\ x \in \mathcal{H}_s\}$ is relatively compact in $\mathcal{H}$. A compact operator is also called *completely continuous*.

We shall denote the set of compact operators on $\mathcal{H}$ by $\mathcal{K}_{comp}(\mathcal{H})$. Note that a compact linear operator is continuous. For discontinuity of A would imply the existence of a sequence $\{x_k\}$ such that $\|x_k\|_{\mathcal{H}} \leqslant 1$ and $\|Ax_k\|_{\mathcal{H}} \to \infty$. This

cannot occur if A is compact. Since $\mathcal{H}$ is a normed space, A is compact if and only if, for each bounded sequence $\{x_k\}$ in $\mathcal{H}$, the sequence $\{Ax_k\}$ contains a subsequence converging to some limit in $\mathcal{H}$.

We illustrate this notion with the following example. Let $a(x, y)$ be a real-valued continuous function defined for $x, y \in [a, b]$. Then the integral operator A defined by

$$(A\Psi)(x) = \int_a^b dy\, a(x, y)\Psi(y)$$

is a compact operator on $C[a, b]$. Note that the identity operator on an infinite-dimensional normed linear space is never compact. As a result, a compact operator on an infinite-dimensional normed linear space cannot have a bounded inverse.

THEOREM *(Hilbert). If $\mathcal{H}$ is a Hilbert space, every compact operator in $\mathcal{B}(\mathcal{H})$ is the uniform limit of operators of finite-rank.*

Hilbert was the first to call attention to an important class of operators that can be approximated by finite-rank operators, namely the compact operators. In 1932, Banach conjectured that this theorem is true when $\mathcal{H}$ is any Banach space. This remained an open question until 1973, when P. Enflo constructed a separable reflexive Banach space $\mathcal{H}$ such that the some compact operators on $\mathcal{H}$ are not the uniform limit of finite-rank operators.

THEOREM. *Let $\mathcal{K}(\mathcal{H})$ be a normed linear space of finite-rank operators. The completion of $\mathcal{K}(\mathcal{H})$ with respect to the operator norm $\| \ \|$ (i.e., the uniform topology) is the space $\mathcal{K}_{comp}(\mathcal{H})$ of compact operators.*

Let us give the basic statements regarding properties of compact (completely continuous) operators.

(1) If A is a finite-rank operator, then A is compact.
(2) If A is a compact operator, then A is bounded.
(3) If A and B are compact operators and $a, b \in \mathbb{C}$, then $aA + bB$ is also a compact operator.
(4) If A is a compact operator, and the operator B is bounded, then AB and BA are compact operators.
(5) If A is a compact operator, then A^* is also compact.
(6) If A is a bounded linear operator defined everywhere in $\mathcal{H}$, and the operator A^*A is compact, then the operator A is also compact.
(7) The sequence of eigenvalues of a compact self-adjoint operator tends to zero.

(8) Any compact self-adjoint operator A has the representation

$$A = \sum_{k=1}^{\infty} a_k |e_k><e_k|,$$

where $|e_k>$ is the orthonormal basis of eigenvectors of A and a_k are the eigenvalues of A.

(9) The unit operator I is compact if and only if $\mathcal{H}$ is finite-dimensional. In general, I is not a compact operator.

(10) If A a compact operator, and let A^{-1} be inverse of A, i.e., $A^{-1}A = AA^{-1} = I$, then A^{-1} is not bounded.

(11) If A is a limit (in the sense of norm convergence in the operator space) of a sequence of compact operators, then A is compact.

Note that properties (3) and (4) express the statement that $\mathcal{K}_{comp}(\mathcal{H})$ is a linear operator algebra.

4.4. Space of trace-class operators

Let $\mathcal{H}$ be a separable Hilbert space. Consider bounded operators which have the diagonal form in a fixed orthonormal basis $|e_k>$ of $\mathcal{H}$,

$$A = \sum_{k=1}^{\infty} a_k |e_k><e_k|, \tag{2}$$

where the series converges strongly. A sequence of operators

$$A_n = \sum_{k=1}^{n} a_k |e_k><e_k| \tag{3}$$

converges to A strongly if

$$\lim_{n\to\infty} \|A_n x - Ax\|_{\mathcal{H}} = 0$$

for all $x \in \mathcal{H}$. For any orthonormal basis $|e_k>$ in $\mathcal{H}$,

$$\sum_{k=1}^{\infty} |e_k><e_k| = I.$$

This is a compact notation for the relation

$$|x> = \sum_{k=1}^{\infty} |e_k><e_k|x>$$

expressing the completeness of the system $\{|e_k>\}$.

Any property of the operator (2) corresponds to a property of the sequence of eigenvalues $\{a_k\}$. For example, A is self-adjoint if and only if a_k are real. The operator A is positive if $a_k > 0$. Restricting to a finite number of k in (2), we get the finite-rank operator. For example, the operator (3) is finite-rank. The operator (2) is compact if $\{a_k\}$ is a null sequences, i.e., $\lim_{k\to\infty} a_k = 0$. An operator that is compact is said to be nuclear or trace-class if

$$\sum_{k=1}^{\infty} a_k < \infty.$$

A trace-class operator on a Hilbert space has the important property that its trace may be defined so that it is finite and is independent of the basis. Given any orthonormal basis $|e_k>$ for the Hilbert space, one may define the trace as

$$Tr[A] = \sum_{k=1}^{\infty} <e_k|A|e_k> = \sum_{k=1}^{\infty} a_k,$$

since the sum converges and is independent of the basis.

The space of all finite-rank operators is an operator analog of the space of all infinite sequences with only a finite number of non-zero terms (sequences with finite support). The space $\mathcal{K}_{comp}(\mathcal{H})$ of all compact operators is an operator analog of the space of null sequences $\{a_k\colon \lim_{k\to\infty} a_k = 0\}$. The l_1 sequence space is defined by

$$\|a\|_1 = \sum_{k=1}^{\infty} |a_k| < \infty.$$

Now we define the operator analog of the space l_1.

We now consider a noncommutative analog of spaces l_1 and $L^1(\mathbb{R})$. For any bounded operator $A \in \mathcal{B}(\mathcal{H})$, we can define the norm $\|A\|_1 = Tr\,|A|$. Here $|A| = \sqrt{A^*A}$ is an operator analog of the formula $|z| = \sqrt{z^*z}$ for $z \in \mathbb{C}$.

DEFINITION. A *trace-class operator* is a linear bounded operator A, such that

$$\|A\|_1 = Tr\,|A| = Tr\,\sqrt{A^*A} < \infty. \tag{4}$$

A trace-class operator is also called the *nuclear operator* or the operator with finite trace.

We illustrate this notion with an example. Let $a(x, y)$ be a real-valued function defined for $x, y \in [a, b]$ such that

$$\int_a^b \int_a^b dx\,dy\,\big|a(x, y)\big| < \infty.$$

Then the integral operator A defined by

$$(A\Psi)(x) = \int_a^b dy\, a(x, y)\Psi(y) \tag{5}$$

is a trace-class operator on $L^1[a, b]$. If A is a trace-class operator and the function $a(x, x)$ is integrable, then

$$Tr[A] = \int_a^b dx\, a(x, x). \tag{6}$$

Let A be a trace-class operator and $\{|e_k>\}$ be an orthonormal basis for $\mathcal{H}$. Then

$$\sum_{k=1}^{\infty} \left| <e_k|Ae_k> \right| < \infty, \qquad Tr[A] = \sum_{k=1}^{\infty} <e_k|Ae_k>,$$

where $Tr[A]$ does not depend on the choice of $\{|e_k>\}$.

The trace is a linear functional on a set of all trace-class operators, such that the following properties are satisfied:

(a) $Tr[A]>0$ for $A > 0$.
(b) $Tr[A] \in \mathbb{R}$ for $A^* = A$.
(c) $Tr[A^*] = (Tr[A])^*$.
(d) $Tr[AB] = Tr[BA]$.
(e) $Tr[ABC] = Tr[CAB] = Tr[BCA]$.

We now describe the relation between the trace and the eigenvalues for a trace-class operator.

THEOREM *(Lidsky). If A is a trace-class operator, then its matrix trace coincides with its spectral trace*

$$Tr[A] = \sum_{k=1}^{\infty} <e_k|A|e_k> = \sum_{k=1}^{\infty} z_k,$$

where $|e_k>$ is an arbitrary orthonormal basis and z_k are the eigenvalues of the operator A.

The trace norm defines a Banach space structure on a set of all trace-class operators.

THEOREM. *The completion of the space $\mathcal{K}(\mathcal{H})$ of all finite-rank operators with respect to the norm (4) is the Banach space $\mathcal{K}^1(\mathcal{H})$ of trace-class operators.*

Any trace-class operators is compact. Note that $\|A\| \leqslant \|A\|_1$. Therefore the completion of $\mathcal{K}(\mathcal{H})$ with respect to $\| \ \|_1$ is contained in the completion with respect to $\| \ \|$:

$$\mathcal{K}(\mathcal{H}) \subset \mathcal{K}^1(\mathcal{H}) \subset \mathcal{K}_{comp}(\mathcal{H}).$$

Any self-adjoint trace-class operator has the spectral representation

$$A = \sum_{k=1}^{\infty} a_k P_k,$$

where $P_k = |e_k><e_k|$ are the projections $P_k^* = P_k$, $P_k^2 = P_k$, and the sum converges in the norm $\| \ \|_1$, since

$$\|P_k\|_1 = 1, \qquad \sum_{k=1}^{\infty} |a_k| = Tr\,|A| < \infty.$$

Any positive operator with finite trace is a trace-class operator such that $a_k \geqslant 0$.

Let $\mathcal{B}(\mathcal{H})$ be a Banach space of all bounded operators with the operator norm $\| \ \|$. The space of continuous linear functionals (the dual space) for $\mathcal{K}^1(\mathcal{H})$ is the space $\mathcal{B}(\mathcal{H})$.

THEOREM *(Dual space of $\mathcal{K}^1(\mathcal{H})$). Let ρ be a trace-class operator. For any $A \in \mathcal{B}(\mathcal{H})$, the map $\rho \to \omega(A) = Tr[\rho A]$ defines a continuous linear functional ω on $\mathcal{K}^1(\mathcal{H})$ with the norm $\|\omega\| = \|A\|$. Conversely, any continuous linear functional on $\mathcal{K}^1(\mathcal{H})$ has this form.*

This is the operator analog of the Riesz–Markov theorem.

STATEMENT. *A Banach operator space $\mathcal{B}(\mathcal{H})$ is a dual space of $\mathcal{K}^1(\mathcal{H})$:* $(\mathcal{K}^1(\mathcal{H}))^* = \mathcal{B}(\mathcal{H})$.

The quantum states are identified with the self-adjoint, positive, linear operators ρ of unit trace. Then ρ is a trace-class operator, such that $|\rho| = \rho$, and $\|\rho\|_1 = Tr\,\rho = 1$. The expectation value of a bounded observable A on a state ρ is computed by the formula

$$<A> = \omega(A) = Tr[\rho A].$$

We may say that the Banach space $\mathcal{K}^1(\mathcal{H})$ is the smallest linear space in which the set of all states can be embedded.

4.5. Space of Hilbert–Schmidt operators

We now consider a noncommutative analog of spaces l_2 and $L^2(\mathbb{R})$. Let $\mathcal{B}(\mathcal{H})$ be an operator space of all bounded operators. For $A, B \in \mathcal{B}(\mathcal{H})$, we define the scalar product

$$(A|B) = Tr[A^*B]. \tag{7}$$

This scalar product determines the norm

$$\|A\|_2 = \sqrt{(A|A)}, \tag{8}$$

which is called the *Hilbert–Schmidt norm* of A.

DEFINITION. A *Hilbert–Schmidt operator* is a linear bounded operator $A \in \mathcal{B}(\mathcal{H})$, such that the norm $\|A\|_2 < \infty$.

A linear bounded operator A is a Hilbert–Schmidt operator, if A^*A is a trace-class operator.

THEOREM. *The completion of $\mathcal{K}(\mathcal{H})$ with respect to Hilbert–Schmidt norm is the Banach space $\mathcal{K}^2(\mathcal{H})$ of all Hilbert–Schmidt operators.*

The scalar product (7) in a Banach space $\mathcal{K}^2(\mathcal{H})$ is representable in the form

$$(A|B) = \sum_{k=1}^{\infty} <Ae_k|Be_k>,$$

where $|e_k>$ is an orthonormal basis for $\mathcal{H}$. This scalar product is independent on the choice of the basis.

THEOREM. *The completion of $\mathcal{K}(\mathcal{H})$ with respect to the scalar product* (7) *is the Hilbert operator space $\mathcal{K}^2(\mathcal{H})$.*

The space $\mathcal{K}^2(\mathcal{H})$ is a separable Hilbert space. By the Riesz–Fréchet theorem, each linear continuous (with respect to the norm $\| \ \|_2$) functional on the Hilbert space $\mathcal{K}^2(\mathcal{H})$ has the form $A \to (\rho|A)$, where ρ is an element of $\mathcal{K}^2(\mathcal{H})$ (and vice versa).

THEOREM *(Dual space of $\mathcal{K}^2(\mathcal{H})$). Let ρ be a Hilbert–Schmidt operator. For any $A \in \mathcal{K}^2(\mathcal{H})$, the map $\rho \to \omega(A) = Tr[\rho A]$ defines a continuous linear functional on $\mathcal{K}^2(\mathcal{H})$. Conversely any continuous linear functional on $\mathcal{K}^2(\mathcal{H})$ has this form.*

We shall denote the space of all continuous linear functionals on $\mathcal{K}^2(\mathcal{H})$ by $\mathcal{K}^{2^*}(\mathcal{H})$. The spaces $\mathcal{K}^{2^*}(\mathcal{H})$ and $\mathcal{K}^2(\mathcal{H})$ are identical except for the names of the elements and operations, such that $\mathcal{K}^{2^*}(\mathcal{H})$ and $\mathcal{K}^2(\mathcal{H})$ are structurally the same. Thus the spaces $\mathcal{K}^{2^*}(\mathcal{H})$ and $\mathcal{K}^2(\mathcal{H})$ are isomorphic.

Let us consider Hilbert–Schmidt operators on $\mathcal{H} = L_2[a, b]$. For $\Psi(x) \in L_2[a, b]$, the integral operator A defined by (5) is a Hilbert–Schmidt operator on $L_2[a, b]$, if the kernel $a(x, y) = <x|A|y>$ is a square-integrable function of two variables $x, y \in [a, b]$. The scalar product is

$$(A|B) = \int_a^b \int_a^b dx\, dy\, a^*(x, y) b(y, x).$$

If A is a trace-class operator and the function $a(x, x) = <x|A|x>$ is integrable, then we have equation (6). Note that it is possible to express a large class of operators A (for example, any bounded operators) in the integral form but with the more general (distribution) kernels.

4.6. Properties of operators from $\mathcal{K}^1(\mathcal{H})$ and $\mathcal{K}^2(\mathcal{H})$

The following are properties of $\mathcal{K}^1(\mathcal{H})$ and $\mathcal{K}^2(\mathcal{H})$.

(1) If A and B are Hilbert–Schmidt operators, then AB and BA are trace-class operators.
(2) If A is bounded and B is a Hilbert–Schmidt operator, then AB and BA are Hilbert–Schmidt operators.
(3) If A is bounded and B is a trace-class operator, then AB and BA are trace-class operators and $Tr[AB] = Tr[BA]$.
(4) A trace-class operator is an operator A of the form

$$A = \sum_{k=1}^{n} B_k C_k,$$

where B_k and C_k are Hilbert–Schmidt operators, and $n < \infty$.
(5) A trace-class operator is a Hilbert–Schmidt operator.
(6) The operator spaces are related by the following inclusions

$$\mathcal{K}(\mathcal{H}) \subset \mathcal{K}^1(\mathcal{H}) \subset \mathcal{K}^2(\mathcal{H}) \subset \mathcal{K}_{comp}(\mathcal{H}) \subset \mathcal{B}(\mathcal{H}).$$

(7) If A is a trace-class operator, then $\|A\|_2 \leqslant \|A\|_1$.
(8) If $A \in \mathcal{K}^1(\mathcal{H})$ and $B \in \mathcal{B}(\mathcal{H})$, then $\|AB\|_1 = \|BA\|_1 \leqslant \|B\|\, \|A\|_1$.
(9) If $A, B \in \mathcal{K}^2(\mathcal{H})$, then $\|AB\|_1 = \|BA\|_1 \leqslant \|A\|_2\, \|B\|_2$.
(10) If $A \in \mathcal{K}^1(\mathcal{H})$, then $|\,Tr\, A| \leqslant \|A\|_1$.
(11) If $A \in \mathcal{K}^1(\mathcal{H})$ and A^* is adjoint of A, then $\|A^*\|_1 = \|A\|_1$.

STATEMENT *(Matrix representation). Each self-adjoint Hilbert–Schmidt operator A on a Hilbert space $\mathcal{H}$ is representable in the form*

$$A = \sum_{k=1}^{\infty} a_k |e_k><e_k| = \sum_{k=1}^{\infty} a_k P_k, \tag{9}$$

where $|e_k>$ is an orthonormal basis for $\mathcal{H}$, and

$$\sum_{k=1}^{\infty} |a_k| < \infty.$$

Each self-adjoint trace-class operator A on a Hilbert space $\mathcal{H}$ is representable in the form (9), where $\{a_k\}$ is a l_2-sequence,

$$\sum_{k=1}^{\infty} |a_k|^2 < \infty.$$

If $\mathcal{H} = L^2(M)$, then there exists a coordinate representation of $A \in \mathcal{K}^2(\mathcal{H})$.

STATEMENT *(Coordinate representation). Let A be a bounded operator on a Hilbert space $\mathcal{H} = L^2(M)$. Then A is a Hilbert–Schmidt operator if and only if there exists a function $a(x, y)$, such that*

$$(A\Psi)(x) = \int_M dy\, a(x, y)\Psi(y),$$

and

$$\|A\|_2^2 = \int_{M\times M} dx\, dy \big|a(x, y)\big|^2 < \infty.$$

If A is a Hilbert–Schmidt operator on $L^2(M)$, then its kernel $a(x, y) \in L^2(M \times M)$.

The kernel $a(x, x') = <x|A|x'>$ of a Hilbert–Schmidt operator A is a square-integrable function, i.e.,

$$Tr\big[A^2\big] = \int dx\, <x|A^2|x> = \int dx\, dx'\, |<x'|A|x>|^2 < \infty.$$

If A is a trace-class operator, then the function $a(x, x) = <x|A|x>$ is integrable, i.e.,

$$Tr[A] = \int dx\, <x|A|x> = \int dx\, a(x, x) < \infty.$$

4.7. Set of density operators

Convex set of density operators

The quantum states can be identified with the self-adjoint, nonnegative linear operators ρ of unit trace.

DEFINITION. A *density operator* is a trace-class operator ρ, such that the following requirements are satisfied:

(1) ρ is nonnegative, i.e., $\rho \geqslant 0$.
(2) ρ is self-adjoint, i.e., $\rho = \rho^*$.
(3) ρ is normalized, i.e., $Tr[\rho] = 1$.

STATEMENT. *A density operator on a separable Hilbert space $\mathcal{H}$ is representable in the form*

$$\rho = \sum_{k=1}^{\infty} p_k |e_k><e_k| = \sum_{k=1}^{\infty} p_k P_k, \tag{10}$$

where $|e_k>$ is an orthonormal basis for $\mathcal{H}$, and

$$0 \leqslant p_k \leqslant 1, \quad p_k^* = p_k, \quad \sum_{k=1}^{\infty} p_k = 1. \tag{11}$$

We shall denote the set of all density operators on $\mathcal{H}$ by $S(\mathcal{H})$. The density operators represent states in quantum mechanics. Then $S(\mathcal{H})$ is a set of all possible quantum states. Note that $S(\mathcal{H})$ is not a linear operator space, since a set of all positive operators is not a linear space.

DEFINITION. A set S is a *convex set* if $\rho_1, \rho_2 \in S$ and $0 < a < 1$ imply $a\rho_1 + (1-a)\rho_2 \in S$.

If $\rho_k \in S(\mathcal{H})$, $k = 1, \ldots, n$, and p_k satisfy (11), then the operator $\sum_{k=1}^{n} p_k \rho_k$ is a density operator. Thus $S(\mathcal{H})$ is a convex set. A set $S(\mathcal{H})$ forms a convex subset of $\mathcal{K}^1(\mathcal{H})$.

DEFINITION. A *convex hull* of S is a set S_{convex} of all convex combinations of elements from S:

$$S_{convex} = \left\{ \sum_{k=1}^{n} r_k \rho_k \colon \rho_k \in S,\ r_k^* = r_k \geqslant 0,\ \sum_{k=1}^{n} r_k = 1,\ n \in \mathbb{N} \right\}.$$

A set $S(\mathcal{H})$ of all density operators on $\mathcal{H}$ is a convex hull.

Pure and mixed states

If $\rho = \rho^2$, then ρ is called the *pure state*, and the density operator ρ has the form $\rho = |e_k><e_k| = P_k$ in some orthonormal basis $|e_k>$. Here

$$P_k^* = P_k, \quad P_k^2 = P_k, \quad \sum_{k=1}^{\infty} P_k = I.$$

Then the pure states of $S(\mathcal{H})$ are the one-dimensional projections. In the general case, any density operator can be expressed as a mixture of the pure states ρ_k:

$$\rho = \sum_{k=1}^{\infty} p_k \rho_k \colon\ 0 \leqslant p_k \leqslant 1,\ p_k^* = p_k,\ \sum_{k=1}^{\infty} p_k = 1.$$

The observables are identified with the self-adjoint linear operators acting on some separable Hilbert space. Then each density operator ρ is an observable. The expectation value of an observable A on a state ρ is computed by the formula

$$<A> = Tr[\rho A].$$

We can consider the expectation value $<\rho> = Tr[\rho^2]$. There exists a natural requirement that must be satisfied by the density operator ρ. The expectation value $<\rho>$ must be finite: $<\rho> < \infty$. Then $Tr[\rho^2] < \infty$, and ρ is a Hilbert–Schmidt operator. Note that any trace-class operator is Hilbert–Schmidt. As a result, any density operator ρ is a Hilbert–Schmidt operator.

If ρ is a pure state ($\rho^2 = \rho$), then

$$<\rho> = Tr\big[\rho^2\big] = Tr[\rho] = 1.$$

In general, ρ can be presented in the form (10). Using (10) and $P_k P_l = \delta_{kl} P_k$, we obtain

$$\begin{aligned} <\rho> = Tr\big[\rho^2\big] &= Tr\left[\left(\sum_{k=1}^{\infty} p_k P_k\right)^2\right] = Tr\left[\sum_{k=1}^{\infty} p_k^2 P_k\right] \\ &= \sum_{k=1}^{\infty} p_k^2\, Tr[P_k] = \sum_{k=1}^{\infty} p_k^2. \end{aligned}$$

As a result, we have $0 \leqslant <\rho> \leqslant 1$. If ρ is a mixed state density operator, then $0 \leqslant <\rho> < 1$. If ρ is a pure state density operator, then $<\rho> = 1$.

Positive cone of density operators

The notion of "positivity" of density operators is very important in quantum theory. Let $\mathcal{M}$ be a set of quantum observables. Suppose there is a binary relation defined for every pair $A, B \in \mathcal{M}$, expressed by $A \leqslant B$, with the properties:

(a) $A \leqslant A$ for all $A \in \mathcal{M}$.
(b) If $A \leqslant B$ and $B \leqslant A$, then $A = B$, for $A, B \in \mathcal{M}$.
(c) If $A \leqslant B$, and $B \leqslant C$, then $A \leqslant C$ for all $A, B, C \in \mathcal{M}$.

Then $\mathcal{M}$ is said to be partially ordered by the relation $\leqslant$.

DEFINITION. An *ordered linear space* is a real linear space $\mathcal{M}$ over $\mathbb{R}$, together with a binary relation $\leqslant$, such that the following properties are satisfied:

(1) $\mathcal{M}$ is partially ordered by the relation $\leqslant$.
(2) If $A \leqslant B$, then $A + C \leqslant B + C$ for all $C \in \mathcal{M}$.
(3) If $A \leqslant B$, $a \in \mathbb{R}$, and $a \geqslant 0$, then $aA \leqslant aB$.

If $\mathcal{M}$ is an ordered linear space, then we can define the *positive cone* $\mathcal{M}_+ = \{A \in \mathcal{M}\colon\ A \geqslant 0\}$.

DEFINITION. A *positive cone* is a set $\mathcal{M}_+$ such that the following requirements are satisfied:

(1) $\mathcal{M}_+$ is a convex set.
(2) If $A \in \mathcal{M}_+$, then $aA \in \mathcal{M}_+$ for all $a \geqslant 0$.
(3) If $A \in \mathcal{M}_+$ and $(-A) \in \mathcal{M}_+$, then $A = 0$.

A positive operator is a linear operator A on $\mathcal{M}_+$ whose domain $D(A)$ and range $R(A)$ both lie in the same positive cone $\mathcal{M}_+$.

If $\mathcal{B}_r(\mathcal{H})$ is a real Banach space of all bounded self-adjoint operators on a Hilbert space $\mathcal{H}$, then the set $\mathcal{B}_{r+}(\mathcal{H}) = \{A \in \mathcal{B}_r(\mathcal{H})\colon\ A \geqslant 0\}$ is a positive cone. For example,

$$\mathcal{K}^1_{r+}(\mathcal{H}) = \left\{A \in \mathcal{K}^1_r(\mathcal{H})\colon\ A \geqslant 0\right\}$$

is a positive cone. Here $\mathcal{K}^1_r(\mathcal{H})$ is a real Banach space of all self-adjoint trace-class operators. As a result, $S(\mathcal{H})$ can be considered as a positive cone $\mathcal{K}^1_{r+}(\mathcal{H})$ of $\mathcal{K}^1_r(\mathcal{H})$: $S(\mathcal{H}) = \{\rho \in \mathcal{K}^1_r(\mathcal{H})\colon\ \rho \geqslant 0\}$.

4.8. Operator Hilbert space and Liouville space

Operator pre-Hilbert and Hilbert spaces

A set of quantum observables can be a Hilbert space.

DEFINITION. A *pre-Hilbert operator space* is a linear operator space $\mathcal{M}$, together with a scalar product $(A|B)$ for each pairs of $A, B \in \mathcal{M}$.

A *scalar operator product* in a linear operator space $\mathcal{M}$ is a complex number $(A|B)$ satisfying the axioms:

(1) $(A + B|C) = (A|C) + (B|C)$ for all $A, B, C \in \mathcal{M}$.
(2) $(A|aB) = a(A|B)$ and $(aA|B) = a^*(A|B)$ for all $A, B \in \mathcal{M}$ and $a \in \mathbb{C}$.
(3) $(A|B) = (B|A)^*$ for all $A, B \in \mathcal{M}$.
(4) $(A|A) > 0$ for $A \neq 0$, and $(A|A) = 0$ if and only if $A = 0$.

DEFINITION. An *operator Hilbert space* is a complete pre-Hilbert operator space.

We illustrate this notions with the following examples.

(1) The most familiar operator Hilbert space is the space $\mathcal{K}^2(\mathcal{H})$ of all Hilbert–Schmidt operators with the scalar product:

$$(A|B) = Tr[A^*B]. \tag{12}$$

The linear space $\mathcal{K}(\mathcal{H})$ of all finite-rank operators on $\mathcal{H}$ is an operator pre-Hilbert space. The completion of $\mathcal{K}(\mathcal{H})$ with respect to the scalar product (12) is the operator Hilbert space $\mathcal{K}^2(\mathcal{H})$ of all Hilbert–Schmidt operators.

(2) Let $\mathcal{M}$ be an operator Banach space. Then $\mathcal{M}$ is an operator Hilbert space if and only if the operator norm $\| \ \|$ of $\mathcal{M}$ satisfies the parallelogram identity

$$\|A + B\|^2 + \|A - B\|^2 = 2\|A\|^2 + 2\|B\|^2 \tag{13}$$

for all $A, B \in \mathcal{M}$. If the parallelogram identity is satisfied for all elements of a Banach operator space $\mathcal{M}$, then the associated scalar product, which makes $\mathcal{M}$ into a Hilbert space, is given by the polarization identity:

$$(A|B) = \frac{1}{4}\sum_{s=0}^{3} i^s \left\| A + i^s B \right\|^2.$$

(3) We can consider a linear operator space $\mathcal{M}$ with the scalar product

$$(A|B)_\omega = \omega(A^*B), \tag{14}$$

where ω is a functional on $\mathcal{M}$. This scalar product is used in the GNS-construction, where the infinite-dimensional Hilbert space in which operators act is defined by a state ω. The infinite-dimensional Hilbert space $\mathcal{H}$ is isomorphic to the operator Hilbert space $\mathcal{M}$.

A Liouville space is an operator Hilbert space with the scalar product (12).

DEFINITION. A *Liouville space* is a set $\mathcal{M}$ of linear operators, such that the following conditions are satisfied.

(1) $\mathcal{M}$ is a linear operator space.

(2) The scalar product $(A|B) = Tr[A^*B]$ is defined for all elements of $\mathcal{M}$.
(3) $\mathcal{M}$ is a complete normed space with the norm $\|A\|_2 = \sqrt{(A|A)}$.

For example, the space $\mathcal{K}^2(\mathcal{H})$ is a Liouville space. In general, we can consider an operator Hilbert space with another scalar product (see, for example, the scalar product (14)).

DEFINITION. An *associated Hilbert space* is a Liouville space $\bar{\mathcal{H}}$, such that all elements of $\bar{\mathcal{H}}$ are operators on a Hilbert space $\mathcal{H}$.

For example, $\mathcal{K}^2(\mathcal{H})$ is an associated Hilbert space. The associated Hilbert space can be considered as a representation of a Liouville space in $\mathcal{B}(\mathcal{H})$.

If the Hilbert space $\mathcal{H}$ is n-dimensional (for example, $\mathcal{H} = \mathbb{C}^n$), the corresponding associated Hilbert space is n^2-dimensional, $\dim \bar{\mathcal{H}} = (\dim \mathcal{H})^2$. If $\mathcal{H} = \mathbb{C}^2$, then an arbitrary element $|A) \in \bar{\mathcal{H}}$ can be presented in the form

$$|A) = a_0\sigma_0 + a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3,$$

where σ_k are Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{15}$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \sigma_0 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{16}$$

Dirac's notations for operator spaces

Suppose $\mathcal{M}$ is an operator Hilbert space. A *dual operator space* of $\mathcal{M}$ is a linear space $\mathcal{M}^*$ of all continuous linear functionals on $\mathcal{M}$. Let us give the basic theorem regarding operator Hilbert spaces.

RIESZ–FRÉCHET THEOREM. *For each element ρ of an operator Hilbert space $\mathcal{M}$ there exists a unique element ω of $\mathcal{M}^*$, such that $\omega(A) = (\rho|A)$ for all $A \in \mathcal{M}$. Conversely, for each element ω of $\mathcal{M}^*$ there exists a unique element ρ of $\mathcal{M}$, such that $\omega(A) = (\rho|A)$ for all $A \in \mathcal{M}$.*

This Riesz–Fréchet theorem establishes the general form of a continuous linear functional on an operator Hilbert space $\mathcal{M}$. Every bounded linear functional on $\mathcal{M}$ has the form $\omega(A) = (\rho|A)$, where ρ is a fixed element of $\mathcal{M}$. Conversely, if $\rho \in \mathcal{M}$, then $\omega(A) = (\rho|A)$ is a bounded linear functional on $\mathcal{M}$.

By the fundamental Riesz–Fréchet theorem, the operator $A \in \mathcal{M}$ can be considered not only as an element of $\mathcal{M}$, but also as an element of the dual space $\mathcal{M}^*$ of continuous linear functionals on the space $\mathcal{M}$. We shall denote A, treated

as an element of $\mathcal{M}$, by $|A)$. This element is called the *ket-vector* of the operator space $\mathcal{M}$. Denote A, treated as an element of $\mathcal{M}^*$, by $(A|$. The elements $(A|$ are called the *bra-vector* of $\mathcal{M}$. Then the map $|A) \to (A|$ is a one-to-one map of $\mathcal{M}$ onto $\mathcal{M}^*$. The symbol for scalar product $(A|B)$ is the graphic junction of the symbols $(A|$ and $|B)$. Note, that the scalar product in an operator Hilbert space satisfies the condition

$$(A|B)^* = (B|A),$$

where $|A), |B) \in \mathcal{M}$. Here we can use $|A)^* = (A|$, and $(A|^* = |A)$.

Note that a map of $\mathcal{M}$ into itself is called the *superoperator*. This Dirac's notation for operator spaces leads to a simple representation of superoperators on $\mathcal{M}$ in terms on an outer product. We shall denote by $\hat{\mathcal{P}}(A, B) = |A)(B|$ the map that assigns to an element $|C)$ of $\mathcal{M}$ the element $|A)(B|C)$:

$$\hat{\mathcal{P}}(A, B)|C) = |A)(B||C) = |A)(B|C).$$

The action of $\hat{\mathcal{P}}(A, B) = |A)(B|$ on $|C)$ is described by a graphic junction of the symbols. Note that $\hat{\mathcal{P}}(A, B)$ maps onto the subspace $\mathcal{M}_A = \{|A)z\colon z \in \mathbb{C}\} \subset \mathcal{M}$. The map $\hat{\mathcal{P}}(A, B) = |A)(B|$ on $\mathcal{M}$ will be called the *ket-bra superoperator*. The adjoint of $\hat{\mathcal{P}}(A, B)$ is defined by

$$\hat{\mathcal{P}}(A, B)^* = \big(|A><B|\big)^* = |B)(A| = \hat{\mathcal{P}}(B, A).$$

Important superoperators in quantum mechanics are the projection superoperators on $\mathcal{M}$. We can define the projection superoperator

$$\mathcal{P}_A = \frac{|A)(A|}{(A|A)}.$$

It projects an arbitrary element $|C)$ of $\mathcal{M}$ onto the element $|A)$, by $\mathcal{P}_A|C) = |A)z$ where $z = (A|C)/(A|A)$. The superoperator $\mathcal{P}_A$ is self-adjoint $\mathcal{P}_A^* = \mathcal{P}_A$, and idempotent $\mathcal{P}_A^2 = \mathcal{P}_A$.

The definition of the projection superoperator can be expanded upon by projecting not onto an element $|A)$, but onto a subspace $\mathcal{M}_N$ of $\mathcal{M}$. If the subspace $\mathcal{M}_N$ is generated by operators E_k, then we can define the superoperator

$$\mathcal{P}_N = \sum_{k=1}^{N} |E_k)(E_k|,$$

such that $\mathcal{P}_N A \in \mathcal{M}_N$ for all $A \in \mathcal{M}_N$.

4.9. Correlation functions

Suppose $\mathcal{M}$ is a Liouville space and I is a unit operator. Then $A|I) = |A)$, and the scalar product $(A|B) = Tr[A^*B]$ in $\mathcal{M}$ can be written in the form $(A|B) = (I|A^*B)$.

Let $\mathcal{M}$ be an operator Hilbert space. The scalar product in this space can be realized in different ways. A particular scalar product can be chosen depending on the given physical problem. If P is a fixed element of $\mathcal{M}$, then we can define the scalar product

$$(A|B)_P = (P|A^*B) = Tr[PA^*B].$$

If $P = I$, the $\mathcal{M}$ is the Liouville space. In quantum mechanics, there exists a natural "fixed" operator P that can be given for a state. We can use a density operator ρ. In this case, we have

$$(A|B)_\rho = (\rho|A^*B) = <A^*B>.$$

Then the scalar product is an expectation value of A^*B.

The following are examples of some scalar products in an operator space.

(1) The *natural correlation function* (correlator) is

$$(A|B)_\rho = <A^*B> = Tr[\rho A^*B].$$

The natural correlator can be defined in the form

$$(A|B)'_\rho = <A^*B> - <A^*><B>.$$

(2) The *lambda-correlation function*

$$(A|B)_{\lambda,\rho} = Tr\left[\rho^\lambda A^* \rho^{1-\lambda} B\right].$$

(3) The *symmetrized correlation function* is

$$(A|B)_{s,\rho} = (A|B)_{1/2,\rho} = Tr\left[\rho^{1/2} A^* \rho^{1/2} B\right].$$

(4) The *canonical correlation function* is

$$(A|B)_{can,\rho} = \int_0^1 d\lambda \, Tr\left[\rho^\lambda A^* \rho^{1-\lambda} B\right].$$

If $\lambda = 1$, then λ-correlation function gives the natural correlation function $(A|B)_\rho$. The value $\lambda = 1/2$ gives the symmetrized correlation function $(A|B)_{s,\rho}$.

The definition of the canonical correlation function may seem to be rather complicated compared to other functions. However, it is adequate for quantum linear

response problems. If ρ describes a canonical equilibrium state, i.e.,

$$\rho = Z^{-1}\exp(-\beta H), \qquad Z = Tr\big[\exp(-\beta H)\big],$$

the canonical correlation function $(A|B)_{can,\rho}$ is called the *Mori product*. This scalar product is temperature dependent due to $\beta = 1/kT$.

Using these correlation functions, the expectation value of an observable A can be written as

$$<A> = (I|A)_\rho = (I|A)_{s,\rho} = (I|A)_{\lambda,\rho} = (I|A)_{can,\rho}.$$

These correlators define different operator Hilbert space.

4.10. Basis for Liouville space

Operator basis and ket-bra operator

Let $\{|x>\}$ be an orthonormal basis such that

$$<x|x'> = \delta(x - x'), \qquad \int dx\, |x><x| = I.$$

Then $\hat{P}(x, y) = |x><y|$ is a ket-bra operator. This operator can be considered as a ket-vector $|xy)$ of an operator space $\mathcal{M}$,

$$|xy) = \big|\hat{P}(x, y)\big) = \big||x><y|\big).$$

The orthonormal basis $\{|x>\}$ generates an orthonormal basis $\{|xy)\}$ of the operator space. We can define a scalar product of the ket-vectors $|xy) = |\hat{P}(x, y))$ by

$$\begin{aligned}(xy|x'y') &= \big(\hat{P}(x, y)|\hat{P}(x', y')\big) = Tr\big[\hat{P}^*(x, y)\hat{P}(x', y')\big] \\ &= Tr\big[\hat{P}(y, x)\hat{P}(x', y')\big] = <x|x'><y'|y> = \delta(x - x')\delta(y' - y).\end{aligned}$$

This means that the basis $\{|xy)\}$ is orthonormal. Using the completeness of $\{|x>\}$, it is not hard to prove that the operator basis $\{|xy)\}$ satisfies the completeness condition

$$\int dx\, dy\, |xy)(xy| = I, \qquad \int dx\, dy\, \hat{P}(x, y)\hat{P}^*(x, y) = I. \tag{17}$$

The operators $\hat{P}(x, y)$ form a basis for $\mathcal{M}$. As a result, each operator $A \in \mathcal{M}$ takes of the form

$$A = \int dx\, dy\, a(x, y)\hat{P}(x, y). \tag{18}$$

Here $a(x, y)$ is a kernel of A in the X-representation, such that

$$a(x, y) = <x|A|y> = Tr\big[\hat{P}(y, x)A\big] = Tr\big[\hat{P}^*(x, y)A\big]$$
$$= \big(\hat{P}(x, y)|A\big) = (xy|A).$$

Using the Dirac's notations, equation (18) has the form

$$|A) = \int dx\, dy\, |xy)(xy|A), \tag{19}$$

where $(xy|A) = a(x, y)$. Equation (19) is a compact notation for the relation

$$(x'y'|A) = \int dx\, dy\, (x'y'|xy)(xy|A)$$

for the kernel $a(x, y) = (xy|A)$. As a result, equations (19) can be interpreted as a completeness condition for the operator basis $\{|xy)\}$.

The trace of A is presented in the form

$$Tr[A] = Tr[I\,A] = \int dx\, dy\, (xy|A|xy)$$
$$= \int dx\, Tr\big[\hat{P}(x, x)A\big] = \int dx\, (xx|A) = \int dx <x|A|x>,$$

where

$$(xy|A|x'y') = \big(\hat{P}(x, y)|A\,\hat{P}(x', y')\big) = a(x, x')\delta(y' - y).$$

Suppose $\mathcal{H} = \mathbb{C}^n$ and $\{|e_k>:\ k = 1, \ldots, n\}$ is a basis for $\mathcal{H}$. Then the elements

$$|kl) = \big|P(e_k, e_l)\big) = \big||e_k><e_l|\big)$$

form a basis of the associated Hilbert space $\bar{\mathcal{H}}$. Each element $|A) \in \bar{\mathcal{H}}$ can be presented in the form

$$|A) = \sum_{k,l=1}^{n^2} |kl)(kl|A),$$

where $(kl|A) = <e_k|A|e_l> = A_{kl}$ is a $n \times n$ matrix of the operator A on the Hilbert space $\mathcal{H} = \mathbb{C}^n$.

Arbitrary orthonormal operator basis

Let $|z) = |E(z))$ be an arbitrary orthonormal operator basis for an operator Hilbert space $\mathcal{M}$, such that

$$(z|z') = \big(E(z)|E(z')\big) = \delta(z - z').$$

This basis is connected with the basis $\{|xy) = \hat{P}(x, y)\}$ by the transformation function

$$(xy|z) = \big(\hat{P}(x, y)|E(z)\big) = Tr\big[\hat{P}^*(x, y)E(z)\big] = <x|E(z)|y>.$$

The completeness of $|z) = |E(z))$ gives

$$\int dz\,(xy|z)(z|x'y') = (xy|x'y'),$$

where $(xy|x'y') = \delta(x - x')\delta(y' - y)$, i.e.,

$$\int dz\,<x|E(z)|y><y'|E^*(z)|x'> = \delta(x - x')\delta(y' - y). \tag{20}$$

Multiplication of (20) by $<y|A|y'>$, and integration over y and y', give

$$\int dz\,E(z)AE^*(z) = Tr[A].$$

If this equation is satisfied for each operator $A \in \mathcal{M}$, then its is equivalent to the completeness condition of the operator basis $\{|E(z))\}$. For $A = I$, we have

$$\int dz<x|E(z)E^*(z)|x'> = \delta(x, x'), \qquad \int dz\,E(z)E^*(z) = I.$$

As a result, each operator $A \in \mathcal{M}$ can be represented by

$$|A) = \int dz\,|z)(z|A) = \int dz\,|z)a(z),$$

where $a(z) = (z|A) = (E(z)|A) = Tr[E^*(z)A]$. The scalar product in the operator Hilbert space $\mathcal{M}$ can be calculated by the formula

$$(A|B) = \int dz\,a^*(z)b(z).$$

If $\mathcal{M}$ is the Liouville space, then we can define multiplication and involution [140–143] by the equations

$$\big|E^*(a)\big) = \int db\,\big|E(b)\big)\big(E(b)|E^*(a)\big),$$

$$|a^*) = \int db\,|b)(b|a^*),$$

$$(b|a^*) = Tr\big[E^*(b)E^*(a)\big] = Tr\big[E^*(a)E^*(b)\big] = (a|b^*).$$

$$\big|E(a)E(b)\big) = \int dc\,\big|E(c)\big)\big(E(c)|E(a)E(b)\big),$$

$$|ab) = \int dc\,|c)(c|ab),$$

$$(c|ab) = Tr\big[E^*(c)E(a)E(b)\big].$$

It is not hard to prove the following statements. Let A be an element of a Liouville space $\mathcal{M}$. Then A satisfies the equation

$$(a|A)^* = \int db\,(a^*|b)(b|A^*).$$

If A and B be elements of a Liouville space $\mathcal{M}$, then AB satisfies the equation

$$(a|AB) = \int da\,db\,(c|ab)(a|A)(b|B).$$

4.11. Rigged Liouville space

Let $\mathcal{M}$ be a Liouville space. An operator Banach space $\mathcal{B} \subset \mathcal{M}$ cannot be complete with respect to convergence in the norm $\|A\|_{\mathcal{M}} = \sqrt{(A|A)}$. However, $\mathcal{B}$ can always be completed with respect to the topology defined by this norm to form an operator Hilbert space $\mathcal{M}$, which is called the Liouville space. By the fundamental Riesz–Fréchet theorem, the space $\mathcal{M}^*$ of all linear functionals on $\mathcal{M}$ is isomorphic to $\mathcal{M}$ itself. On the other hand, functionals in $\mathcal{M}^*$ are also bounded linear functionals on $\mathcal{B} \subset \mathcal{M}$. The space $\mathcal{B}^*$ of all linear functionals on $\mathcal{B}$ is bigger than $\mathcal{M}^*$. The space $\mathcal{B}^*$ includes the Liouville space $\mathcal{M}^* = \mathcal{M}$. The embedded spaces $\mathcal{B}$, $\mathcal{M} = \mathcal{M}^*$, $\mathcal{B}^*$ form a rigged Liouville space.

DEFINITION. A *rigged Liouville space* is the triplet $\mathcal{B} \subset \mathcal{M} = \mathcal{M}^* \subset \mathcal{B}^*$, where $\mathcal{M}$ is a Liouville space, $\mathcal{B}$ is an operator Banach space, and $\mathcal{B}^*$ is dual of $\mathcal{B}$.

As a result, we have a rigged operator Hilbert space.

Let A be a bounded operator on the function Hilbert space $\mathcal{H} = L^2(M)$. Then A is an element of the Liouville space $\mathcal{M} = \mathcal{K}^2(\mathcal{H})$ if and only if there exists a function $a(x, y)$, such that

$$(A\Psi)(x) = \int_M dy\,a(x, y)\Psi(y),$$

and

$$(A|B) = \int_M \int_M dx\,dy\,(A|xy)(xy|B) = \int_M \int_M dx\,dy\,a^*(x, y)b(x, y).$$

The kernel $a(x, y) = (xy|A) = <x|A|y>$ of each element $|A)$ of the Liouville space $\mathcal{M} = \mathcal{K}^2(\mathcal{H})$ is a square-integrable function, i.e., $(xy|A) \in L^2(M \times M)$.

Then

$$Tr\big[A^2\big] = \int\limits_M dx\,\big(xx|A^2\big) = \int\limits_M \int\limits_M dx\,dy\,|<y|A|x>|^2 < \infty.$$

As a result, the Liouville space can be represented as the space $L^2(M \times M)$ of square-integrable functions on $M \times M$.

Example of a rigged Liouville space is the following triple of spaces:

$$\mathcal{J}(M \times M) \subset L^2(M \times M) \subset \mathcal{J}^*(M \times M).$$

This triplet consists of the Banach space $\mathcal{J}(M \times M)$ of test functions, the Liouville space $L^2(M \times M)$ of square integrable functions, and the Banach space $\mathcal{J}^*(M \times M)$ of the linear functionals on $\mathcal{J}(M \times M)$.

As a result, a rigged operator Hilbert space (*rigged Liouville space*) can be considered as a rigged function Hilbert space for operator kernels.

Let $\mathcal{M}$ be a Liouville space. Suppose $\mathcal{B} \subset \mathcal{M}$ is a Banach operator space with norm $\| \ \|_{\mathcal{B}}$. Denote by J the embedding operator $J : \mathcal{B} \to \mathcal{M}$. The operator J will be assumed to be bounded, such that $\|A\|_{\mathcal{M}} \leqslant C\|A\|_{\mathcal{B}}$ for all $A \in \mathcal{B}$ and some positive constant C.

We introduce the space $\mathcal{B}^*$ of continuous linear functionals on $\mathcal{B}$. If $\omega \in \mathcal{B}^*$, then

$$\omega(aA + bB) = a\omega(A) + b\omega(B)$$

for all $A, B \in \mathcal{B}$ and $a, b \in \mathbb{C}$, and $|\omega(A)| \leqslant C\|A\|_{\mathcal{B}}$ for some $C > 0$. The value of a functional ω on an element $A \in \mathcal{B}$ will be also expressed as

$$(\omega|A) = \omega(A).$$

We can define addition and multiplication by a number in $\mathcal{B}^*$ by setting

$$(a\omega_1 + b\omega_2|A) = a^*(\omega_1|A) + b^*(\omega_2|A)$$

for all $\omega_1, \omega_2 \in \mathcal{B}^*$ and $A \in \mathcal{B}$.

There exists a natural linear map J^*: $\mathcal{M} = \mathcal{M}^* \to \mathcal{B}^*$, such that

$$J^*\omega(A) = \omega(JA)$$

for all $A \in \mathcal{B} \subset \mathcal{M}$. Then to each element $B \in \mathcal{M}$ exits a functional $J^*B \in \mathcal{B}^*$ defined by the formula $(J^*B|A) = (B|JA) = (B|A)$ for all $A \in \mathcal{B} \subset \mathcal{M}$.

We can define the norm in $\mathcal{B}^*$ by the formula

$$\|\omega\|_{\mathcal{B}^*} = \sup\big\{\big|(\omega|A)\big|\colon\ \|A\|_{\mathcal{B}} = 1,\ A \in \mathcal{B}\big\}.$$

It is not hard to prove that J^* is a bounded linear map from $\mathcal{M} = \mathcal{M}^*$ into $\mathcal{B}^*$.

As a result, we have the triple of operator spaces $\mathcal{B} \subset \mathcal{M} = \mathcal{M}^* \subset \mathcal{B}^*$, where $\mathcal{M}$ is a Liouville space, $\mathcal{B}$ is a Banach operator space densely embedded in $\mathcal{M}$ and $\mathcal{B}^*$ is the space of continuous linear functionals on $\mathcal{B}$.

To each $\omega \in \mathcal{B}^*$ and $A \in \mathcal{B}$, there exists the value $(\omega|A) = \omega(A)$ of ω at A. This value is an extension of the scalar product in the Liouville space $\mathcal{M}$, that is, if $\omega \in \mathcal{M}^* \subset \mathcal{B}^*$, then the scalar product $(\omega|A)$ in $\mathcal{M}$ equals to the value of the functional ω at A.

We define

$$(A|\omega) = (\omega|A)^* = \big(\omega(A)\big)^*.$$

Then $(A|\omega)$ is the complex conjugate of $\omega(A) = (\omega|A)$. This definition is a generalization of the property $(A|B) = (B|A)^*$ of the scalar product in the Liouville space $\mathcal{M}$.

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Chapter 5

Algebras of Quantum Observables

5.1. Linear algebra

A linear space consists of a set $\mathcal{M}$, together with two binary operations of addition and multiplication by real (or complex) numbers. A linear algebra is a generalization of this notion. The linear space $\mathcal{M}$ is a linear algebra if $\mathcal{M}$ is equipped with a multiplication law which associates the product AB to each pair $A, B \in \mathcal{M}$. The product is assumed to be distributive.

DEFINITION. A *linear algebra* is a linear space $\mathcal{M}$ over a field F, together with a binary operation g of multiplication on $\mathcal{M}$, such that the following conditions are satisfied:

$$g(A, aB + bC) = ag(A, B) + bg(A, C),$$
$$g(aA + bB, C) = ag(A, C) + bg(B, C),$$

for all $A, B, C \in \mathcal{M}$ and $a, b \in F$.

We consider $F = \mathbb{C}$ or $F = \mathbb{R}$.

DEFINITION. An algebra $\mathcal{M}$ is a *unital algebra* if there exists an element $I \in \mathcal{M}$ such that $g(I, A) = g(A, I) = A$ for all $A \in \mathcal{M}$. This element I is an identity element (*unity*) for g on $\mathcal{M}$.

An algebra $\mathcal{M}$ over a field F is a *division algebra* over F if $\mathcal{M}$ has a unity for multiplication and contains a multiplicative inverse of each nonzero element.

DEFINITION. Let $\mathcal{M}$ be an algebra and let $A_k \in \mathcal{M}$ for $k = 1, \ldots, n$. The smallest subalgebra of $\mathcal{M}$ containing $\{A_k\colon\ k = 1, \ldots, n\}$ is the *subalgebra generated by* $\{A_k\colon\ k = 1, \ldots, n\}$. If this subalgebra is all of $\mathcal{M}$, then $\{A_k\colon\ k = 1, \ldots, n\}$ generates $\mathcal{M}$ and the A_k are *generators of* $\mathcal{M}$.

A free algebra is an algebra generated by finite linear combinations and finite powers of the elements $\{A_k\colon\ k = 1, \ldots, n\}$ and the identity I.

5.2. Associative algebra

If A, B, C are elements of a linear algebra $\mathcal{M}$, then we define the associator of these elements as

$$(A, B, C) = g\big(g(A, B), C\big) - g\big(A, g(B, C)\big).$$

DEFINITION. An *associative algebra* is a linear algebra $\mathcal{M}$, such that the associator $(A, B, C) = 0$ for all $A, B, C \in \mathcal{M}$.

If A, B are elements of a linear algebra $\mathcal{M}$, then we define the commutator of these elements as

$$[A, B] = g(A, B) - g(B, A).$$

DEFINITION. A *commutative algebra* is a linear algebra $\mathcal{M}$, such that the commutator $[A, B] = 0$ for all $A, B \in \mathcal{M}$.

Let $\mathcal{B}(\mathcal{H})$ be a linear operator space of all bounded operators on $\mathcal{H}$. For $A, B \in \mathcal{B}(\mathcal{H})$, we define the product $g(A, B)$ as the linear bounded operator such that $g(A, B)x = A(Bx)$ for all $x \in \mathcal{H}$. With this definition of multiplication, $\mathcal{B}(\mathcal{H})$ becomes a linear operator algebra. This algebra is associative. In general, $\mathcal{B}(\mathcal{H})$ is not a commutative algebra.

5.3. Lie algebra

If A, B, C are elements of a linear algebra $\mathcal{M}$, then we define the Jacobian

$$J(A, B, C) = g\big(g(A, B), C\big) + g\big(g(B, C), A\big) + g\big(g(C, A), B\big).$$

DEFINITION. A *Lie algebra* is a linear algebra $\mathcal{M}$, such that its bilinear multiplicative operation g satisfies the following conditions:

(1) The operation g is anticommutative: $g(A, B) = -g(B, A)$ for all $A, B \in \mathcal{M}$.
(2) The operation g satisfies the Jacobi identity $J(A, B, C) = 0$ for all $A, B, C \in \mathcal{M}$.

The classic notation to denote the binary operation $g(A, B)$ of a Lie algebra is $A \cdot B$. Using $A \cdot B = -B \cdot A$, the Jacobi identity can be presented in the form

$$(A \cdot B) \cdot C - A \cdot (B \cdot C) = -(C \cdot A) \cdot B,$$

i.e., the associator is not equal to zero in general. Then Lie algebras are nonassociative.

Let $\mathcal{M}$ be a linear algebra over a field F. In the linear space of this algebra let us choose a basis $\{E_k\}$. Every element $A \in \mathcal{M}$ has a unique expression of the form

$$A = \sum_k a_k E_k,$$

where $a_k \in F$. Then the addition of elements of $\mathcal{M}$ and their multiplication reduce to the addition and the multiplication of the corresponding coefficients. The multiplication $g(E_k, E_l)$, being an element of $\mathcal{M}$, also has an expression in terms of the basis $\{E_k\}$,

$$g(E_k, E_l) = \sum_m c_{kl}^m E_m.$$

The system of numbers c_{kl}^m of the field F completely determines the multiplication in the algebra $\mathcal{M}$. The coefficients c_{ij}^k are called the *structure constants* of the algebra. If $\mathcal{M}$ is a Lie algebra, then the structure constants satisfy the conditions

$$c_{kl}^m = -c_{lk}^m, \qquad c_{kj}^i c_{lm}^j + c_{lj}^i c_{mk}^j + c_{mj}^i c_{kl}^j = 0. \tag{1}$$

Let us give the basic theorem regarding Lie algebras.

THEOREM. *Let $\mathcal{M} = <M, g>$ be an associative algebra that consists of a linear space M, together with a binary operation g of multiplication on the set M. Then $\mathcal{M}^{(-)} = <M, g_->$ is a Lie algebra with respect to the multiplication*

$$g_-(A, B) = g(A, B) - g(B, A).$$

Note that the Jacobian $J(A, B, C)$ is a linear combination of associators of the form

$$\begin{aligned} J(A, B, C) &= \big[[A, B], C\big] + \big[[B, C], A\big] + \big[[C, A], B\big] \\ &= (A, B, C) - (B, A, C) + (B, C, A) - (C, B, A) \\ &\quad + (C, A, B) - (A, C, B). \end{aligned}$$

If $(A, B, C) = 0$ for all $A, B, C \in \mathcal{M}$, then $J(A, B, C) = 0$ for all $A, B, C \in \mathcal{M}^{(-)}$. The algebra $\mathcal{M}^{(-)}$ is called the special Lie algebra. The theorem have the following converse statement.

POINCARÉ–BIRKHOFF–WITT THEOREM. *For each Lie algebra L, there exists an associative algebra $\mathcal{M}$, such that L is isomorphic to some subalgebra of the Lie algebra $\mathcal{M}^{(-)}$.*

This theorem states that each Lie algebra is isomorphic to some special Lie algebra.

DEFINITION. An *enveloping algebra* of a Lie algebra L is an associative algebra $\mathcal{M}$, such that L is a subalgebra of $\mathcal{M}^{(-)}$. Suppose L is a Lie algebra and $\{E_k\}$ is a basis of L such that

$$E_k \cdot E_l = \sum_m c_{kl}^m E_m. \tag{2}$$

A *universal enveloping algebra* of L is an associative unital algebra $U(L)$ that is generated by $\{E_k\}$ such that (2) with $E_k \cdot E_l = E_k E_l - E_l E_k$ is satisfied.

If $\{E_k\colon\ k = 1, \ldots, n\}$ is a basis of a Lie algebra L, then the monomials $E_1^{k_1} \ldots E_n^{k_n}$, where $k_1, \ldots, k_n \in \mathbb{N}$, form a basis of $U(L)$. It is easy to see, that the universal enveloping algebra $U(L)$ is infinite-dimensional. The map from L into $U(L)$ assigns to the finite-dimensional nonassociative algebra L an infinite-dimensional associative algebra $U(L)$.

DEFINITION. Let $\mathcal{M}$ be a Lie algebra and let $\mathcal{H}$ be a Hilbert space. A *representation of the Lie algebra* $\mathcal{M}$ on the Hilbert space $\mathcal{H}$ is a homomorphism π of $\mathcal{M}$ into the set of linear operators on $\mathcal{H}$ such that

(1) $\pi(aA + bB) = a\pi(A) + b\pi(B)$ for all $A, B \in \mathcal{M}$ and $a, b \in \mathbb{C}$.
(2) $\pi(A \cdot B) = [\pi(A), \pi(B)] = \pi(A)\pi(B) - \pi(B)\pi(A)$ for all $A, B \in \mathcal{M}$.

If the space $\mathcal{H}$ is infinite dimensional, then we assume in addition that the operators $\pi(A)$ for all $A \in \mathcal{M}$ have a common linear invariant domain D which is dense in $\mathcal{H}$.

5.4. Jordan algebra

If A, B, C are elements of a linear algebra $\mathcal{M}$, then we define the Jordanian

$$I(A, B) = g\big(g\big(g(A, A), B\big), A\big) - g\big(g(A, A), g(B, A)\big).$$

DEFINITION. A *Jordan algebra* is a linear algebra $\mathcal{M}$, such that its bilinear multiplicative operation g satisfies the following conditions:

(1) The operation g is commutative: $g(A, B) = g(B, A)$ for all $A, B \in \mathcal{M}$.
(2) The operation g satisfies the Jordan identity $I(A, B) = 0$ for all $A, B \in \mathcal{M}$.

The classic notation to denote the binary operation $g(A, B)$ is $A \circ B$. In general, the Jordan algebra is not associative.

Let us give the basic theorem regarding Jordan algebras.

THEOREM. *Let $\mathcal{M} = <M, g>$ be an associative algebra that consists of a linear space M, together with a binary operation g of multiplication on the set M. Then $\mathcal{M}^{(+)} = <M, g_+>$ is a Jordan algebra with respect to the multiplication*

$$g_+(A, B) = \frac{1}{2}\big(g(A, B) + g(B, A)\big).$$

Any Jordan algebra of this type is called special.

DEFINITION. A Jordan algebra, which is isomorphic to a subalgebra of $\mathcal{M}^{(+)}$ for some associative algebra $\mathcal{M}$, is called the *special Jordan algebra*. The Jordan algebras that are not special are called the *exceptional Jordan algebras*.

In contrast to the theory of Lie algebras, in which the Poincaré–Birkhoff–Witt theorem states that every Lie algebra is isomorphic to a subalgebra of $\mathcal{M}^{(-)}$ for some associative algebra $\mathcal{M}$, exceptional Jordan algebras do exists.

The following are examples of some Jordan algebras.

(1) The set of self-adjoint real, complex, or quaternionic matrices with the multiplication $(1/2)(AB + BA)$ form a special Jordan algebra.
(2) The set of 3×3 self-adjoint matrices over the octonions forms an exceptional Jordan algebra $H_3(\mathbb{O})$.

Let us define a linear algebra with two multiplication operations.

DEFINITION. A *Lie–Jordan algebra* $<\mathcal{M}, \cdot, \circ, \hbar>$ is a linear space $\mathcal{M}$, together with two bilinear multiplicative operations $\cdot$ and $\circ$, such that the following conditions are satisfied:

(1) $<\mathcal{M}, \cdot>$ is a Lie algebra.
(2) $<\mathcal{M}, \circ>$ is a Jordan algebra.
(3) The operations $<\cdot, \circ>$ are connected by the Leibnitz rule,

$$A \cdot (B \circ C) = (A \cdot B) \circ C + B \circ (A \cdot C).$$

(4) The associators of the operations $<\cdot, \circ>$ are connected by the equation

$$(A \circ B) \circ C - A \circ (B \circ C) = \frac{\hbar^2}{4}\big((A \cdot B) \cdot C - A \cdot (B \cdot C)\big),$$

where $\hbar$ is a positive real number.

Requirement (4) expresses the statement that

$$(A, B, C)_{Jordan} = \frac{\hbar^2}{4}(A, B, C)_{Lie}.$$

If $\hbar = 0$, then $<\mathcal{M}, \circ>$ is an associative Jordan algebra.

5.5. Involutive, normed and Banach algebras

Let $\mathcal{M}$ be a linear algebra. An *involution* is a map that assigns to each element A of $\mathcal{M}$ exactly one element A^* of $\mathcal{M}$, such that the following conditions are satisfied:

$$(A^*)^* = A, \qquad (aA + bB)^* = a^*A^* + b^*B^*, \qquad (AB)^* = B^*A^*,$$

where $a, b \in \mathbb{C}$, and a^* is the complex conjugate of a. In general, the involution is not a linear operation, since $(aA+bB)^* \neq aA^*+bB^*$. The linear algebra with an involution is called the involutive algebra, or $*$-algebra.

DEFINITION. An *involutive algebra* is a linear algebra $\mathcal{M}$, together with a unary operation g_* on $\mathcal{M}$, such that the following requirements are satisfied:

(1) $g_*(g_*(A)) = A$ for all $A \in \mathcal{M}$.
(2) $g_*(aA + bB) = a^*g_*(A) + b^*g_*(B)$ for all $A, B \in \mathcal{M}$, and $a \in \mathbb{C}$.
(3) $g_*(g(A, B)) = g(g_*(B), g_*(A))$ for all $A, B \in \mathcal{M}$.

Let $\mathcal{M}$ be an involutive algebra and let $\mathcal{M}^* = \{A^*\colon\ A \in \mathcal{M}\}$. Then $\mathcal{M}$ is a *self-adjoint algebra* if $\mathcal{M}^* = \mathcal{M}$. Suppose $\mathcal{M}$ is an involutive algebra and A is in $\mathcal{M}$. Then A is a *self-adjoint element* if $A^* = A$.

Let $\mathcal{M}$ be a linear algebra over the field $\mathbb{C}$. The algebra $\mathcal{M}$ is a normed algebra, if to each element A there is associated a real number $\|A\|$, called the norm of A, satisfying the requirements:

(1) $\|A\| \geqslant 0$.
(2) $\|A\| = 0$ if and only if $A = 0$.
(3) $\|A + B\| \leqslant \|A\| + \|B\|$.
(4) $\|aA\| = |a|\|A\|$, where $a \in \mathbb{C}$.
(5) $\|AB\| \leqslant \|A\|\|B\|$.

The norm represents the greatest possible absolute value for the observable.

DEFINITION. A *normed algebra* is a set $\mathcal{M}$, such that the following requirements are satisfied:

(1) $\mathcal{M}$ is a normed space.

(2) $\mathcal{M}$ is a linear algebra.
(3) $\|AB\| \leqslant \|A\|\|B\|$ for all $A, B \in \mathcal{M}$.

Let $\mathcal{M}$ be a normed algebra. The norm defines a norm topology on $\mathcal{M}$ which is referred to as the uniform topology. If $\mathcal{M}$ is complete with respect to the norm (i.e., if $\mathcal{M}$ is a Banach space), then it is a Banach algebra. As a result, the set $\mathcal{M}$ of quantum observables is a complete space with respect to the metric determined by the norm. A Banach algebra is a Banach space $\mathcal{M}$, together with a binary operation such that $\|AB\| \leqslant \|A\|\|B\|$ for all $A, B \in \mathcal{M}$.

DEFINITION. A *Banach algebra* is a set $\mathcal{M}$, such that the following requirements are satisfied:

(1) $\mathcal{M}$ is a Banach space.
(2) $\mathcal{M}$ is a linear algebra.
(3) $\|AB\| \leqslant \|A\|\|B\|$ for all $A, B \in \mathcal{M}$.

All bounded operators on a Banach space $\mathcal{H}$ form the Banach algebra $\mathcal{B}(\mathcal{H})$.

A Banach algebra with involution, which has the property $\|A^*\| = \|A\|$, is an involutive Banach algebra. The involutive Banach algebra is a Banach algebra with a norm preserving involution. It is also referred as the *B^*-algebra*.

DEFINITION. An *involutive Banach algebra* is a set $\mathcal{M}$, such that the following requirements are satisfied:

(1) $\mathcal{M}$ is a Banach algebra.
(2) $\mathcal{M}$ is an involutive algebra.
(3) $\|A^*\| = \|A\|$ for all $A \in \mathcal{M}$.

If a Banach algebra $\mathcal{M}$ admits an involution with the property $\|A^*\| = \|A\|$ for all $A \in \mathcal{M}$, then $\mathcal{M}$ is an involutive Banach algebra.

We can assume that a Banach algebra has a unit I (i.e., a multiplicative identity), such that $IA = AI = A$ for all A and such that $\|I\| = 1$.

DEFINITION. A *unital Banach algebra* is a Banach algebra $\mathcal{M}$ with unity I, such that $\|I\| = 1$.

Concrete Banach algebras commonly consist either of complex-valued function or of linear operators. The operations of addition and scalar multiplication are defined pointwise, but there are three different types of multiplication: pointwise multiplication of functions, convolution of functions, and composition of operators. The corresponding algebras are often referred to as function algebras, group algebras, and operator algebras.

The following are examples of some Banach algebras.

(1) The simplest Banach algebra is the complex field $\mathbb{C}$ with $\|z\| = |z|$.

(2) The most important example of a commutative associative Banach algebra is the Banach space $C(M)$ of all bounded continuous complex-valued functions on a separable topological space M, with multiplication defined pointwise.

(3) If $\mathcal{H}$ is a Hilbert space, then $\mathcal{B}(\mathcal{H})$ is a Banach algebra with the operator norm and operator multiplication. If $\mathcal{H} = \mathbb{C}^n$ is finite dimensional, then $\mathcal{B}(\mathbb{C}^n)$ can be identified with the algebra $M_n(\mathbb{C})$ of all $n \times n$ matrices with complex entries. Under this identification, operator multiplication corresponds to matrix multiplication.

Suppose $\mathcal{M}$ is a unital Banach algebra and A is in $\mathcal{M}$. An element A of $\mathcal{M}$ is *invertible* if there exists an element A^{-1} of $\mathcal{M}$ such that $AA^{-1} = A^{-1}A = I$. Note that the set $Inv(\mathcal{M}) = \{A \in \mathcal{M}\colon\ A \text{ is invertible}\}$ is a group under multiplication. The *spectrum* of A, denoted by $\sigma(A)$, is the set of all complex numbers z such that $(zI - A)$ is not invertible in $\mathcal{M}$. Note that the notion of the spectrum is purely algebraic. It only depends on the algebraic structure of the Banach algebra $\mathcal{M}$.

Recall that an algebra whose nonzero elements are invertible is called the *division algebra*. If a Banach algebra $\mathcal{M}$ is a division algebra, then $\mathcal{M}$ is isomorphic to the complex field $\mathbb{C}$. This statement is usually called the Gelfand–Mazur theorem.

THEOREM *(Gelfand–Mazur). Let $\mathcal{M}$ be a unital Banach algebra. If every nonzero elements in $\mathcal{M}$ is invertible, then $\mathcal{M}$ is isomorphic to the algebra $\mathbb{C}$ of complex numbers.*

PROOF. Suppose A is in $\mathcal{M}$ and let $z \in \sigma(A)$. Since $zI - A$ is not invertible, it must be 0. Hence $A = zI$. We see that A is just the set of scalar multiples of I. We define the map $\varphi\colon \mathcal{M} \to \mathbb{C}$ by $\varphi(A) = zI$. Then φ is a linear, one-to-one, and onto map. Moreover, φ preserves multiplication and norm. Then φ is an isomorphism. □

COROLLARY. *If every nonzero elements in a unital Banach algebra $\mathcal{M}$ is invertible, then $\mathcal{M}$ is commutative.*

DEFINITION. Suppose $\mathcal{M}$ is a unital Banach algebra and A is in $\mathcal{M}$. The number

$$r(A) = \sup\bigl\{|z|\colon\ z \in \sigma(A)\bigr\}$$

is called the *spectral radius* of A.

THEOREM. *Suppose $\mathcal{M}$ is a unital Banach algebra and A is in $\mathcal{M}$. Then $\sigma(A)$ is compact in $\mathbb{C}$ and is contained in the closed disk $\{z \in \mathbb{C}\colon\ \|z\| \leqslant \|A\|\}$.*

If $\mathcal{M}$ is a Banach algebra, then the spectrum $\sigma(A)$ of any element $A \in \mathcal{M}$ is compact, and hence the spectral radius is always finite.

COROLLARY. *Let $\mathcal{M}$ be a unital Banach algebra and let $r(A)$ be a spectral radius of $A \in \mathcal{M}$. Then $r(A) \leqslant \|A\|$.*

Note that we always have $r(AB) = r(BA)$.

5.6. C^*-algebra

Definitions and properties

C^*-algebras are a special class of Banach algebras. A C^*-algebra $\mathcal{M}$ is an involutive Banach algebra, such that $\|A^*A\| = \|A\|^2$ for all $A \in \mathcal{M}$.

DEFINITION. A *C^*-algebra* is a set $\mathcal{M}$, such that the following requirements are satisfied:

(1) $\mathcal{M}$ is a Banach algebra.
(2) $\mathcal{M}$ is an involutive algebra.
(3) $\|A^*A\| = \|A\|^2$ for all $A \in \mathcal{M}$.

The norm property that characterizes a C^*-algebra gives the following statement.

STATEMENT. *If A is an element of a C^*-algebra $\mathcal{M}$, then $\|A^*\| = \|A\|$ for all $A \in \mathcal{M}$.*

PROOF. Using

$$\|A\|^2 = \|A^*A\| \leqslant \|A^*\|\|A\|,$$

we obtain $\|A\| \leqslant \|A^*\|$. Replacing A by A^*, we conclude that $\|A^*\| \leqslant \|A\|$ and hence $\|A^*\| = \|A\|$. □

COROLLARY. *If A is an element of a C^*-algebra $\mathcal{M}$, then*

$$\|A^*A\| = \|AA^*\|, \qquad \|A^*A\| = \|A^*\|\|A\|$$

for all $A \in \mathcal{M}$.

Let A be an element of a C^*-algebra $\mathcal{M}$. We say that A is *normal* if $A^*A = AA^*$. We say that A is *self-adjoint* if $A^* = A$. It is clear that a self-adjoint element is normal.

THEOREM. *If A is a normal element of a unital C^*-algebra $\mathcal{M}$, then $r(A) = \|A\|$. If A is self-adjoint, then $r(A) = \|A\|$.*

As a consequence of this theorem is that the norm in a C^*-algebra is unique.

THEOREM. *If A is a self-adjoint element of a C^*-algebra $\mathcal{M}$, then $\sigma(A) \subset \mathbb{R}$.*

Let A be a normal element of a C^*-algebra $\mathcal{M}$. Then A is self-adjoint if and only if $\sigma(A) \subset \mathbb{R}$.

Positive elements

Let A be an element of a C^*-algebra $\mathcal{M}$. We say that A *positive* if $A = B^*B$ for some $B \in \mathcal{M}$. It is clear that positive elements are self-adjoint.

There are various equivalent characterizations of positivity but the most important definition appears to be in terms of the spectrum. We can assume that an element A of a C^*-algebra $\mathcal{M}$ is positive when $A^* = A$ and its spectrum is positive, i.e., $\sigma(A) \subset \mathbb{R}_+$. The set of all positive elements of $\mathcal{M}$ is denoted by $\mathcal{M}_+$. We write $A \in \mathcal{M}_+$ where

$$\mathcal{M}_+ = \big\{A \in \mathcal{M}\colon\ \sigma(A) \subset \mathbb{R}_+\big\} = \{B^*B\colon\ B \in \mathcal{M}\}.$$

This notion of positivity allows us to define the *modulus* of a self-adjoint element A of a C^*-algebra $\mathcal{M}$ as a unique positive element B of $\mathcal{M}$ such that $B^2 = A^*A$. The modulus is denoted by $|A|$.

We collect these statements in the following theorem.

THEOREM. *For a self-adjoint element A of C^*-algebra $\mathcal{M}$, the following three conditions are equivalent*:

(a) $\sigma(A) \subset [0, +\infty)$.
(b) $A = B^*B$ *for some* $B \in \mathcal{M}$.
(c) $A = B^2$ *for some self-adjoint* $B \in \mathcal{M}$.

If A is a self-adjoint element of a C^*-algebra $\mathcal{M}$, then we can define the positive operators

$$A_\pm = \frac{1}{2}\big(|A| \pm A\big). \tag{3}$$

Then $|A| = A_+ + A_-$, and $A = A_+ - A_-$. Every self-adjoint element A has a decomposition $A = A_+ - A_-$, where $A_+A_- \in \mathcal{M}_+$ and $A_+A_- = A_-A_+ = 0$. This decomposition is often referred to as the orthogonal decomposition of A. As a result, we have the following basis theorem regarding self-adjoint elements.

THEOREM. *Let A be a self-adjoint element of a C^*-algebra $\mathcal{M}$. Then there exist unique self-adjoint elements A_+ and A_- in $\mathcal{M}$ such that*

(a) $A = A_+ - A_-$.
(b) $A_+A_- = A_-A_+ = 0$.
(c) *A_+ and A_- are positive, and* $\sigma(A_\pm) \subset \mathbb{R}_+$.
(d) $\|A_\pm\| \leqslant \|A\|$.

Note that statements (a) and (b) can be proves by using (3) and the fact that A commutes with $|A|$.

COROLLARY. *Each bounded quantum observable can be uniquely expressed as a linear combination of positive observables.*

The notion of positivity allows us to introduce an order relation between elements of a C^*-algebra. We can introduce an order relation $A \geqslant B$ between self-adjoint elements. The relation $A \geqslant B$ is interpreted to mean that $A - B \geqslant 0$, i.e., $(A - B) \in \mathcal{M}_+$.

We say that A is *projection* if $A^* = A = A^2$. It is clear that projections are positive. Suppose A is a normal element of a C^*-algebra $\mathcal{M}$. Then A is projection if and only if $\sigma(A) \subset \{0; 1\}$. The self-adjoint projection operators can be associated with physical question whose answer is either "yes" or "no".

Gelfand and Gelfand–Naimark theorems

Let $\mathcal{H}$ be a Hilbert space and let $\mathcal{B}(\mathcal{H})$ be a set of all bounded operators on $\mathcal{H}$. Define sums and multiplications of elements of $\mathcal{B}(\mathcal{H})$ in the standard manner and equip this set with the operator norm. The adjoint operation in $\mathcal{H}$ defines an involution on $\mathcal{B}(\mathcal{H})$. Then $\mathcal{B}(\mathcal{H})$ is a C^*-algebra with respect to these operations and this operator norm. As a result, uniformly closed self-adjoint algebras of bounded operators on a Hilbert space are C^*-algebras. The following theorem states [64] that this particular case in fact describes the general situation.

GELFAND–NAIMARK THEOREM. *Each C^*-algebra is isomorphic to a norm-closed self-adjoint algebra of bounded operators on a Hilbert space.*

Let $\mathcal{B}(\mathcal{H})$ be a C^*-algebra of all bounded linear operators on a separable Hilbert space $\mathcal{H}$. By the Gelfand–Naimark theorem, each C^*-algebra is isomorphic to some subalgebra $\mathcal{M}_0$ of the C^*-algebra $\mathcal{B}(\mathcal{H})$ such that the following properties are satisfied:

(1) $\mathcal{M}_0$ is closed with respect to operator norm topology.
(2) $\mathcal{M}_0$ is closed under the involution operation.

Function algebras also provide examples of C^*-algebras. Let M be a locally compact space. Suppose $C_0(M)$ is a set of all the continuous functions over M which vanish at infinity. By this we mean that for each $A(x) \in C_0(M)$ and $\varepsilon > 0$ there is a compact subspace $M_0 \subset M$ such that $|A(x)| < \varepsilon$ for all $x \in M/M_0$, the complement of M_0 in M. Define the algebraic operations by

$$(A + B)(x) = A(x) + B(x), \quad (aA)(x) = aA(x),$$
$$(AB)(x) = A(x)B(x),$$

and the involution $(A^*)(x) = (A(x))^*$. Introduce the norm $\|A\| = \sup\{|A(x)|: x \in \mathcal{M}\}$. It follows that function algebra $C_0(M)$ is a commutative C^*-algebra. The following theorem states [64] that this example describes the general situation for commutative case.

GELFAND THEOREM. *Let $\mathcal{M}$ be a commutative C^*-algebra. Then $\mathcal{M}$ is isomorphic to the algebra $C_0(M)$ of continuous functions over a locally compact Hausdorff space M, which vanish at infinity.*

The algebra $M_n(\mathbb{C})$ of $n \times n$ matrices over $\mathbb{C}$ is a C^*-algebra if we consider matrices as operators on the space $\mathbb{C}^n$. The involution is given by the adjoint transpose. More generally, one can consider finite direct sums of matrix algebras $M_n(\mathbb{C})$.

THEOREM. *Every finite-dimensional C^*-algebra $\mathcal{M}$ is isomorphic to a finite direct sum of the matrix algebras $M_n(\mathbb{C})$.*

Suppose $\mathcal{B}(\mathcal{H})$ is a C^*-algebra of all bounded linear operators on a Hilbert space $\mathcal{H}$. A set $\mathcal{K}(\mathcal{H})$ of all finite-rank operators is an involutive subalgebra of $\mathcal{B}(\mathcal{H})$. The completion of $\mathcal{K}(\mathcal{H})$ with respect to the operator norm is a C^*-algebra $\mathcal{K}_{comp}(\mathcal{H})$ of all compact operators on $\mathcal{H}$. The algebra $\mathcal{K}_{comp}(\mathcal{H})$ is a C^*-subalgebra of $\mathcal{B}(\mathcal{H})$. A set $\mathcal{K}^2(\mathcal{H})$ of all Hilbert–Schmidt operators is a Banach algebra with respect to the norm $\|A\|_2 = (Tr[A^*A])^{1/2}$.

5.7. *W**-algebra

W^*-algebra and weak operator topology

Every C^*-algebra can be represented by an algebra of bounded operators on a separable Hilbert space. This algebra is closed in the uniform operator topology. We can complete the operator algebra in some topology which is weaker than the uniform topology. At least five useful operator topologies can be defined on $\mathcal{B}(\mathcal{H})$. All are distinct when $\mathcal{H}$ is infinite-dimensional and coincide otherwise.

(1) The *uniform operator topology* is the topology induced on $\mathcal{B}(\mathcal{H})$ by the operator norm:

$$\|A\| = \sup\{\|Ax\|_{\mathcal{H}}\colon \|x\|_{\mathcal{H}} \leqslant 1\}.$$

It is also referred as the *operator norm topology*. Suppose that A_n and A are in $\mathcal{B}(\mathcal{H})$ and that $\|A_n - A\| \to 0$. This is equivalent to the statement that $\|A_n x - Ax\|_{\mathcal{H}} \to 0$ uniformly for all $x \in \mathcal{H}$ such that $\|x\|_{\mathcal{H}} \leqslant 1$. For this reason the topology for $\mathcal{B}(\mathcal{H})$ defined by the operator norm is often called the uniform topology.

(2) The *strong operator topology* is the topology induced on $\mathcal{B}(\mathcal{H})$ by the set of all seminorms of the form:

$$\|A\|_{S,x} = \|Ax\|_{\mathcal{H}},$$

where $x \in \mathcal{H}$. It is also referred as the *S-topology*.

(3) The *weak operator topology* is the topology induced on $\mathcal{B}(\mathcal{H})$ by the set of all seminorms of the form:

$$\|A\|_{W,x,y} = |<x|Ay>|$$

for all $x, y \in \mathcal{H}$. It is also referred as the *W-topology*.

(4) The *ultraweak operator topology* is the topology induced on $\mathcal{B}(\mathcal{H})$ by the set of all seminorms of the form:

$$\|A\|_{\sigma} = \sum_{k=1}^{\infty} |<x_k|Ay_k>|,$$

where $x_k, y_k \in \mathcal{H}$, and

$$\sum_{k=1}^{\infty} \|x_k\|_{\mathcal{H}}^2 < \infty, \qquad \sum_{k=1}^{\infty} \|y_k\|_{\mathcal{H}}^2 < \infty.$$

It is also called the *σ-weak topology*.

(5) The *ultrastrong operator topology* is the topology induced on $\mathcal{B}(\mathcal{H})$ by the set of all seminorms of the form:

$$\|A\|_{\sigma} = \left(\sum_{k=1}^{\infty} \|Ax_k\|_{\mathcal{H}}^2\right)^{1/2} : \sum_{k=1}^{\infty} \|x_k\|_{\mathcal{H}}^2 < \infty.$$

It is also called the *σ-strong topology*.

The uniform operator topology is stronger than the strong operator topology. The strong operator topology is stronger than the weak operator topology. By the Cauchy–Schwarz inequality, strong operator convergence implies weak operator convergence. The weak operator topology is the weakest topology. The uniform operator topology is strongest operator topology.

For $A \in \mathcal{M}$, let L_A, R_A be the maps of $\mathcal{M}$ into itself given by

$$L_A B = AB, \qquad R_A B = BA$$

for all $B \in \mathcal{M}$. We can think of L_A (or R_A) as meaning left (or right) multiplication by A. We mention that the maps $L_A : A \to AB$ and $R_A : A \to BA$ with fixed B are continuous for all five topologies. However, the maps $A, B \to AB$ are not continuous except for uniform topology. Note that the map $J : A \to A^*$ is continuous for the uniform, the weak, and the ultraweak operator topologies but not for the strong nor ultrastrong topologies.

Note that an involutive subalgebra of $\mathcal{B}(\mathcal{H})$, which is closed with respect to the uniform operator topology, is a C^*-algebra.

DEFINITION. A W^*-*algebra* is an involutive subalgebra of $\mathcal{B}(\mathcal{H})$, which is closed with respect to the weak operator topology (W-topology).

If $\mathcal{M}$ is a C^*-subalgebra of $\mathcal{B}(\mathcal{H})$, then the weak or strong operator closure of $\mathcal{M}$ is a W^*-algebra. Note that the weak operator closure of $\mathcal{M}$ coincides with the strong operator closure of $\mathcal{M}$ in $\mathcal{B}(\mathcal{H})$.

In this definition the weak operator topology can be replaced by almost any other operator topology other than the uniform topology, in particular by the strong, ultrastrong or ultraweak topologies. Note that the involutive algebras of bounded operators that are closed in the uniform operator topology are C^*-algebras. In particular, any W^*-algebra is a C^*-algebra.

There are two following basic examples of W^*-algebras:

(1) The algebra $B(\mathcal{H})$ of all bounded operators on a Hilbert space $\mathcal{H}$ is a W^*-algebra. This algebra is noncommutative if the Hilbert space $\mathcal{H}$ has dimension at least 2.

(2) Let $\mathcal{H} = L^2(\mathbb{R})$ be the Hilbert space of all square integrable functions on $\mathbb{R}$. The algebra $L^\infty(\mathbb{R})$ of bounded measurable functions on $\mathbb{R}$ (modulo null functions) is a commutative W^*-algebra, which acts by pointwise multiplication on $L^2(\mathbb{R})$. For $A(x) \in L^\infty(\mathbb{R})$, let $L_{A(x)}$ be the mapping of $L^2(\mathbb{R})$ into $L^2(\mathbb{R})$ given by $L_{A(x)}B(x) = A(x)B(x)$ for $B(x) \in L^2(\mathbb{R})$. We can think of $L_{A(x)}$ as meaning left multiplication by $A(x)$. These operators form a commutative W^*-algebra.

The relationship between commutative W^*-algebras and measure spaces is analogous to that between commutative C^*-algebras and locally compact Hausdorff spaces. Every commutative W^*-algebra is isomorphic to $L^\infty(M)$ for some measure space (M, μ). Conversely, for every σ-finite measure space M, the set $L^\infty(M)$ is a W^*-algebra. As a result, the theory of W^*-algebras can be considered as a noncommutative measure theory.

W^*-algebra and predual Banach space

A W^*-algebra as a Banach space is a dual of some Banach space [132]. This property is characteristic and can serve as a definition of the algebra.

THEOREM *(Sakai). A C^*-algebra $\mathcal{M}$ is isomorphic to a W^*-algebra if and only if the space of $\mathcal{M}$ is a dual space of some Banach space.*

We can define W^*-algebra as a set of operators on a Hilbert space. A W^*-algebra can also be defined abstractly as a C^*-algebra that have a predual space. In other words the W^*-algebra, considered as a Banach space, is the dual of some other Banach space called the *predual*. The predual is unique up to isomorphism.

As a result, W^*-algebras are a special class of C^*-algebras.

DEFINITION. A *W^*-algebra* is a set $\mathcal{M}$, such that the following requirements are satisfied:

(1) $\mathcal{M}$ is a C^*-algebra.
(2) A Banach space of $\mathcal{M}$ is dual of some Banach space.

A W^*-algebra is a set $\mathcal{M}$, such that the following requirements are satisfied:

(a) $\mathcal{M}$ is a Banach space.
(b) $\mathcal{M}$ is dual of a Banach space.
(c) $\mathcal{M}$ is an involutive algebra.
(d) $\|A^*A\| = \|A\|^2$ for all $A \in \mathcal{M}$.

Some authors use "von Neumann algebra" for the operator algebras on a Hilbert space, and "W^*-algebra" for the abstract concept, so a von Neumann algebra is a W^*-algebra, together with a Hilbert space and a representation by operators on this space. The concrete and abstract definitions of a W^*-algebra are similar to the concrete and abstract definitions of a C^*-algebra, which can be defined either as a norm-closed involutive algebra of operators on a Hilbert space, or as an involutive Banach algebra, such that $\|AA^*\| = \|A\|\|A^*\|$.

W^*-algebra and bicommutant

A W^*-algebra can be considered as a subset of the bounded operators closed under involution and equal to its *double commutant*, or equivalently as a commutant of some subset closed under involution.

Let $\mathcal{M}$ be a subset of $\mathcal{B}(\mathcal{H})$. Suppose $\mathcal{M}'$ is the set of all bounded operators on $\mathcal{H}$ commuting with every operator in $\mathcal{M}$. Then the set

$$\mathcal{M}' = \{A \in \mathcal{M}\colon\ AB = BA \text{ for all } B \in \mathcal{M}\}$$

is called the *commutant* of $\mathcal{M}$. The *double commutant* (or *bicommutant*) of $\mathcal{M}$, denoted by $\mathcal{M}''$, is simply the commutant of $\mathcal{M}'$.

THEOREM. *If $\mathcal{M}$ is invariant under the involution, that is, if $A \in \mathcal{M}$ implies $A^* \in \mathcal{M}$, then $\mathcal{M}'$ is a C^*-algebra, which is closed with respect to the weak operator topology.*

For a subset $\mathcal{M}$ of $\mathcal{B}(\mathcal{H})$, we let $\mathcal{M}^* = \{A^*\colon\ A \in \mathcal{M}\}$. We say that $\mathcal{M}$ is *self-adjoint* if $\mathcal{M}^* = \mathcal{M}$.

THEOREM. *$\mathcal{M}'$ is a W^*-algebra if $\mathcal{M}$ is self-adjoint.*

Suppose $\mathcal{M}$ is a unital self-adjoint subalgebra of $\mathcal{B}(\mathcal{H})$. Then $\mathcal{M}''$ is the weak (or strong) operator closure of $\mathcal{M}$. As a result, $\mathcal{M}$ is dense in $\mathcal{M}''$ with respect to the weak (or strong) operator topology.

Let us give the basic theorem regarding commutants.

THE DOUBLE COMMUTANT THEOREM. *Let $\mathcal{M}$ be a C^*-subalgebra of $\mathcal{B}(\mathcal{H})$. Then $\mathcal{M}$ is a W^*-algebra if and only if $\mathcal{M} = \mathcal{M}''$.*

As a result, a W^*-algebra is an involutive subalgebra $\mathcal{M}$ of $\mathcal{B}(\mathcal{H})$ such that $\mathcal{M} = \mathcal{M}''$.

Functionals on W^*-algebra

Suppose ω is a linear functional on $\mathcal{B}(\mathcal{H})$. Then the following conditions are equivalent:

(a) ω is weakly continuous.
(b) ω is strongly continuous.
(c) There exists elements x_k, y_k, $k = 1, \ldots, n$, in $\mathcal{H}$ such that $\omega(A) = \sum_{k=1}^{n} <x_k|Ay_k>$ for $A \in \mathcal{B}(\mathcal{H})$.

We can introduce several topologies in $\mathcal{B}(\mathcal{H})$, based on the duality between the Banach space $\mathcal{B}(\mathcal{H})$ and $\mathcal{B}(\mathcal{H})^*$. Since $\mathcal{B}(\mathcal{H})$ is the dual space of the Banach space $\mathcal{B}(\mathcal{H})^*$, we can define the ultraweak and ultrastrong topologies in the following form.

The *ultraweak operator topology* can be defined by the set of all seminorms of the form:

$$\|A\|_{\sigma,\rho} = \big|\omega(A)\big|,$$

where $\omega \in \mathcal{B}(\mathcal{H})^*$. If $\omega \in \mathcal{B}(\mathcal{H})^*$ is nonnegative functional on $\mathcal{B}(\mathcal{H})^*$, i.e., $\omega(A^*A) \geqslant 0$ for $A \in \mathcal{B}(\mathcal{H})$, then

$$\|A\|_\omega = \left(\omega(A^*A)\right)^{1/2}$$

is a seminorm in $\mathcal{B}(\mathcal{H})$. The topology determined by the family of these seminorms is a *ultrastrong operator topology* in $\mathcal{B}(\mathcal{H})$.

In quantum mechanics, C^*-algebras and W^*-algebras are considered as algebras of quantum observables. A W^*-algebra has the following important property: If a state on a W^*-algebra of observables is continuous with respect to the ultraweak topology, then a kinematical postulate becomes the theorem.

THEOREM. *Let $\mathcal{M}$ be a unital W^*-algebra, and let ω be a nonnegative linear functional on $\mathcal{M}$ with $\omega(I) = 1$. If ω is continuous with respect to the ultraweak topology, then there exists a density operator $\rho \in \mathcal{M}$, such that*

$$\omega(A) = Tr[\rho A].$$

This theorem is a generalization of the Riesz–Fréchet theorem from Liouville spaces into W^*-algebras.

5.8. *JB*-algebra

A Jordan algebra is defined by the identities:

$$A \circ B = B \circ A, \quad (A \circ B) \circ B^2 = \left(A \circ B^2\right) \circ B.$$

The algebra obtained from an associative algebra on replacing the product AB by $A \circ B = (1/2)(AB + BA)$ is a Jordan algebra. Any subalgebra of a Jordan algebra of this type is called special.

A *JB*-algebra is a real Jordan algebra $\mathcal{M}$ which is also a Banach space the norm on which satisfies some conditions.

DEFINITION. A *JB-algebra* is a set $\mathcal{M}$, such that the following requirements are satisfied:

(1) $\mathcal{M}$ is a Jordan algebra over $\mathbb{R}$.
(2) $\mathcal{M}$ is a Banach space over $\mathbb{R}$.
(3) $\|A^*A\| = \|A\|^2$ for all $A \in \mathcal{M}$.
(4) $\|A^2 - B^2\| \leqslant \max\{\|A^2\|, \|B^2\|\}$ for all A and B in $\mathcal{M}$.

An example of a *JB*-algebra is the self-adjoint part of a C^*-algebra. The bounded observables of a quantum system are identified with a real linear space of bounded self-adjoint operators. We can assume that this space is a Jordan algebra

of self-adjoint operators which is closed in the operator topology. A uniformly closed Jordan algebra of self-adjoint operators on a Hilbert space is called the *JC-algebra*. This algebra is an example of *JB*-algebra. The classical example of a *JB*-algebra which lacks a Hilbert space representation is M_3^8 the 3×3 Hermitian matrices over the octonions.

5.9. Hilbert algebra

Let us define an involutive operator algebra with some scalar product. An involutive algebra $\mathcal{M}$ over $\mathbb{C}$ is called the *left Hilbert algebra*, if $\mathcal{M}$ admits a scalar product satisfying the following conditions:

(1) Each fixed $A \in \mathcal{M}$ generates the bounded map L_A: $B \in \mathcal{M} \to AB \in \mathcal{M}$ by multiplying from the left.
(2) $(AB|C) = (B|A^*C)$ for all $A, B, C \in \mathcal{M}$.
(3) The subalgebra, denoted by $\mathcal{M}^2$, linearly generated (spanned) by all products AB of $A, B \in \mathcal{M}$ is dense in $\mathcal{M}$.

A right Hilbert algebra is defined similarly. An involutive algebra $\mathcal{M}$ over $\mathbb{C}$ is called the *right Hilbert algebra*, if $\mathcal{M}$ admits a scalar product satisfying the following conditions:

(1) Each fixed $A \in \mathcal{M}$ generates the bounded map $R_A : B \in \mathcal{M} \to BA \in \mathcal{M}$ by multiplying from the right.
(2) $(BA|C) = (B|CA^*)$ for all $A, B, C \in \mathcal{M}$.
(3) The subalgebra, denoted by $\mathcal{M}^2$, linearly generated by all products AB of $A, B \in \mathcal{M}$ is dense in $\mathcal{M}$.

The involution is an isometry, if $(A|B) = (B^*|A^*)$ for all $A, B \in \mathcal{M}$. If the involution of a left Hilbert algebra $\mathcal{M}$ is an isometry, then it is also a right Hilbert algebra. In this case, we say that $\mathcal{M}$ is a (unimodular) Hilbert algebra.

DEFINITION. A *Hilbert algebra* is an involutive algebra $\mathcal{M}$, such that the following conditions are satisfied.

(1) $\mathcal{M}$ is a pre-Hilbert space with respect to a scalar product $(A|B)$.
(2) $(A|B) = (B^*|A^*)$ for all $A, B \in \mathcal{M}$.
(3) $(CA|B) = (A|C^*B)$ for all $A, B, C \in \mathcal{M}$.
(4) For each fixed $A \in \mathcal{M}$, the mapping $L_A : B \to AB$ is continuous.
(5) The subalgebra, denoted by $\mathcal{M}^2$, linearly generated by all products AB of $A, B \in \mathcal{M}$ is dense in $\mathcal{M}$.

Note that a scalar product of Hilbert algebra cannot be defined by the correlation functions, since requirements (4)–(5) are not satisfied. If a set $\mathcal{M}$ of operators

is a Liouville space and an involutive algebra, then $\mathcal{M}$ is a Hilbert algebra. As an example of a Hilbert algebra, we can consider an involutive Banach algebra $\mathcal{K}^2(\mathcal{H})$ of Hilbert–Schmidt operators that equipped with the scalar product $(A|B) = Tr[A^*B]$.

The theory of Hilbert algebras is the noncommutative counter part of the algebra of all bounded square integrable functions on a measure space.

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Chapter 6

Mathematical Structures on State Sets

6.1. State as functional on operator algebra

Let $\mathcal{M}$ be a set of observables, and let $\mathcal{M}^*$ be a set of all functionals on $\mathcal{M}$. A state must be some sort of linear functional on the observables. If $\mathcal{M}$ is a set with unit observable I, then there exists a rule that assigns to each bounded observable $A \in \mathcal{M}$ its expectation value in the state $\omega \in \mathcal{M}^*$:

$$<A> = \omega(A)/\omega(I).$$

If ω is a normalized functional such that $\omega(I) = 1$, then the expectation value is $<A> = \omega(A)$.

DEFINITION. A functional ω is *nonnegative* if $\omega(A^2) \geqslant 0$ for all $A \in \mathcal{M}$.

A nonnegative linear functional ω does not necessarily take nonnegative values all the time, but only for $A \geqslant 0$.

DEFINITION. A functional is *positive* if the following two conditions are satisfied:

(1) $\omega(A^2) > 0$ for all $A \neq 0$.
(2) $\omega(A^2) = 0$ if and only if $A = 0$.

These conditions mean that ω is positive on positive elements of $\mathcal{M}$. If ω is a positive functional, then ω is nonnegative. In general, a nonnegative functional is not positive.

As a result, a state can be considered as a nonnegative (or positive) normalized linear functional on a set of observables.

DEFINITION. Let $\mathcal{M}$ be a set of all observables, and let $\mathcal{M}^*$ be a set of all functionals on $\mathcal{M}$. A *state* is an element ω of $\mathcal{M}^*$, such that the following requirements are satisfied:

(1) $\omega(aA + bB) = a\omega(A) + b\omega(B)$ for all $A, B \in \mathcal{M}$ and $a, b \in \mathbb{R}$.
(2) $\omega^*(A) = \omega(A^*)$ for all $A \in \mathcal{M}$.
(3) $\omega(I) = 1$.
(4) $\omega(0) = 0$.
(5) $\omega(A^2) > 0$ for all $A \neq 0$.

An example of a state is provided by the functional $\omega(A) = Tr[\rho A]$, where ρ is a positive self-adjoint operator with unit trace. Such states ω are described by the operators ρ. These operators ρ are called the *density operators*. In general, a state cannot be described by a density operator. We use a postulate that assigns to each quantum state exactly one density operator.

POSTULATE. For each state $\omega \in \mathcal{M}^*$, there exists a density operator $\rho \in \mathcal{M}$, such that

$$<A> = \omega(A) = Tr[\rho A]. \tag{1}$$

From the Riesz–Fréchet theorem, each state ω on a Liouville space $\mathcal{M}$ can be presented by (1). The given postulate generalizes the statement of the Riesz–Fréchet theorem from an operator Hilbert space $\mathcal{M}$ with the scalar product $(A|B) = Tr[A^*B]$ into arbitrary operator algebras.

Let $\mathcal{M}$ be a set of quantum observables and let S be a set of quantum states. Note that $\omega(A)$ is the expectation value of A in the state ω. We say that $A \leqslant B$ whenever $\omega(A) \leqslant \omega(B)$ for all $\omega \in S$. In particular, we write $A \geqslant 0$ if and only if $\omega(A) \geqslant 0$ for all $\omega \in S$. The relation $\leqslant$ defined above is a partial ordering relation on $\mathcal{M}$.

POSTULATE OF ORDER STRUCTURE. The inequality $A \leqslant B$ between any two elements A and B of $\mathcal{M}$ holds if and only if A and B satisfy the inequality $\omega(A) \leqslant \omega(B)$ for all states $\omega \in S$. In particular, $A \leqslant B$ and $B \leqslant A$ implies $A = B$.

As a result, the set of states S is such that $\omega(A) = \omega(B)$ for all $\omega \in S$ implies $A = B$. Hence the postulate assumes that there are enough states in S so that we can distinguish between two observables by measuring their expectation values. The set of observables $\mathcal{M}$ can be equipped with the algebraic structure of a linear space over $\mathbb{R}$.

POSTULATE OF ALGEBRAIC STRUCTURE.

(1) For any pair of observables A and B in $\mathcal{M}$ and real numbers $a, b \in \mathbb{R}$ there exists an element $(aA + bB)$ in M, such that $\omega(aA + bB) = a\omega(A) + b\omega(B)$ for all $\omega \in S$.

(2) There exists in $\mathcal{M}$ two elements 0 and I such that $\omega(0) = 0$ and $\omega(I) = 1$ for all $\omega \in S$.

By virtue of the postulate of order structure, we have that 0, I, aA, and $(A + B)$ are uniquely defined. For the same reason, we conclude that the sum is distributive with respect to the multiplication by real numbers and is both commutative and associative.

6.2. State on C^*-algebra

State as a linear functional

States on a C^*-algebra are important component in the description of both classical and quantum systems. Let $\mathcal{M}$ be a C^*-algebra. We denote the dual of $\mathcal{M}$ by $\mathcal{M}^*$. Then $\mathcal{M}^*$ is a space of continuous linear functionals on $\mathcal{M}$. We can define the norm of any functional ω on $\mathcal{M}$ by

$$\|\omega\| = \sup_{A \in \mathcal{M}} \{|\omega(A)|: \|A\|_{\mathcal{M}} = 1\}.$$

A linear functional ω on an involutive algebra $\mathcal{M}$ is nonnegative if $\omega(A^*A) \geqslant 0$ for all $A \in \mathcal{M}$.

DEFINITION. A nonnegative linear functional ω on a C^*-algebra $\mathcal{M}$ with $\|\omega\| = 1$ is called a *state*.

In case ω' is only a nonnegative linear functional on $\mathcal{M}$, we define $\omega = \|\omega'\|^{-1}\omega'$, which is a state on $\mathcal{M}$.

DEFINITION. A *state on a C^*-algebra* $\mathcal{M}$ is a functional ω on $\mathcal{M}$, such that the following conditions are satisfied:

(1) ω is a linear functional on $\mathcal{M}$.
(2) ω is a nonnegative functional on $\mathcal{M}$.
(3) ω is normalized: $\|\omega\| = 1$.

A *state on a unital C^*-algebra* $\mathcal{M}$ is a linear nonnegative functional ω on $\mathcal{M}$, such that $\omega(I) = 1$.

In these definitions, we have not required that the nonnegative functionals be continuous, i.e., the statement that there exists $c > 0$ such that $|\omega(A)| < c\|A\|_{\mathcal{M}}$ for all $A \in \mathcal{M}$. For a C^*-algebra the continuity is a consequence of positivity. Note also that every positive element of a C^*-algebra is of the form A^*A and hence positivity of ω is equivalent to ω being positive on positive elements.

The following are examples of some states.

(a) Positive measures on function algebras are positive linear functionals. Probability measures are states.
(b) The mapping $A \to Tr[\rho A]$ of $n \times n$ matrices A if ρ is positive in the sense that all of its eigenvalues are positive. If in addition $Tr[\rho] = 1$, then it is a state.

The set of all states on $\mathcal{M}$ will be denoted by $S(\mathcal{M})$.

STATEMENT. *$S(\mathcal{M})$ is a subset of $\mathcal{M}^*$.*

Suppose $\mathcal{M}$ is a C^*-algebra and ω is a linear functional on $\mathcal{M}$. We say that ω is a *Hermitian functional* if $\omega(A^*) = \omega(A)^*$ for all $A \in \mathcal{M}$.

STATEMENT. *All positive functionals on a C^*-algebra are Hermitian.*

A linear functional ω on a C^*-algebra $\mathcal{M}$ is Hermitian if and only if $\omega(A)$ is real for each self-adjoint $A \in \mathcal{M}$.

Positive, continuous, bounded

A state ω on $\mathcal{M}$ defines a scalar product $< ; >$ on $\mathcal{M}$ through the formula

$$<A; B> = \omega(A^*B),$$

which implies the general Cauchy–Schwarz inequality. If ω is a nonnegative linear functional on a C^*-algebra $\mathcal{M}$, then

$$\left|\omega(A^*B)\right|^2 \leqslant \omega(A^*A)\omega(B^*B), \qquad \left(\omega(A^*B)\right)^* = \omega(B^*A) \tag{2}$$

for all $A, B \in \mathcal{M}$.

STATEMENT. *Let ω be a linear functional on a C^*-algebra $\mathcal{M}$. Then the following conditions are equivalent*:

(1) *ω is nonnegative.*
(2) *ω is continuous.*

Then each state ω on a C^*-algebra $\mathcal{M}$ is continuous. It is well known that the necessary and sufficient condition for the continuity of a linear functional is its boundedness $\|\omega\| < \infty$. From the inequality $\|\omega(A)\| \leqslant \|A\|_{\mathcal{M}}$, we see that ω is bounded and hence continuous with $\|\omega\| \leqslant 1$.

An algebra $\mathcal{M}$ is unital if there exists a unit I such that $\|I\|_{\mathcal{M}} = 1$. A state on a unital C^*-algebra $\mathcal{M}$ is a linear functional ω that is nonnegative, i.e., $\omega(A^*A) \geqslant 0$ for all $A \in \mathcal{M}$, and normalized: $\omega(I) = 1$.

STATEMENT. *Let ω be a linear functional on a unital C^*-algebra $\mathcal{M}$. Then ω is nonnegative if and only if ω is bounded and $\|\omega\| = \omega(I)$.*

A continuous linear functional ω on a unital C^*-algebra $\mathcal{M}$ is positive if and only if $\|\omega\| = \omega(I) < \infty$. If $\omega(I) = 1$, then $\|\omega\| = 1$. Then a linear functional ω on a unital C^*-algebra $\mathcal{M}$ is a state if and only if $\|\omega\| = \omega(I) = 1$.

STATEMENT. *Suppose $\mathcal{M}$ is a C^*-algebra and A is in $\mathcal{M}$. For each $z \in \sigma(A)$ there exists a state ω on $\mathcal{M}$ such that $\omega(A) = z$.*

The set of all states on $\mathcal{M}$ will be denoted by $S(\mathcal{M})$. The following result shows that the set $S(\mathcal{M})$ of a C^*-algebra is not only empty, it is also large enough to reveal many properties of an element in the algebra.

STATEMENT. *Suppose $\mathcal{M}$ is a C^*-algebra and A is in $\mathcal{M}$.*

(a) $A = 0$ *if and only if* $\omega(A) = 0$ *for all* $\omega \in S(\mathcal{M})$.
(b) $A = A^*$ *if and only if* $\omega(A) \in \mathbb{R}$ *for all* $\omega \in S(\mathcal{M})$.
(c) $A \geqslant 0$ *if and only if* $\omega(A) \geqslant 0$ *for all* $\omega \in S(\mathcal{M})$.
(d) *If A is normal* ($A^*A = AA^*$), *then there exists* $\omega \in S(\mathcal{M})$ *such that* $\|A\|_{\mathcal{M}} = |\omega(A)|$.

Convex set

Let ω_1 and ω_2 be nonnegative linear functionals on a C^*-algebra $\mathcal{M}$. If ω_1 and ω_2 are states, then $\omega = \lambda\omega_1 + (1 - \lambda)\omega_2$ is positive for $0 \leqslant \lambda \leqslant 1$, and

$$\|\omega\| = \lambda\|\omega_1\| + (1 - \lambda)\|\omega_2\| = \lambda + (1 - \lambda) = 1.$$

Then ω is a state. As a result, convex combinations of states are states. If ω_1 and ω_2 are states on $\mathcal{M}$ and $0 < a < 1$, then

$$\omega = a\omega_1 + (1 - a)\omega_2 \tag{3}$$

is a state. The set $S = \{\omega \in S(\mathcal{M})\colon \|\omega\| \leqslant c\}$ is a *convex set* if $\omega_1, \omega_2 \in S$ and $0 < a < 1$ implies $a\omega_1 + (1 - a)\omega_2 \in S$.

STATEMENT. *The states on $\mathcal{M}$ form a convex subset of the dual of $\mathcal{M}$.*

The property of nonnegativity introduces a natural ordering of functionals. If ω_1 and ω_2 are nonnegative linear functionals, we write $\omega_1 \geqslant \omega_2$ whenever $\omega_1 - \omega_2$ is nonnegative.

DEFINITION. A *convex hull* of S is a set S_{convex} of all convex combinations of elements from S:

$$S_{convex} = \left\{ \sum_{k=1}^{n} a_k \omega_k \colon \omega_k \in S,\ a_k \geqslant 0,\ \sum_{k=1}^{n} a_k = 1,\ n \in \mathbb{N} \right\}.$$

STATEMENT. *A set $S(\mathcal{M})$ of all states on $\mathcal{M}$ is a convex hull.*

Note that a set $S(\mathcal{M})$ is a convex hull if $\omega_k \in S(\mathcal{M})$, $a_k \geqslant 0$, $\sum_{k=1}^{n} a_k = 1$ implies $\sum_{k=1}^{n} a_k \omega_k \in S(\mathcal{M})$.

Extreme elements and pure states

We call a state pure whenever it cannot be written as a convex combination of other states. A state ω is a *pure state* if it cannot be decomposed into a non-trivial convex combination, i.e., if for $0 \leqslant a \leqslant 1$ and $\omega_1, \omega_2 \in S(\mathcal{M})$, the relation (3) implies that $\omega_1 = \omega_2 = \omega$. The set of all pure states is denoted by $P(\mathcal{M})$.

The following are examples of some pure states.

(a) Consider the commutative C^*-algebra of continuous functions on a compact set. The state are probability measures, and the pure states are integrals with Dirac delta-functions.
(b) The map $A \to Tr[\rho A]$ on $n \times n$ matrices A, where all eigenvalues ρ are positive and $Tr[\rho] = 1$, is a state. Then the trace map with one-dimensional projections is pure state, i.e., the state $A \to <n|A|n>$ is pure.

Let S be a subset of a real or complex linear space $\mathcal{M}$. A subset $S_0 \subset S$ is said to be an *extremal subset* of S, if a convex combination $a\omega_1 + (1-a)\omega_2$, $0 < a < 1$, of two elements ω_1 and ω_2 of S lies in S_0 only if both ω_1 and ω_2 are in S_0. An element ω of S is called *extreme element* of S_0 if ω cannot be written as $\omega = a\omega_1 + (1-a)\omega_2$, with $a \in (0, 1)$ and ω_1, ω_2 being different elements of S_0.

For example, in a three-dimensional Euclidean space, the surface of a solid ball (sphere) is an extremal subset of the ball, and every point of the surface is an extreme element. For the unit sphere $S = \{\Psi \in \mathcal{H} \colon \|\Psi\|_{\mathcal{H}} \leqslant 1\}$ in a Hilbert space $\mathcal{H}$ the extreme elements of S are precisely those on the surface of S, i.e., those of norm 1.

THEOREM. *Let $\mathcal{M}$ be a C^*-algebra, and let $S_0(\mathcal{M})$ be a set of positive linear functionals on $\mathcal{M}$ with norm less than or equal to one. Then $S_0(\mathcal{M})$ is a convex subset of the dual $\mathcal{M}^*$ whose extreme elements are* 0 *and the pure states $P(\mathcal{M})$.*

As a result, each pure state on a C^*-algebra $\mathcal{M}$ is an extreme element of $S(\mathcal{M})$, and $P(\mathcal{M})$ is an extremal subset of $S(\mathcal{M})$.

Weak-star topology on states

Let $\mathcal{M}$ be a Banach space and let $\mathcal{M}^*$ be dual of $\mathcal{M}$. The weak topology on $\mathcal{M}$ induced by $\mathcal{M}^*$ is the weakest (smallest) topology on $\mathcal{M}$, which makes every map in $\mathcal{M}^*$ continuous. By the weak topology on $\mathcal{M}$, we mean the topology induced by the family of all bounded linear functionals on $\mathcal{M}$. Thus a set $\{A_k\}$ converges to A in $\mathcal{M}$ weakly (i.e., in the weak topology) if and only if $\omega(A_k)$ converges to $\omega(A)$ for every ω in $\mathcal{M}^*$.

The *weak-star topology* (or W^*-topology) on $\mathcal{M}^*$ is simply the weak topology on $\mathcal{M}^*$ induced by the family $\{l_A^*\colon\ A \in \mathcal{M}\}$, where for each A in $\mathcal{M}$ the map $l_A^* : \mathcal{M}^* \to \mathbb{C}$ is defined by $l_A^*\omega = \omega(A)$ for all $\omega \in \mathcal{M}^*$. Thus a set $\{\omega_n\}$ in $\mathcal{M}^*$ converges to ω in $\mathcal{M}^*$ in the weak-star topology if and only if $\omega_n(A)$ converges to $\omega(A)$ for every A in $\mathcal{M}$. We say that a set of continuous functionals ω_n on $\mathcal{M}$ converges in the weak-star topology to $\omega \in \mathcal{M}^*$ if $\lim_{n\to\infty} \omega_n(A) = \omega(A)$ for all $A \in \mathcal{M}$.

For every C^*-algebra $\mathcal{M}$, we let $S(\mathcal{M})$ denote the set of all states on $\mathcal{M}$. The state set $S(\mathcal{M})$ is a subset of $\mathcal{M}^*$ that is closed both with respect to the norm and the weak-star topology. The set $S(\mathcal{M})$, together with the weak-star topology will be called the state (topological) space of $\mathcal{M}$. The topological space $P(\mathcal{M})$ of pure states is the weak-star closure of a set of pure states on $\mathcal{M}$.

Weak-star compact set

A linear topological space $\mathcal{M}$ over $\mathbb{R}$ is called a *locally convex* (*linear topological*) *space* if any of its open subsets contains convex, balanced and absorbing open sets:

(1) M is convex if $A, B \in M$ and $0 < a < 1$ imply $aA + (1-a)B \in M$.
(2) M is balanced if $A \in M$ and $|a| \leqslant 1$ imply $aA \in M$.
(3) M is absorbing if for any $A \in M$, there exists $a > 0$ such that $a^{-1}A \in M$.

Let S be a compact convex subset of a locally convex linear topological space $\mathcal{M}$. Suppose E is a set of the extreme elements of S. Then S coincides with the smallest closed set containing every convex combination $\sum_{k=1}^n a_k\omega_k$, where $a_k \geqslant 0$, $\sum_{k=1}^n a_k = 1$ and $\omega_k \in E$, i.e., S is equal to the closure of the convex hull of E.

THEOREM. *A nonvoid compact convex subset S_0 of a locally convex linear topological space S has at least one extreme element.*

The Krein–Milman theorem say that a nonvoid convex compact subset S of a locally convex linear topological space is equal to the closure of the convex hull of

the extreme elements of S. The theorem assures the existence of extreme elements for compact convex subset of a locally convex space.

Since the state space $S(\mathcal{M})$ is convex and weak-star compact, it has extreme points. By the Krein–Milman theorem, $S(\mathcal{M})$ is the weak-star closed convex hull of the set $P(\mathcal{M})$ of its extreme points. Elements of $P(\mathcal{M})$ are called pure states of $\mathcal{M}$. Thus every ω in $S(\mathcal{M})$ can be approximated in the weak-star topology by elements of the form $\sum_{k=1}^{n} a_k\omega_k$, where each ω_k is in $P(\mathcal{M})$, each a_k in $[0, 1]$, and $\sum_{k=1}^{n} a_k = 1$.

Let us give the important theorem regarding pure states.

THEOREM. *Suppose $\mathcal{M}$ is a C^*-algebra and A is in $\mathcal{M}$.*

(a) $A = 0$ *if and only if* $\omega(A) = 0$ *for all* $\omega \in P(\mathcal{M})$.
(b) $A = A^*$ *if and only if* $\omega(A) \in \mathbb{R}$ *for all* $\omega \in P(\mathcal{M})$.
(c) $A \geqslant 0$ *if and only if* $\omega(A) \geqslant 0$ *for all* $\omega \in P(\mathcal{M})$.
(d) *If A is normal, then there exists* $\omega \in P(\mathcal{M})$ *such that* $\|A\|_{\mathcal{M}} = |\omega(A)|$.

This theorem shows that the set of pure states of a C^*-algebra is sufficiently large enough to reveal many properties of an element in the algebra.

Closed unit ball

A *closed unit ball* in $\mathcal{M}^*$ is a set of all bounded linear functionals on $\mathcal{M}$ whose norms are less that or equal to 1.

A set $S(\mathcal{M})$ is a subset of the unit ball $\mathcal{B}^* = \{\omega \in \mathcal{M}^*\colon \|\omega\| \leqslant 1\}$ in $\mathcal{M}^*$. A set $S(\mathcal{M})$ is a compact with respect to weak-star topology on $\mathcal{M}^*$. This property is a corollary of the following theorem.

THEOREM *(Alaoglu). Let $\mathcal{M}$ be a Banach space, and let $\mathcal{M}^*$ be a dual space of $\mathcal{M}$. If $\mathcal{B}^*$ is a closed unit ball in $\mathcal{M}^*$, then $\mathcal{B}^*$ is compact in the weak-star topology.*

A set $S(\mathcal{M})$ is a subset of the closed unit ball in the dual space of $\mathcal{M}$. We can collect the properties of $S(\mathcal{M})$ in the following statement.

STATEMENT. *Let $S(\mathcal{M})$ be a set of all states on a C^*-algebra $\mathcal{M}$. Then the following properties are satisfied*:

(1) $S(\mathcal{M})$ *is a subset of* $\mathcal{M}^*$.
(2) $S(\mathcal{M})$ *is a convex set.*
(3) $S(\mathcal{M})$ *is a convex hull of its extreme elements.*
(4) $S(\mathcal{M})$ *is a unit ball in* $\mathcal{M}^*$.
(5) $S(\mathcal{M})$ *is compact subset of* $\mathcal{M}^*$.

This statement describe the mathematical structures on the set $S(\mathcal{M})$ of states.

6.3. Representations C^*-algebra and states

Let us introduce the basic definition of representation theory.

DEFINITION. A *representation of a C^*-algebra* $\mathcal{M}$ is a pair $(\mathcal{H}, \pi)$, where $\mathcal{H}$ is a complex Hilbert spaces and π is a linear map from $\mathcal{M}$ into $\mathcal{B}(\mathcal{H})$ satisfying the following conditions:

(1) $\pi(AB) = \pi(A)\pi(B)$ for all $A, B \in \mathcal{M}$.
(2) $\pi(A^*) = \pi(A)^*$ for all $A \in \mathcal{M}$.
(3) if $\mathcal{M}$ is unital, then $\pi(I) = I$.

The kernel of a representation $(\mathcal{H}, \pi)$ of a C^*-algebra $\mathcal{M}$ is $Ker(\pi) = \{A \in \mathcal{M}\colon\ \pi(A) = 0\}$. The representation $(\mathcal{H}, \pi)$ is said to be *faithful* if and only if $Ker(\pi) = 0$. A representation is faithful if $\pi(A) = 0$ implies $A = 0$. In this case π is a bijective map from $\mathcal{M}$ to $\pi(\mathcal{M}) = \{\pi(A)\colon\ A \in \mathcal{M}\}$. Hence we can define a morphism π^{-1} from the range $\pi(\mathcal{M})$ into $\mathcal{M}$ by $\pi^{-1}\pi(A) = A$ for all $A \in \mathcal{M}$.

Each representation $(\mathcal{H}, \pi)$ of a C^*-algebra $\mathcal{M}$ defines a faithful representation of the quotient algebra $\mathcal{M}_\pi = \mathcal{M}/\,Ker(\pi)$. Let us give the basic theorem presenting the following criteria for faithfulness.

THEOREM. *Let $(\mathcal{H}, \pi)$ be a representation of a C^*-algebra $\mathcal{M}$. This representation is faithful if and only if it satisfies one of the following equivalent conditions*:

(a) $Ker(\pi) = 0$.
(b) $\|\pi(A)\| = \|A\|_{\mathcal{M}}$ *for all* $A \in \mathcal{M}$.
(c) $\pi(A) > 0$ *for all* $A > 0$.

Requirement (b) expresses the statement that π is a norm preserving map. Requirement (c) is a statement of the fact that π is positive on positive elements.

A representation can be nontrivial ($\pi \neq 0$), but nevertheless have the trivial part: $\mathcal{H}_0 = \{\Psi \in \mathcal{H}\colon\ \pi(A)\Psi = 0 \text{ for all } A \in \mathcal{M}\}$. A representation $(\mathcal{H}, \pi)$ is said to be *nondegenerate* if $\mathcal{H}_0 = 0$. An important class of nondegenerate representations is the class of cyclic representations.

DEFINITION. Let $(\mathcal{H}, \pi)$ be a representation of a C^*-algebra $\mathcal{M}$. A *cyclic vector* is an element Ψ of $\mathcal{H}$, such that $\|\Psi\|_{\mathcal{H}} = 1$ and the set $\{\pi(A)\Psi\colon\ A \in \mathcal{M}\}$ is dense in $\mathcal{H}$.

A cyclic representation is a representation with a cyclic vector.

DEFINITION. A *cyclic representation of a C^*-algebra $\mathcal{M}$* is a triple $(\mathcal{H}, \pi, \Psi)$, where $(\mathcal{H}, \pi)$ is a representation of $\mathcal{M}$ and Ψ is a cyclic vector in $\mathcal{H}$.

Here the set $\{\pi(A)\Psi\colon\ A \in \mathcal{M}\}$ is dense in $\mathcal{H}$ with respect to the strong topology on $\mathcal{H}$, i.e., that induced by the norm. Cyclic representations play an important role in the theory of representations. In particular, each representation is the direct sum of cyclic representations.

THEOREM. *Let $(\mathcal{H}, \pi)$ be a nondegenerate representation of a C^*-algebra $\mathcal{M}$. Then π is the direct sum of a set of cyclic representations.*

If $(\mathcal{H}, \pi)$ is a nondegenerate representation of a C^*-algebra $\mathcal{M}$, and Ψ is a cyclic vector of $\mathcal{H}$, then there exists the linear functional

$$\omega_\Psi(A) = <\Psi|\pi(A)\Psi>. \tag{4}$$

This is the *vector functional*. Note that ω_Ψ is a positive linear functional such that

$$\omega_\Phi(I) = <\Psi|\Psi> = \|\Psi\|^2_{\mathcal{H}} = 1.$$

Every positive linear functional obtained in this way is said to be a *vector state* associated to the representation $(\mathcal{H}, \pi)$.

STATEMENT. *If $(\mathcal{H}, \pi, \Psi)$ is a nondegenerate cyclic representation of a C^*-algebra $\mathcal{M}$, then the vector functional* (4) *is a state on $\mathcal{M}$.*

It is important to consider the converse statement: every state on a C^*-algebra $\mathcal{M}$ is a vector state for some nondegenerate representation. Then starting from a state ω we must construct a cyclic representation $(\mathcal{H}_\omega, \pi_\omega, \Psi_\omega)$ such that ω is a vector state ω_{Ψ_ω}. This representations $(\mathcal{H}_\omega, \pi_\omega, \Psi_\omega)$ is called the Gelfand–Naimark–Segal construction.

6.4. Gelfand–Naimark–Segal construction

Let $\mathcal{M}$ be a C^*-algebra. The GNS-construction associates to every state ω on $\mathcal{M}$ a cyclic representation $(\mathcal{H}_\omega, \pi_\omega, \Psi_\omega)$ of $\mathcal{M}$.

THEOREM *(Gelfand–Naimark–Segal). Let ω be a state on a C^*-algebra $\mathcal{M}$, then there exists a cyclic representation $(\mathcal{H}_\omega, \pi_\omega, \Psi_\omega)$ of $\mathcal{M}$ such that*

$$\omega(A) = \left(\Psi_\omega, \pi_\omega(A)\Psi_\omega\right)$$

for all $A \in \mathcal{M}$.

PROOF. The proof is constructive. This construction is usually called the GNS-construction.

1. A scalar product. The idea of the proof is to turn $\mathcal{M}$ into a Hilbert operator space by introducing the scalar product

$$(A;\, B)_\omega = \omega(A^* B). \tag{5}$$

This is the natural correlation function (correlator). The set $\mathcal{M}$ is an operator Banach space. It may be converted into a pre-Hilbert operator space by introducing the positive semidefined scalar product (5).

2. A seminorm. Now define the seminorm

$$\|A\|_\omega = (A;\, A)_\omega^{1/2} = \left[\omega(A^* A)\right]^{1/2}.$$

In general, the given seminorm is not a norm.

3. From a seminorm into a norm. The seminorm and scalar product (5) can be degenerate. Therefore we divide $\mathcal{M}$ by its kernel

$$\mathcal{M}_0 = \left\{A \in \mathcal{M}:\ \|A\|_\omega = \omega(A^* A) = 0\right\}$$

to obtain a set $\mathcal{M}/\mathcal{M}_0$. Note that the set $\mathcal{M}_0$ is a left ideal of $\mathcal{M}$, i.e., $\mathcal{M}_0$ is invariant under left multiplication by element of $\mathcal{M}$: $L_A C = AC \in \mathcal{M}_0$ whenever $A \in \mathcal{M}$ and $C \in \mathcal{M}_0$. Because ω is norm-continuous, $\mathcal{M}_0$ is a norm-closed subspace of $\mathcal{M}$.

We say that two elements $A_1, A_2 \in \mathcal{M}$ are equivalent modulo $\mathcal{M}_0$ if $(A_1 - A_2) \in \mathcal{M}_0$, and write this fact symbolically by $A_1 \sim A_2$. We shall denote the set of all elements of $\mathcal{M}$ equivalent modulo $\mathcal{M}_0$ to a fixed element A by $[A]$. Here $[A]$ is called a class of equivalent elements. We can consider the classes as elements in a new linear space, where we define the operations

$$z[A] = [zA], \qquad [A] + [B] = [A + B].$$

The linear space obtained in this way is called the factor space of $\mathcal{M}$ modulo $\mathcal{M}_0$ and its denoted by $\mathcal{M}/\mathcal{M}_0$. The elements of the set $\mathcal{M}/\mathcal{M}_0$ are the subsets

$$[A] = \{A + C:\ C \in \mathcal{M}_0\}.$$

Suppose $\omega(A^* A) = 0$ if and only if $A = 0$, i.e., $\mathcal{M}_0 = 0$. Then $[A] = A$.

Note that the scalar product (5) does not change its value when we replace A by $A + C_1$ with $C_1 \in \mathcal{M}_0$, and, similarly, we replace B by $B + C_2$ with $C_2 \in \mathcal{M}_0$:

$$\begin{aligned}\omega\big((A + C_1)^*(B + C_2)\big) &= \omega(A^* B) + \omega(C_1^* B) + \omega(A^* C_2) + \omega(C_1^* C_2)\\ &= \omega(A^* B) + \big(\omega(B^* C_1)\big)^* + \omega(A^* C_2) + \omega(C_1^* C_2)\\ &= \omega(A^* B).\end{aligned}$$

Here we use that $BC_k \in \mathcal{M}_0$, $k = 1, 2$, and $\omega(C) = 0$ if $C \in \mathcal{M}_0$.

We define the scalar product

$$\big([A],[B]\big) = (A;\,B)_\omega = \omega(A^*B), \tag{6}$$

and the norm

$$\big\|[A]\big\|_\omega = \big([A],[A]\big)^{1/2} = \big(\omega(A^*A)\big)^{1/2}, \tag{7}$$

where $[A] \in \mathcal{M}/\mathcal{M}_0$. As a result, $\mathcal{M}/\mathcal{M}_0$ is a pre-Hilbert operator space with respect to this scalar product.

4. A Hilbert space. A pre-Hilbert space may be completed, i.e., linearly embedded as a dense subspace of a Hilbert space in a manner which preserves the scalar product. Let $\mathcal{H}_\omega$ be a completion of $\mathcal{M}/\mathcal{M}_0$ with respect to the norm (7). Then $\mathcal{H}_\omega$ is a Hilbert operator space.

Let $|A)_\omega$ be an element of $\mathcal{H}_\omega$ that corresponds to $[A]$. The scalar product (6) on $\mathcal{H}_\omega$ has the form $(|A)_\omega, |B)_\omega) = \omega(A^*B)$. As a result, a linear map from a C^*-algebra $\mathcal{M}$ into a dense linear subspace $\mathcal{M}/\mathcal{M}_0$ is a Hilbert space $\mathcal{H}_\omega$.

5. Representation π_ω of $\mathcal{M}$. Let us consider the definition of the map π_ω from $\mathcal{M}$ into an algebra $\mathcal{B}(\mathcal{H}_\omega)$. If $A \in \mathcal{M}$, then there exists a linear operator $\pi_\omega(A) = L_{[A]}$ on $\mathcal{H}_\omega$ such that

$$\pi_\omega(A)|B)_\omega = |AB)_\omega, \tag{8}$$

for all $|B)_\omega \in \mathcal{H}_\omega$, i.e., $\pi_\omega(A)[B] = [AB]$.

For $|A)_\omega \in \mathcal{H}_\omega$, let $\pi_\omega(A)$ be the mapping of $\mathcal{H}_\omega$ into itself given by (8). We can think of $L_{[A]} = \pi_\omega(A)$ as meaning *left multiplication by* A. A map $\pi_\omega(A)$ assigns to each class $[B]$ of $\mathcal{M}/\mathcal{M}_0$ exactly one class $[AB]$ of $\mathcal{M}/\mathcal{M}_0$. A map L_A assigns to each operator B of $\mathcal{M}$ exactly one operator $L_AB = AB$ of $\mathcal{M}$. It is known that a map from an operator space into itself is called *superoperator*. Then $L_{[A]} = \pi_\omega(A)$ *is a superoperator on the factor space* $\mathcal{M}/\mathcal{M}_0$, and L_A is a superoperator on $\mathcal{M}$. If $\mathcal{M}_0 = 0$, then $\mathcal{H}_\omega = \mathcal{M}$ and $\pi_\omega(A) = L_A$. A set of all superoperators $\pi_\omega(A)$ form a C^*-algebra $\mathcal{B}(\mathcal{H}_\omega)$ of bounded superoperators on an operator Hilbert space $\mathcal{H}_\omega$. Then $\mathcal{B}(\mathcal{H}_\omega)$ is the left regular representation of $\mathcal{M}$.

6. $\pi_\omega(A)$ is bounded. Using

$$\omega(B^*AB) \leqslant \|A\|_{\mathcal{M}}\omega(B^*B), \qquad \big(|B)_\omega, \pi_\omega(A)|B)_\omega\big) = \omega(B^*AB),$$

we obtain

$$\begin{aligned}\big\|\pi_\omega(A)|B)_\omega\big\|^2 &= (AB,\,AB)_\omega = \omega(B^*A^*AB) \leqslant \|A\|^2_{\mathcal{M}}\omega(B^*B)\\ &= \|A\|^2_{\mathcal{M}}\,\big\|[B]\big\|^2_\omega.\end{aligned}$$

Hence the norm of $\pi_\omega([A]) \in \mathcal{B}(\mathcal{H}_\omega)$ satisfies the inequality $\|\pi_\omega([A])\| \leqslant \|A\|_\omega$. Then $\pi_\omega(A)$ has a bounded closure, which we also denote by $\pi_\omega(A)$.

7. Cyclic vector Ψ_ω. If $\mathcal{M}$ contains the unit I, then we define the cyclic vector

$$\Psi_\omega = |I)_\omega,$$

i.e., $\Psi_\omega = [I]$ and $\Psi_\omega \in \mathcal{H}_\omega$. Then we obtain the vector state

$$\omega_{\Psi_\omega}(A) = \big(\Psi_\omega, \pi_\omega(A)\Psi_\omega\big) = \omega(A).$$

This ends the proof. □

The GNS-construction associates to every state ω of a C^*-algebra $\mathcal{M}$ some regular representation of $\mathcal{M}$. An operator $A \in \mathcal{M}$ is represented by the left superoperator, i.e., the left multiplication by A. The algebra $\mathcal{M}$ is considered as an operator Hilbert space $\mathcal{H}_\omega$. As a result, we realize a Hilbert space as an operator Hilbert space and operators on this space as superoperators (operators on an operator space). From the point of view of general theory difference between infinite-dimensional Hilbert spaces is unessential, since these spaces are isomorphic and any statement about one of the spaces can be in principle translated into the terms of another.

STATEMENT. *Each C^*-algebra $\mathcal{M}$ is isomorphic to a norm-closed algebra of self-adjoint bounded operators on a Hilbert space.*

This GNS-representation is unique up to unitary equivalence.

Note that the Stinespring factorization theorem [148] characterizing completely positive maps is an important generalization of the GNS-construction for quantum non-Hamiltonian systems.

The notions of purity of a state and irreducibility of the representation associated with ω are related. Let $(\mathcal{H}, \pi)$ be a representation of C^*-algebra $\mathcal{M}$. A subset $\mathcal{H}_0$ of $\mathcal{H}$ is called the *invariant* (or stable) with respect to all $\pi(A)$, if $\pi(A)\Psi \in \mathcal{H}_0$ for all $A \in \mathcal{M}$ and all $\Psi \in \mathcal{H}_0$.

DEFINITION. A representation $(\mathcal{H}, \pi)$ of C^*-algebra $\mathcal{M}$ is said to be *irreducible* if the only subspaces of $\mathcal{H}$ invariant with respect to all $\pi(A)$, $A \in \mathcal{M}$, are the trivial subspaces $\{0\}$ and $\mathcal{H}$.

A *commutant* $\mathcal{M}'$ of $\mathcal{M}$ is a set of all elements of $\mathcal{M}$ which commute with all $A \in \mathcal{M}$. Then $A \in \mathcal{M}'$ if and only if $A \in \mathcal{M}$ and $[A, B] = 0$ for all $B \in \mathcal{M}$.

THEOREM. *Let $(\mathcal{H}, \pi)$ be a representation of a C^*-algebra $\mathcal{M}$. The following conditions are equivalent*:

(a) *$(\mathcal{H}, \pi)$ is irreducible.*
(b) *The commutant $\pi(\mathcal{M})'$ of $\pi(\mathcal{M}) = \{\pi(A)\colon\ A \in \mathcal{M}\}$ consists of multiples of the identity operator I, i.e., $\pi(\mathcal{M})' = \{zI\colon\ z \in \mathbb{C}\}$.*

(c) *Each nonzero element* $\Psi \in \mathcal{H}$ *is a cyclic vector of* $\mathcal{H}$.

Let us give the basic theorem which makes the connections between pure states and irreducible representations.

THEOREM. *Let* ω *be a state on a* C^**-algebra* $\mathcal{M}$. *A cyclic representation* $(\mathcal{H}_\omega, \pi_\omega, \Psi_\omega)$ *of* $\mathcal{M}$, *is irreducible if and only if* ω *is a pure state.*

Hence, each vector state associated with an irreducible representation of a C^*-algebra $\mathcal{M}$ is a pure state.

6.5. State on W^*-algebra

A W^*-algebra is a C^*-algebra. Then all properties of states on a C^*-algebra are valid for a W^*-algebra. Note that there exists an important theorem for a W^*-algebra. This theorem says that if a state is continuous with respect to ultra-weak topology, then the kinematical postulate (1) is a theorem.

For W^*-algebras, we can formulate an analog of the Riesz–Fréchet theorem, which gives an equivalence of a Hilbert space $\mathcal{H}$ and a dual space $\mathcal{H}^*$.

THEOREM. *Let* $\omega \in \mathcal{M}^*$ *be a state on a* W^**-algebra* $\mathcal{M}$. *Then the following conditions are equivalent*:

(1) ω *is continuous with respect to ultra-weak topology.*
(2) *There exists a positive self-adjoint operator* $\rho \in \mathcal{M}$ *with unit trace, such that* $\omega(A) = Tr[\rho A]$ *for all* $A \in \mathcal{M}$.

By this theorem, each state ω on a W^*-algebra has the form $\omega(A) = (\rho|A) = Tr[\rho A]$ for all $A \in \mathcal{M}$. Note that condition (2) is equivalent to the requirement: ω is a normal state. A state ω is *normal* if $\omega(\sum_{k=1}^{n} P_k) = \sum_{k=1}^{n} \omega(P_k)$ for all sets $\{P_k\}$ of orthogonal projection operators $P_k \in \mathcal{M}$. As a result, each state on a W^*-algebra is normal.

Chapter 7

Mathematical Structures in Classical Kinematics

7.1. Symplectic structure

The phase-space of the classical system can be the Euclidean space $\mathbb{R}^n$. However, this is not always the case. Some problems involve phase-spaces which are more complicated manifolds. A manifold is a topological space that is locally Euclidean. Every point $x \in \mathcal{M}$ has a neighborhood that is topologically the same as an open set in $\mathbb{R}^n$. A manifold is a topological space in which every point has a neighborhood which is similar to the Euclidean space, but in which the global structure may be more complicated. The spherical Earth is described using flat maps or charts, collected in an atlas. Similarly, a smooth manifold can be described using coordinate charts collected in a mathematical atlas. It is not generally possible to describe a manifold with just one chart, because the global structure of the manifold is different from the simple structure of the charts. For example, no single flat map that can represent the entire Earth.

We shall consider here an important class of manifolds [60].

DEFINITION. A *symplectic manifold* (M, ω) is a smooth manifold M endowed with a closed nondegenerate differential 2-form ω.

In local coordinates, we have

$$\omega = \omega_{kl}(x)\, dx^k \wedge dx^l,$$

where $\wedge$ is the wedge product such that $dx^k \wedge dx^l = -dx^l \wedge dx^k$, $dx^k \wedge dx^k = 0$. The nondegeneracy condition means that $\det[\omega_{kl}(x)] \neq 0$ at every point of M, so that there exists an inverse antisymmetric matrix $\Psi^{kl}(x) = \omega^{kl}(x)$. It follows that the dimension of M is even.

The condition for ω to be closed, $d\omega = 0$, is expressed in local coordinates as

$$\partial_k \omega_{lm} + \partial_l \omega_{mk} + \partial_m \omega_{kl} = 0.$$

This is the Jacobi identity for ω_{kl}.

All symplectic manifolds have locally the same structure. A precise formulation of this statement is given by the following theorem.

DARBOUX'S THEOREM. *For any point x of a symplectic manifold (M, ω) there exists a local coordinate system $(q, p) = (q_1, \ldots, q_n, p_1, \ldots, p_n)$ in a neighbourhood of x such that the symplectic form ω has the canonical expression $\omega = dq_k \wedge dp_k$.*

By this theorem, any statement of local nature which is invariant under symplectic transformations and has been proved for the canonical coordinates can be extended to all symplectic manifolds.

Symplectic manifolds have some specific topological properties. We shall note here only one of them. Suppose (M, ω) is a compact symplectic manifold of dimension $2n$. Then the nth power ω^n of the symplectic form ω is a volume form on M. Moreover, it should be noted that all the powers of ω up to ω^n must be nonzero.

7.2. Poisson manifold and Lie–Jordan algebra

In the classical mechanics an observable is represented by a function. A mathematical structure is obtained by taking a set of observables and equipping this set with a structure by defining relations between these observables.

DEFINITION. Let M be a manifold. A classical observable is a real-valued function on M.

We shall denote the linear space of all classical observables on M by $\mathcal{F}(M)$. Let us give the basic mathematical structures on $\mathcal{F}(M)$.

(1) $\mathcal{F}(M)$ *is a linear space*. Let $\mathcal{F}(M)$ be a linear space of all smooth square-integrable functions on M. The scalar product

$$(A, B) = \int dq\, dp\, A(q, p)B(q, p)$$

is defined for all $A, B \in \mathcal{F}(M)$. Note that $(A, A) \leqslant \infty$, since $A \in \mathcal{F}(M)$ is square-integrable. Then $\mathcal{F}(M)$ is a pre-Hilbert space. Every linear space with scalar product is a normed space with the norm $\|A\| = \sqrt{(A, A)}$. We can always complete $\mathcal{F}(M)$ to a Hilbert space.

(2) $\mathcal{F}(M)$ *is a commutative associative algebra*. An algebra consists of a linear space $\mathcal{F}(M)$ over a field $\mathbb{R}$, together with a binary operation of pointwise multiplication on the set $\mathcal{F}(M)$ such that for all $a \in \mathbb{R}$ and $A, B, C \in \mathcal{F}(M)$, the following conditions are satisfied:

$$(aA)B = A(aB) = a(AB), \quad (A + B)C = AC + BC,$$

$$A(B + C) = AB + AC.$$

Also, $\mathcal{F}(M)$ is an associative commutative algebra if, in addition to the preceding three conditions, we have $AB - BA = 0$, and $(AB)C - A(BC) = 0$.

(3) $\mathcal{F}(M)$ *is a Jordan algebra*. We can define the Jordan multiplication $A \circ B = A(x)B(x)$, where AB is the usual pointwise multiplication. Then $\mathcal{F}(M)$ is a special Jordan associative algebra.

(4) $\mathcal{F}(M)$ *is a Lie algebra*. Let $\mathcal{F}(M)$ be a linear space of all smooth functions on M. We say that M is endowed with a Poisson structure if we are given an operation assigning to every pair of functions $A, B \in \mathcal{F}(M)$ a new function $\{A, B\} \in \mathcal{F}(M)$, which is linear in A and B and satisfies the following conditions:

(a) the skew-symmetry condition $\{A, B\} = -\{B, A\}$,
(b) the Jacobi identity $\{\{A, B\}, C\} + \{\{B, C\}, A\} + \{\{C, A\}, B\} = 0$,
(c) the Leibnitz rule $\{A, BC\} = \{A, B\}C + B\{A, C\}$.

Requirements (a) and (b) are the axioms of a Lie algebra. In this way, the space $\mathcal{F}(M)$, together with the Poisson bracket becomes a Lie algebra with the multiplication $A \cdot B = \{A, B\}$.

Requirement (c) expresses that the Lie operation is connected with the Jordan multiplication by

$$A \cdot (B \circ C) = (A \cdot B) \circ C + B \circ (A \cdot C).$$

Let us consider the Poisson bracket of the form

$$\{A, B\} = \Psi^{kl}(x)\partial_k A(x)\partial_l B(x).$$

The skew-symmetry condition and the Jacobi identity give

$$\Psi^{kl}(x) = -\Psi^{lk}(x), \qquad \Psi^{ki}\partial_i\Psi^{lm} + \Psi^{li}\partial_i\Psi^{mk} + \Psi^{mi}\partial_i\Psi^{kl} = 0. \tag{1}$$

This is Jacobi identity for $\Psi^{kl}(x)$. We note that Poisson bracket obeys the Leibnitz rule and so is completely determined by the Poisson brackets of the coordinates functions

$$\left\{x^k, x^l\right\} = \Psi^{kl}(x).$$

The following are examples of some Poisson brackets.

(a) In the simplest case, the tensor $\Psi^{kl}(x)$ does not depend on x, i.e., $\Psi^{kl}(x) = \Psi^{kl}$. Let $M = \mathbb{R}^{2n}$ and $x = (q, p)$. Then the expression

$$\{A, B\} = \sum_{k=1}^{n}\left(\frac{\partial A}{\partial q^k}\frac{\partial B}{\partial p^k} - \frac{\partial A}{\partial p^k}\frac{\partial B}{\partial q^k}\right)$$

determines the canonical Poisson structure on $\mathcal{F}(M)$. The conditions

$$\{q^k, q^l\} = \{p^k, p^l\} = 0, \qquad \{q^k, p^l\} = \delta^{kl}$$

combined with the Leibnitz rule determine a Poisson structure.

(b) Let M be a linear space. The next simplest case is that of the linear coefficients $\Psi^{kl}(x) = C^{kl}_m x^m$, where C^{kl}_m are constants. The Poisson bracket becomes

$$\{A, B\} = C^{kl}_m x^m \partial_k A(x) \partial_l B(x).$$

This is the *Lie–Poisson bracket*. It is not hard to prove that (1) coincide respectively with the skew-symmetry condition and the Jacobi identity for the structure constants C^{kl}_m of a Lie algebra. Then C^{kl}_m form a set of structure constants for some Lie algebra.

(5) $\mathcal{F}(M)$ *is a Lie–Jordan algebra*. We can define two bilinear multiplication on $\mathcal{F}(M)$ denoted by symbols $\{\ ,\ \}$ and $\circ$, and satisfying the conditions:

(a) $<\mathcal{F}(M), \{\ ,\ \}>$ is a Lie algebra:

$$\{A, B\} = -\{B, A\},$$
$$\big\{\{A, B\}, C\big\} + \big\{\{B, C\}, A\big\} + \big\{\{C, A\}, B\big\} = 0;$$

(b) $<\mathcal{F}(M), \circ>$ is a special Jordan algebra:

$$A \circ B = B \circ A, \quad ((A \circ A) \circ B) \circ A = (A \circ A) \circ (B \circ A);$$

(c) $<\mathcal{F}(M), \circ>$ is an associative Jordan algebra:

$$(A \circ B) \circ C - A \circ (B \circ C) = 0;$$

(d) $\{\ ,\ \}$ is a derivation on $<\mathcal{F}(M), \circ>$:

$$\big\{A, (B \circ C)\big\} = \{A, B\} \circ C + B \circ \{A, C\}.$$

In this case, the Lie–Jordan algebra on $\mathcal{F}(M)$ is defined. We shall also assume that there exists a unity I in $\mathcal{F}(M)$ such that $A \circ I = A$ and $\{A, I\} = 0$.

DEFINITION. A *Poisson manifold* is a manifold M equipped with two bilinear operations $\{\ ,\ \}$ and $\circ$ from $\mathcal{F}(M) \times \mathcal{F}(M)$ into $\mathcal{F}(M)$ with the property that $<\mathcal{F}(M), \circ, \{\ ,\ \}>$ is a Lie–Jordan algebra.

If $\det[\Psi^{kl}(x)] = 0$ then the Poisson structure is called degenerate. Note that each general Poisson manifold with a degenerate Poisson structure stratified into symplectic submanifolds on which the tensor $\Psi^{kl}(x)$ is nondegenerate. For each Poisson manifold there exists a family of symplectic manifolds. The fact that an arbitrary Poisson manifold is stratified into symplectic submanifolds is somewhat analogous to the decomposition of a finite-dimensional C^*-algebra as a direct sum of matrix algebras.

(6) $\mathcal{F}(M)$ *is a commutative* C^**-algebra*. If M is a locally compact Hausdorff space, then the set of all continuous complex valued functions on M vanishing at infinity equipped with the supremum norm $\|f\| = \sup\{|f(x)|\colon\ x \in X\}$ is a commutative C^*-algebra. The Gelfand theorem states that each commutative C^*-algebra is of this form $C(M)$. The C^*-algebra is unital if and only if M is compact.

The concepts of C^*-algebra and Lie–Jordan algebra allows us to formulate classical and quantum theories by the same mathematical structures.

7.3. Classical states

Classical states as functionals

Let $\mathcal{F}(M)$ be a linear space of smooth functions on a manifold M.

DEFINITION. A *classical state* is a linear nonnegative functional ω_c on $\mathcal{F}(M)$, such that

(a) $\omega_c(A^*) = (\omega_c(A))^*$ for all $A \in \mathcal{F}(M)$,
(b) $\omega_c(1) = 1$.

If ω_c is nonnegative, then $\omega_c(A^2) \geqslant 0$ for all $A \in \mathcal{F}(M)$. A linear functional ω_c is positive if the following conditions are satisfied:

(a) $\omega_c(A^*) = (\omega_c(A))^*$ for all $A \in \mathcal{F}(M)$.
(b) $\omega_c(A) = 0$ if and only if $A = 0$.

Requirement (a) means that $\omega_c(A) \in \mathbb{R}$ for all real-valued functions $A \in \mathcal{F}(M)$.

If ω_c is a classical states, then the following requirements are satisfied:

(1) $\omega_c(aA + bB) = a\omega_c(A) + b\omega_c(B)$ for all $A, B \in \mathcal{F}(M)$ and $a, b \in \mathbb{R}$.
(2) $\omega_c(A^*) = (\omega_c(A))^*$ for all $A \in \mathcal{F}(M)$.
(3) $\omega_c(1) = 1$.
(4) $\omega_c(0) = 0$, and $\omega_c(A^2) > 0$ for all $A \neq 0$.

Conditions (4) give that $\omega_c(A) = 0$ if and only if $A = 0$.

Classical states as Borel measures

Let M be a set. A pair $(M, \mathcal{B})$ is called a *sigma-ring* of sets if $\mathcal{B}$ is a family of subsets of M such that:

(1) $M \subset \mathcal{B}$.
(2) $B \subset \mathcal{B}$ implies $(M - B) \subset \mathcal{B}$.

(3) $B_k \in \mathcal{B}$ $(k = 1, 2, \ldots)$ implies $\bigcup_{k=1}^{\infty} B_k \in \mathcal{B}$.

DEFINITION. Let $(M, \mathcal{B})$ be a sigma-ring of sets in M. Then a triple $(M, \mathcal{B}, \mu)$ is called a *measure space* if μ is a nonnegative, sigma-additive measure defined on $\mathcal{B}$:

(1) $\mu(B) \geqslant 0$ for every $B \in \mathcal{B}$.
(2) the sigma-additivity of μ: $\mu(\sum_{k=1}^{\infty} B_k) = \sum_{k=1}^{\infty} \mu(B_k)$ for any disjoint sequence $\{B_k,\ k \in \mathbb{N}\}$ of sets in $\mathcal{B}$.
(3) M is expressible as a countable union of sets $B_k \in M$ such that $\mu(B_k) < \infty$.

The value $\mu(B)$ is called the *measure* of the set B.

Let M be a *locally compact space*, i.e., a closed subset of the n-dimensional Euclidean space $\mathbb{R}^n$. The *Borel subsets* of M are the elements of the smallest sigma-ring of subsets of M, which contains every compact set of M.

A nonnegative *Borel measure* on M is a sigma-additive measure defined for every Borel subset of M such that the measure of every compact set is finite. The Borel measure μ is called *regular* if for each Borel set B, we have $\mu(B) = \inf\{\mu(U)\colon\ B \subset U\}$, where the infimum is taken over all open sets E containing B. If μ is a Borel measure, then $\mu(B) < \infty$ for every compact subset B of M.

Note that classical states can be presented by measures on a manifold. A real-valued function A defined on the locally compact space M is said to have *compact support* if there exists a compact set B of M such that $A = 0$ on $(M - B)$. We denote by $\mathcal{F}_0(M)$ the class of all continuous functions A from M into $\mathbb{R}$ with compact support.

STATEMENT. *For each Borel measure μ on a smooth real manifold M there exists exactly one nonnegative linear functional ω_c on $\mathcal{F}_0(M)$, such that*

$$\omega_c(A) = \int_M A(x)\, d\mu(x). \tag{2}$$

Hence, classical states can be described by Borel measures on M.

RIESZ–MARKOV THEOREM. *To every positive linear functional ω_c on $\mathcal{F}_0(M)$ corresponds a unique regular Borel measure μ such that (2) holds for all A in $\mathcal{F}_0(M)$ and conversely.*

The Riesz–Markov theorem establishes the general form of a positive linear functional on $\mathcal{F}_0(M)$. This theorem is some analog of the fundamental Riesz–Fréchet theorem. As a result, we have the correspondence between states and measures.

Classical states as distribution functions

Let M be an oriented $2n$-dimensional smooth manifold M. A measure on M can be defined by a differential $2n$-form ω_{2n}. This form is called the volume form. In the local coordinates, this form can be presented by

$$\omega_{2n} = \omega_{12\ldots 2n}\, dx^1 \wedge dx^2 \wedge \cdots \wedge dx^{2n}.$$

Each volume form ω_{2n} defines a measure $\mu(B)$ on a Borel set B by

$$\mu(B) = \int_B \omega_{2n}.$$

The volume form ω_{2n} on M generates the continuous linear functional

$$\omega_c(A) = \int_M A(x)\omega_{2n}.$$

Each symplectic manifold (M, ω) has a natural volume form. If M is a $2n$-dimensional manifold, then there exists the volume form $\omega_{2n} = (\omega)^n$, where $(\omega)^n$ is nth power of the symplectic form ω. For canonical coordinates (q, p),

$$\omega_{2n} = (\omega)^n = dq_1 \wedge dp_1 \wedge dq_2 \wedge dp_2 \wedge \cdots \wedge dq_n \wedge dp_n.$$

This is the *Liouville measure*.

The smooth requirement gives that the volume form ω_{2n} is defined by a non-negative measurable density function $\rho(x)$, such that

$$\omega_{2n} = \rho(x)\, dx^1 \wedge dx^2 \wedge \cdots \wedge dx^{2n}.$$

We use more compact notation $\omega_{2n} = \rho(x)\, dx$. Then there locally exists a non-negative measurable function $\rho(x)$, such that the measure is defined by

$$\mu(B) = \int_B \rho(x)\, dx$$

for all measurable set B. As a result, a classical state can be defined by the density function $\rho(x)$, which is often called the distribution function. Then the classical state is described by a distribution function $\rho(q, p)$ on M, such that

$$\omega_c(A) = \int_M A(q, p)\rho(q, p)\, dq\, dp,$$

where $dq\, dp = dq_1 \wedge dp_1 \wedge dq_2 \wedge dp_2 \wedge \cdots \wedge dq_n \wedge dp_n$. The normalization requirement $\mu(M) = 1$ gives

$$\omega_c(1) = \int_M \rho(q, p)\, dq\, dp = 1.$$

A pure state of classical system is defined as a measure that is concentrated at some point x_0 of M. The distribution function of the pure state is then the Dirac delta-function $\rho_0(x) = \delta(x - x_0)$. This pure state is defined by the point x_0 of M. Then the phase space M can be considered as a space of all pure states. An expectation value of an observable $A(x)$ on a pure state x_0 is equal to the value of $A(x)$ at this point:

$$\omega_c(A) = \int_M A(x)\rho_0(x)\,dx = \int_M A(x)\delta(x - x_0)\,dx = A(x_0).$$

For this pure state, the variance $\mathcal{D}(A) = \omega_c(A^2) - \omega_c^2(A)$ is equal to zero: $\mathcal{D}(A) = 0$.

7.4. Classical observables and C^*-algebra

Let $\mathcal{M}$ be a unital Banach algebra. A *homomorphism* from $\mathcal{M}$ into a set $\mathcal{M}'$ is a linear mapping Φ such that $\Phi(AB) = \Phi(A)\Phi(B)$ for $A, B \in \mathcal{M}$. We illustrate this notion with the following example. Let $\mathcal{M}$ be a Banach algebra, and for each $A \in \mathcal{M}$, define a mapping L_A by

$$L_A B = AB$$

for $B \in \mathcal{M}$. Clearly L_A is a linear map from $\mathcal{M}$ into itself. It is easily to see that the correspondence $A \to L_A$ is a linear mapping that also preserves the operation of multiplication. For example, we have

$$L_{AB}C = (AB)C = A(BC) = L_A(BC) = L_A L_B C$$

for $A, B, C \in \mathcal{M}$. Hence $L_{AB} = L_A L_B$ and then the left multiplication is a homomorphism. The mapping $A \to L_A$ is called the left regular representation of $\mathcal{M}$. We shall denote the linear space of all left multiplications on $\mathcal{M}$ by $\mathcal{A}_l(\mathcal{M})$. Then the left regular representation of $\mathcal{M}$ is an example of a homomorphism of $\mathcal{M}$ into $\mathcal{M}' = \mathcal{A}_l(\mathcal{M})$.

A homomorphism ω of $\mathcal{M}$ into the algebra $\mathcal{M}' = \mathbb{C}$ of complex numbers is called a *multiplicative linear functional* with the added property that

$$\omega(AB) = \omega(A)\omega(B) \tag{3}$$

for all $A, B \in \mathcal{M}$. We can define the norm of any functional ω on $\mathcal{M}$ by

$$\|\omega\| = \sup_{A \in \mathcal{M}} \{|\omega(A)|\colon \|A\|_{\mathcal{M}} = 1\}.$$

THEOREM. *If ω is a multiplicative linear functional on a Banach algebra $\mathcal{M}$, then $\|\omega\| = 1$.*

A linear functional ω on a unital Banach algebra $\mathcal{M}$ is a multiplicative if and only if $\omega(I) = 1$ and $\omega(A) \neq 0$ whenever A is invertible in $\mathcal{M}$.

Let $\mathcal{M}$ be a commutative C^*-algebra. A *character* ω of $\mathcal{M}$ is a nonzero linear map $\omega : A \in \mathcal{M} \to \omega(A) \in \mathbb{C}$ such that condition (3) holds for all $A, B \in \mathcal{M}$. A character is a multiplicative functional on C^*-algebra.

For example, the characters of the algebra of $n \times n$ diagonal matrices are the maps $A \to A_{mm}$, where $1 \leqslant m \leqslant n$. The *spectrum* $\sigma(\mathcal{M})$ of $\mathcal{M}$ is defined to be the set of all characters on $\mathcal{M}$. The spectrum $\sigma(\mathcal{M})$ of $\mathcal{M}$ is a subset of the dual $\mathcal{M}^*$ of $\mathcal{M}$. The introduction of characters is quite conventional but, in fact, characters are nothing other than pure states.

THEOREM. *Let ω be a nonzero linear functional on a commutative C^*-algebra $\mathcal{M}$. Then the following conditions are equivalent*:

(a) *ω is a pure state.*
(b) *ω is a character.*

DEFINITION. Let $\mathcal{M}$ be a commutative Banach algebra with a unit. The *carrier space* of $\mathcal{M}$ is the set $\mathcal{M}^*_{car}$ of all nonzero multiplicative linear functionals (characters) on $\mathcal{M}$, endowed with the topology of pointwise convergence on $\mathcal{M}$.

If $\mathcal{M}^*$ is a set of all linear functionals on $\mathcal{M}$, then $\mathcal{M}^*_{car} \subset \mathcal{M}^*$.

DEFINITION. For all $A \in \mathcal{M}$, the (left) *Gelfand transform* of A is the map L^*_A defined on $\mathcal{M}^*_{car}$ by

$$L^*_A \omega = \omega(A)$$

for $\omega \in \mathcal{M}^*_{car}$.

We shall denote the linear space of all (left) Gelfand transforms on $\mathcal{M}^*_{car}$ by $\mathcal{A}_l(\mathcal{M}^*_{car})$.

STATEMENT. *Let $\mathcal{M}$ be a commutative Banach algebra with a unit. Then the carrier space $\mathcal{M}^*_{car}$ is a compact Hausdorff space.*

The correspondence $A \to L^*_A$ is called the *Gelfand representation* of $\mathcal{M}$. The mapping is obviously linear. It is also multiplicative because, if $A, B \in \mathcal{M}$ and $\omega \in \mathcal{M}^*_{car}$, then

$$L^*_{AB}\omega = \omega(AB) = \omega(A)\omega(B) = (L^*_A\omega)(L^*_B\omega).$$

Thus the Gelfand representation is a homomorphism of $\mathcal{M}$ onto a subalgebra $\hat{\mathcal{M}}$ of $\mathcal{A}_l(\mathcal{M}^*_{car})$. Denoting the norm in $\mathcal{A}_l(\mathcal{M}^*_{car})$ by $\| \ \|_{\mathcal{N}}$, we have

$$\|L^*_A\|_{\mathcal{N}} = \sup\{L^*_A\omega\colon\ \omega \in \mathcal{N}\} = \sup\big\{\omega(A)\colon\ \omega \in \mathcal{N}\big\}.$$

Using $\|L^*_A\|_{\mathcal{N}} \leqslant \|A\|_{\mathcal{M}}$, we obtain that the Gelfand representation is norm-decreasing and hence continuous.

THEOREM. *Let $\mathcal{M}$ be a commutative Banach algebra with a unit I, and let $\mathcal{M}^*_{car}$ be its carrier space. The Gelfand representation $A \to L^*_A$ is a norm-decreasing homomorphism of $\mathcal{M}$ onto an algebra $\hat{\mathcal{M}}$ of continuous functions on the compact Hausdorff space $\mathcal{M}^*_{car}$ such that $L^*_I\omega = \omega(I) = 1$.*

THEOREM. *Let $\mathcal{M}$ be a commutative Banach algebra with a unit. Then $\hat{\mathcal{M}}$ is isometrically isomorphic to $\mathcal{M}$ if and only if $\|A\|^2_{\mathcal{M}} = \|A^2\|_{\mathcal{M}}$ for all $A \in \mathcal{M}$.*

A *uniform algebra* is a closed subalgebra of $C(\mathcal{M})$ that contains the constant functions and separates the points of $\mathcal{M}$, where $\mathcal{M}$ is a compact Hausdorff space.

THEOREM. *Let $\mathcal{M}$ be a* (*commutative or noncommutative*) *unital Banach algebra. Then $\mathcal{M}$ is isometrically isomorphic to a uniform algebra if and only if $\|A\|^2_{\mathcal{M}} = \|A^2\|_{\mathcal{M}}$ for all $A \in \mathcal{M}$.*

Note that the Gelfand representation replace abstract algebra by certain algebras of functions.

GELFAND'S THEOREM. *Let $\mathcal{M}$ be a commutative B^*-algebra, with carrier space $\mathcal{M}^*_{car}$. Then the mapping $A \to L^*_A$ is an isometric $*$-isomorphism of $\mathcal{M}$ onto $C(\mathcal{M}^*_{car})$.*

An immediate consequence of the above theorem is that the self-adjoint elements in a commutative B^*-algebra are precisely those whose Gelfand transforms are real-valued.

Let $\mathcal{M}$ be a commutative C^*-algebra and $\mathcal{M}^*_{car}$ the set of characters of $\mathcal{M}$ equipped with the weak topology. It follows that $\mathcal{M}^*_{car}$ is a locally compact Hausdorff space which is compact if and only if $\mathcal{M}$ contains the identity. Moreover, $\mathcal{M}$ is isomorphic to the algebra $C_0(\mathcal{M}^*_{car})$ of continuous functions over $\mathcal{M}^*_{car}$ which vanish at infinity.

The Gelfand's theorem was proved in [64]. In the same paper the authors also proved that an arbitrary (and possibly noncommutative) B^*-algebra $\mathcal{M}$ is isometrically $*$-isomorphic to a C^*-algebra of operators on some Hilbert space. This is the Gelfand–Naimark theorem.

Chapter 8

Quantization in Kinematics

8.1. Quantization and its properties

Semi-quantization and prequantization

Setting quantization means establishing a general rule assigning a quantum system to each classical system. Quantum and classical systems consist essentially of two elements, a kinematical structure describing the instantaneous observables and states, and a dynamical structure describing the change of these observables and states with time. There exist natural requirements that must be satisfied by the quantization:

(1) A quantization of the kinematical structure of the system is a rule that assigns a quantum observable (or state) to each classical observable (or state).
(2) A quantization of the dynamical structure of the system is a rule that assigns a quantum equation of motion to each classical equation of motion.
(3) An interconsistency of these quantizations must be exists.

In quantum kinematics, there exist many quantization schemes. A common basis of all these methods is an assumption that *classical and quantum kinematical structures are different representations of the same totality of mathematical structures*. This is the *Dirac's correspondence principle* [45].

A quantization in kinematics is a general rule assigns a quantum observable $A(Q, P)$ to each classical observable $A(q, p)$ which is a function on the phase space. Here a quantum observable can be an operator on a Hilbert space $\mathcal{H}$. The function $A(q, p)$ itself is called in this case the symbol of the operator $A(Q, P)$.

DEFINITION. A *quantization* is a mapping π from a set of classical observables into a set of quantum observables that to each classical observable $A(q, p)$ there corresponds a linear self-adjoint operator $A(Q, P) = \pi(A(q, p))$ on a Hilbert space.

There exist a requirement that must be satisfied by the quantization $\pi : A(q, p) \to A(Q, P)$. First of all, this procedure should satisfy the Dirac's correspondence

principle. For a more accurate formulation of this principle, we note the following conditions:

(1) Let $g_c^{(2)}$ be a binary operation on a set of classical observables. For a given quantization, there is a binary operation $g_q^{(2)}$ on the set of quantum observables corresponding to the operation $g_c^{(2)}$, i.e.,

$$g_c^{(2)}\big(A(q,p), B(q,p)\big) \to g_q^{(2)}\big(A(Q,P), B(Q,P)\big).$$

(2) If $g_c^{(1)}$ is a unary operation on a set of classical observables, then there exists a unary operation $g_q^{(1)}$ on the set of quantum observables corresponding to the operation $g_c^{(1)}$, i.e.,

$$g_c^{(1)}\big(A(q,p)\big) \to g_q^{(1)}\big(A(Q,P)\big).$$

(3) If $g_c^{(0)}$ is a nullary operation on a set of classical observables, then there exists a nullary operation $g_q^{(0)}$ on the set of quantum observables corresponding to $g_c^{(0)}$, i.e., $g_c^{(0)} \to g_q^{(0)}$.

DEFINITION. Let $\mathcal{M}_c$ be a set of all classical observables, and let $\mathcal{M}_q$ be a set of all quantum observables. A *semi-quantization* is a mapping π from a set $\mathcal{M}_c$ into a set $\mathcal{M}_q$, such that the following properties are satisfied:

(1) $\pi(aA + bB) = a\pi(A) + b\pi(B)$ for all $A, B \in \mathcal{M}_c$, and $a, b \in \mathbb{R}$.
(2) $\pi(A^*) = [\pi(A)]^*$ for all $A \in \mathcal{M}_c$.
(3) $\pi(1) = I$.
(4) $\pi(0) = 0$.

Requirement (1) express the mathematical statement that π is a linear map. Then π is a map from a linear space $\mathcal{M}_c$ into a linear space $\mathcal{M}_q$. In this way, there exists a binary operation $g_q^{(2)}(\pi(A), \pi(B)) = \pi(A)+\pi(B)$ on $\mathcal{M}_q$ corresponding to the binary operation $g_c^{(2)}(A, B) = A + B$ on $\mathcal{M}_c$.

Requirement (2) expresses the statement that π is a map from a set of real-valued functions into a set of self-adjoint operators. Then there exists a unary operation $g_q^{(1)}(\pi(A)) = [\pi(A)]^*$ on $\mathcal{M}_q$ corresponding to the unary operation $g_c^{(1)}(A) = A^*$ on $\mathcal{M}_c$.

Requirements (3) and (4) are obvious. They are a statement of the fact that there are the nullary operations I and 0 on $\mathcal{M}_q$ corresponding to the operation 1 and 0 on $\mathcal{M}_c$.

DEFINITION. A *prequantization* (or *Dirac quantization*) is a semi-quantization π from a set $\mathcal{M}_c$ into a set $\mathcal{M}_q$, such that

$$\pi\big(\{A, B\}\big) = (1/i\hbar)\big[\pi(A), \pi(B)\big],$$

where $\{A, B\}$ is a Poisson brackets of $A, B \in \mathcal{M}_c$.

This requirement is a statement that there exists a Lie operation $g_q^{(2)}$ on $\mathcal{M}_q$ corresponding to a Lie operation $g_c^{(2)}$ on $\mathcal{M}_c$. These operations are defined by the equations

$$g_q^{(2)}\big(\pi(A), \pi(B)\big) = \pi(A) \cdot \pi(B) = \frac{1}{i\hbar}\big[\pi(A), \pi(B)\big],$$
$$g_c^{(2)}(A, B) = A \cdot B = \{A, B\}$$

for $A, B \in \mathcal{M}_c$.

DEFINITION. A *Jordan quantization* is a semi-quantization π from a set $\mathcal{M}_c$ into a set $\mathcal{M}_q$, such that for any function $f : \mathbb{R} \to \mathbb{R}$ for which $\pi(f(A))$ and $f(\pi(A))$ are well defined, we have

$$\pi\big(f(A)\big) = f\big(\pi(A)\big).$$

In the special case, the Jordan quantization is defined by the monomials $f(A) = A^n$, where $n \in \mathbb{N}$. Then we have the requirement $\pi(A^n) = (\pi(A))^n$ for all $A \in \mathcal{M}_c$ and $n \in \mathbb{N}$.

Properties of semi-quantization

The following properties are satisfied for the semi-quantization procedure.

(1) Each finite linear combination of observables is an observable, i.e., $\pi(\sum_{k=1}^n a_i A_i) = \sum_{k=1}^n a_i \pi(A_i)$, where a_i are real numbers.

(2) If A and B are two arbitrary elements of $\mathcal{M}_c$, then $\pi(A)\pi(B)$ is *not* a quantum observable. In general, $\pi(A)\pi(B)$ does not belong to $\mathcal{M}_q$ since it is not a self-adjoint operator: $(\pi(A)\pi(B))^* = \pi(B)\pi(A)$. In the general case, a multiplication of two self-adjoint operators is not a self-adjoint operator.

(3) A semi-quantization cannot be defined as a map that assigns to a pointwise multiplication of $A, B \in \mathcal{M}_c$ exactly one multiplication of $\pi(A), \pi(B) \in \mathcal{M}_q$. In general,

$$\pi(AB) \neq \pi(A)\pi(B).$$

(4) If $\pi(A)$ is a self-adjoint operator, then $\pi(A)^2$ is self-adjoint. A semi-quantization can be defined as a map that assigns to each function f of $A \in \mathcal{M}_c$ exactly one function $f(\pi(A))$ of $\pi(A) \in \mathcal{M}_q$:

$$\pi\big(f(A)\big) = f\big(\pi(A)\big).$$

For example, $\pi(A^2) = [\pi(A)]^2$. This requirement is a statement that there exists a binary operation $g^{(2)}(\pi(A), \pi(A)) = \pi(A)\pi(A)$ on $\mathcal{M}_q$ corresponding to the

binary operation $g^{(2)}(A, A) = AA$ on $\mathcal{M}_c$. In this case, the semi-quantization is called Jordan quantization. Note that this requirement is *not* valid for so-called Weyl quantization. In general,

$$\pi(AA) \neq \pi(A)\pi(A), \qquad \pi(A^n) \neq \big[\pi(A)\big]^n.$$

(5) The symmetrized multiplication (anticommutator)

$$\pi(A) \circ \pi(B) = \frac{1}{2}\big(\pi(A)\pi(B) + \pi(B)\pi(A)\big) \tag{1}$$

is a self-adjoint operator. If the condition $\pi(A^2) = [\pi(A)]^2$ is valid, then the Jordan multiplication (1) of self-adjoint operators can be defined. The definition of $\pi(A) \circ \pi(B)$ does not require, as we did in (1), the knowledge of the ordinary product of two observables. The Jordan multiplication can be defined by the equality

$$\pi(A) \circ \pi(B) = \frac{1}{4}\Big(\big(\pi(A) + \pi(B)\big)^2 - \big(\pi(A) - \pi(B)\big)^2\Big).$$

The right hand side of this expression contains only those operation that we have already defined in the Jordan quantization. If $\pi(A^2) = \pi(A)^2$ for all $A \in \mathcal{M}_c$, then $\pi(A \circ B) = \pi(A) \circ \pi(B)$ for all $A, B \in \mathcal{M}_c$. Note that $A \circ B = AB$.

(6) For the Jordan quantization, we have the requirement

$$\pi(A^n) = \big(\pi(A)\big)^n, \tag{2}$$

where $A \in \mathcal{M}_c$ and $n \in \mathbb{N}$. Unfortunately, the axioms of Jordan quantization are not quite consistent. Using these axioms it is possible to express $\pi(A)$ for $A(q, p) = q^2p^2 = (qp)^2$ in two ways with two different results. Namely, by the rule (2) for the squaring function, we obtain

$$\begin{aligned}\pi(qp) &= \frac{1}{2}\pi\big((q+p)^2 - q^2 - p^2\big) = \frac{1}{2}\big((Q+P)^2 - Q^2 - P^2\big)\\ &= \frac{1}{2}(QP + PQ).\end{aligned}$$

Similarly,

$$\begin{aligned}\pi\big(q^2p^2\big) &= \frac{1}{2}\pi\big(\big(q^2+p^2\big)^2 - q^4 - p^4\big) = \frac{1}{2}\big(\big(Q^2+P^2\big)^2 - Q^4 - P^4\big)\\ &= \frac{1}{2}\big(Q^2P^2 + P^2Q^2\big).\end{aligned}$$

However, it is not hard to prove by using the canonical commutation relations that

$$\left(\frac{1}{2}(QP + PQ)\right)^2 \neq \frac{1}{2}\big(Q^2P^2 + P^2Q^2\big).$$

Then, $\pi(A^2) \neq (\pi(A))^2$ for $A = qp$, and

$$\pi(A \circ A) \neq \pi(A) \circ \pi(A).$$

As a result, we see that the Jordan quantization does not work in general.

(7) An algebra of classical observables is a Lie algebra with respect to Poisson brackets. An algebra $\mathcal{M}_q$ is a Lie algebra with respect to the self-adjoint commutator:

$$A \cdot B = \frac{1}{i\hbar}[A, B] = \frac{1}{i\hbar}(AB - BA),$$

where $A, B \in \mathcal{M}_q$. If A and B are self-adjoint operators, then $A \cdot B$ is self-adjoint:

$$\begin{aligned}(A \cdot B)^* &= \left(\frac{1}{i\hbar}(AB - BA)\right)^* = -\frac{1}{i\hbar}\big((AB)^* - (BA)^*\big) \\ &= -\frac{1}{i\hbar}(B^*A^* - A^*B^*) = -\frac{1}{i\hbar}(BA - AB) = \frac{1}{i\hbar}(AB - BA) \\ &= A \cdot B.\end{aligned}$$

This Lie operation on a set of quantum observables maps this set into itself.

A prequantization is a semi-quantization from $\mathcal{M}_c$ into a set of self-adjoint operators acting on some Hilbert space, such that

$$\pi(A \cdot B) = \pi(A) \cdot \pi(B) \tag{3}$$

for all $A, B \in \mathcal{M}_c$. If π is a one-to-one mapping $\mathcal{M}_c$ onto $\mathcal{M}_q$, then equation (3) means that prequantization is an isomorphism of a Lie algebra $\mathcal{M}_c^{(-)}$ with a Lie algebra $\mathcal{M}_q^{(-)}$. However, requirement (3) will caused the difficulty. If two Lie algebras $\mathcal{M}_c^{(-)}$ and $\mathcal{M}_q^{(-)}$ are isomorphic then so are their derivation algebras $Der(\mathcal{M}_c^{(-)})$ and $Der(\mathcal{M}_q^{(-)})$. A derivation algebra is a Lie algebra $Der(\mathcal{M}^{(-)})$ of all linear maps $\mathcal{L}$ on $\mathcal{M}^{(-)}$ which satisfies $\mathcal{L}(A \cdot B) = (\mathcal{L}A) \cdot B + A \cdot (\mathcal{L}B)$. A derivation $\mathcal{L}$ is said to be inner if there exists $H \in \mathcal{M}^{(-)}$ such that $\mathcal{L}A = H \cdot A$, otherwise $\mathcal{L}$ is said to be outer. If one Lie algebra has outer derivations and the other not, then they cannot be isomorphic. In general, prequantization π cannot form an isomorphism of the Lie algebra $\mathcal{M}_c^{(-)}$ and the Lie algebra $\mathcal{M}_q^{(-)}$ since one algebra admits outer derivations while the other does not.

We illustrate this problem with an example. Using $\{q^3, p^2\} = 6q^2p$, we obtain

$$\pi\big(q^2p\big) = \frac{1}{6}\pi\big(\{q^3, p^2\}\big) = \frac{1}{6i\hbar}\big[Q^3, P^2\big] = \frac{1}{2}\big(Q^2P + PQ^2\big). \tag{4}$$

Similarly,

$$\pi\big(qp^2\big) = \frac{1}{2}\big(QP^2 + P^2Q\big). \tag{5}$$

Finally, we have on the one hand $\{q^3, p^3\} = 9q^2p^2$, gives

$$\pi(q^2p^2) = \frac{1}{9}\pi(\{q^3, p^3\}) = \frac{1}{9i\hbar}[Q^3, P^3]$$
$$= Q^2P^2 - 2i\hbar QP - \frac{2\hbar^2}{3}. \tag{6}$$

On the other hand, for the equation $\{q^2p, qp^2\} = 3q^2p^2$, we have

$$\pi(q^2p^2) = \frac{1}{3}\pi(\{q^2p, qp^2\}) = \frac{1}{3i\hbar}[\pi(q^2p), \pi(qp^2)].$$

Substitution of (4) and (5) into this relation gives

$$\pi(q^2p^2) = \frac{1}{12i\hbar}[Q^2P + PQ^2, QP^2 + P^2Q] = Q^2P^2 - 2i\hbar QP - \frac{\hbar^2}{3}.$$

This equation contradicts (6). As a result, we see that the Dirac quantization does not work in general.

(8) Let the set of observables form a linear space $\mathcal{M}_0$ over $\mathbb{R}$. If $\mathcal{M}_0$ is $\mathcal{M}_c$, then $\mathcal{M}_0$ is a set of classical observables. If $\mathcal{M}_0$ is $\mathcal{M}_q$, then we have a set of quantum observables. We can define two bilinear multiplication operations on the set $\mathcal{M}_0$ denoted by symbols $\cdot$ and $\circ$, and satisfying the conditions:

(a) $<\mathcal{M}_0, \cdot>$ is a Lie algebra:

$$A \cdot B = -B \cdot A, \quad (A \cdot B) \cdot C + (B \cdot C) \cdot A + (C \cdot A) \cdot B = 0;$$

(b) $<\mathcal{M}_0, \circ>$ is a special Jordan algebra:

$$A \circ B = B \circ A, \quad \big((A \circ A) \circ B\big) \circ A = (A \circ A) \circ (B \circ A);$$

(c) the Leibnitz rule

$$A \cdot (B \circ C) = (A \cdot B) \circ C + B \circ (A \cdot C);$$

(d) the equation for associators

$$(A \circ B) \circ C - A \circ (B \circ C) = \frac{\hbar^2}{4}\big((A \cdot B) \cdot C - A \cdot (B \cdot C)\big). \tag{7}$$

In this case, the Lie–Jordan algebra is said to be defined. We shall also assume that there exists a unity I in $\mathcal{M}_0$ such that $A \circ I = A$ and $A \cdot I = 0$. We denote as $\mathcal{M}$ a free Lie–Jordan algebra over $\mathbb{R}$ with unity I and generators Q_k and P_k, where $k = 1, \ldots, n$ and

$$Q_k \cdot P_l = \delta_{kl} I, \qquad Q_k \cdot Q_L = 0, \qquad P_k \cdot P_l = 0.$$

The smallest subalgebra of $\mathcal{M}$ containing $\mathcal{G} = \{Q_k, P_k\colon\ k = 1, \ldots, n\}$ is the subalgebra generated by $\mathcal{G}$. If this subalgebra is all of $\mathcal{M}$, then $\mathcal{G}$ generates $\mathcal{M}$ and

the Q_k, P_k are generators of $\mathcal{M}$. A *free algebra* is an algebra generated by finite linear combinations and finite powers of the elements Q_k, P_k $(k = 1, \dots, n)$ and the identity I.

For the classical observables $A(q, p)$ and $B(q, p)$, the operations $\cdot$ and $\circ$ can be defined in terms of the Poisson bracket in $\mathbb{R}^{2n}$ and the usual pointwise multiplication

$$A(q, p) \cdot B(q, p) = \big\{A(q, p), B(q, p)\big\},$$
$$A(q, p) \circ B(q, p) = A(q, p)B(q, p).$$

For the quantum observables $A = A(Q, P)$ and $B = B(Q, P)$, the Lie and Jordan multiplication are defined by

$$A \cdot B = \frac{1}{i\hbar}(AB - BA), \qquad A \circ B = \frac{1}{2}(AB + BA).$$

As a result, $\mathcal{M}_c$ and $\mathcal{M}_q$ can be considered as Lie–Jordan algebras over $\mathbb{R}$.

The Lie–Jordan algebra is an algebraic structure that gives a uniform description of classical and quantum systems. The case $\hbar = 0$ corresponds to transition from a nonassociative Jordan algebra into associative. Common algebraic properties of classical and quantum systems are not depend on relation (7).

(9) Let $\mathcal{M}^{(\pm)}$ be a Lie–Jordan algebra. Then there exists an associative algebra such that the multiplication is defined by

$$g_a(A, B) = A \circ B + \frac{i\hbar}{2} A \cdot B.$$

In the classical mechanics ($\hbar = 0$), the second term is equal to zero, i.e., $g_a(A, B) = A \circ B$.

(10) Let M be a Hausdorff space, which is locally compact (in that each point has a compact neighbourhood). The space $C_0(M)$ consists of all continuous functions on M which vanish at infinity in the sense that for each $\varepsilon > 0$ there is a compact subset $M_\varepsilon \subset M$ such that $|A(x)| < \varepsilon$ for all x outside M_ε. The space $C_0(M)$ can be considered as an associative C^*-algebra of classical observables.

The semi-quantization can be considered as the map $\pi : C_0(M) \to \mathcal{B}(\mathcal{H})$, where $\mathcal{B}(\mathcal{H})$ is a C^*-algebra of bounded operators on a Hilbert space $\mathcal{H}$.

(11) In the general case, it is desirable (though not strictly necessary) that the semi-quantization π preserves positivity:

$$\pi(A) \geqslant 0$$

for all $A \geqslant 0$.

Then quantization can be considered as the positive map $\pi : C_0(M) \to \mathcal{B}(\mathcal{H})$, where $C_0(M)$ and $\mathcal{B}(\mathcal{H})$ are regarded as associative C^*-algebras. An element A of a C^*-algebra is called positive (nonnegative) when $A^* = A$ and its spectrum is positive, i.e., $\sigma(A) \subset \mathbb{R}_+$. We write $A \geqslant 0$. A positive map π between two

C^*-algebras is a linear map such that $A \geqslant 0$ implies $\pi(A) \geqslant 0$. Every self-adjoint element A has a decomposition

$$A = A_+ - A_-, \tag{8}$$

where $A_\pm \geqslant 0$ and $A_+A_- = 0$. It follows from (8) that a positive map automatically preserves self-adjointness. Let us give the basic statement regarding properties of positivity.

STATEMENT. *If π is a positive map between two C^*-algebras $C_0(M)$ and $\mathcal{B}(\mathcal{H})$, then $A^* = A$ implies $\pi(A)^* = \pi(A)$ for all $A \in C_0(M)$.*

This theorem means that $A(x) \in C_0(M)$ is mapped into a self-adjoint operator $\pi(A) \in \mathcal{B}(\mathcal{H})$.

(12) By properties (6) and (7), the Dirac and Jordan quantizations do not work in general. To solve this problem, we define the Weyl quantization as a consistent quantization.

DEFINITION. A *Weyl quantization* is a semi-quantization π from a set $\mathcal{M}_c$ into a set $\mathcal{M}_q$, such that

$$\pi(A * B) = \pi(A) * \pi(B).$$

If $A = A(q, p)$ and $B = B(q, p)$, then

$$A(q, p) * B(q, p) = A\big(L_q^+, L_p^+\big)B(q, p) = A\big(L_q^+, L_p^+\big)B\big(L_q^+, L_p^+\big)1,$$

where L_q^+, L_p^+ are Jordan left multiplications by q and p.

It can be proved that

$$\pi\big(A\big(L_q^+, L_p^+\big)\big) = A\big(L_Q^+, L_P^+\big)$$

for all $A \in \mathcal{M}_c$. Here L_Q^+, L_P^+ are Jordan left multiplications by Q and P. In general,

$$L_{Q_k}^+ L_{Q_l}^+ - L_{Q_l}^+ L_{Q_k}^+ = 0, \quad L_{P_k}^+ L_{P_l}^+ - L_{P_l}^+ L_{P_k}^+ = 0,$$
$$L_{Q_k}^+ L_{P_l}^+ - L_{P_l}^+ L_{Q_k}^+ = 0,$$

if $[Q_k, Q_l] = [P_k, P_l] = 0$ and $[Q_k, P_l] = i\hbar\delta_{kl} I$. Note that the operators

$$A(Q, P) = A\big(L_Q^+, L_P^+\big)I$$

are Weyl ordered. The multiplication $\pi(A) * \pi(B)$ is defined by

$$\begin{aligned}\pi(A) * \pi(B) &= A(Q, P) * B(Q, P) = A\big(L_Q^+, L_P^+\big)B(Q, P)\\ &= A\big(L_Q^+, L_P^+\big)B\big(L_Q^+, L_P^+\big)I,\end{aligned}$$

and will be called the Weyl multiplication.

For the theory of Weyl quantization see, for instance, [15–19,49].

8.2. Heisenberg algebra

If algebraic operations for quantum observables are defined, then an algebra of observables are determined by generators. Each element of this algebra can be derived by application of algebraic operations to generators. Let $\{Q_1, \ldots, Q_n, P_1, \ldots, P_n, I\}$ be a basis for $(2n+1)$-dimensional linear operator space H. Consider now a Lie algebra $H_n = <H, \cdot>$ generated by finite linear combinations of Q, P, and its multiplications, where $Q_k \cdot P_l = \delta_{kl} I$, and other products of the basis elements are equal to zero. The algebra H_n is called the Heisenberg algebra.

DEFINITION. A *Heisenberg algebra* is a Lie algebra H_n generated by $\{Q_k, P_k, I: k = 1, \ldots, n\}$, such that

$$[Q_k, P_l] = i\hbar\delta_{kl} I, \qquad [Q_k, Q_l] = [P_k, P_l] = [I, Q_k] = [I, P_k] = 0, \quad (9)$$

where $k, l = 1, 2, \ldots, n$.

Equations (9) are called the *canonical commutation relations* (*CCR*). An element of algebra H_n can be presented by

$$A = aQ + bP + cI,$$

where $aQ = \sum_{k=1}^{n} a_k Q_k$, $bP = \sum_{k=1}^{n} b_k P_k$, and $a_k, b_k \in \mathbb{R}$. If $A, A' \in H_n$, then

$$\begin{aligned} A \cdot A' &= (aQ + bP + cI) \cdot (a'Q + b'P + c'I) \\ &= (ac' + ca')Q + (bc' + cb')P + (cc' + ab' - a'b)I. \end{aligned}$$

The universal enveloping algebra U_n of the Lie algebra H_n is an associative algebra of polynomials in Q_k, P_k, $k = 1, \ldots, n$. A set of all elements $Q_1^{i_1} P_1^{j_1} \ldots Q_n^{i_n} P_n^{j_n}$ generates a linear operator space U_n. The set of these elements forms a basis for this space.

STATEMENT. *Let U_n be a universal enveloping algebra of Heisenberg algebra H_n. Then the operators*

$$E_{ij} = Q^i P^j = \prod_{k=1}^{n} (Q_k)^{i_k} \prod_{l=1}^{n} (P_l)^{j_l}, \quad Q_k^0 = I, \quad P_k^0 = I,$$

where $i = (i_1, \ldots, i_n)$ and $j = (j_1, \ldots, j_n)$ form a basis for U_n.

For each polynomial

$$A(q, p) = \sum_{|i|,|j|<m} a_{ij} q^i p^j,$$

there exists the operator

$$A(Q, P) = \sum_{|i|,|j|<m} a_{ij} Q^i P^j,$$

where $q^i = q_1^{i_1} \cdots q_n^{i_n}$, $p^j = p_1^{j_1} \cdots p_n^{j_n}$, and $Q^i = Q_1^{i_1} \cdots Q_n^{i_n}$, $P^j = P_1^{j_1} \cdots P_n^{j_n}$.

DEFINITION. We say that a pair (Q_k, P_k) of self-adjoint operators acting on a separable Hilbert space $\mathcal{H}$ form a *Heisenberg kinematical representation* of the CCR, if there exists a dense set D in $\mathcal{H}$, such that $D \subset D(Q) \cap D(P)$ and the CCR are realized on D.

A Heisenberg kinematical representation, as formulated in the definition, concentrates its requirement essentially on the local aspects of the CCR, neglecting the physics contained in the boundary conditions. Consequently, if we want any uniqueness theorem, we need to impose some conditions that are more stronger than those required in the definition of Heisenberg kinematical representation. One way to achieve this is to impose conditions on the domains and properties of the self-adjoint operators Q and P. For example, it is necessary and sufficient that there exists a dense set D in a Hilbert space $\mathcal{H}$, such that the following conditions are satisfied

(1) $D \subset D(QP - PQ)$,
(2) $(Q \pm iI)A \in D(Q) \cap D(P)$ for all $A \in D$,
(3) $(P \pm iI)A \in D(Q) \cap D(P)$ for all $A \in D$.

Note that at least one of the operators Q or P must be unbounded. The operators Q and P cannot both be bounded.

THEOREM. *There is no representation of the canonical commutation relations by bounded operators.*

This theorem means that it is impossible to realize the Heisenberg kinematical representation by bounded operators. Elements of U_n are unbounded operators $A(Q, P)$.

Consider now the question of what should be the bounded observables associated with Q and P. In general, there exists an operator algebra that is generated

by basic operators, and regard the self-adjoint elements of this algebra as observables. This operator algebra consists of all bounded operator functions of the basic operators.

The algebra of operators generated by Q and P may be defined as the set of all limits in the weak operator topology of the algebra of all linear combinations of the operators

$$W(a,b) = \exp\left\{\frac{i}{\hbar}(aQ + bP)\right\}.$$

If $\tilde{A}(a,b)$ is an integrable function of the real variables a and b, then

$$A(Q,P) = \int da\, db\, \tilde{A}(a,b) \exp\left\{\frac{i}{\hbar}(aQ + bP)\right\} \tag{10}$$

will be well-defined bounded operator. The operator $A(Q,P)$ is called the *Weyl ordered operator function*. It is clear that $A(Q,P)$ is constructed from Q and P in a relatively explicit manner and so may be defined as an operator function of Q and P. The collection of all such $A(Q,P)$, together with their uniform limits form an operator algebra $\mathcal{M}_W$ of Weyl ordered operators. The operators $W(a,b)$ are generators of this algebra.

8.3. Weyl system and Weyl algebra

Weyl system

Observables are usually considered as bounded self-adjoint operators on a separable Hilbert space. Consider now the question of what should be the bounded observables associated with Q_k and P_k. In general, there exists an operator algebra that is generated by the basic operators, and regard the self-adjoint elements of this algebra as observables. This operator algebra consists of all bounded operator functions of Q_k and P_k. We consider the following bounded functions of Q_k and P_k:

$$U_k(a) = e^{\frac{i}{\hbar}aQ_k}, \qquad V_k(b) = e^{\frac{i}{\hbar}bP_k}. \tag{11}$$

We can define a representation of the CCR as follows: for each k and l there are two continuous, one-parameter groups $\{U_k(a), V_l(b) |\ a, b \in \mathbb{R}\}$ of unitary operators acting on some separable Hilbert space $\mathcal{H}$, such that

$$\big[U_k(a), U_l(b)\big] = \big[V_k(a), V_l(b)\big] = 0,$$
$$U_k(a)V_l(b) = V_l(b)U_k(a) \exp\frac{i}{\hbar}ab\delta_{kl}.$$

We now define the following unitary bounded operators

$$U(a) = e^{\frac{i}{\hbar}aQ}, \qquad V(b) = e^{\frac{i}{\hbar}bP},$$

where $aQ \equiv \sum_{k=1}^{n} a_k Q_k$, $bP \equiv \sum_{k=1}^{n} b_k P_k$. Commutation relations (9) give

$$U(a)V(b) = V(b)U(a)e^{-\frac{i}{\hbar}ab}, \tag{12}$$

$$U(a)U(a') = U(a+a'), \quad V(b)V(b') = V(b+b'). \tag{13}$$

Here we use the Baker–Campbell–Hausdorff formula

$$e^A e^B = e^{A+B} e^{\frac{1}{2}[A,B]},$$

for A and B such that $[[A, B], A] = [[A, B], B] = 0$. The representation of CCR in the exponential form (12) and (13) is called the *Weyl system*.

A Weyl system may be defined as a pair of unitary representations $U(a)$ and $V(b)$ of two n-parameter commutative groups, which are weakly continuous and satisfy the Weyl relations (12). For any such Weyl system there exists by Stone's theorem self-adjoint operators Q_k and P_k such that equations (11) are valid. These operators can be called the canonical variables of the system. The existence of a Weyl system is clear from the existence of the following representation.

Since Q is self-adjoint, it generates a weakly continuous, one-parameter group $\{U(a)|a \in \mathbb{R}\}$ of the unitary operators $U(a)$ defined on $L^2(\mathbb{R})$ by

$$\big(U(a)\Psi\big)(q) = e^{\frac{i}{\hbar}aq}\Psi(q).$$

We also consider the weakly continuous one-parameter group $\{V(b)\colon\ b \in \mathbb{R}\}$ of the unitary operators $V(b)$ defined on $L^2(\mathbb{R})$ by

$$\big(V(b)\Psi\big)(q) = q\Psi(q+b).$$

This is the Weyl's form of the Schrödinger representation of the CCR.

DEFINITION. A *Schrödinger kinematical representation* of CCR on $L^2(\mathbb{R}^n)$ is a representation of operators $U(a)$ and $V(b)$ on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n)$, such that

$$U(a)\Psi(q) = e^{\frac{i}{\hbar}aq}\Psi(q), \qquad V(b)\Psi(q) = \Psi(q+b) \tag{14}$$

for all functions $\Psi(q) = <q|\Psi> \in L^2(\mathbb{R}^n)$.

Using the Dirac's notations, equations (14) give

$$U(a)|q> = |q>e^{\frac{i}{\hbar}aq}, \qquad V(b)|q> = |q-b>, \tag{15}$$

and

$$<q|U(a) = e^{-\frac{i}{\hbar}aq}<q|, \qquad <q|V(b) = <q+b|. \tag{16}$$

The uniqueness problem can be reduced to the uniqueness of the representation of the CCR in Weyl's form. This question is answered by the following von Neumann theorem.

THEOREM *(von Neumann). Let $\mathcal{H}$ be a separable Hilbert space, and $\{U(a)|\ a \in \mathbb{R}^n\}$ and $\{V(b)\colon\ b \in \mathbb{R}^n\}$ be two weakly continuous n-parameter groups of unitary operators acting on $\mathcal{H}$, such that equations* (12) *and* (13) *hold for all $a, b \in \mathbb{R}^n$. Then a set $\{U(a), V(b)|\ a, b \in \mathbb{R}^n\}$ is unitary equivalent to a direct sum of the Schrödinger kinematical representations.*

This theorem states that *each irreducible Weyl system for a quantum system with n degrees of freedom is unitary equivalent to the Schrödinger kinematical representation on $L^2(\mathbb{R}^n)$*. Any two irreducible representations of the Weyl system are unitary equivalent.

For each Weyl system $\{U(a), V(b)|\ a, b \in \mathbb{R}^n\}$ there exists by Stone's theorem, the self-adjoint operators Q_k and P_k, $k = 1, \ldots, n$, such that

$$U(a) = \exp \frac{i}{\hbar} a Q, \qquad V(b) = \exp \frac{i}{\hbar} b P.$$

If $U(a)$ and $V(b)$ are weakly continuous with respect to a_k and b_k, then

$$Q_k = -i\hbar \frac{\partial U(a)}{\partial a_k}, \qquad P_k = -i\hbar \frac{\partial V(b)}{\partial b_k}.$$

STONE'S THEOREM. *Any strongly (or weakly) continuous unitary group $\{U(a)\colon\ a \in \mathbb{R}\}$ has the form $U(a) = \exp(i a Q)$, where Q is a uniquely defined self-adjoint operator.*

Let $\mathcal{H}$ be a Hilbert space. The strong continuity of $\{U(a)\colon\ a \in \mathbb{R}\}$ means that

$$\lim_{a \to 0} \| U(a)x - x \|_{\mathcal{H}} = 0$$

for all $x \in \mathcal{H}$. Note that $U(a)$ is a unitary operator if $<U(a)x|U(a)y> = <x|y>$ for all $x, y \in \mathcal{H}$.

Weyl algebra

The operators

$$W(a, b) = \exp \frac{i}{\hbar}(aQ + bP)$$

are called the *Weyl operators*. For each Weyl system $\{U(a), V(b)\colon\ a, b \in \mathbb{R}^n\}$,

$$W(a, b) = U(a)V(b)e^{-\frac{i}{2\hbar}ab} = V(b)U(a)e^{\frac{i}{2\hbar}ab}.$$

The Weyl operators satisfy the composition law

$$W(a_1, b_1)W(a_2, b_2) = W(a_1 + a_2, b_1 + b_2)e^{-\frac{i}{2\hbar}[a_1 b_2 - a_2 b_1]}. \tag{17}$$

We refer to this law as the *Weyl's form of CCR*. Using $W(a, 0) = U(a)$, $W(0, b) = V(b)$, we obtain that equations (17) gives (13) and (12). Then equation (17) summarizes relations (13) and (12) of the Weyl system.

We notice that as a consequence of the Weyl's form of CCR the complex linear space W_n of all finite linear combinations

$$\sum_{i=1}^{m} c_i W(a_i, b_i) \tag{18}$$

is stable under the product of any two its elements. Then it is an algebra, which we refer to as the Weyl algebra. Using

$$W^*(a, b) = W(-a, -b), \qquad W^*(a, b)W(a, b) = I, \tag{19}$$

it is not hard to prove that this algebra is stable with respect to the involution. The ordinary operator norm provides the norm on W_n, which that becomes an involutive normed algebra.

DEFINITION. A *Weyl algebra* W_n is a normed involutive algebra that is determined by relations (17) and (19).

Let $\mathcal{B}(\mathcal{H})$ be a C^*-algebra of all bounded operators on a Hilbert space $\mathcal{H}$. Note that W_n is a subalgebra of $\mathcal{B}(\mathcal{H})$. It is possible to construct a C^*-algebra, which is generated by the Weyl's form of CCR. An algebra $\mathcal{M}$ of observables is usually defined as a smallest C^*-subalgebra of $\mathcal{B}(\mathcal{H})$, that contains $\{W(a, b)\colon a, b \in \mathbb{R}^n\}$. The algebra $\mathcal{M}$ may also be defined as the set of all limits in the weak operator topology of the algebra of all finite linear combinations (18). Then $\mathcal{M}$ is a closure of W_n in the weak operator topology. Note that each state ω on this Weyl C^*-algebra $\mathcal{M}$ is completely defined by the functions $\omega_{ab} = \omega(W(a, b))$. These are the *characteristic functions*.

8.4. Weyl and Wigner operator bases

Weyl operator basis

The Weyl operators

$$W(a, b) = e^{\frac{i}{\hbar}(aQ + bP)} \tag{20}$$

can be considered as a basis for an operator space with the scalar product $(A|B) = Tr(A^*B)$. These operators are similar to the functions

$$w(a, b) = \exp i(aq + bp), \tag{21}$$

which form a generalized basis for the function space $\mathcal{J}(\mathbb{R}^{2n}) \subset L^2(\mathbb{R}^{2n}) \subset \mathcal{J}^*(\mathbb{R}^{2n})$ with the scalar product

$$(\Psi_1, \Psi_2) = \int dq\, dp\, \Psi_1^*(q, p)\Psi_2(q, p).$$

It is not hard to prove that

$$\big(w(a, b), w(a', b')\big) = (2\pi)^{2n}\delta(a - a')\delta(b - b').$$

If $A(q, p) \in L^2(\mathbb{R}^{2n})$, then there is

$$\tilde{A}(a, b) = \frac{1}{(2\pi\hbar)^n} \int da\, db\, A(q, p)w(-a, -b),$$

such that

$$A(q, p) = \frac{1}{(2\pi\hbar)^n} \int da\, db\, \tilde{A}(a, b)w(a, b). \tag{22}$$

The Weyl operators $W(a, b)$ can be considered as a Weyl quantization of $w(a, b)$, such that

$$\pi\big(w(a, b)\big) = W(\hbar a, \hbar b).$$

From the definition of $W(a, b)$, it immediately follows that

$$Tr\big[W(a, b)\big] = (2\pi\hbar)^n\delta(a)\delta(b).$$

Taking the trace of the composition law

$$W(a, b)W(a', b') = W(a + a', b + b') \exp \frac{i}{2\hbar}(ab' - ba'), \tag{23}$$

we find

$$Tr\big[W(-a, -b)W(a', b')\big] = (2\pi\hbar)^n\delta(a' - a)\delta(b' - b). \tag{24}$$

Let us define the normalized Weyl operators by

$$\overline{W}(a, b) = \frac{1}{(2\pi\hbar)^{n/2}} W(a, b).$$

STATEMENT. *A set of all normalized Weyl operators forms an orthonormal operator basis, such that*

$$\big(\overline{W}(a, b)|\overline{W}(a', b')\big) = \delta(a' - a)\delta(b' - b).$$

This statement is proved by equation (24).

STATEMENT. *Each orthonormal operator basis* $\{\overline{W}(a,b)\colon\ a,b\in\mathbb{R}^n\}$ *for a Liouville space is a complete basis. A requirement of completeness of the basis gives the relation*

$$\big(\overline{W}(a,b)|A|\overline{W}(a,b)\big)=\frac{1}{(2\pi\hbar)^n}\,Tr[A].$$

PROOF.

$$\begin{aligned}\big(\overline{W}(a,b)|A|\overline{W}(a,b)\big)&=Tr\big[\overline{W}^*(a,b)A\overline{W}(a,b)\big]\\&=Tr\big[\overline{W}(-a,-b)A\overline{W}(a,b)\big]\\&=Tr\big[A\overline{W}(a,b)\overline{W}(-a,-b)\big]\\&=\frac{1}{(2\pi\hbar)^{n/2}}\,Tr\big[A\overline{W}(0,0)\big]=\frac{1}{(2\pi\hbar)^n}\,Tr[A].\end{aligned}\qquad\square$$

The requirement of completeness for the basis $\{\overline{W}(a,b)\colon\ a,b\in\mathbb{R}^n\}$ is similar to the requirement for an operator basis $\{E(a)\colon\ a\in\mathbb{R}\}$, and it is of the form:

$$\begin{aligned}\big(\overline{W}(a,b)|A|\overline{W}(a,b)\big)&=\int da\,db\,\overline{W}(a,b)A\overline{W}(a,b)\\&=\int\frac{da\,db}{(2\pi\hbar)^n}W(a,b)AW(a,b)=Tr[A].\end{aligned}$$

STATEMENT. *If* $W(a,b)$ *is a Weyl operator, then*

$$\big[P^k,W(a,b)\big]=a^kW(a,b),\qquad\big[Q^k,W(a,b)\big]=b^kW(a,b).$$

Let $W(a,b)$ be a Weyl operator, and let $\mathcal{M}$ be an operator space. Then a wide class of the bounded operator $A\in\mathcal{M}$ can be uniquely expressed in the form

$$A=\frac{1}{(2\pi\hbar)^n}\int da\,db\,\tilde{A}(a,b)W(a,b),$$

where $\tilde{A}(a,b)$ is an integrable function of the real variables $a,b\in\mathbb{R}^n$. This is operator analog of the Fourier representation (22) of the function $A(q,p)\in\mathcal{J}(\mathbb{R}^{2n})$.

The composition law expresses the product of two Weyl operators as a single Weyl operator. This can be used to obtain the composition law for the function $\tilde{C}(a,b)$ associated with the operator $C=AB$ in the terms of the functions $\tilde{A}(a,b)$, $\tilde{B}(a,b)$ associated with the operators A, B. Express A, B, and C in terms of $W(a,b)$, and derive the expansion coefficients using the composition law (23).

As a result, we obtain

$$\tilde{C}(a,b) = \frac{1}{\hbar^{2n}} \int da'\, db'\, \tilde{A}(a',b') B(a-a', b-b') \exp \frac{-i}{2\hbar}(ab' - ba'). \tag{25}$$

Using the variables $s = a/\hbar$, $t = b/\hbar$, we find

$$\tilde{C}(s,t) = \int ds'\, dt'\, \tilde{A}(s',t') B(s-s', t-t') \exp \frac{-i\hbar}{2}(st' - ts').$$

We notice that if $\hbar = 0$, we obtain the usual convolution expression as expected for the Fourier coefficients.

Wigner operator basis

The Wigner basis is defined as

$$\begin{aligned} \mathcal{W}(q,\, p) &= \frac{1}{(2\pi\hbar)^n} \int da\, db\, W(a,b) \exp \frac{-i}{\hbar}(aq + bp) \\ &= \frac{1}{(2\pi\hbar)^n} \int da\, db \exp \frac{i}{\hbar}\big(a(Q - qI) + b(P - pI)\big). \end{aligned}$$

This is the *Wigner operator*. In this basis the operator $A(Q,\, P)$ can be written

$$A(Q,\, P) = \frac{1}{(2\pi\hbar)^n} \int dq\, dp\, \mathcal{W}(q,\, p) A(q,\, p).$$

We now establish the dual basis, and then specify the composition law. Using the definition of $\mathcal{W}(q,\, p)$ in terms of $W(a,b)$ and the expression for the trace of $W(a,b)$, we obtain

$$\begin{aligned} &Tr\big[\mathcal{W}(q,\, p)\big] = 1, \\ &Tr\big[\mathcal{W}(q,\, p)\mathcal{W}(q',\, p')\big] = (2\pi\hbar)^n \delta(q - q')\delta(p - p'). \end{aligned}$$

Consequently $\mathcal{W}(q,\, p)/(2\pi\hbar)^n$ is a dual basis of $\mathcal{W}(q,\, p)$. The normalized Wigner basis

$$\overline{\mathcal{W}}(q,\, p) = \frac{1}{(2\pi\hbar)^{n/2}} \mathcal{W}(q,\, p)$$

is dual of itself, and

$$\big(\overline{\mathcal{W}}(q,\, p) | \overline{\mathcal{W}}(q',\, p')\big) = \delta(q - q')\delta(p - p').$$

We can express the product of $\mathcal{W}(q,\, p)$ operators using the composition law (23):

$$\mathcal{W}(q,\, p)\mathcal{W}(q',\, p') = \frac{2^n}{(\pi\hbar)^n} \int dq''\, dp''\, \mathcal{W}(q'',\, p'') J(q,\, p,\, q',\, p',\, q'',\, p''),$$

where

$$J(q, p, q', p', q'', p'') = \exp\frac{-2i}{\hbar}\big(p(q'-q'') - q(p'-p'') + (p'q''-q'p'')\big).$$

Note that the product of the Weyl operators is proportional to a single operator. The product of two Wigner operators is a linear combination of an infinite number of the Wigner operators.

This formula can be used to obtain the composition law for a function associated with the product of two operators, in terms of the functions associated with the operators in the product. This way one finds that if $C = AB$, then

$$C(q, p) = \frac{1}{(\pi\hbar)^{2n}}\int dq'\,dq''\,dp'\,dp''\,A(q, p)B(q, p) \times J(q', p', q'', p'', q, p),$$

where we use

$$A(q, p) = \big(\mathcal{W}(q, p)|A(Q, P)\big) = Tr\big[\mathcal{W}(q, p)A(Q, P)\big],$$
$$B(q, p) = \big(\mathcal{W}(q, p)|B(Q, P)\big) = Tr\big[\mathcal{W}(q, p)B(Q, P)\big].$$

Let us find the operator $\mathcal{W}(q, p)$ in the q-representation. This is easily found from the q-representation of the Weyl operator:

$$<q'|W(a, b)|q''> = \delta(b + q' - q'')\exp\left(\frac{i}{\hbar}a\frac{(q'+q'')}{2}\right).$$

As a result, we obtain

$$<q'|\mathcal{W}(q, p)|q''> = \delta\left(q - \frac{q'+q''}{2}\right)\exp\frac{i}{\hbar}p(q'-q''),$$

and $A(q, p)$ can be written

$$A(q, p) = \int dq'\,dq''\,<q'|\mathcal{W}(q, p)|q''><q''|A|q'> = \int dx\,<q - \frac{1}{2}x|A|q + \frac{1}{2}x>e^{\frac{i}{\hbar}xp}.$$

We note that $A(q, p)$ will be real-valued function if $A(Q, P)$ is a self-adjoint operator. In the special case, when $A(Q, P)$ is the density operator, we have the usual definition of Wigner's function

$$\rho_W(q, p) = \frac{1}{(2\pi\hbar)^n}\int dx\,<q - \frac{1}{2}x|\rho|q + \frac{1}{2}x>e^{\frac{i}{\hbar}xp}.$$

8.5. Differential operators and symbols

Let A be a linear operator on $M \subset \mathbb{R}^n$.

DEFINITION. A *linear differential operator* is an operator A that is defined on $M \subset \mathbb{R}^n$ and has the form

$$A = \sum_{|k| \leqslant m} a_k(q) D^k, \quad D^k = D_1^{k_1} D_2^{k_2} \dots D_n^{k_n}, \; D_j = -i\,\partial/\partial q^j, \tag{26}$$

where k is a multi-index, i.e., $k = (k_1, \dots, k_n)$, k_j are integer numbers, $|k| = k_1 + \dots + k_n$, and $a_k(q)$ are functions on M.

DEFINITION. A *symbol* of the linear differential operator (26) is the function

$$A(q, p) = \sum_{|k| \leqslant m} a_k(q) p^k.$$

It is not hard to prove the following statement.

STATEMENT. *The function $A(q, p)$ defined by the equation*

$$A(q, p) = e^{-iqp} A e^{iqp}$$

is the symbol of the operator A.

For $\Psi(q) \in \mathcal{J}(\mathbb{R}^n)$, we define its Fourier transform $\tilde{\Psi}(p)$ by

$$\tilde{\Psi}(p) = \frac{1}{(2\pi)^{n/2}} \int e^{-iqp} \Psi(q)\, dq. \tag{27}$$

We also define the inverse Fourier transform

$$\Psi(q) = \frac{1}{(2\pi)^{n/2}} \int e^{iqp} \tilde{\Psi}(p)\, dp. \tag{28}$$

Differentiation of (28) with respect to q_j gives

$$-i \frac{\partial}{\partial q_j} \Psi(q) = \frac{1}{(2\pi)^{n/2}} \int e^{iqp} p_j \tilde{\Psi}(p)\, dp.$$

The application of the differential operator (26) to equation (28) gives

$$A\Psi(q) = \frac{1}{(2\pi)^{n/2}} \int e^{iqp} A(q, p) \tilde{\Psi}(p)\, dp, \tag{29}$$

where $A(q, p)$ is the symbol of A. It is easy to see, that $A(q, p) \in C^\infty(M \times \mathbb{R}^n)$ and $A(q, p)$ is a polynomial in p. Substituting of (27) into (29), we obtain

$$A\Psi(q) = \frac{1}{(2\pi)^n} \iint e^{i(q-y)p} A(q, p) \Psi(y)\, dy\, dp. \tag{30}$$

Equations (29) and (30) can be considered as a definition of the differential operator, if $A(q, p)$ is a polynomial in p. These equation make it possible to define the operator A for a broad class of functions $A(q, p)$. As a result, we obtain a generalization of differential operator that is usually called the *pseudodifferential operator*.

For example, if a symbol $A(q, p)$ is such that $A(q, p) \in C^\infty(M \times \mathbb{R}^n)$ and

$$\left|\partial_p^k \partial_q^l A(q, p)\right| \leqslant C_{kl}(1 + |p|)^{m-|k|} \tag{31}$$

for certain fixed m and for all k and l, then equations (29) and (30) makes it possible to define the pseudodifferential operator A.

We shall denote the space of all symbols $A(q, p) \in C^\infty(M \times \mathbb{R}^n)$, which satisfy inequality (31), by S^m. If $A(q, p)$ is the polynomial of degree m, then (31) is valid, and $A(q, p) \in S^m$. Another example of $A(q, p) \in S^m$ is defined by the Fourier transform of a smooth kernel. If $a(x, y) \in C^\infty(M \times M)$, then the integral operator

$$A\Psi(q) = \int a(q, y)\Psi(y)\, dy, \tag{32}$$

can be presented in the form (29) or (30) with $A(q, p) \in S^m$. It is not hard to prove this statement by the following transformations

$$\begin{aligned} A\Psi(q) &= \int a(q, y)\Psi(y)\, dy = \int a(q, y)\left(\frac{1}{(2\pi)^{n/2}} \int e^{iyp}\tilde{\Psi}(p)\, dp\right) dy \\ &= \frac{1}{(2\pi)^{n/2}} \int e^{iqp}\left(\int e^{i(y-q)p} a(q, y)\, dy\right)\tilde{\Psi}(p)\, dp. \end{aligned}$$

Using (29), we obtain

$$A(q, p) = \int e^{i(y-q)p} a(q, y)\, dy.$$

Then $A(q, p)$ for all fixed q is a Fourier transform of $a(q, y) \in C^\infty(M \times M)$ up to $\exp(-iqp)$.

DEFINITION. A *canonical pseudodifferential operator* of the order m on M is a linear operator A, such that (29) holds for all $A(q, p) \in S^m$ and $\Psi(q) \in \mathcal{D}(M)$. This operator A is the linear mapping form a space $\mathcal{D}(M)$ into $C^\infty(M)$.

If $A(q, p) \in S^m$ and $m < -n$, then equation (30) gives (32) with

$$a(q, y) = \frac{1}{(2\pi)^n} \int e^{i(q-y)p} A(q, p)\, dp.$$

The function $a(q, y)$ is called the *kernel of operator* A.

If the linear operator (32) is a mapping from $\mathcal{D}(M)$ into $\mathcal{D}^*(M)$, then its kernel is a generalized function, $K_A(x, y) = a(x, y) \in \mathcal{D}^*(M \times M)$, such that the equation

$$<A\Psi, \Phi> = <K_A, \Phi \otimes \Psi> \tag{33}$$

is valid for all $\Psi \in \mathcal{D}(M)$ and $\Phi \in \mathcal{D}(M)$. Here $\mathcal{D}(M)$ is a space of all smooth functions with compact support, and $\mathcal{D}^*(M)$ is a dual space of $\mathcal{D}(M)$.

SCHWARZ KERNEL THEOREM. *For each continuous linear operator* $A : \mathcal{D}(M) \to \mathcal{D}^*(M)$ *there exists exactly one generalized function* $a(x, y) = K_A(x, y) \in \mathcal{D}^*(M \times M)$, *such that A can be represented by equation* (32) *for all* $\Psi \in \mathcal{D}(M)$.

Note that equation (33) is a rule that assigns to each kernel $a(x, y) \in \mathcal{D}^*(M \times M)$ exactly one operator A from $\mathcal{D}(M)$ into $\mathcal{D}^*(M)$. The kernel $a(x, y)$ is uniquely defined by the operator A. Hence, we obtain the one-to-one correspondence between the linear continuous operators $A : \mathcal{D}(M) \to \mathcal{D}^*(M)$ and the generalized functions $a(x, y) \in \mathcal{D}^*(M \times M)$. For example, if I is an identity operator, then $a(x, y) = \delta(x - y)$ is the Dirac delta-function. The differential operator (26) on $M \subset \mathbb{R}^n$ has the kernel

$$a(q, y) = \sum_{|k| \leqslant m} a_k(q) D^k \delta(q - y).$$

8.6. Weyl quantization mapping

A quantization is a map that assigns to each classical observable $A(q, p)$, which is a real-valued function, exactly one quantum observable $A(Q, P)$, which is a self-adjoint operator. Let us introduce Weyl quantization for classical observables $A(q, p)$. To do this, we consider the function $A(q, p)$ given by the Fourier transform according to the equation

$$A(q, p) = \frac{1}{(2\pi)^n} \int ds\, dt\, \tilde{A}_c(s, t) e^{i(sq+tp)},$$

and

$$\tilde{A}_c(s, t) = \frac{1}{(2\pi)^n} \int dq\, dp\, A(q, p) e^{-i(sq+tp)}.$$

Introducing, instead of s and t, the new integration variables $a = \hbar s$, $b = \hbar t$, and $\tilde{A}(a, b) = \tilde{A}_c(a/\hbar, b/\hbar)/\hbar^n$, we obtain

$$A(q, p) = \frac{1}{(2\pi\hbar)^n} \int da\, db\, \tilde{A}(a, b) e^{\frac{i}{\hbar}(aq+bp)},$$

and

$$\tilde{A}(a,b) = \frac{1}{(2\pi\hbar)^n}\int dq\,dp\,A(q,p)e^{-\frac{i}{\hbar}(aq+bp)}. \tag{34}$$

Then $A(Q,P) = \pi(A(q,p))$ can be defined by the formula

$$A(Q,P) = \frac{1}{(2\pi\hbar)^n}\int da\,db\,\tilde{A}(a,b)e^{\frac{i}{\hbar}(aQ+bP)}. \tag{35}$$

Using the Weyl operator (20), this equation can be presented in the form

$$A(Q,P) = \frac{1}{(2\pi\hbar)^n}\int da\,db\,\tilde{A}(a,b)W(a,b).$$

The operator $A(Q,P)$ called the *Weyl (symmetric) ordered operator*.

Substitution of (34) into (35) gives

$$A(Q,P) = \frac{1}{(2\pi\hbar)^{2n}}\int da\,db\,dq\,dp\,A(q,p) \times \exp\frac{i}{\hbar}\big(a(Q-qI)+b(P-pI)\big). \tag{36}$$

Note that this equation can be rewritten in the form

$$A(Q,P) = \frac{1}{(2\pi)^{2n}}\int ds\,dt\,dq\,dp\,A(q,p)\exp i\big(s(Q-qI)+t(P-pI)\big).$$

As a result, we obtain the one-to-one correspondence between the operators $A(Q,P)$ and the functions $A(q,p)$.

DEFINITION. A *Weyl quantization* is a mapping that assigns to each function $A(q,p)$ exactly one operator $A(Q,P)$, which is defined by equation (36).

We illustrate this notion in the following examples.

(1) If $A(q,p) = qp$, then $A(Q,P) = \frac{1}{2}(QP+PQ)$.
(2) If $A(q,p) = q^2p$, then $A(Q,P) = (1/3)(Q^2P+QPQ+PQ^2)$.
(3) If $A(q,p) = q^2p^2$, then $A(Q,P) = (1/4)(Q^2P^2+2QP^2Q+P^2Q^2)$.

Note that $QP^2Q = PQ^2P$.

There exist QP and PQ ordered maps:

$$A_{QP}(Q,P) = \frac{1}{(2\pi\hbar)^{2n}}\int da\,db\,dq\,dp\,A(q,p)e^{\frac{i}{\hbar}a(Q-qI)}e^{\frac{i}{\hbar}b(P-pI)},$$

$$A_{PQ}(Q,P) = \frac{1}{(2\pi\hbar)^{2n}}\int da\,db\,dq\,dp\,A(q,p)e^{\frac{i}{\hbar}a(P-pI)}e^{\frac{i}{\hbar}a(Q-qI)}.$$

For these maps, $\pi(qp)$ gives QP and PQ. These operators are not self-adjoint and cannot be considered as observables. Therefore QP and PQ ordered maps

from a set of functions into a set of operators cannot be considered as a quantization of observables. There exists natural requirement that must be satisfied by the quantization: if $A^* = A$, then $[\pi(A)]^* = \pi(A)$.

8.7. Kernel and symbol of Weyl ordered operator

Let $a(q', q'') = <q'|A|q''>$ be a kernel of $A(Q, P)$ in the coordinate representation, and let $A(q, p)$ be a symbol of $A(Q, P)$. There exists a correspondence between $A(q, p)$ and $a(q', q'')$. The kernel of $A(Q, P)$ is defined by the equation

$$\begin{aligned} a(q', q'') &= <q'|A|q''> = \int dp\, <q'|A|p><p|q''> \\ &= \frac{1}{(2\pi\hbar)^{n/2}} \int dp\, <q'|A|p> e^{-\frac{i}{\hbar} q'' p}. \end{aligned} \tag{37}$$

For QP-ordered operator $A(Q, P)$, we can use the relation

$$<q'|A(Q, P)|p> = A(q', p)<q'|p> = A(q', p) \frac{1}{(2\pi\hbar)^{n/2}} e^{\frac{i}{\hbar} q' p}. \tag{38}$$

Substitution of this relation into (37), we obtain

$$a(q', q'') = \frac{1}{(2\pi\hbar)^n} \int dp\, A(q', p) e^{-\frac{i}{\hbar}(q''-q')p}.$$

It is not hard to prove that $a(q', q'')$ is a Fourier transform of (38) with respect to p and $(q'' - q')$. Then

$$A(q, p) = \int dq''\, a(q, q'') e^{\frac{i}{\hbar}(q''-q)p}.$$

As a result, we obtain the correspondence between the kernel $a(q', q'') = <q'|A|q''>$ and the symbol $A(q, p)$ of the QP-ordered operator A.

To describe this correspondence for Weyl ordered operators, we use the Baker–Campbell–Hausdorff formula

$$W(a, b) = e^{\frac{i}{\hbar}(aQ+bP)} = e^{\frac{i}{\hbar} aQ} e^{\frac{i}{\hbar} bP} e^{\frac{i}{2\hbar} ab}.$$

This is the QP-ordered form of $W(a, b)$. Then the kernel of the Weyl operator $W(a, b)$ can be written in the form

$$\begin{aligned} <q'|W(a, b)|q''> &= <q'|e^{\frac{i}{\hbar}(aQ+bP)}|q''> = <q'|e^{\frac{i}{\hbar} aQ} e^{\frac{i}{\hbar} bP} e^{\frac{i}{2\hbar} ab}|q''> \\ &= e^{\frac{i}{\hbar} aq'} <q'|e^{\frac{i}{\hbar} bP}|q''> e^{\frac{i}{2\hbar} ab} \\ &= e^{\frac{i}{\hbar} a(q'+\frac{1}{2}b)} \delta(b + q' - q'') \\ &= e^{\frac{i}{\hbar} a\frac{1}{2}(q'+q'')} \delta(b + q' - q''). \end{aligned}$$

As a result, we obtain

$$a(q', q'') = \frac{1}{(2\pi\hbar)^n} \int dp\, A\left(\frac{q'+q''}{2}, p\right) e^{\frac{i}{\hbar}(q'-q'')p}.$$

Using the variables $q = (q'+q'')/2$, $x = -(q'-q'')$, we rewrite this equation in the form

$$a\left(q - \frac{1}{2}x, q + \frac{1}{2}x\right) = \frac{1}{(2\pi\hbar)^n} \int dp\, A(q, p) e^{-\frac{i}{\hbar}xp}.$$

Then

$$A(q, p) = \int dx\, a\left(q - \frac{1}{2}x, q + \frac{1}{2}x\right) e^{\frac{i}{\hbar}xp}.$$

It can be easily verified that in this way, we obtain the one-to-one correspondence between the kernel $a(q', q'')$ and the symbol $A(q, p)$ of the Weyl ordered operator $A(Q, P)$.

8.8. Weyl symbols and Wigner representation

A Weyl quantization is a rule that assigns a self-adjoint operator $A(Q, P)$ to each classical observable $A(q, p)$ by the formula

$$A(Q, P) = \frac{1}{(2\pi\hbar)^{2n}} \int da\, db\, dq\, dp\, A(q, p) W(a, b) e^{-\frac{i}{\hbar}(aq+bp)}.$$

If ρ is a density operator, then

$$\begin{aligned} <A(Q, P)> &= Tr\big[\rho A(Q, P)\big] \\ &= \int \frac{da\, db\, dq\, dp}{(2\pi\hbar)^{2n}} A(q, p) e^{-\frac{i}{\hbar}(aq+bp)}\, Tr\big[\rho W(a, b)\big]. \end{aligned}$$

If ρ and A are Weyl ordered operators, then the trace of ρA has the form

$$Tr[\rho A] = \frac{1}{(2\pi\hbar)^n} \int dq\, dp\, \rho(q, p) A(q, p),$$

where $\rho(q, p)$ and $A(q, p)$ are the Weyl symbols of ρ and A. As a result, we obtain

$$\rho(q, p) = \frac{1}{(2\pi\hbar)^n} \int da\, db\, e^{-\frac{i}{\hbar}(aq+bp)}\, Tr\big[\rho W(a, b)\big].$$

DEFINITION. A *characteristic function* is an expectation value of the Weyl operator $W(a, b)$, i.e.,

$$\omega\big(W(a, b)\big) = <W(a, b)> = \big(\rho | W(a, b)\big) = Tr\big[\rho W(a, b)\big].$$

STATEMENT. *The Weyl operator $W(a, b)$ can be presented in the form*

$$W(a,b) = \int |q' - \frac{1}{2}b> dq' \, e^{\frac{i}{\hbar}aq'} <q' + \frac{1}{2}b|. \tag{39}$$

PROOF. Using (15) and (16), it is not hard to prove this statement:

$$\begin{aligned}
W(a,b) &= e^{\frac{i}{\hbar}(aQ+bP)} = e^{\frac{i}{\hbar}aQ} \, e^{\frac{i}{\hbar}bP} e^{\frac{i}{2\hbar}ab} \\
&= \int dq\, dp\, |q><q|e^{\frac{i}{\hbar}aQ} \, e^{\frac{i}{\hbar}bP}|p><p|e^{\frac{i}{2\hbar}ab} \\
&= e^{\frac{i}{2\hbar}ab} \int dq\, dp\, |q>e^{\frac{i}{\hbar}aq}<q|p><p|e^{\frac{i}{\hbar}bp}<p| \\
&= e^{\frac{i}{2\hbar}ab} \int dq\, dp\, dq'\, |q>e^{\frac{i}{\hbar}(aq+bp)}<q|p><p|q'><q'| \\
&= e^{\frac{i}{2\hbar}ab} \frac{1}{(2\pi\hbar)^n} \int dq\, dp\, dq'\, |q>e^{\frac{i}{\hbar}(aq+bp+qp-pq')}<q'| \\
&= e^{\frac{i}{2\hbar}ab} \int dq\, dq'\, |q>e^{\frac{i}{\hbar}aq}<q'|\frac{1}{(2\pi\hbar)^n} \int dp\, e^{\frac{i}{\hbar}(b+q-q')p} \\
&= e^{\frac{i}{2\hbar}ab} \int dq\, dq'\, |q>e^{\frac{i}{\hbar}aq}<q'|\delta(b+q-q') \\
&= e^{\frac{i}{2\hbar}ab} \int dq\, |q>e^{\frac{i}{\hbar}aq}<b+q|.
\end{aligned}$$

Using $q = q' - (1/2)b$, we obtain (39). □

Let $A = A(Q, P)$ be a self-adjoint operator. A *Weyl symbol* of A is the function

$$A(q,p) = \int dx \, <q - \frac{1}{2}x|A|q + \frac{1}{2}x>e^{\frac{i}{\hbar}xp}. \tag{40}$$

Equation (40) describes a map from a set of operators into a set of symbols $A(q, p) = symb(A(Q, P))$. It is not hard to prove the following relations

$$\begin{aligned}
&<q|A(Q,P)|q> = \frac{1}{(2\pi\hbar)^n} \int dp\, A(q,p), \\
&<p|A(Q,P)|p> = \frac{1}{(2\pi\hbar)^n} \int dq\, A(q,p), \\
&Tr[A] = \int dq <q|A|q> = \frac{1}{(2\pi\hbar)^n} \int dq\, dp\, A(q,p).
\end{aligned}$$

DEFINITION. Let ρ be a density operator. A *Wigner distribution function* is a Weyl symbol of $\rho/(2\pi\hbar)^n$, which is defined by Fourier transformation of nondiagonal elements of the kernel $<x|\rho|y>$:

$$\rho_W(q,\,p) = \frac{1}{(2\pi\hbar)^n}\int dy\, <q - \frac{1}{2}y|\rho|q + \frac{1}{2}y> e^{\frac{i}{\hbar}yp}. \tag{41}$$

Equation (41) is a special case of (40) for $A = \rho/(2\pi\hbar)^n$. As a result, $\rho_W(p, q)$ is a symbol of the operator $\rho/(2\pi\hbar)^n$.

The Wigner distribution function satisfies to the following properties:

(1) $\rho_W(p, q)$ is a real-valued function.
(2) If we integrate the Wigner function over p, or q, we obtain the probability density for the coordinate q, or the momentum p:

$$\int dp\, \rho_W(p, q) = <q|\rho|q>, \qquad \int dq\, \rho_W(p, q) = <p|\rho|p>.$$

(3) Integration of the Wigner function over q and p gives a unit:

$$\iint dq\, dp\, \rho_W(p, q) = Tr[\rho] = 1.$$

(4) The Wigner function is *not* a positive defined function.
(5) The estimate $|\rho_W(q,\, p)| \leqslant 1/(\pi\hbar)^n$ is valid for the Wigner function.

Using the Wigner distribution function (41), the expectation value $<A> = Tr[\rho A]$ can be written in the form

$$<A> = \int dp\, dq\, A(p, q)\rho_W(p, q), \tag{42}$$

where $A(p, q)$ is a symbol of the Weyl ordered operator A. It allows us to formulate quantum mechanics in the form, which is similar to classical mechanics. We may be interested in the expectation values of certain powers of A. For example, the mean square of an observable A is the expectation $<A^2>$. In general, the operator A^2 is not in the Weyl ordered form, so that equation (42) cannot be directly applied to it. If, however, we bring it into Weyl ordered form by means of the commutation relations to find its Weyl symbol, then $symb(A^2) \neq (symb\, A)^2$. Therefore,

$$<A^2> \neq \int dp\, dq\, \big(A(p, q)\big)^2 \rho_W(p, q).$$

Let A and B be Weyl ordered operators, and let $C = AB$. Then

$$C_W(p, q) = A_W(p, q)\left(\exp -\frac{i\hbar\mathcal{P}}{2}\right)B_W(p, q), \tag{43}$$

where

$$\mathcal{P} = \overleftarrow{\partial_p}\overrightarrow{\partial_q} - \overleftarrow{\partial_q}\overrightarrow{\partial_p}, \quad A_W(p,q)\overleftarrow{\partial_p}\overrightarrow{\partial_q}B_W(p,q) = \partial_p A_W \partial_q B_W,$$

and $A_W \mathcal{P} B_W = -\{A_W, B_W\}$. Equation (43) gives

$$symb(AB) \neq symb(A)symb(B).$$

Using (43), we obtain the following Weyl symbols for the Lie and Jordan multiplications

$$(A \cdot B)_W(p,q) = -\frac{2}{\hbar} A_W(p,q)\left(\sin\frac{\hbar\mathcal{P}}{2}\right)B_W(p,q),$$
$$(A \circ B)_W(p,q) = A_W(p,q)\left(\cos\frac{\hbar\mathcal{P}}{2}\right)B_W(p,q).$$

Then

$$symb(A \cdot B) \neq symb(A) \cdot symb(B),$$
$$symb(A \circ B) \neq symb(A) \circ symb(B).$$

Note that these inequalities are connected with the following properties of the Weyl quantization

$$\pi(A \cdot B) \neq \pi(A) \cdot \pi(B), \qquad \pi(A \circ B) \neq \pi(A) \circ \pi(B)$$

for some $A = A(q, p)$ and $B = B(q, p)$.

8.9. Inverse of quantization map

Let A be a self-adjoint operator. The equation

$$A(q,p) = symb(A)(q,p) = \int dx \, <q - \frac{1}{2}x|A|q + \frac{1}{2}x> e^{\frac{i}{\hbar}xp} \tag{44}$$

describes a map *symb* from a set of operators into a set of functions (of symbols). This map is inverse of π: $symb = \pi^{-1}$. Using the operator

$$P(q,p) = \int dy \, |p - \frac{1}{2}y> e^{\frac{i}{\hbar}yq} <p + \frac{1}{2}y|$$

equation (44) can be rewritten in the form

$$A(q,p) = Tr\big[P(q,p)A\big].$$

The Weyl symbol of $P(q, p)$ is

$$\big(P(q,p)\big)_W(q',p') = (2\pi\hbar)^n \delta(q-q')\delta(p-p').$$

As a result, *symb* assigns to the operator $P(q, p)$ a Dirac delta-function.

We introduce new, more compact notations. Let $z = q, p$ be a point of phase space, and $dz = (2\pi\hbar)^{-n}\, dq\, dp$ be an elementary volume element. The following properties of $P(z)$ are satisfied.

(1) $\int dz P(z) = I$, or $(I|P(z)) = Tr[P(z)] = 1$.
(2) $P^*(z) = P(z)$.
(3) $(P(z)|P(z')) = \delta(z - z')$, or $(P(z))_W(z') = \delta(z - z')$.
(4) $A_W(z) = (P(z)|A)$.

Here a Weyl symbol of A is a scalar product of A and $P(q, p)$, i.e., $A_W(z) = (P(z)|A)$.

There is the Dirac's notation $|z)$ for $P(z)$ that can be used. Then the following properties of the ket-vectors $|z) = |P(z))$ are satisfied:

(1) $\int |z) dz (z| = I$.
(2) $(I|z) = 1$.
(3) $(z|z') = \delta(z - z')$.
(4) $A_W(z) = (z|A)$.

The scalar product $(A|B) = Tr[A^*B]$ can be presented by

$$(A|B) = \int dz\, A_W^*(z) B_W(z).$$

As a result, the operators $P(q, p)$ form an operator basis.

8.10. Symbols of operators and Weyl quantization

Quantization and symbols

Setting quantization in kinematics means establishing a general rule assigning a quantum observable $A(Q, P)$ to each classical observable $A(q, p)$ which is a real-valued function on the phase space. Here a quantum observable is a self-adjoint operator on a Hilbert space $\mathcal{H}$. The function $A(q, p)$ itself is called in this case the *symbol of the operator* $A(Q, P)$.

Consider a system with n degrees of freedom, such that the phase space is the space $\mathbb{R}^{2n}$. We can set $\mathcal{H} = L^2(\mathbb{R}^n)$ and make correspond to the function q_k, the operator Q_k of multiplication by q_k and to the function p_k, the operator $P_k = -i\hbar\partial_{q_k}$:

$$\pi(q_k) = Q_k, \qquad \pi(p_k) = P_k.$$

In general, quantization is not uniquely defined by this correspondence. For example, the product $q_k^2 p_k^2$ can be associated with the self-adjoint operators $P_k Q_k^2 P_k$,

or $(1/2)(Q_k^2P_k^2 + P_k^2Q_k^2)$ or also $(1/4)(Q_k^2P_k^2 + 2P_kQ_k^2P_k + P_k^2Q_k^2)$. These correspond to different quantizations and different ordering rules. Note that

$$\frac{1}{2}\big(Q_k^2P_k^2 + P_k^2Q_k^2\big) = P_kQ_k^2P_k - \hbar^2 I.$$
$$\frac{1}{4}\big(Q_k^2P_k^2 + 2P_kQ_k^2P_k + P_k^2Q_k^2\big) = P_kQ_k^2P_k - \frac{\hbar^2}{2}I.$$

The simplest operators in $L^2(\mathbb{R}^n)$ are differential operators with polynomial coefficients

$$A(Q, P) = \sum_{|a|,|b|\leqslant m} c_{ab}Q^aP^b = \sum_{|a|,|b|\leqslant m} c_{ab}q^a(-i\hbar\partial_q)^b, \tag{45}$$

where c_{ab} are constants, a and b are multi-indices ($a = (a_1, \dots, a_n)$, $|a| = a_1 + \cdots + a_n$), and $Q^a = Q_1^{a_1}\cdots Q_n^{a_n}$, $P^b = P_1^{b_1}\cdots P_n^{b_n}$. The operators $A(Q, P)$ of the form (45) are, in a sense, dense in the set of all the operators on $L^2(\mathbb{R}^n)$. Therefore, the symbols with a reasonably defined continuous dependency on a set of operators must be uniquely defined by the action on the operators of the form (45). This implies that the correspondence between operators and symbols is completely defined by the formulas expressing the symbols of the operators $Q_kA(Q, P)$, $A(Q, P)Q_k$, $P_kA(Q, P)$, $A(Q, P)P_k$ in terms of the symbol $A(q, p)$ of the operator $A(Q, P)$. This quantization is called linear if the formulas have linear differential operators.

DEFINITION. A *linear quantization* is a semi-quantization that is defined by the formulas:

$$Q_kA(Q, P) \leftrightarrow L_{q_k}^{(1)}A(q, p), \qquad A(Q, P)Q_k \leftrightarrow L_{q_k}^{(2)}A(q, p),$$
$$P_kA(Q, P) \leftrightarrow L_{p_k}^{(3)}A(q, p), \qquad A(Q, P)P_k \leftrightarrow L_{p_k}^{(4)}A(q, p),$$

where $L_{q_k}^{(1)}$, $L_{q_k}^{(2)}$, $L_{p_k}^{(3)}$, $L_{p_k}^{(3)}$ are linear differential operators of the first order with constant coefficients:

$$L_{q_k}^{(m)} = \sum_{l=1}^{n}\big(a_{kl}^{(m)}q_l + b_{kl}^{(m)}p_l + c_{kl}^{(m)}\partial_{q_l} + h_{kl}^{(m)}\partial_{p_l}\big) \quad (m = 1, 2),$$
$$L_{p_k}^{(m)} = \sum_{l=1}^{n}\big(a_{kl}^{(m)}q_l + b_{kl}^{(m)}p_l + c_{kl}^{(m)}\partial_{q_l} + h_{kl}^{(m)}\partial_{p_l}\big) \quad (m = 1, 2).$$

The matrices $a_{kl}^{(s)}$, $b_{kl}^{(s)}$, $c_{kl}^{(s)}$, $h_{kl}^{(s)}$, where $s = 1, 2, 3, 4$, are not arbitrary. They must be satisfied the relations resulting from the canonical commutation relations (9).

Symmetric product and Jordan multiplication

To describe the Weyl quantization, we first introduce the symmetric product of noncommuting operators.

DEFINITION. The *symmetric product* $(A_1^{k_1}\cdots A_n^{k_n})_s$ of noncommuting operators $A_1^{k_1},\dots,A_n^{k_n}$ is defined by the formula

$$(a_1A_1+\cdots+a_nA_n)^k=\sum_{k_1+\cdots+k_n=k}\frac{k!}{k_1!\cdots k_n!}a_1^{k_1}\cdots a_n^{k_n}\big(A_1^{k_1}\cdots A_n^{k_n}\big)_s, \tag{46}$$

where $a_k\in\mathbb{C}$, and the sum is taken over all the sets $(k_1,\dots,k_n)$.

As a result, $(A^{k_1}\cdots A^{k_1})_s$ is the coefficient of $k!/(k_1!\cdots k_n!)a_1^{k_1}\cdots a_n^{k_n}$ of the expansion (46).

In the case of $n=2$ and $A_1=Q$, $A_2=P$, equation (46) gives

$$(aQ+bP)^k=\sum_{l+m=k}\frac{k!}{l!m!}a^lb^m\big(Q^lP^m\big)_s.$$

For example,

$$(QP)_s=\frac{1}{2}(QP+PQ),\qquad \big(Q^2P\big)_s=\frac{1}{3}\big(Q^2P+QPQ+PQ^2\big).$$

The notation of the symmetric product $(Q^lP^k)_s$ is somewhat ambiguous since it is impossible to denote Q^l (or P^k) by one letter. For example, $(Q^2P)_s\neq(AP)_s$ for $A=Q^2$.

Consider now an associative algebra generated by finite linear combinations and finite powers of operators Q, P, where $QP-PQ=i\hbar I$. Then the symmetric product $(Q^lP^m)_s$ can be presented through the Jordan multiplication $A\circ B=(1/2)(AB+BA)$. In general, this multiplication is not associative, i.e., $(A\circ B)\circ C\neq A\circ(B\circ C)$.

THEOREM. *The symmetric product $(Q^lP^m)_s$ is an operator monomial with respect to the Jordan multiplication such that all the left brackets "(" are more to the left of all right brackets ")". All the right brackets ")" more to the right of left "(".*

$$\begin{aligned}\big(Q^lP^m\big)_s&=\big(Q\circ\big(\cdots\circ\big(P\circ(P\circ P)\big)\cdots\big)\big)\\&=\big(\big(\cdots\big((Q\circ Q)\circ Q\big)\circ\cdots\big)\circ P\big).\end{aligned}$$

For the case of $k=l=2$,

$$\big(Q^2P^2\big)_s=\big(Q\circ\big(Q\circ(P\circ P)\big)\big).$$

Moreover, we have

$$\big(Q\circ\big(Q\circ(P\circ P)\big)\big)=\big(Q\circ\big(P\circ(Q\circ P)\big)\big)=\big(P\circ\big(P\circ(Q\circ Q)\big)\big),$$

and

$$\big(Q\circ\big(Q\circ(P\circ P)\big)\big)=\big((P\circ P)\circ Q\big)\circ Q=\big((Q\circ P)\circ Q\big)\circ P.$$

The symmetric product $(Q^l P^m)_s$ is an element of an operator Jordan algebra with the left brackets on the left of the right brackets. Note that

$$\big(Q^2P^2\big)_s\neq(Q\circ Q)\circ(P\circ P),\qquad \big(Q^2P^2\big)_s\neq(Q\circ P)\circ(Q\circ P).$$

As a result, the symmetric multiplication is defined by Jordan left multiplications by Q and P. Suppose $\mathcal{M}_W$ is a set of all Weyl ordered self-adjoint operators. For $A(Q,P)\in\mathcal{M}_W$, let L_Q^+ and L_P^+ be the maps given by

$$L_Q^+A(Q,P)=Q\circ A(Q,P),\qquad L_P^+A(Q,P)=P\circ A(Q,P).\tag{47}$$

We can think of L_Q^+ and L_P^+ as meaning Jordan left multiplications by Q and P. Note that

$$L_Q^+L_P^+=L_P^+L_Q^+.$$

Let us give the important statement regarding symmetric multiplications of operators.

STATEMENT. *The symmetric multiplication $(Q^l P^m)_s$ is expressed by*

$$\big(Q^lP^m\big)_s=\big(L_Q^+\big)^l\big(L_P^+\big)^mI,$$

where I is the identity operator.

Let $\mathcal{M}_W$ be a set of all Weyl ordered self-adjoint operators. Then L_Q^+ and L_P^+ are maps from $\mathcal{M}_W$ into itself. A superoperator is a map from an operator set $\mathcal{M}_W$ into itself. Then the maps L_Q^+ and L_P^+ are superoperators on $\mathcal{M}_W$.

Weyl ordered operators and Weyl symbols

Let us consider the polynomial

$$A(q,p)=\sum_{|a|,|b|\leqslant m}c_{ab}q^ap^b,\tag{48}$$

and put in correspondence to it the operator

$$A(Q,P)=\sum_{|a|,|b|\leqslant m}c_{ab}\big(Q_1^{a_1}P_1^{b_1}\big)_s\cdots\big(Q_n^{a_n}P_n^{b_n}\big)_s,\tag{49}$$

where $(Q_k^{a_k} P_k^{b_k})_s$ are the symmetric product

$$\left(Q_k^{a_k} P_k^{b_k}\right)_s = \left(L_{Q_k}^+\right)^{a_k} \left(L_{P_k}^+\right)^{b_k} I.$$

Then $A(Q, P)$ is called the Weyl ordered operator, and $A(q, p)$ is called the Weyl symbol of the operator $A(Q, P)$.

Let us introduce Weyl symbols for more general operators. To do this, we consider a function $A(q, p)$ given by the Fourier transform

$$A(q, p) = \frac{1}{(2\pi\hbar)^n} \int da\, db\, \tilde{A}(a, b) \exp \frac{i}{\hbar}(aq + bp),$$

where $a, b \in \mathbb{R}^n$. Then the operator $A(Q, P)$ with the symbol $A(q, p)$ is given by the equation

$$A(Q, P) = \frac{1}{(2\pi\hbar)^n} \int da\, db\, \tilde{A}(a, b) \exp \frac{i}{\hbar}(aQ + bP).$$

It is not hard to prove that this agrees with (49). Representing the exponential in the series form

$$W(a, b) = \exp \frac{i}{\hbar}(aQ + bP) = \sum_{k=0}^{\infty} \frac{i^k}{\hbar^k k!}(aQ + bP)^k,$$

we see that it suffices to verify that the Weyl quantization of $(aq + bp)^k$ gives the operator $(aQ + bP)^k$, i.e.,

$$\pi\left((aq + bp)^k\right) = (aQ + bP)^k.$$

To do this, we use the equation

$$(aq + bp)^k = \sum_{k_1 + \cdots + k_n = k} \frac{k!}{k_1! \cdots k_n!}(a_1 q_1 + b_1 p_1)^{k_1} \cdots (a_n q_n + b_n p_n)^{k_n}.$$

In this equation we can substitute q_k for Q_k and p_k for P_k, since the operators $a_k Q_k + b_k P_k$ and $a_l Q_l + b_l P_l$ commute. It now sufficient to prove that

$$\pi\left((a_k q_k + b_k p_k)^m\right) = (a_k Q_k + b_k P_k)^m,$$

which is obvious from the definition of symmetric product.

The Weyl quantization of (48) gives the Weyl ordered operator (49). It can be easily verified that in this way, we obtain the one-to-one correspondence between the polynomials (48), and the Weyl ordered operator (49). We can extend this correspondence to functions and operators of a more general form. For this purpose, we formulate the following theorem.

STATEMENT. *If the operator $A(Q, P)$ corresponds to the polynomial $A(q, p)$, then we have the correspondences*

$$Q_k A(Q,P) \leftrightarrow \left(q_k + \frac{i\hbar}{2}\frac{\partial}{\partial p_k}\right)A(q,p),$$

$$A(Q,P)Q_k \leftrightarrow \left(q_k - \frac{i\hbar}{2}\frac{\partial}{\partial p_k}\right)A(q,p),$$

$$P_k A(Q,P) \leftrightarrow \left(p_k - \frac{i\hbar}{2}\frac{\partial}{\partial q_k}\right)A(q,p),$$

$$A(Q,P)P_k \leftrightarrow \left(p_k + \frac{i\hbar}{2}\frac{\partial}{\partial q_k}\right)A(q,p).$$

If $A(q, p)$ is a polynomial, then to prove this theorem it is sufficient to verify the formulas for the monomials $A(q, p) = q^a p^b$, which is not difficult to perform by induction on a_k and b_k.

Let us derive the kernel of a Weyl ordered operator $A(Q, P)$ with the symbol $A(q, p)$. For this purpose, we calculate explicitly the action of the operator $W(a, b) = \exp(i/\hbar)(aQ + bP)$ in the coordinate representation, i.e., for $Q_k\Psi(q) = q_k\Psi(q)$, and $P_k\Psi(q) = -i\hbar\partial\Psi(q)/\partial q_k$ in $L^2(\mathbb{R}^n)$. As a result, we obtain

$$A(Q,P)\Psi(q) = \frac{1}{(2\pi\hbar)^n}\int dy\,dp\,A\left(\frac{q+y}{2}, p\right)e^{\frac{i}{\hbar}(q-y)p}\Psi(y).$$

This is the equation that defines the action of the Weyl ordered operator $A(Q, P)$ having the symbol $A(q, p)$. Using (32), the kernel of this operator is

$$a(x,y) = \frac{1}{(2\pi\hbar)^n}\int dp\,A\left(\frac{x+y}{2}, p\right)\exp\left\{\frac{i}{\hbar}(x-y)p\right\}. \tag{50}$$

Thus $a(x, y)$ is obtained as the Fourier transform $p \to (x - y)$ of the function $A((x + y)/2, p)$. Using the inversion formula, we obtain

$$A(q,p) = \int dz\,a(q - z/2, q + z/2)\exp\frac{i}{\hbar}pz. \tag{51}$$

One of the advantages of Weyl ordering over other orderings is that the Weyl symbol $A(q, p)$ of the Weyl ordered operator $A(Q, P)$ is related to the Weyl symbol $A_*(q, p)$ of the operator $A^*(Q, P)$ by the simple formula

$$A_*(q,p) = A^*(q,p),$$

which is a consequence of (51). In particular, *real-valued Weyl symbols $A(q, p)$ correspond to self-adjoint Weyl ordered operators $A(Q, P)$.*

Composition formula for Weyl symbols

Let $A(Q, P)$ and $B(Q, P)$ be Weyl ordered operators. In the general case, $A(Q, P)B(Q, P)$ is not a symmetric product, and $symb(AB) \neq symb(A)symb(B)$. We now derive the composition formula for Weyl symbols. To do this, we use equations (50) and (51). The kernel $c(x, y)$ of the operator $C(Q, P) = A(Q, P)B(Q, P)$ is expressed in terms of the kernels $a(x, y)$, $b(x, y)$ of the operators $A(Q, P)$ and $B(Q, P)$ by the equation

$$c(x, y) = \int dz\, a(x, z)b(z, y).$$

Using

$$a(x, z) = \frac{1}{(2\pi\hbar)^n} \int dp_1\, A\left(\frac{x+z}{2}, p_1\right) \exp \frac{i}{\hbar}(x - z)p_1,$$
$$b(z, y) = \frac{1}{(2\pi\hbar)^n} \int dp_2\, B\left(\frac{z+y}{2}, p_2\right) \exp \frac{i}{\hbar}(z - y)p_2,$$

we obtain

$$c(x, y) = \frac{1}{(2\pi\hbar)^{2n}} \int dz\, dp_1\, dp_2 \times e^{\frac{i}{\hbar}[(x-z)p_1+(z-y)p_2]} A\left(\frac{x+z}{2}, p_1\right) B\left(\frac{z+y}{2}, p_2\right).$$

Equation (51) can be rewritten as

$$C(q, p) = 2^n \int ds\, c(q - s, q + s) \exp \frac{2i}{\hbar} ps.$$

Therefore the Weyl symbol $C(q, p)$ of the operator $C(Q, P)$ has the form

$$C(q, p) = \frac{1}{2^n(\pi\hbar)^{2n}} \int dp_1\ dp_2\, dz\, ds\, A\left(\frac{q - s + z}{2}, p_1\right) \times B\left(\frac{q + s + z}{2}, p_2\right) \exp \frac{i}{\hbar}\big[(q - s - z)p_1 - (q + s - z)p_2 + 2sp\big].$$

Introducing, instead of z and s, the new integration variables

$$q_1 = \frac{1}{2}(q - s + z), \qquad q_1 = \frac{1}{2}(q + s + z),$$

and taking into account the value 2^{-n} of the Jacobian, we obtain

$$C(q, p) = \frac{1}{(2\pi\hbar)^{2n}} \int dp_1\, dp_2\, dq_1\, dq_2\, A(q_1, p_1) \times B(q_2, p_2) \exp \frac{i}{\hbar}\big[(q_1 - q_2)p_1 + (q_1 - q)p_2 + (q_2 - q_1)p\big]. \tag{52}$$

This is the so-called *composition formula for Weyl symbols*. Equation (52) can be rewritten as

$$C(q,\,p)=\left[A\left(q+\frac{i\hbar}{2}\frac{\partial}{\partial p_2},\,p-\frac{i\hbar}{2}\frac{\partial}{\partial q_2}\right)B(q_2,\,p_2)\right]_{q_2=q,\,p_2=p}.$$

Expanding A in this equation into a Taylor series at the point $(q,\,p)$, we obtain the formal equality

$$C(q,\,p)=\sum_{a,b}^{\infty}\frac{(-1)^{|b|}}{a!b!}\left(\frac{i\hbar}{2}\right)^{|a+b|}\big[\partial_q^a\partial_p^b A(q,\,p)\big]\big[\partial_q^b\partial_p^a B(q,\,p)\big],$$

where the sum is taken over all pairs of multi-indices a, b. This equation can be rewritten as

$$C(q,\,p)=\left(\exp\left\{\frac{i\hbar}{2}\mathcal{P}_{12}\right\}\big[A(q_1,\,p_1)B(q_2,\,p_2)\big]\right)_{\substack{q_1=q_2=q\\ p_1=p_2=p}},$$

where

$$\mathcal{P}_{12}=\frac{\partial^2}{\partial q_1\partial p_2}-\frac{\partial^2}{\partial q_2\partial p_1},\qquad \frac{\partial^2}{\partial q\,\partial p}=\sum_{k=1}^{n}\frac{\partial^2}{\partial q_k\partial p_k}.$$

From (50) it follows that the trace of an operator $A(Q,\,P)$ is expressed in terms of the Weyl symbol $A(q,\,p)$ by the equation

$$Tr\big[A(Q,\,P)\big]=\int dx\,a(x,\,x)=\frac{1}{(2\pi\hbar)^n}\int dq\,dp\,A(q,\,p). \tag{53}$$

If we have two Weyl ordered operators $A(Q,\,P)$, $B(Q,\,P)$ with Weyl symbols $A(q,\,p)$, $B(q,\,p)$, then we obtain from (53) the formula

$$(A|B)=Tr[A^*B]=\frac{1}{(2\pi\hbar)^n}\int dq\,dp\,A_*(q,\,p)B(q,\,p),$$

where $A_*(q,\,p)$ is the Weyl symbol of $A^*(Q,\,P)$. The norm $\|A(Q,\,P)\|_2$ of an operator $A(Q,\,P)$ is expressed in terms of its Weyl symbol by the equation

$$\big\|A(Q,\,P)\big\|_2=\frac{1}{(2\pi\hbar)^n}\int dq\,dp\,|A(q,\,p)|^2.$$

We see that $A(Q,\,P)$ is a Hilbert–Schmidt operator if and only if $A(q,\,p)\in L^2(\mathbb{R}^{2n})$.

8.11. Generalization of Weyl quantization

The general form of the quantization map

Let us consider canonical coordinates q, p and the corresponding operators Q, P. For an exponential function of q and p, we can define a correspondence rule in the following general form

$$\pi\left(\exp\frac{i}{\hbar}(aq+bp)\right) = W_F(a,b) = F(a,b)\exp\frac{i}{\hbar}(aQ+bP),$$

where $F(a,b)$ is a function of the auxiliary variables a, b. The function $F(a,b)$ defines the ordering rule.

There exist a natural requirement that must be satisfied by the quantization $\pi : A(q,p) \to A(Q,P)$. This map must be a rule that assigns a self-adjoint operator to each real-valued function. Then

$$F^*(a,b) = F(-a,-b). \tag{54}$$

Note that QP-ordered map has $F(a,b) = \exp(iab/2)$ and requirement (54) is not satisfied. The following are examples of some quantizations.

(1) The Weyl quantization $F(a,b) = 1$.
(2) The Rivier quantization $F(a,b) = \cos(ab/2\hbar)$.
(3) The Born–Jordan quantization $F(a,b) = 2\hbar/(ab)\sin(ab/2\hbar)$.

We can describe the general form of quantization directly. The operator $A_F(Q,P)$ that corresponds to a function $A(q,p)$ is given by the formula

$$A_F(Q,P) = \frac{1}{(2\pi\hbar)^{2n}}\int da\,db\,dq\,dp\,A(q,p)F(a,b) \times \exp\frac{i}{\hbar}\big(a(Q-qI)+b(P-pI)\big).$$

This is a generalization of the Weyl quantization (36).

Basis operators

Consider a set of all self-adjoint operators that are operator functions of Q and P. We can multiply them with scalars, and we can add them together. Thus, they form a linear operator space $\mathcal{M}$. In this case, we must find a complete basis for this operator space. If we have an operator basis, then we can write any operator as a linear combination of the basis. The expansion coefficients are the functions associated with the operators.

All bases always depend on Q, P. Suppose $B(a, b, Q, P)$ is a basis for $\mathcal{M}$. This basis is enumerated by the variables a, b. Then

$$A(Q, P) = \int da\, db\, B(a, b, Q, P) A(a, b),$$

where the expansion coefficients $A(a, b)$ are the associated functions. As a result, we write any operator $A(Q, P)$ as a linear combination of a set of operators $B(a, b, Q, P)$ which form a basis set.

Let $\mathcal{M}^*$ be a set of all linear functionals on $\mathcal{M}$. For any $A \in \mathcal{M}$ and $\beta \in \mathcal{M}^*$, we shall denote by $(\beta|A)$ the value of the functional β at the element A. The pair $\beta(a, b, Q, P) \in \mathcal{M}^*$, $B(a', b', Q, P) \in \mathcal{M}$ is called the biorthogonal system if

$$\big(\beta(a, b, Q, P)|B(a', b', Q, P)\big) = \delta(a - a')\delta(b - b').$$

The basis $\beta(a, b, Q, P)$ is called the *dual basis* of $B(a', b', Q, P)$. In general, the basis $|B(a, b, Q, P))$ must have a dual basis $\beta(a, b, Q, P)$. If there exists the scalar product $(A|B) = Tr[A^*B]$, then $\beta(a, b, Q, P)$ should be defined by an operator $B_\beta(a, b, Q, P) \in \mathcal{M}$ such that

$$Tr\big[B^*_\beta(a, b, Q, P) B(a', b', Q, P)\big] = \delta(a - a')\delta(b - b').$$

Note that

$$Tr[AC] = \int da\, db\, A(a, b) C_*(a, b),$$

where $A, C \in \mathcal{M}$, and

$$A(a, b) = Tr\big[B(a, b, Q, P) A(Q, P)\big],$$
$$C_*(a, b) = Tr\big[B^*_\beta(a, b, Q, P) C(Q, P)\big].$$

As particular examples of the basis $B(a, b, Q, P)$, we have the following operators.

(a) The Weyl basis:

$$B(a, b, Q, P) = \overline{W}(a, b) = \frac{1}{(2\pi\hbar)^{n/2}} \exp \frac{i}{\hbar}(aQ + bP). \tag{55}$$

(b) The Wigner basis

$$\begin{aligned} B(q, p, Q, P) &= \overline{\mathcal{W}}(a, b) \\ &= \frac{1}{(2\pi\hbar)^{n/2}} \int da\, db\, \overline{W}(a, b) \exp \frac{-i}{\hbar}(aq + bp) \\ &= \frac{1}{(2\pi\hbar)^n} \int da\, db\, \exp \frac{i}{\hbar}\big(a(Q - qI) + b(P - pI)\big). \end{aligned}$$

This basis is a Fourier transform of the Weyl basis (55).

(c) The generalized Weyl basis:

$$B(a, b, Q, P) = F(a, b)\overline{W}(a, b).$$

(d) The generalized Wigner basis:

$$\begin{aligned} &B(q, p, Q, P) \\ &\quad = \frac{1}{(2\pi\hbar)^{n/2}} \int da\, db\, \overline{W}(a, b) F(a, b) \exp \frac{-i}{\hbar}(aq + bp) \\ &\quad = \frac{1}{(2\pi\hbar)^{n}} \int da\, db\, F(a, b) \exp \frac{i}{\hbar}\big(a(Q - qI) + b(P - pI)\big). \end{aligned}$$

This basis is a Fourier transform of $\overline{W}(a, b)F(a, b)$.

(e) The Rivier basis is a generalized Weyl basis with the function $F(a, b) = \cos(ab/2\hbar)$, and the Born–Jordan basis is defined by $F(a, b) = (2\hbar/ab)\sin(ab/2\hbar)$.

If $B(a, b, Q, P)$ is a generalized Weyl basis, then

$$B_\beta(a, b, Q, P) = \frac{1}{F(a, b)}\overline{W}(a, b)$$

is dual of $B(a, b, Q, P)$. Then the function $F(a, b)$ should be such that $F(a, b) \neq 0$ for all $a \in \mathbb{R}^n$ and $b \in \mathbb{R}^n$. If $F(a, b) = 0$ for some points $(a, b) \in \mathbb{R}^{2n}$, then the generalized Weyl basis do not lead to a correct basis, since the basis have no dual.

If we introduce new bases, then we can introduce new ordering since each new basis corresponds to a new ordering. However, not all orderings are suitable for the generation of a basis, since we may not be able to construct the dual basis. For example, the Rivier basis is an operator basis such that there is no dual basis due to the zeros in the cosine factor. Another basis which has the same problem is the Born–Jordan basis. Again no dual basis exists because of the zeros in the function $F(a, b)$. As a result, the Rivier and Born–Jordan basis are not correct bases.

As a result, we have a restriction for $F(a, b)$ used in the definition of the generalized Weyl basis. The function $F(a, b)$ can have no zeros on the finite real a, b axis. Each new choice of $F(a, b)$ which satisfies the above conditions will generate a new basis, a new ordering, and a new quantization.

In general, quantum analogs of classical notions are not "covariant". For example, the commutator is just a Poisson bracket in lowest order with respect to $\hbar$. The correction terms of higher order in $\hbar$ depend on the choice of basis and hence are not unique [11]. Of course the higher order terms become unique once an operator basis is chosen. As a result, the correction terms to Poisson brackets are not "covariant" notion. It then makes no sense in the abstract to ask what are the quantum corrections to Poisson brackets without specifying the operator basis.

Wavelets quantization

A wavelet is a kind of function used to divide a given function into different components and study each component with a resolution that matches its scale. The wavelets are scaled and translated copies of a fast-decaying oscillating function (known as the "mother wavelet"). A wavelet transform is the representation of a function by wavelets. In formal terms, this representation is a wavelet series representation of a square integrable function with respect to either a complete, orthonormal set of basis functions for the Hilbert space of square integrable functions. Wavelet transforms have advantages over usual Fourier transforms for representing functions that have discontinuities and sharp peaks.

Let $\Psi(x)$ be a square-integrable function on $\mathbb{R}$, i.e., $\Psi(x) \in L_2(\mathbb{R})$. For $A, B \in L_2(\mathbb{R})$, we use the scalar product

$$(A, B) = \int dx\, A^*(x)B(x).$$

We can define the following two-parameter family of wavelets by using translations and dilations

$$\Psi_{a,b}(x) = |a|^{-1/2}\Psi\left(\frac{x-b}{a}\right),$$

where $a, b \in \mathbb{R}$, and $a \neq 0$. The suggested normalization of $\Psi_{a,b}(x)$ such that

$$\left\|\Psi_{a,b}(x)\right\|_2 = \left\|\Psi(x)\right\|_2,$$

where $\|A(x)\|_2 = \sqrt{(A, A)}$. The functions $\Psi_{a,b}(x)$ are called the *wavelets*, and $\Psi(x)$ is a mother wavelet. For example, the Mexican hat wavelet

$$\Psi(x) = \frac{1}{\sqrt{2\pi}}\left(1 - x^2\right)\exp\left(-x^2/2\right)$$

is the normalized second derivative of a Gauss function.

The continuous wavelet transform is the function

$$T(a, b) = \left(\Psi_{a,b}(x), A(x)\right) = \int_{\mathbb{R}} dx\, \Psi^*_{a,b}(x)A(x)$$

$$= |a|^{-1/2}\int_{\mathbb{R}} dx\, \Psi\left(\frac{x-b}{a}\right)A(x).$$

The magnitude of $T(a, b)$ is called the *scaleogram*. The inverse wavelet transform is defined by

$$A(x) = C_\Psi^{-1}\int_0^\infty \frac{da}{a}\int_{\mathbb{R}} db\, T(a, b)\Psi_{a,b}(x),$$

where C_Ψ is defined by the admissibility condition

$$C_\Psi = 2\pi \int \frac{dy}{|y|} \big|\tilde{\Psi}(y)\big|^2 < \infty.$$

Here $\tilde{\Psi}(y)$ is a Fourier transform of $\Psi(x)$. In many cases, this condition is equivalent to

$$\int dx\, \Psi(x) = 0.$$

If $A \in L_2(\mathbb{R})$, then

$$\int_0^\infty \frac{da}{a^2} \int_{\mathbb{R}} db\, \big|T(a,b)\big|^2 = \int dx\, \big|A(x)\big|^2.$$

Let $\Psi \in L_2(\mathbb{R}^{2n})$ and $\Psi(q,p) = \Psi(q^2+p^2)$,

$$q^2 = q_1^2 + \cdots + q_n^2, \qquad p^2 = p_1^2 + \cdots + p_n^2.$$

Then $\tilde{\Psi}(y) = \tilde{\Psi}(|y|)$, and

$$\Psi_{a,b}(q,p) = |a|^{-n} \Psi\left(\frac{q-b}{a}, \frac{p-b}{a}\right),$$

where $a > 0$, and $b \in \mathbb{R}^{2n}$. If $A(q,p) \in L_2(\mathbb{R}^{2n})$ is a classical observable, then the continuous wavelet transform is the function

$$T(a,b) = \big(\Psi_{a,b}(q,p), A(q,p)\big) = \int_{\mathbb{R}^{2n}} dq\, dp\, \Psi^*_{a,b}(q,p) A(q,p). \tag{56}$$

The inverse wavelet transform for $L_2(\mathbb{R}^{2n})$ is defined by

$$A(q,p) = C_\Psi^{-1} \int_0^\infty \frac{da}{a^{n+1}} \int_{\mathbb{R}^{2n}} db\, T(a,b) \Psi_{a,b}(q,p).$$

The admissibility condition is

$$C_\Psi = (2\pi)^{2n} \int_0^\infty \frac{dy}{y} \big|\tilde{\Psi}(y)\big|^2 < \infty.$$

Let us define a wavelet operator $\Psi(Q,P)$ for $\Psi(q,p)$. For example, the Mexican hat wavelet operator

$$\Psi(Q,P) = \frac{1}{\sqrt{2\pi}} \big(1 - Q^2 - P^2\big) \exp(-1/2)\big(Q^2 + P^2\big).$$

Then we can define the operator

$$A(Q,P) = C_\Psi^{-1} \int_0^\infty \frac{da}{a^{n+1}} \int_{\mathbb{R}^{2n}} db\, T(a,b) \Psi_{a,b}(Q,P), \tag{57}$$

where $T(a,b)$ is defined by (56). Substitution of (56) into (57) gives

$$A(Q,P) = C_\Psi^{-1} \int_0^\infty \frac{da}{a^{n+1}} \int_{\mathbb{R}^{2n}} db \int_{\mathbb{R}^{2n}} dq\, dp\, A(q,p) \Psi_{a,b}^*(q,p) \Psi_{a,b}(Q,P).$$

This equation defines the *wavelet quantization* of $A(q,p)$.

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Chapter 9

Spectral Representation of Observable

9.1. Spectrum of quantum observable

Spectrum of operator

The determination of the eigenvalues and eigenvectors of an operator is important in quantum theory. A linear operator can be considered to act on a ket-vector to change it, usually changing both its magnitude and its direction. An eigenvector of a given operator is a ket-vector which is simply multiplied by a constant called the eigenvalue. The direction of the eigenvector is either unchanged (for positive eigenvalues) or reversed (for negative eigenvalues).

DEFINITION. Let A be a linear operator on a Hilbert space $\mathcal{H}$. An *eigenvalue problem* for A is a determination of nonzero elements $|x>$ of $\mathcal{H}$ and complex numbers z, such that the following equation is satisfied:

$$(zI - A)|x> = 0. \tag{1}$$

In other words, it is necessary to find elements $|x> \in \mathcal{H}$, such that the action of operator A can be reduced to multiplication on number z, i.e., to solve the equation

$$A|x> = |x>z.$$

A nonzero element $|x> \in \mathcal{H}$ satisfied equation (1) is called the *eigenvector* of A. The number $z \in \mathbb{C}$, for which equation (1) has a solution, is called the *eigenvalue* of A.

An example of the eigenvalue problem is the following: Find a function $\Psi(x)$ satisfying

$$\frac{d^2\Psi(x)}{dx^2} = -z\Psi(x), \quad \Psi(0) = \Psi(1) = 0.$$

For most values of z, there is only the solution $\Psi(x) = 0$. If $z = (n\pi)^2$, $n \in \mathbb{N}$, then $\Psi(x) = \sin(\sqrt{z}x)$ is a solution. Moreover, any function satisfying this equation and the boundary conditions can be written as an infinite linear combination of these eigenvectors.

Let A be a linear operator whose domain $D(A)$ and range $R(A)$ both lie in the same Hilbert space $\mathcal{H}$. We consider the linear operator $A(z) = zI - A$, where z is a complex number and I the identity operator. The distribution of the values of z for which $A(z)$ has an inverse and the properties of the inverse when it exists, are called the spectral theory for the operator A.

If z such that the range $R(A(z))$ is dense in $\mathcal{H}$ and $A(z)$ has a bounded inverse $(zI - A)^{-1}$, we say that z is in the *resolvent set* $\rho(A)$ of A. We denote this inverse $(zI - A)^{-1}$ by $R(z, A)$ and call it the *resolvent* of A. All complex numbers z not in $\rho(A)$ form a set $\sigma(A)$ called the *spectrum* of A. Then $\sigma(A) \cup \rho(A) = \mathbb{C}$, and $\sigma(A) \cap \rho(A) = \emptyset$.

The spectrum $\sigma(A)$ is decomposed into the following disjoint sets.

(1) A *point spectrum* $P_\sigma(A)$ of an operator A is a set of eigenvalues of the operator. The point spectrum $P_\sigma(A)$ is a set of $z \in \mathbb{C}$, for which there exists a nonzero solution of the equation $A|x> = |x>z$. *$P_\sigma(A)$ is the totality of complex numbers z for which $A(z)$ does not have an inverse.*

(2) A *continuous spectrum* $C_\sigma(A)$ of an operator A is a set of $z \in \mathbb{C}$, such that the operator $A(z)$ has an unbounded inverse operator

$$R(z, A) = (zI - A)^{-1}$$

with a dense domain of definition. Here the operator $R(z, A)$ is unbounded, and the domain $D(R(z, A))$ does not coincide with entire space $\mathcal{H}$. For finite-dimensional cases, a continuous spectrum is empty. *$C_\sigma(A)$ is the totality of complex numbers z for which $A(z)$ has a unbounded inverse with domain dense in $\mathcal{H}$.*

(3) A *residual spectrum* $R_\sigma(A)$ of an operator A is a set of $z \in \mathbb{C}$, such that the operator $A(z) = zI - A$ has a bounded (or unbounded) inverse operator $R(z, A) = (zI - A)^{-1}$, such that its domain is not dense in $\mathcal{H}$. For many operators, which are used in quantum mechanics, the residual spectrum is empty. For example, self-adjoint operators have only $P_\sigma(A)$ and $C_\sigma(A)$. *$R_\sigma(A)$ is the totality of complex numbers z for which $A(z)$ has an inverse whose domain is not dense in $\mathcal{H}$.*

As a result, we obtain $\sigma(A) = P_\sigma(A) \cup C_\sigma(A) \cup R_\sigma(A)$. A necessary and sufficient condition for $z \in P_\sigma(A)$ is that the equation $A|x> = |x>z$ has a solution $|x> \neq |0>$. In this case, z is called the eigenvalue of A, and $|x>$ the corresponding eigenvector. The null space $N(A(z)) = \{|x> \in D(A(z))\colon\ A(z)|x> = 0\}$ of $A(z)$ is called the *eigenspace* of A corresponding to the eigenvalue z of A. It consists of the ket-vector $|0>$ and the totality of eigenvectors corresponding to z. The dimension of the eigenspace corresponding to z is called the *multiplicity of the eigenvalue z.*

Resolvent and its properties

Let A be a linear operator on a Hilbert space $\mathcal{H}$. We consider the linear operator $A(z) = zI - A$, where z is a complex number and I the identity operator.

DEFINITION. The *resolvent set* of A is the set $\rho(A)$ of all $z \in \mathbb{C}$ such that the range of $A(z) = zI - A$ is dense in $\mathcal{H}$ and $A(z) = zI - A$ has a bounded inverse. For z in the resolvent set $\rho(A)$, the operator

$$R(z, A) = (zI - A)^{-1}$$

is called the *resolvent operator* of A, or *resolvent*.

The resolvent is a family of operators depending on the complex parameter $z \in \rho(A)$. Then $R(z, A)$ is an operator-valued function of the complex variable z defined on $\rho(A) \subset \mathbb{C}$. According to the definition of $\rho(A)$, the resolvent $R(z, A)$ for $z \in \rho(A)$ is a bounded operator with domain dense in $\mathcal{H}$. Let us give the basic theorem regarding resolvents.

THEOREM. *Let A be a bounded (or closed) linear operator. Then the resolvent operators $R(z, A)$ for all z_1 and z_2 in $\rho(A)$ satisfy the following equations*:

(1) *The first resolvent equation*

$$R(z_1, A) - R(z_2, A) = (z_2 - z_1)R(z_1, A)R(z_2, A).$$

(2) *The commutativity equation*

$$R(z_1, A)R(z_2, A) = R(z_2, A)R(z_1, A).$$

The first resolvent equation is also called the Hilbert identity. The resolvent $R(z, A)$ can be considered as a function of A. There exists the second resolvent equation presented by the following theorem.

THEOREM. *Let A and B be operators of a unital Banach algebra. Then resolvent operators $R(z, A)$ and $R(z, B)$ satisfy the second resolvent equation*

$$R(z, A) - R(z, B) = R(z, A)(A - B)R(z, B)$$

for all z in $\rho(A) \cap \rho(B)$.

Let us give the important theorems regarding commuting operators.

THEOREM. *Suppose $\mathcal{M}$ is a Banach algebra with unity, and A, B are in $\mathcal{M}$. Then A commutes with B if and only if the operator A commutes with $R(z, B)$ for all $z \in \rho(B)$.*

This theorem means, that $AB = BA$ if and only if $AR(z, B) = R(z, B)A$ for all $z \in \rho(B)$.

THEOREM. *Suppose $\mathcal{M}$ is a unital Banach algebra, and A, B are in $\mathcal{M}$. Then A and B commute if and only if its resolvents $R(z_1, A)$ and $R(z_2, B)$ commute for all z_1, z_2 in $\rho(A) \cap \rho(B)$.*

This theorem means that $[A, B] = 0$ if and only if $[R(z_1, A), R(z_2, B)] = 0$ for all $z_1, z_2 \in \rho(A) \cap \rho(B)$.

Each resolvent $R(z, A)$ on $\rho(A)$ is an analytic function of z, i.e., there exists an element $R'(z, A)$, such that

$$\lim_{z' \to z} \left\| \frac{R(z', A) - R(z, A)}{z' - z} - R'(z, A) \right\| = 0,$$

where the Hilbert identity gives $R'(z, A) = -R(z, A)^2$.

Spectrum of bounded and self-adjoint operators

It is important to find the smallest r such that $|z| < r$ if $z \in \sigma(A)$.

DEFINITION. A *spectral radius* of a bounded operator A is the real number

$$r(A) = \sup_{z \in \sigma(A)} |z|.$$

We know that $R(z, A)$ is an analytic function when $|z| > r(A)$. Then $R(z, A)$ can be presented as a series.

THEOREM. *If $\mathcal{H}$ is a complex Hilbert space and $A \in \mathcal{B}(\mathcal{H})$, then the resolvent operator is given by*

$$R(z, A) = \sum_{n=1}^{\infty} z^{-n} A^{n-1}$$

if $|z| \geqslant r(A)$. This series also represents $R(z, A)$ if the series converges and $|z| = r(A)$. The series diverges if $|z| < r(A)$.

The following theorem gives a formula for the spectral radius of $A \in \mathcal{B}(\mathcal{H})$.

THEOREM. *If A is a bounded operator on a complex Hilbert space $\mathcal{H}$, then*

$$r(A) = \lim_{n \to \infty} \sqrt[n]{\|A^n\|}.$$

The estimate $r(A) \leqslant \|A\|$ holds.

A linear operator A with domain and range in the Hilbert space $\mathcal{H}$ is said to be *symmetric* if $<x|Ay> = <Ax|y>$ for each x and y in $D(A)$. If A is symmetric, then $<x|Ax>$ is real, even when $\mathcal{H}$ is a complex space. We define

$$m(A) = \inf\{<x|Ax>:\ \|x\|_{\mathcal{H}} = 1\},$$
$$M(A) = \sup\{<x|Ax>:\ \|x\|_{\mathcal{H}} = 1\}.$$

In general, the possibilities $m(A) = -\infty$ and $M(A) = +\infty$ are not excluded.

THEOREM. *If A is a symmetric operator, then all its eigenvalues z are real, and $m(A) \leqslant z \leqslant M(A)$. Eigenvectors corresponding to distinct eigenvalues are orthogonal.*

As a result, there is a complete orthogonal basis, $\{|e_k>\}$, for $\mathcal{H}$ such that $A|e_k> = |e_k>z_k$, and

$$A = \sum_{k=0}^{\infty} z_k |e_k><e_k|.$$

If A is a symmetric operator defined on the whole space $\mathcal{H}$, then A is bounded if and only if $m(A)$ and $M(A)$ are both finite. In this case, $\|A\| = \max\{|m(A)|, |M(A)|\}$. It is easy to see that the norm represents the greatest possible absolute value for the observable.

Spectrum of unbounded operator

Many important operators are unbounded. Consider, for example, the operator $A = -d^2/dx^2$ on the Hilbert space $\mathcal{H} = L^2[0, \pi]$. Let the domain $D(A)$ of the operator A consists of the infinitely differentiable functions $\Psi(x)$ on the closed interval $[0, \pi]$ satisfying the conditions $\Psi(0) = \Psi(\pi) = 0$. Then the functions $\Psi_n(x) = \sin(nx)$, where $n \in \mathbb{N}$, belong to the domain of definition, and

$$A\Psi_n(x) = z_n \Psi_n(x),$$

where $z_n = n^2$. Hence the operator A has arbitrary large eigenvalues, and it is not bounded. Thus the operator on a Hilbert space $\mathcal{H}$ is a linear mapping of some set $D(A)$ of $\mathcal{H}$ into the space $\mathcal{H}$. Therefore in order to define an unbounded operator one must first describe its domain of definition, and then know how it acts on this domain.

HELLINGER–TOEPLITZ THEOREM. *Each self-adjoint linear operator A, which is defined on whole Hilbert space $\mathcal{H}$, is bounded, i.e., if $D(A) = \mathcal{H}$, then A is bounded.*

The Hellinger–Toeplitz theorem says that an everywhere-defined operator A, which satisfies $<Ax|y> = <x|Ay>$, is necessarily a bounded operator. This theorem means that a unbounded operator will only be defined on a subset of the Hilbert space.

In study of unbounded operators the graph of an operator plays an important role.

DEFINITION. The *graph* of a linear operator A on $D(A) \subset \mathcal{H}$ is the set

$$G(A) = \{(\Psi, A\Psi)\colon\ \Psi \in D(A)\} \subset \mathcal{H} \times \mathcal{H}.$$

The graph $G(A)$ of A is also denoted by $graph(A)$.

DEFINITION. Let A be a linear operator on a Hilbert space $\mathcal{H}$. Then A is called the *closed operator* if $graph(A)$ is a closed subset of $\mathcal{H} \times \mathcal{H}$.

If A is a linear unbounded operator, then A is not continuous. In general, the fact $x_k \to x$ does not leads to the existence of a limit for Ax_k. However, many of the unbounded linear operators have a property that in some respects compensates for the absence of the continuity.

STATEMENT. *Suppose A is a linear operator, and $\{x_k\}$ is in $D(A)$. Then A is a closed operator if*

$$\lim_{k\to\infty} \|x_k - x\|_{\mathcal{H}} = 0, \qquad \lim_{k\to\infty} \|Ax_k - Bx\|_{\mathcal{H}} = 0$$

for all $\{x_k\} \subset D(A)$ implies $x \in D(A)$, and $A = B$.

An important set of unbounded operators is a set of operators with bounded resolvents.

THEOREM. *Let A be a self-adjoint operator. Then the following conditions are satisfied*:

(a) *For $z \in \rho(A)$, the resolvent $R(z, A) = (zI - A)^{-1}$ is bounded.*
(b) *The spectrum of A belongs to $\mathbb{R}$.*
(c) *The estimate $\|R(z, A)\| \leqslant [\mathrm{Im}(z)]^{-1}$ is valid for all $z \in \rho(A)$.*
(d) *The resolvent set $\rho(A)$ of A contains $\mathbb{C}_+ \cup \mathbb{C}_- = \{z \in \mathbb{C}\colon\ \mathrm{Im}(z) \neq 0\}$.*

A spectrum of each self-adjoint operator lays on $\mathbb{R}$, a residual spectrum is empty, the upper and lower half-planes are in a resolvent set.

THEOREM. *Suppose A is a closed operator on a Hilbert space $\mathcal{H}$, and z is in $\rho(A)$. Then the resolvent $R(z, A) = (zI - A)^{-1}$ is a bounded operator on $\mathcal{H}$.*

To define convergence of self-adjoint and closed unbounded operators A_k, we use the fact that its resolvents $R(z, A_k)$ are bounded operators.

DEFINITION. Let A_k and A be self-adjoint (or closed) operators. Then A_k is said to converge to A in the *norm resolvent sense* if

$$\lim_{k\to\infty} \| R(z, A_k) - R(z, A) \| = 0$$

for all $z \in \rho(A)$.

The notions of weak and strong resolvent convergences of self-adjoint (and closed) unbounded operators also can be defined. If

$$\lim_{k\to\infty} \| R(z, A_k)x - R(z, A)x \|_{\mathcal{H}} = 0$$

for all $x \in \mathcal{H}$ and $z \in \rho(A)$, then A_k is said to converge to A in the *strong resolvent sense*.

The following theorem shows that norm resolvent convergence is a generalization of norm convergence for bounded operators.

THEOREM. *Let A_k and A be bounded self-adjoint (or closed) operators. Then $A_k \to A$ in the norm resolvent sense if and only if $A_k \to A$ in the norm sense.*

The convergence of resolvents is related with a convergence of other bounded operator functions by the following theorems.

THEOREM. *Let A_k and A be self-adjoint operators. If $A_k \to A$ in the norm resolvent sense and $f(z)$ is a continuous function on $\mathbb{R}$ vanishing at $z \to \infty$, then $f(A_k) \to f(A)$ with respect to operator norm. If $A_k \to A$ in the strong resolvent sense and $f(z)$ is a bounded continuous function on $\mathbb{R}$, then $f(A_k)$ strongly converges to $f(A)$.*

For example, if $A_k \to A$ in the norm resolvent sense, then $\exp(-aA_k)$ converges in norm to $\exp(-aA)$ for each positive a. Suppose A_k and A are self-adjoint operators. Then $A_k \to A$ in the strong resolvent sense if and only if $\exp(iaA_k)$ strongly converges to $\exp(iaA)$ for all $a \in \mathbb{R}$. This statement is called the Trotter theorem.

9.2. Algebra of operator functions

Let A be a bounded operator. Using the polynomial

$$p(z) = \sum_{k=0}^{n} a_k z^k,$$

where $a_k \in \mathbb{C}$, we define the operator polynomial

$$p(A) = \sum_{k=0}^{n} a_k A^k.$$

If $\mathcal{H}$ is a complex Banach space and A is a closed operator with domain and range in $\mathcal{H}$, the fact that the resolvent operator $R(z, A)$ is an analytic function of z enables us to obtain some important results using contour integrals in the complex plane. The completeness of $\mathcal{H}$ (and hence of $\mathcal{B}(\mathcal{H})$) provides the existence of these integrals.

The correspondence $p(z) \leftrightarrow p(A)$ between the polynomials $p(z)$ and the operators $p(A)$ can be presented in the form

$$p(A) = \frac{1}{2\pi i} \oint_{C_A} p(z)(zI - A)^{-1}\, dz, \tag{2}$$

where $z \in \rho(A)$. It can be easy verified that in this way, we obtain the one-to-one correspondence between the polynomials $p(z)$ and the operator polynomials $p(A)$. Equation (2) allows us to extend this correspondence to functions (and operators) of a more general form.

Let $f(z)$ be an analytic function. We now propose to define a certain set of complex-valued analytic functions on $\mathbb{C}$ and to associate with each such function $f(z)$ an operator. The operator associated with $f(z)$ will be denoted by $f(A)$, and is called the *operator function*. To this purpose, we denote by K_A the set of all single-valued functions $f(z)$, which are analytic in some neighborhood of the spectrum $\sigma(A)$. Let $f(z) \in K_A$, and let $\sigma(A)$ be contained inside of the curve C_A. Then the operator $f(A)$ on a Banach space $\mathcal{H}$ will be defined by

$$f(A) = \frac{1}{2\pi i} \oint_{C_A} f(z) R(z, A)\, dz, \tag{3}$$

where $z \in \mathbb{C}$, and $R(z, A) = (zI - A)^{-1}$. This formula gives a correspondence between functions from K_A and operators on $\mathcal{H}$. By Cauchy's integral theorem, the value $f(A)$ depends only on the function $f(z)$ and the operator A, but not on the choice of the contour C_A.

The feature of greatest importance in this association is that this correspondence between $f(z)$, where $z \in \sigma(A)$, and $f(A)$ preserves the basic algebraic operations:

(1) If $f(z) = 1$, then $f(A) = I$.
(2) If $f(z) = a_1 f_1(z) + a_2 f_2(z)$, where $a_1, a_2 \in \mathbb{C}$, then $f(A) = a_1 f_1(A) + a_2 f_2(A)$.
(3) If $f(z) = f_1(z) f_2(z)$, then $f(A) = f_1(A) f_2(A)$.

(4) If $f_k(z) \to f(z)$, then $f_k(A) \to f(A)$.

As a result, we have the following theorem.

DUNFORD'S THEOREM. *Let $f_1(z)$ and $f_2(z)$ be analytic functions on $\sigma(A)$, i.e., $f_1, f_2 \in K_A$, and let a and b be complex numbers. Then functions (af_1+bf_2) and $f_1 f_2$ are analytic on $\sigma(A)$, and for the operators $f_1(A)$ and $f_2(A)$, the following relations are satisfied*:

$$(af_1 + bf_2)(A) = af_1(A) + bf_2(A), \qquad (f_1 f_2)(A) = f_1(A) f_2(A).$$

It is possible to consider the association of $f(A)$ with $f(z)$ as an algebraic homomorphism. But in order to be precise about this, it is necessary to convert K_A into an algebra by an appropriate equivalence relation. We define two functions $f_1(z)$, $f_2(z)$ as being equivalent if $f_1(z) = f_2(z)$ on some open set containing $\sigma(A)$. Then K_A is divided into equivalence classes, and these classes form an operator algebra with a unit element, if we define the algebraic operations in an obvious way.

THEOREM. *The mapping $f(z) \to f(A)$ by equation (3) is an algebraic homomorphism of the algebra of the equivalence classes of K_A into a linear operator algebra $\mathcal{M}$. This mapping transforms the function $f(z) = 1$ into I, and the function $f(z) = z$ into A.*

For example, the function $\exp(az)$ corresponds to the operator $\exp(aA)$.
If $f(z) \in K_A$, then the relation $\sigma(f(A)) = f(\sigma(A))$ holds.

9.3. Spectral projection and spectral decomposition

Spectral projection

We now describe the Riesz projection (the spectral projection), which is an important tool of spectral theory of operators.

Suppose A is a closed operator on a Hilbert space $\mathcal{H}$. Let the spectrum $\sigma(A)$ of A be divided into two nonintersecting closed subsets $\sigma_1(A)$ and $\sigma_2(A)$ with $\Delta = \sigma_1(A)$ compact. Then there exists a continuous piecewise smooth closed contour $C(\Delta)$ on $\mathbb{C}$, such that $C(\Delta)$ does not intersect $\sigma(A)$ and the part of $\sigma(A)$ situated inside $C(\Delta)$ coincides with $\sigma_1(A)$. We will assume that $C(\Delta)$ is oriented counter-clockwise.

DEFINITION. A *spectral projection*, or *Riesz projection*, corresponding to a set Δ of the spectrum $\sigma(A)$ is the operator

$$P_\Delta = \frac{1}{2\pi i} \oint\limits_{C(\Delta)} R(z, A)\, dz,$$

where $R(z, A) = (zI - A)^{-1}$.

Note, that P_Δ does not depend on the choice of $C(\Delta)$ for a given $\Delta = \sigma_1(A)$. Since the resolvent $R(z, A)$ is an analytic operator-valued function in $z \in \mathbb{C}$, it follows that the Riesz projection P_Δ is a bounded linear operator on $\mathcal{H}$. It is not hard to prove that P_Δ is a projection, i.e., $P_\Delta^2 = P_\Delta$ and $P_\Delta^* = P_\Delta$ if $A^* = A$.

THEOREM. *Let A be a self-adjoint operator, and let P_Δ be a Riesz projection corresponding to the compact subset Δ of $\sigma(A)$. If $\theta(z)$ is the characteristic function of Δ, i.e., $\theta(z) = 1$ for $z \in \Delta$ and $\theta(z) = 0$ for $z \notin \Delta$, then $P_\Delta = \theta(A)$.*

For example, if $a, b \in \mathbb{R}/\sigma(A)$ and $\Delta = \sigma(A) \cap (a, b)$, then

$$P_\Delta = \int\limits_a^b P(x)\, dx,$$

where $P(x) = |x><x|$.

Spectral decomposition

Using the Riesz projections, we can realize a decomposition of a self-adjoint operator A that is corresponded to decomposition of $\sigma(A)$ into disjoint subsets.

Suppose $\mathcal{M}$ is a Banach operator algebra and A is in $\mathcal{M}$. A *spectral set* of A is a subset σ of $\sigma(A)$, such that σ is closed in $\mathbb{C}$, and σ is open in $\sigma(A)$.

Let $C(\sigma)$ be a closed contour such that the following requirements are satisfied:

(1) $C(\sigma)$ consists of a finite number closed simple rectifiable curves.
(2) $C(\sigma)$ is in $\rho(A)$.
(3) $C(\sigma)$ encloses an open set D such that $\sigma \subset D$.
(4) $C(\sigma)$ is oriented in positive sense.

The following theorem assigns to each decomposition of $\sigma(A)$ exactly one decomposition of A.

THEOREM. *Let A be a self-adjoint linear operator, and let $\sigma(A)$ be a spectrum of A, such that*

$$\sigma(A) = \bigcup_{k=1}^{m} \sigma_k(A), \tag{4}$$

where $\sigma_k(A)$ are bounded disjoint spectral sets of A, i.e., $\sigma_k(A) \cap \sigma_l(A) = \emptyset$, for $k \neq l$. Then the operators

$$P_k = \frac{1}{2\pi i} \oint_{C_k} R(z, A)\, dz, \tag{5}$$

where C_k is a disjoint contour enclosing the spectral set $\sigma_k(A)$, form a system of orthogonal projections, such that the following equations are satisfied

$$\sum_{k=1}^{m} P_k = I, \qquad P_k P_l = \delta_{kl} P_k.$$

Moreover, the operator A can be presented as

$$A = \sum_{k=1}^{m} A_k,$$

where $A_k = P_k A$ are bounded operators, such that

$$A_k A_l = 0 \ (k \neq l), \qquad \sigma(A_k) = \sigma_k(A) \cup \{0\}.$$

In order to prove this theorem, we consider the function

$$f_k(z) = \begin{cases} 1 & \text{if } z \text{ is inside of } C_k, \\ 0 & \text{if } z \text{ is outside of } C_k. \end{cases}$$

These functions belong to K_A. By the Dunford's theorem, we define the operators

$$P_k = f_k(A) = \frac{1}{2\pi i} \oint_{C} f_k(z) R(z, A)\, dz = \frac{1}{2\pi i} \oint_{C_k} R(z, A)\, dz.$$

The functions $f_k(z)$ satisfy the conditions

$$\sum_{k=1}^{m} f_k(z) = 1, \qquad f_k(z) f_l(z) = \delta_{kl} f_k(z).$$

Then the operators $P_k = f_k(A)$ satisfy equations (5). The projection P_k is a spectral projection that corresponds to the spectral set $\sigma_k(A)$. The set $\{P_k\colon\ k = 1, \ldots, m\}$ of all operators P_k is a decomposition of unity I.

Equation (5) gives $P_k A = A P_k$. Hence, each subspace $\mathcal{H}_k = P_k \mathcal{H}$ of a Banach space $\mathcal{H}$ is invariant with respect to A. A spectrum of the operator $A_k = P_k A$ on $\mathcal{H}_k$ is the spectral set $\sigma_k(A)$. As a result, the Banach space $\mathcal{H}$ is a direct sum of $\mathcal{H}_k$.

9.4. Symmetrical and self-adjoint operators

It is a fact that many of the most important operators which are used in quantum mechanics are not bounded. In general, a unbounded operator is defined on a subset of the Hilbert space.

Let A be a linear (unbounded) operator defined on the domain $D(A)$ of a Hilbert space $\mathcal{H}$ and taking its values in $\mathcal{H}$. $D(A)$ is said to be the *domain* of A and the subset $R(A) = \{A|x>: |x> \in D(A)\}$ of $\mathcal{H}$ is said to be the *range* of A.

DEFINITION. An operator is a triple (D, R, A) consisting of a set $D = D(A)$, a second set $R = R(A)$, and a mapping A from D into R. The set $D(A)$ is called the domain of A, and $R(A)$ the range of A.

A linear operator is said to be *densely defined* if the norm-closure of $D(A)$ in $\mathcal{H}$ coincides with $\mathcal{H}$ itself.

DEFINITION. Let A and B be two linear operators respectively defined on $D(A)$ and $D(B)$ in $\mathcal{H}$. If $D(A)$ is contained in $D(B)$ and $A|x> = B|x>$ for all $|x>$ in $D(A)$, then A is said to be the *restriction* of B to $D(A)$, and B is said to be an *extension* of A to $D(B)$.

The operators A and B are said to be *adjoint to each other* if

$$<x|Ay> = <Bx|y>$$

for all $|y> \in D(A)$ and all $|x> \in D(B)$. If A is densely defined, there exists a *unique* linear operator A^*, called the *adjoint* of A, such that every operator B adjoint to A is the restriction of A^* to some subset $D(B)$ contained in $D(A^*)$.

A bounded operator A on a Hilbert space $\mathcal{H}$ is called symmetric, if $<Ax|y> = <x|Ay>$ for all $x, y \in \mathcal{H}$. However, the most important operators are not bounded, and its are not defined on all of $\mathcal{H}$. A general unbounded operator A can only be defined on a subset $D(A)$ of $\mathcal{H}$. An operator A, which satisfies $<Ax|y> = <x|Ay>$ for all $x, y \in D(A)$ and $D(A)$ is a dense subset of $\mathcal{H}$, is called the symmetric, or Hermitian.

DEFINITION. A linear operator A on a Hilbert space $\mathcal{H}$ is called *symmetric*, if its domain of definition $D(A)$ is dense in $\mathcal{H}$, and $<Ax|y> = <x|Ay>$ for all $x, y \in D(A)$.

Equivalently, the operator A is symmetric if its domain of definition $D(A)$ is dense in $\mathcal{H}$, and $D(A) \subset D(A^*)$. We can conclude from this that a symmetric operator always admits a closure.

STATEMENT. *Let A be a symmetric operator on a Hilbert space $\mathcal{H}$. Then the following conditions are satisfied*:

(1) $D(A)$ *is dense in* $\mathcal{H}$.
(2) $D(A) \subset D(A^*)$.
(3) $A|x> = A^*|x>$ *for all* $|x> \in D(A)$.

For symmetric operators, we have the inclusions $D(A) \subset D(A^{**}) \subset D(A^*)$.

For closed symmetric operators, $D(A) = D(A^{**}) \subset D(A^*)$. A linear operator A is said to be self-adjoint if an addition to being symmetric it satisfies $D(A^*) = D(A)$.

DEFINITION. A *self-adjoint operator* is a symmetric operator A, such that $D(A) = D(A^*)$, i.e., $A^* = A$.

For self-adjoint operators, the following requirements are satisfied:

(1) $D(A)$ is dense in $\mathcal{H}$.
(2) $D(A) = D(A^*)$.
(3) $A|x> = A^*|x>$ for all $|x> \in D(A)$.

If A is a self-adjoint operator, then $D(A) = D(A^{**}) = D(A^*)$.

THEOREM. *A closed symmetric operator A is self-adjoint if and only if A^* is symmetric.*

A bounded symmetric operator is self-adjoint. The distinction between closed symmetric operators and self-adjoint operators is very important. It is only for self-adjoint operators that the spectral theorem holds. It is only self-adjoint operators that may be exponentiated to give the one-parameter unitary group. Each self-adjoint operator has a complete set of eigenvectors. In general, we cannot find a complete set of eigenvectors for arbitrary symmetric operator.

9.5. Resolution of the identity

Let M be a set. A pair $(M, \mathcal{M})$ is called the *σ-algebra*, if $\mathcal{M}$ is a family of subsets of M, such that the following conditions are satisfied:

(1) $\emptyset \in \mathcal{M}$.
(2) If $\Delta_k \in \mathcal{M}$, then $\bigcup_{k=1}^{\infty} \Delta_k \in \mathcal{M}$.
(3) If $\Delta_k \in \mathcal{M}$, then $\bigcap_{k=1}^{\infty} \Delta_k \in \mathcal{M}$.

Suppose $(M, \mathcal{M})$ is a σ-algebra. A *measure* on M is a mapping $\mu : \mathcal{M} \to [0; +\infty)$, such that the following properties are realized:

(1) $\mu(\emptyset) = 0$.
(2) $\mu(M) = 1$.
(3) $\mu(\bigcup_{k=1}^{\infty} \Delta_k) = \sum_{k=1}^{\infty} \mu(\Delta_k)$, if $\Delta_k \cap \Delta_l = \emptyset$ for all $k \neq l$.

DEFINITION. A *spectral measure* is a mapping E from $\mathcal{M}$ into $\mathcal{B}(\mathcal{H})$, such that the following conditions are satisfied:

(1) $E(\Delta)$ is a self-adjoint projection if $\Delta \in \mathcal{M}$.
(2) $E(\emptyset) = 0$, and $E(M) = I$.
(3) $E(\Delta_1 \cap \Delta_2) = E(\Delta_1)E(\Delta_2)$ if $\Delta_1, \Delta_2 \in \mathcal{M}$.
(4) $E(\Delta_1 \cup \Delta_2) = E(\Delta_1) + E(\Delta_2)$, if $\Delta_1 \cap \Delta_2 = \emptyset$.
(5) $\mu(\Delta) = E_{x,y}(\Delta) = <x|E(\Delta)y>$ is a complex measure on M for all $x, y \in \mathcal{H}$.

To every spectral measure on $\mathbb{R}$ there exists a *spectral family* of projections E_z with $z \in \mathbb{R}$. For $\Delta = (-\infty, z]$, we define $E_z = E(z) = E(\Delta)$. This spectral family satisfies the relations:

(1) $E_{z_1} \leqslant E_{z_2}$ for $z_1 < z_2$.
(2) $E_{z+0} = E_z$.
(3) $E_{-\infty} = 0$, and $E_{+\infty} = I$.

If the spectral family is known, the spectral measure can be reconstructed by the equation

$$E(\Delta) = \int_{\Delta} dE_z$$

for any set $\Delta \in \mathcal{M}$. This formula is a short notation for the integral

$$<\Psi|E(\Delta)\Psi> = \int_{-\infty}^{+\infty} \theta(z, \Delta)\, d<\Psi|E_z\Psi> = \int_{\Delta} d<\Psi|E_z\Psi>$$

valid for any $\Psi \in \mathcal{H}$, where $\theta(\Delta) = 1$ for $z \in \Delta$ and $\theta(\Delta) = 0$ for $z \notin \Delta$. If $\Delta = (z_1, z_2]$, then the operator $E(\Delta) = E(z_2) - E(z_1)$ is a spectral measure.

Let $E(z) = E_z$ be a spectral family, and let Ψ an element of $\mathcal{H}$. Then we define the spectral density function

$$\mu_\Psi(z) = <\Psi | E(z)\Psi>.$$

First we list a few properties of any function $\mu(z) = <\Psi | E(z)\Psi>$ which follow directly from the basis properties of the spectral family $E(z)$:

(1) $\mu(z_1) \leqslant \mu(z_2)$ for $z_1 < z_2$.
(2) $\mu(z + 0) = \mu(z)$.
(3) $\mu(-\infty) = 0$.
(4) $\mu(+\infty) = 1$ if $\|\Psi\|_{\mathcal{H}} = 1$.

Let A be a self-adjoint operator. A spectral set of A is a set Δ, such that $\Delta \cap \sigma(A)$ is open in $\mathbb{C}$ and $\Delta \cap \sigma(A)$ is closed in $\sigma(A)$. Suppose $\mathcal{M}$ is a σ-algebra of subsets of $\mathbb{C}$. For each $\Delta \in \mathcal{M}$, we can define the self-adjoint projection

$$E(\Delta) = \frac{1}{2\pi i} \oint_{C(\Delta)} R(z_0, A)\, dz_0,$$

where $C(\Delta)$ is a rectifiable curve enclosing $\Delta \cap \sigma(A)$ such that other points of $\sigma(A)$ are outside of $C(\Delta)$. As a result, the map $\Delta \to E(\Delta)$ is a spectral measure.

The Heaviside step function $\theta(z - \lambda)$ is a characteristic function of the interval $(-\infty; z)$. This function is a discontinuous function whose value is zero for $\lambda \geqslant z$ and one for $\lambda < z$. By Dunford's theorem, we obtain

$$E_z = E(z, A) = \frac{1}{2\pi i} \oint_C \theta(z - \lambda)\, R(\lambda, A)\, d\lambda = \frac{1}{2\pi i} \oint_{C((-\infty; z])} R(\lambda, A)\, d\lambda.$$

The operator E_z can be denoted by $\theta(zI - A)$. Using $\theta(z)\theta(z) = \theta(z)$, $\theta(z)^* = \theta(z)$, and the Dunford's theorem, we obtain

$$E^2(z, A) = E(z, A), \qquad E^*(z, A) = E(z, A).$$

As a result, $E(z, A)$ is a projection.

DEFINITION. A *resolution of the identity* is a set of projections $\{E_z\colon z \in \mathbb{R}\}$, such that the following requirements are satisfied:

(1) $E_{z_1} E_{z_2} = E_{z_2} E_{z_1} = E_{z_1}$ for all $z_1 \leqslant z_2$, i.e., $E(z_1)E(z_2) = E(\min\{z_1, z_2\})$.
(2) E_z is strongly continuous with respect to z at the left, i.e.,

$$\lim_{\varepsilon \to 0+} \|E_{z+\varepsilon} x - E_z x\|_{\mathcal{H}} = 0$$

for all $x \in \mathcal{H}$.

(3) $E_{-\infty} = 0$, and $E_{+\infty} = I$ in the strong operator topology, i.e.,

$$\lim_{z\to-\infty} \|E_z x\|_{\mathcal{H}} = 0, \qquad \lim_{z\to\infty} \|E_z x - x\|_{\mathcal{H}} = 0$$

for all $x \in \mathcal{H}$.

If A is a self-adjoint operator, then the operator $E_z = E(z, A)$ and the resolvent $R(z_0, A)$ are connected by the equations

$$R(z_0, A) = \int_{-\infty}^{+\infty} \frac{1}{z_0 - z}\, dE_z, \qquad E(z, A) = \frac{1}{2\pi i} \oint_{C(\Delta)} R(z_0, A)\, dz_0. \tag{6}$$

Here $C(\Delta)$ is a rectifiable curve that encloses all points of spectrum $\sigma(A)$ from the set $\Delta = (-\infty; z]$, and we have not other points of $\sigma(A)$ inside of $C(\Delta)$.

Let us consider the spectral projection

$$P_\Delta = \frac{1}{2\pi i} \oint_{C(\Delta)} R(z, A)\, dz. \tag{7}$$

Here $C(\Delta)$ is a rectifiable curve that encloses all points of the spectrum $\sigma(A)$ from the set $\Delta \subset \mathbb{R}$. Suppose that $\Delta = (z_1, z_2)$ has an isolated set of $\sigma(A)$ and $z_1, z_2 \notin \sigma(A)$. Let $C(\Delta)$ be a circle, such that the segment $[z_1, z_2]$ is a diameter, and let z be a variable point of the contour $C(\Delta)$. Using (6) and (7), we obtain

$$\begin{aligned} P_\Delta &= \frac{1}{2\pi i} \oint_{C(\Delta)} R(z_0, A)\, dz_0 = \frac{1}{2\pi i} \oint_{C(\Delta)} dz_0 \int_{-\infty}^{+\infty} \frac{1}{z_0 - z}\, dE_z \\ &= \int_{-\infty}^{+\infty} \left(\frac{1}{2\pi i} \oint_{C(\Delta)} \frac{1}{z_0 - z}\, dz_0 \right) dE_x = E_{z_2} - E_{z_1} = E(\Delta), \end{aligned}$$

where

$$\frac{1}{2\pi i} \oint_{C(\Delta)} \frac{1}{z_0 - z}\, dz_0 = \begin{cases} 1 & \text{if } z \text{ is inside of } C(\Delta), \\ 0 & \text{if } z \text{ is outside of } C(\Delta). \end{cases}$$

As a result, $P_\Delta = E(\Delta)$ is a spectral projection.

9.6. Spectral theorem

By the spectral theorem, the eigenvalues and eigenvectors characterize a linear operator in a unique way. In its simplest version, the spectral theorem states that,

under precise conditions, a linear transformation of a ket-vector can be expressed as the linear combination of the eigenvectors. The coefficients are equal to the eigenvalues.

Bounded self-adjoint operator

There exists the following spectral theorem for a self-adjoint operator on a finite-dimensional Hilbert space.

THEOREM. *To every self-adjoint operator A on a finite-dimensional Hilbert space $\mathbb{C}^n$ there corresponds a spectral family of orthogonal projections $E(z_k)$, where $k = 1, 2, \ldots, m \leqslant n$, and $z_1, \ldots, z_m$ are the eigenvalues of the operator A, having the properties*:

(1) $E(z_k) \leqslant E(z_l)$ *if* $z_k \leqslant z_l$.
(2) $E(z_m) = I$, *and* $E(z_0) = 0$.
(3) *Using* $E(z_k)$, *the operator* A *can be represented in the form*

$$A = \sum_{k=1}^{m} z_k \big[E(z_k) - E(z_{k-1})\big].$$

This formula is called the spectral decomposition *of the self-adjoint operator* A *on* $\mathbb{C}^n$.

The simplest generalization of this spectral theorem for finite-dimensional case is its analog for bounded self-adjoint operators.

THEOREM. *Let* A *be a bounded self-adjoint operator on a complex Hilbert space. Then there exists a spectral family of orthogonal projections* $E(z) = E(z, A)$ *defined for each real* z, *with the following properties*:

(a) $E(z_1)E(z_2) = E(z_2)E(z_1)$ *if* $z_1 \leqslant z_2$.
(b) $\lim_{z_1 \to z_2} E_{z_1} = E_{z_2}$.
(c) $E(z) = 0$ *if* $z < m(A)$.
(d) $E(z) = I$ *if* $z \geqslant M(A)$.
(e) $E(z)A = AE(z)$.
(f) *Using* $E(z)$, *the operator* A *is represented in the form*

$$A = \int_a^b z \, dE(z),$$

where $a < m(A)$ *and* $b \geqslant M(A)$.

The family of projections $E(z)$ is unique. Because of this uniqueness, the operator A fully determines the family $E(z)$, and is fully determined by the family. This family of projections is called the *resolution of the identity* corresponding to A.

Unbounded self-adjoint operator

Let A be a unbounded self-adjoint operator whose domain $D(A)$ and range $R(A)$ both lie in the same Hilbert space $\mathcal{H}$.

SPECTRAL THEOREM. *For each self-adjoint linear operator A on a separable Hilbert space $\mathcal{H}$, there exists a resolution of the identity $\{E_z\colon\ z \in \mathbb{R}\}$ such that A can be presented by $E_z = E(z, A)$ in the form*

$$<x|Ay> = \int_{-\infty}^{+\infty} z<x|dE_z y>, \quad y \in D(A). \tag{8}$$

The element $x \in \mathcal{H}$ belongs to $D(A)$ if and only if

$$\|Ax\|_{\mathcal{H}}^2 = \int_{-\infty}^{+\infty} z^2\, d<x|E_z x> < \infty. \tag{9}$$

The integral representation (8) of the self-adjoint operator A with the spectral family $E_z = E(z, A)$ can be presented in the form

$$A = \int_{-\infty}^{+\infty} z\, dE_z.$$

The operator A is bounded if and only if the integral of equation (9) exists for all $x \in \mathcal{H}$. If A is unbounded, then the domain of definition $D(A)$ is given by the set of elements $|x> \in \mathcal{H}$ for which (9) holds.

For unit operator I, we have

$$I = \int_{-\infty}^{+\infty} dE_z.$$

This equation means, that each element $|x>$ of a Hilbert space $\mathcal{H}$ can be presented as

$$|x> = \int_{-\infty}^{+\infty} |z>\, dE_z.$$

Note that this formula is a generalization of the decomposition

$$|x> = \sum_{k=1}^{\infty} |e_k> x_k$$

of an element $|x> \in \mathcal{H}$, where $x_k = <e_k|x>$, and $\{|e_k>\}$ are eigenvectors of a bounded self-adjoint operator.

9.7. Spectral operator through ket-bra operator

Spectral operators through ket-bra operators

The operators $E_z = E(z, A)$ can be defined through the ket-bra operators

$$P(x) = \hat{P}(x, x) = |x><x|.$$

If eigenvalues of a self-adjoint operator A form a discrete set, then we can define the operator

$$E(z, A) = \sum_{k:\, z_k<z} P(e_k) = \sum_{k=1}^{\infty} \theta(z - z_k) P(e_k).$$

Here $\theta(z)$ is a Heaviside step function, such that $\theta(z) = 1$ for $z > 0$ and $\theta(z) = 0$ for $z \leqslant 0$. Then the decomposition

$$A = \sum_{k=1}^{\infty} z_k P(e_k)$$

can be presented as the integral

$$A = \int_{-\infty}^{+\infty} z \, dE_z.$$

In the general case, it is possible to define $E(z, A)$ by the formula

$$E(z, A) = \int_{-\infty}^{z} P(x) \, dx = \int_{-\infty}^{+\infty} \theta(z - x) P(x) \, dx. \tag{10}$$

Differentiation (10) with respect to z gives

$$dE_z = P(z) \, dz.$$

Then

$$E(dz) = dE_z = P(z) \, dz = P(z, z) \, dz = |z> dz <z|.$$

Using (10), the operator $E(\Delta) = E_{z_2} - E_{z_1}$ is of the form

$$E(\Delta) = E(z_2, A) - E(z_1, A) = \int_{-\infty}^{z_2} P(x)\,dx - \int_{-\infty}^{z_1} P(x)\,dx = \int_{z_1}^{z_2} P(x)\,dx.$$

As a result, we obtain

$$E(\Delta) = \int_{z_1}^{z_2} P(x)\,dx.$$

Ket-bra operator through spectral operator

The operator $P(x)$ can be defined by the equation

$$P(x) = \left(\frac{dE_z}{dz}\right)_{z=x}. \tag{11}$$

The condition

$$E(z_1, A)E(z_2, A) = E\big(\min\{z_1, z_2\}, A\big)$$

can be presented in the form

$$E(z_1, A)E(z_2, A) = \theta(z_1 - z_2)E(z_2, A) + \theta(z_2 - z_1)E(z_2, A). \tag{12}$$

Differentiation of (12) with respect to z_1 and z_2 at $z_1 = x$, $z_2 = x'$ gives

$$P(x)P(x') = \delta(x - x')P(x).$$

For each operator $P(x)$, there exists a ket-bra operator $\hat{P}(x, y)$ that is defined by the polarization procedure

$$\hat{P}(x, y) = \frac{1}{4}\sum_{s=0}^{n=3} i^s P(x + i^s y). \tag{13}$$

Substitution of (13) into (11) gives

$$\hat{P}(x, y) = \frac{1}{4}\sum_{s=0}^{n=3} i^s \left(\frac{dE_z}{dz}\right)_{z=x+i^s y}.$$

This equation assigns to each operator $E_z = E(z, A)$ exactly one operator $\hat{P}(x, y)$.

A set of ket-bra operators $\hat{P}(x, y)$ forms an operator basis. Each operator A can be uniquely presented as the decomposition

$$A = \int dx\,dy\,a(x, y)\hat{P}(x, y), \quad a(x, y) = <x|A|y> = Tr\big[\hat{P}(y, x)A\big].$$

If A is a self-adjoint operator, such that $A|x> = |x>z(x)$, then

$$a(x, y) = z(x)\delta(x - y), \qquad A = \int z(x)\, dP(x),$$

where $dP(x) = P(x)\, dx$.

9.8. Function of self-adjoint operator

Bounded self-adjoint operators

We consider an integral of $f(z)$ over z from a to b, where $f(z)$ is an arbitrary complex-valued continuous function defined on the interval $m(A) \leqslant z \leqslant M(A)$. We extend the definition of $f(z)$ by setting $f(z) = f(m(A))$ if $a \leqslant z \leqslant m(A)$, and $f(z) = f(M(A))$ if $b \geqslant z \geqslant M(A)$. There exists a uniquely determined self-adjoint operator, which is denoted by $f(A)$, such that

$$<x|f(A)y> = \int_a^b f(z)\, d<x|E(z)y>$$

for all $x, y \in \mathcal{H}$. We use the following more compact notation

$$f(A) = \int_a^b f(z)\, dE(z). \tag{14}$$

The correspondence between the continuous function $f(z)$ and the operator $f(A)$ induced by this equation has the properties:

(1) $(f + g)(A) = f(A) + g(A)$ and $(af)(A) = af(A)$.
(2) $(fg)(A) = f(A)g(A)$.
(3) $f(A)$ is self-adjoint if $f(z)$ is real-valued.
(4) $f(A)$ is nonnegative if $f(z) \geqslant 0$ for all z.

These properties exhibit a homomorphism of the algebra of continuous functions on $[m(A), M(A)]$ into the algebra $\mathcal{B}(\mathcal{H})$.

The integral (14) is defined by

$$\int_a^b f(z)\, dE_z = \lim_{N\to\infty} \sum_{k=0}^{N} f(z_k)(E_{z_{k+1}} - E_{z_k}), \tag{15}$$

$a \leqslant z_1 \leqslant \cdots \leqslant z_N \leqslant b$, and $z_0 = a$, $z_{N+1} = b$, and

$$E(\Delta_k) = E_{z_{k+1}} - E_{z_k}, \quad \Delta_k = [z_k, z_{k+1}].$$

A definition of the integral (15) can be formulated with respect to the uniform, strong operator and weak operator topologies.

(a) The operators E_z are bounded, and we can define the integral (15) for the measures $\mu(z) = \|E_z\|$ if finite function $f(z)$ is measurable with respect to all measures $\mu(z) = \|E_z\|$.

(b) The limit (15) can be realized in the strong operator topology for $f(z)$ measurable with respect to all measures generated by

$$\mu_x(z) = \mu_{x,x}(z) = E_{x,x}(z) = <x|E_z x> = \|E_z x\|^2_{\mathcal{H}}.$$

(c) The limit (15) can be realized in the weak operator topology for $f(z)$ measurable with respect to all measures generated by

$$\mu_{x,y}(z) = E_{x,y}(z) = <x|E_z y> \quad (z \in \mathbb{R}).$$

Unbounded self-adjoint operators

The spectral decomposition allows us to define a wide class of operator functions. Let $f(z)$ be a bonded function that is measurable with respect to

$$\mu_x(z) = <x|E_z x> = \|E_z x\|^2_{\mathcal{H}},$$

where $x \in \mathcal{H}$. If A is a self-adjoint unbounded operator, then we can define the operator

$$f(A) = \int_{-\infty}^{+\infty} f(z)\, dE_z, \tag{16}$$

where $\{E_z = E(z, A)\colon\ z \in \mathbb{R}\}$ is a spectral resolution of the identity for A. This equation means

$$<x|f(A)x> = \int_{-\infty}^{+\infty} f(z)\, d\|E_z x\|^2_{\mathcal{H}},$$

where $x \in D(f(A))$. The operator $f(A)$ is unbounded. The domain $D(f(A))$ of $f(A)$ is a set of all elements x, such that

$$\int_{-\infty}^{+\infty} \big|f(z)\big|^2\, d\|E_z x\|^2_{\mathcal{H}} < \infty.$$

The set $D(f(A))$ is dense in $\mathcal{H}$.

The following are examples of some operator functions.

(1) If $f(z) = 1$, then $f(A) = I$.

(2) If $f(z) = z$, then $f(A) = A$.
(3) If $f(z)$ is a real-valued function, then $f(A)$ is self-adjoint.
(4) If $f(z)$ is a bounded function, then $f(A)$ is a bounded operator.
(5) If $f(z) = \exp(iz)$, then

$$\exp(iA) = \int_{-\infty}^{+\infty} e^{iz}\, dE_z$$

is a unitary operator.
(6) If $z_0 \in \rho(A)$ and $f(z) = (z_0 - z)^{-1}$, then $f(A) = R(z_0, A)$ is a resolvent, i.e.,

$$R(z_0, A) = \int_{-\infty}^{+\infty} \frac{1}{z_0 - z}\, dE_z.$$

These equations express the resolvent $R(z, A)$ through the operator $E_z = E(z, A)$.
(7) If $f(z) = \theta(z_0 - z)$ is a Heaviside function, then $f(A) = E(z_0, A)$ such that

$$E(z_0, A) = \int_{-\infty}^{+\infty} \theta(z_0 - z)\, dE_z = \int_{-\infty}^{z_0} dE_z.$$

9.9. Commutative and permutable operators

Commutativity of operators is a widely used notion that refers to the ability to change the order of these operators without changing the end result.

DEFINITION. Let A and B be bounded operators on a Hilbert space $\mathcal{H}$. Then A and B are *commutative operators*, if $AB|x> = BA|x>$ for all $|x> \in \mathcal{H}$.

If we accept this definition for all operators, then even a bounded operator A on $\mathcal{H}$ is not commutative with inverse A^{-1}, if A^{-1} is defined on a linear subspace $D(A^{-1})$ of $\mathcal{H}$. In this case, $A^{-1}A|x> = |x>$ for all $|x> \in \mathcal{H}$, that is $A^{-1}A = I$. However the relation $AA^{-1}|x> = |x>$ takes place only for $|x> \in D(A^{-1})$, therefore $AA^{-1} \neq I$. To avoid this inconvenience, we use the following definition.

DEFINITION. A bounded operator A is called *permutable* with an operator B, if the following conditions are satisfied:

(1) $A|x> \in D(B)$ for all $|x> \in D(B)$.

(2) $AB|x> = BA|x>$ for all $|x> \in D(B)$.

These conditions give $D(AB) \subset D(BA)$. Here A is bounded and $D(A) = \mathcal{H}$.

STATEMENT. *Let A be a self-adjoint operator and let B be a bounded operator on a Hilbert space $\mathcal{H}$. Then the operators A and B are permutable if and only if $D(BA) \subset D(AB)$.*

It seems that two unbounded operators A and B can be called permutable, if the following requirements are satisfied:

(1) $A|x> \in D(B)$ for all $|x> \in D(A)$.
(2) $B|x> \in D(A)$ for all $|x> \in D(B)$.
(3) $AB|x> = BA|x>$ for all $|x> \in D(A) \cap D(B)$.

However the intersection of the domains $D(A)$ and $D(B)$ can be empty $D(A) \cap D(B) = \emptyset$. It is possible to avoid this difficulty for unbounded operators that have bounded resolvents. Note that all self-adjoint and closed operators have bounded resolvents. Two self-adjoint operators A and B can be called permutable, if its resolvents $R(z, A)$ and $R(z, A)$ commute.

The resolvents $R(z, A)$ of a self-adjoint operator A are related with the bounded operators $E_z = E(z, A)$ which are used in the resolution of the identity generated by A. It is possible to introduce a permutability for self-adjoint unbounded operators by the spectral projections E_z. For this purpose, we give the following statements.

THEOREM. *A bounded operator B is permutable with a self-adjoint operator A if and only if B commutes with each projection $E(z, A)$ from the spectral family of A.*

COROLLARY. *Bounded self-adjoint operators A and B are permutable if and only if any two projections $E(z, A)$ and $E(z, B)$ from the spectral families of these operators commute.*

For arbitrary unbounded operators it is not clear how to introduce a notion of permutability. However, for self-adjoint operators we can give the following definition.

DEFINITION. Unbounded self-adjoint operators are *permutable* if projections from the spectral families of these operators commute.

If $E(z_1, A)E(z_1, B) = E(z_2, B)E(z_1, A)$ for $z_1 \in \rho(A)$, $z_2 \in \rho(B)$ and $A^* = A$, $B^* = B$, then A and B are permutable.

9.10. Spectral representation

This is a section which reviews the basic facts of spectral representation. For the theory of spectral representations with accurate proof can be found in the book [19].

Let $\mathcal{H} = L^2(\mathbb{R}^n)$ be the space of functions in n real variables that are square integrable with respect to a measure μ. Clearly any multiplication operator by a bounded measurable function commutes with any other multiplication operator by a bounded measurable function. It turns out that the converse statement is also true.

THEOREM. *Any bounded operator A on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n)$ commuting with all multiplication operators by a bounded measurable function is the multiplication operator by a bounded measurable function. If A is self-adjoint, then the function is real-valued.*

Let A be a self-adjoint operator on a Hilbert space $\mathcal{H}$, and let $E(x, A)$ be a spectral family of A. Then a *cyclic vector* for A is an element $|\Psi>$ of $\mathcal{H}$, such that $\{E(x, A)|\Psi>: x \in \mathbb{R}\}$ coincides with $\mathcal{H}$. The cyclic vector is also called the generating vector. There is a generalization of this definition for permutable operators. A cyclic vector for a system of permutable self-adjoint operators $X_1, \ldots, X_n$ is an element $|\Psi>$ of a Hilbert space $\mathcal{H}$, such that

$$\left\{E(x_1, X_1) \ldots E(x_n, X_n)|\Psi>: x_1, \ldots, x_n \in \mathbb{R}\right\} = \mathcal{H}.$$

The vector Ψ is a cyclic for the unbounded operator X, if the set $\{g(X)\Psi: g(x) \in C^\infty(\mathbb{R})\}$ is dense in $\mathcal{H}$. Note that the cyclic vector can be defined by resolvents.

DEFINITION. Let $X_1, \ldots, X_n$ be permutable self-adjoint operators on a Hilbert space $\mathcal{H}$, and $R(x_1, X_1), \ldots, R(x_n, X_n)$ be resolvents of these operators. A ket-vector $|\Psi> \in \mathcal{H}$ is a *cyclic vector* for a system of operators $X_1, \ldots, X_n$, if the minimal closed subspace in $\mathcal{H}$ containing $|\Psi>$ and invariant with respect to all $R(x_1, X_1), \ldots, R(x_n, X_n)$ coincides with $\mathcal{H}$.

The cyclic vector allows us to define a special class of permutable self-adjoint operators.

DEFINITION. A system of permutable self-adjoint operators $X_1, \ldots, X_n$ has *simple joint spectrum* if there exists a cyclic vector for this system. If the system consisting of a single operator X has a cyclic vector, then X is an operator with *simple spectrum*.

Let A be a self-adjoint operator with simple spectrum on a Hilbert space $\mathcal{H}$. There is an isomorphism of $\mathcal{H}$ and $L^2(\mathbb{R})$. Under this isomorphism the operator A corresponds to the operator of multiplication by the variable x. Using this isomorphism it is easy to describe all bounded self-adjoint operators that are permutable with A.

THEOREM. *Let the self-adjoint operator A be the multiplication operator by x on the space $L^2(\mathbb{R})$. Then any bounded operator permutable with A is the multiplication operator by a bounded measurable function. Any self-adjoint operator permutable with A is the multiplication operator by a real-valued measurable function.*

The operator of multiplication by x on the space $L^2(\mathbb{R})$ is an operator with simple spectrum. As a cyclic vector we can take the function identically equal to 1.

Consider a system of permutable operators $X_1, \ldots, X_n$ with simple joint spectrum. Let $E(x_k, X_k)$, $k = 1, \ldots, n$, be a spectral family of these operators, and let $|\Psi>$ be a cyclic vector. We define the measure

$$d\mu(x) = <\Psi | E(x_1, X_1) \cdots E(x_n, X_n)\Psi> \tag{17}$$

where $x \in \mathbb{R}^n$.

THEOREM. *There exists a unique isomorphism between a Hilbert space $\mathcal{H}$ in which self-adjoint operators $X_1, \ldots, X_n$ with simple joint spectrum act and the space $L^2(\mathbb{R}^n)$ with the measure* (17)*, such that the following conditions are satisfied*:

(a) *the cyclic vector $|\Psi> \in \mathcal{H}$ corresponds to the function identically equal to* 1.
(b) *the operator X_k, $k = 1, \ldots, n$, corresponds to the multiplication operator by the variable x_k, which maps $f(x_1, \ldots, x_n) \in L^2(\mathbb{R}^n)$ into $x_k f(x_1, \ldots, x_n)$.*

As a result, we have the following definition of a spectral representation.

DEFINITION. Let $X_1, \ldots, X_n$ be permutable self-adjoint operators on a Hilbert space $\mathcal{H}$. Then there is an isomorphism of $\mathcal{H}$ with the space $L^2(\mathbb{R}^n)$ of complex-valued square-integrable functions on $\mathbb{R}^n$, such that $X_1, \ldots, X_n$ are mapped to multiplication operators by real-valued measurable and almost everywhere finite functions on $\mathbb{R}^n$. This isomorphism from a Hilbert space $\mathcal{H}$ into $L^2(\mathbb{R}^n)$ is called the *spectral representation* or X-representation.

Suppose $X_1, \ldots, X_n$ is a system of permutable self-adjoint operators with simple joint spectrum. In the spectral representation, any bounded operator A permutable with all $X_1, \ldots, X_n$ becomes the multiplication operator by a bounded

measurable function. Any self-adjoint operator A that is permutable with all $X_1, \ldots, X_n$ becomes the multiplication operator by a real-valued measurable function.

Consider a system $X_1, \ldots, X_n$ of permutable self-adjoint operator on a Hilbert space $\mathcal{H}$. Let $E(x_1, X_1), \ldots, E(x_n, X_n)$ be a spectral family of $X_1, \ldots, X_n$, and let $f(x_1, \ldots, x_n)$ be a function in n real variable $x_1, \ldots, x_n$ that is measurable and almost everywhere finite with respect to the measure (17). The operator $f(X_1, \ldots, X_n)$ on $\mathcal{H}$ is the operator that under the realization of $\mathcal{H}$ as the space $L^2(\mathbb{R}^n)$ turns into the multiplication operator by $f(x_1, \ldots, x_n)$. The domain of $f(X_1, \ldots, X_n)$ is the set

$$D\big(f(X_1, \ldots, X_n)\big) = \left\{ |\Psi> \in \mathcal{H}\colon \int\limits_{\mathbb{R}^n} \big|f(x_1, \ldots, x_n)\big|^2 \, d\mu(x) < \infty \right\}.$$

For any $|\Psi_1> \in \mathcal{H}$ and any $|\Psi_2> \in D(f(X_1, \ldots, X_n))$, we have the relation

$$<\Psi_1|f(X_1, \ldots, X_n)\Psi_2> = \int\limits_{\mathbb{R}^n} f(x_1, \ldots, x_n) <\Psi_1|dE(x_1, X_1) \cdots dE(x_n, X_n)|\Psi_2>.$$

This equation is usually expressed more compactly:

$$f(X_1, \ldots, X_n) = \int\limits_{\mathbb{R}^n} f(x_1, \ldots, x_n)\, dE(x_1, X_1) \cdots dE(x_n, X_n).$$

If $f(x_1, \ldots, x_n) = x_k$, then $f(X_1, \ldots, X_n) = X_k$. If $f(x_1, \ldots, x_n)$ is a bounded function, then $f(X_1, \ldots, X_n)$ is a bounded operator. If $f(x_1, \ldots, x_n)$ is a real-valued function, then $f(X_1, \ldots, X_n)$ is self-adjoint.

THEOREM. *Let $X_1, \ldots, X_n$ be permutable self-adjoint operators with a simple joint spectrum. If B is a self-adjoint or bounded operator that is permutable with each of the operators $X_1, \ldots, X_n$, then there exists a function $f(x_1, \ldots, x_n)$, such that $B = f(X_1, \ldots, X_n)$.*

Let A be a self-adjoint operator and let $f(x)$ be a bounded real-valued function. Then the set of all bounded self-adjoint operators $f(A)$ forms an algebra $\mathcal{M}$. This is the algebra generated by A. We denote by $\mathcal{M}'$ the set of all bounded operators which commute with A. Note that the algebra generated by A is then the set $\mathcal{M}'' = \mathcal{M}$. If $\mathcal{M}' = \mathcal{M}$, then the algebra is called *maximal commutative*. There is the following important statement: *The operator A has simple spectrum if the algebra $\mathcal{M}$ is a maximal commutative algebra: $\mathcal{M}' = \mathcal{M}$.*

9.11. Complete system of commuting observables

For one-dimensional quantum system, we need one number to label the basis vectors of a Hilbert space. For a basis ket-vector $|x>$, there exists an operator X, such that $|x>$ is an eigenvector of X. For a quantum system with n degrees of freedom, we need n numbers to enumerate the basis ket-vectors $|x_1, \ldots, x_n>$. A set of all permutable self-adjoint operators $X_1, \ldots, X_n$, such that

$$X_k|x_1, \ldots, x_n> = |x_1, \ldots, x_n>x_k, \tag{18}$$

is called the complete system of commuting observables (CSCO). The eigenvalues $x_1, \ldots, x_n$ of $X_1, \ldots, X_n$ are called the quantum numbers.

A system of permutable self-adjoint operators that specifies the (generalized) basis system completely is called a complete system of commuting observables (CSCO). The (generalized) eigenvalues of a CSCO are *quantum numbers*. For different quantum systems and different algebras of observables we usually have different complete systems of commuting observables. The question of what constitutes a complete system of commuting observables is not a mathematical question but can only be answered by experiment. The physical problem is not to find a CSCO for a given operator algebra, but is usually the reverse. From the experimental data we find out how many quantum numbers are required, and what are the possible values of these quantum numbers. This gives the complete system of commuting observables $\{X_1, \ldots, X_n\}$ and its spectrum.

DEFINITION. A *complete system of commuting observables* (CSCO) is a set of self-adjoint operators $X_1, \ldots, X_n$, such that the following requirements are satisfied:

(1) X_i and X_j are permutable for all i and j.
(2) X_k cannot be presented as a function of $X_1, \ldots, X_{k-1}, X_{k+1}, \ldots, X_n$.
(3) If A is permutable with $X_1, \ldots, X_n$, then there exists a function $f(x_1, \ldots, x_n)$ such that $A = f(X_1, \ldots, X_n)$.

The algebra of observables should have a complete system of commuting observables. The problem of determining for which operator involutive algebra there exists a CSCO is unsolved. The requirement of the existence of a CSCO is a restrictive condition. For certain classes of involutive operator algebras $\mathcal{M}$ there do exist CSCO. For example, if $\mathcal{M}$ is the enveloping algebra of a nilpotent or semisimple group, then complete systems of commuting observables exist.

The question of what is a CSCO for a particular quantum system and the question of when a system of permutable operators is complete are physical questions. If an experiment gives more values than can be supplied by a given system of permutable operators, then this system is not complete. Then one has to introduce

a new quantum number, i.e., enlarge the system of commuting operators. This usually requires a further enlargement of the algebra.

In quantum mechanics, *we must postulate that for the algebra of observables $\mathcal{M}$ for a given quantum system one always has a CSCO*. Thus for the algebra $\mathcal{M}$ there exists a set of permutable operators $X_1, \ldots, X_n$ in $\mathcal{M}$, which have a set of (generalized) eigenvectors $|x_1, \ldots, x_n>$ (see equation (18)), such that every element $|\Psi>$ in $\mathcal{H}$ can be represented as

$$|\Psi> = \int d\mu(x_1, \ldots, x_n)|x_1, \ldots, x_n><x_1, \ldots, x_n|\Psi>.$$

This means that the conditions of the spectral theorem are fulfilled. Here the set $\{x_1, \ldots, x_n\}$ is the spectrum of the CSCO $X_1, \ldots, X_n$ with x_k in the spectrum $\sigma(X_k)$ of the observable X_k.

All infinite-dimensional separable Hilbert spaces are isomorphic to each other. Then each Hilbert space can be described as an abstract Hilbert space. However, it is often convenient to use the Hilbert space $L^2(\mathbb{R}^n)$. It is similar to use a coordinate frame instead of general (vector) forms of description. If CSCO is defined, then a Hilbert space $\mathcal{H}$ can be realized as a space of functions $\Psi(x_1, \ldots, x_n) = <x_1, \ldots, x_n|\Psi>$ with the scalar product,

$$<\Psi_1|\Psi_2> = \int\limits_{\mathbb{R}^n} \Psi^*(x_1, \ldots, x_n)\Psi(x_1, \ldots, x_n)\, d\mu(x_1, \ldots, x_n),$$

where $\mu(x_1, \ldots, x_n)$ is a measure. Then $X_1, \ldots, X_n$ are the multiplication operators

$$X_k\Psi(x_1, \ldots, x_n) = x_k\Psi(x_1, \ldots, x_n).$$

This is the *X-representation*. This realization of $\mathcal{H}$ by $L^2(\mathbb{R}^n)$ is also called the *spectral representation* that is generated by CSCO. As a result, the Hilbert space $\mathcal{H}$ is a space of functions on a spectrum of commuting observables.

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PART II

QUANTUM DYNAMICS

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Chapter 10

Superoperators and its Properties

10.1. Mathematical structures in quantum dynamics

Until now we have not mentioned time and have completely ignored the time evolution of the state of a system and the time development of an observable. We have restricted ourselves to properties of systems defined at one instant. In general, one should specify not only the physical values obtained in a measurement but also the time at which the observation is made. In this part we consider the time evolution—the dynamics—of quantum systems. We make the assumption that time is a continuous real parameter t that labels sequences of states and observables. That is, we make the idealizing assumption that observables and states can be defined at a succession of arbitrary small time interval, and that at any instant of time the specification of a complete set of observables is possible.

To formulate quantum kinematics the mathematical language of operator algebra and functional analysis was considered. Quantum dynamics, too, has its mathematical language. This is the language of superoperators, operator differential equations, one-parameter semi-groups, etc. Although one might obtain some understanding of quantum dynamics without knowing its mathematical language, the precise and deep meaning of the physical notions in their full generality cannot be achieved without using its mathematical structures. Modern mathematics distinguishes three basic kinds of structures: algebraic, topological, and ordering. The mathematical structures of quantum dynamics are complicated combinations of these three.

Dynamical structure and differential equations

Quantum mechanics consists essentially of two physical structures, a kinematical structure describing the initial states and observables of the system, and a dynamical structure describing the evolution of these states and observables with time. The observables and states can be given by operators. The dynamical structures are given by maps of the underlying kinematical structure, which represents the evolution of the system with time.

In the physical theories, the dynamical structure can be introduced by the differential equations, which represent the evolution of the observables $A \in \mathcal{M}$ and states $\rho \in \mathcal{S}$ with time. These differential equations will be presented in the form of $E_{\mathcal{S}}(\rho) = 0$ and $E_{\mathcal{M}}(A) = 0$. In quantum theory, we can restricted ourselves to these linear operator differential equations with

$$E_{\mathcal{S}} = d/dt - \Lambda_t, \qquad E_{\mathcal{M}} = d/dt - \mathcal{L}_t,$$

where Λ_t is called the *Liouville superoperator*, and $\mathcal{L}_t$ is the *Heisenberg superoperator*. These equations, as a rule, are subjected to some fundamental principles, which have geometrical, algebraic, or analytic nature. These principles determine mathematical structures of dynamics.

POSTULATE *(Dynamical structure).* A dynamical structure $\mathcal{D}_{eq}$ is a dynamical set D_{eq}, together with mathematical structures on D_{eq}.

(1) D_{eq} is a totality $D_{eq} = (D_M, D_S, D_B)$ of the following sets:
  (1.1) D_M is a set of all equations $E_{\mathcal{M}}(A) = 0$ for $A \in \mathcal{M}$. The solutions of these equations are interpreted as a time evolution of observables.
  (1.2) D_S is a set of all equations $E_{\mathcal{S}}(\rho) = 0$ for $\rho \in \mathcal{S}$. The solutions of these equations are interpreted as a time evolution of states.
  (1.3) D_B is a set of all equations $E_{\mathcal{B}}[(\rho|A)] = 0$ for expectation values $(\rho|A) \in B$. The solutions of these equations are interpreted as a time evolution of expectation values.
(2) The given dynamical set $D_{eq} = (D_M, D_S, D_B)$ is equipped with mathematical structures.

A kinematical structure describes the instantaneous states and observables of the system. Then it can be considered as a set of all initial conditions for equations of motion. As a result, the time evolution of the kinematical structure $\mathcal{K}$ is a map from a kinematical set K into K_t. The set K_t is a totality of all solutions $K_t = Sol\{E_{\mathcal{M}}, E_{\mathcal{S}}, E_{\mathcal{B}}\}$.

In the conventional formulations of quantum theories the dynamical structure is introduced by the linear operator differential equation

$$\frac{dA_t}{dt} = \mathcal{L}_t A_t \tag{1}$$

under a variety of conditions and assumptions. In each example, the operator A_t describes an observable, or state, of the quantum system and will be represented by an element of some suitable operator space, or algebra, $\mathcal{M}$. The map $t \in \mathbb{R} \to A_t \in \mathcal{M}$ describes the motion of A, and $\mathcal{L}_t$ is a superoperator on $\mathcal{M}$, which generates the infinitesimal change of A. A superoperator is a map from a set of operators into itself. The derivative $dA(t)/dt$ is understood to be the limit, in the norm of the space $\mathcal{M}$, of the difference quotient $\tau^{-1}[A(t+\tau) - A(t)]$ as $\tau \to 0$.

The dynamics can be defined by solution of the operator differential equation. The existence of a sensible, non-catastrophic, time development of the system is equivalent to the existence of global solutions of the equation of motion satisfying the initial conditions.

A Cauchy problem is the problem of finding a solution A_t of equation (1) in which the initial condition is given by $A_0 \in \mathcal{M}$ at the time t_0.

We say that the Cauchy problem is correctly formulated if the following conditions are satisfied:

(1) The unique solution A_t of the Cauchy problem exists for arbitrary A_0 belongs to the domain $D(\mathcal{L})$ of definition of $\mathcal{L}$.
(2) This solution depends continuously on initial conditions in the sense that if A_k tend to 0, then for the corresponding solutions $A_k(t)$ of (1) it follows that $A_k(t) \to 0$.

If the Cauchy problem for equation (1), in which the initial condition is given by $A_0 \in D(\mathcal{L})$, is correctly formulated, then its solution can be presented by the formula

$$A(t) = \Phi(t, t_0)A_0,$$

where $\Phi(t, t_0)$ is a superoperator.

Dynamical structure and dynamical maps

Let us denote by A_0 the observable of a system that is defined at the time $t = t_0$. We then expect that A_0 will uniquely determine another observable A_t at any later time $t > t_0$. During the evolution the system may be subjected to external influences, so that the manner of evolution will depend explicitly upon the interval from t_0 to t.

Our understanding of the time evolution suggests that we can impose the following requirements on the map $\Phi(t, t_0) : A_0 \to A_t$.

(1) $\Phi(t, t_0)$ is a transformation of the set $\mathcal{M}$ of observables, satisfying the initial condition

$$\Phi(t_0, t_0) : A_0 \to A_0. \tag{2}$$

(2) If $\Phi(t_1, t_0)$ and $\Phi(t, t_1)$ are maps with

$$\Phi(t_1, t_0) : A_0 \to A_1, \qquad \Phi(t, t_1) : A_1 \to A_t,$$

where $0 < t_0 < t_1 < t$, then there is a natural transformation $\Phi(t, t_0)$ mapping A_0 into A_t satisfying the following composition law

$$\Phi(t, t_1)\Phi(t_1, t_0) = \Phi(t, t_0). \tag{3}$$

The map $\Phi(t, t_0)$ is said to be a *dynamical map* of a physical system if the described conditions are satisfied.

Requirement (1) is intuitively obvious. Requirement (2) means that the evolution of the observable in the time interval (t_0, t) can be constructed by evolution in the two intervals (t_0, t_1) and (t_1, t), where t_1 is an arbitrary time point between t_0 and t. In general, an evolution process is called the *Markov process* if it satisfies condition (3). The time development of an observable is a Markov process.

In the mathematical terminology, equations (2), (3) are a statement of the fact that the time evolution form a two-parameter semi-group.

That the time evolution of an observable defined by operator differential equation (1) with $\mathcal{L}_t = \mathcal{L}$ is Markovian is a consequence of the fact that this equation is first order with respect to t.

Let $\mathcal{M}$ be a set of quantum observables. An evolution $\Phi(t, t_0)$ from a set $\mathcal{M}$ into itself is a surjection (is onto $\mathcal{M}$) since each element A_t of $\mathcal{M}$ has at least one element A_0 of $\mathcal{M}$ evolved into it. To show that $\Phi(t, t_0)$ is a surjection, we can show that for each A_t, there exists A_0 such that $\Phi(t, t_0)A_0 = A_t$. In general, the evolution $\Phi(t, t_0)$ is not an injection (a one-to-one map). To show that $\Phi(t, t_0)$ is injection, you show that $A_t = B_t$ implies $A_0 = B_0$. In the general case, the evolution cannot be considered as an automorphism (isomorphism with itself) of the kinematical structure.

POSTULATE *(Dynamical structure).* A dynamical structure $\mathcal{D}_{map}$ is a set D_{map} of all dynamical maps on a kinematical structure, together with mathematical structures on D_{map}.

(1) A dynamical set D_{map} is a totality $(\Phi_{\mathcal{M}}, \Phi_{\mathcal{S}}, \Phi_{\mathcal{B}}, T)$ of the following sets.
  (1.1) $\Phi_{\mathcal{M}}$ is a set of all dynamical maps on $\mathcal{M}$. The element of $\Phi_{\mathcal{M}}$ is interpreted as an evolution of observable $A \in \mathcal{M}$.
  (1.2) $\Phi_{\mathcal{S}}$ is a set of all dynamical maps on $\mathcal{S}$. The element of $\Phi_{\mathcal{S}}$ is interpreted as an evolution of state $\rho \in \mathcal{S}$.
  (1.3) $\Phi_{\mathcal{B}}$ is a set of all dynamical maps on $\mathcal{B}$. The element of $\Phi_{\mathcal{B}}$ is interpreted as an evolution of measured numerical value $(\rho|A) \in \mathcal{B}$.
  (1.4) T is a set of all possible instants of time.
(2) Mathematical structures are defined on the given dynamical set $D_{map} = (\Phi_{\mathcal{M}}, \Phi_{\mathcal{S}}, \Phi_{\mathcal{B}}, T)$.

A map $\Phi(t, t_0)$ is said to be temporarily homogeneous if $\Phi(t, t_0)$ is a function of $t - t_0$ only. In this case, equation (3) takes the form $\Phi_t \Phi_s = \Phi_{t+s}$, where $\Phi_t = \Phi(t + t_0, t_0)$. This equation is intuitively obvious. It is a statement of the fact that letting an observable evolve first for a period of length s and then letting the resultant observable evolve for a period of length t leads to the same result as letting the original observable evolve for a period of length $t + s$.

In general, dynamical maps $\Phi(t, t_0)$ on a kinematical structure $\mathcal{K}$ cannot be considered as endomorphisms. For non-Hamiltonian systems, there exist A and B such that

$$\Phi(t, t_0)g(A, B) \neq g\big(\Phi(t, t_0)A, \Phi(t, t_0)B\big), \tag{4}$$

where $g(\cdot,\cdot)$ is a binary operation. This inequality is satisfied for associative, Lie and Jordan algebras in the theory of non-Hamiltonian and dissipative systems. We have an equality in (4) for Hamiltonian systems. The evolution of such systems is a group of automorphisms of the underlying kinematical structure. In non-Hamiltonian dynamics, the time evolution cannot be considered as an endomorphism of an operator algebra. In general, the evolution of non-Hamiltonian and dissipative systems is not an endomorphism of a linear space, since these exist strange attractors that cannot be considered as the linear spaces. It is possible to generalize a kinematical structure such that it will be "invariant" with respect to time evolution. In general, the conservation ("invariance") of algebraic structures for dissipative and non-Hamiltonian systems is an open question. The "noninvariant" kinematical set can be considered only as a set of all possible initial and boundary conditions for equations of motion and dynamical maps.

This is a chapter which reviews the basic facts of superoperator on operator spaces.

10.2. Definition of superoperator

Quantum theories consist essentially of two parts, a kinematical structure describing the initial states and observables of the system, and a dynamical structure describing the change of these states and observables with time. In the quantum mechanics the states and observables are given by operators. The dynamical description of the system is given by a superoperator, which is a map from a set of operators into itself.

Let $\mathcal{M}$ be an operator space. We shall denote by $\mathcal{M}^*$ the dual space of $\mathcal{M}$. Thus $\mathcal{M}^*$ is the set of all linear functionals on $\mathcal{M}$. The classic notations to denote an element of $\mathcal{M}$ are $|B)$ and B. The symbols $(A|$ and ω denote the elements of $\mathcal{M}^*$. By the Riesz–Fréchet theorem, any linear continuous (with respect to the norm $\|\ \|$) functional on a Liouville space $\mathcal{M}$ has the form $\omega(B) = (A|B)$ for all $B \in \mathcal{M}$, where $|A)$ is an element from $\mathcal{M}$. Therefore the element A can be considered not only as an element $|A)$ of $\mathcal{M}$, but also as an element $(A|$ of the dual space $\mathcal{M}^*$. The symbol $(A|B)$ for a value of the functional $(A|$ on the operator $|B)$ is the graphic junction of the symbols $(A|$ and $|B)$.

DEFINITION. Let $\mathcal{M}$ be a set of operators. A *superoperator* on $\mathcal{M}$ is a mapping $\mathcal{L}$ from $\mathcal{M}$ into itself. In other words, a superoperator $\mathcal{L}$ is a rule that assigns to each operator A exactly one operator $\mathcal{L}(A)$.

A superoperator may be pictured as a "black box" that generates an operator at the output in response to an operator at the input. It is said that a superoperator applied to an operator generates a new operator.

The superoperator $\mathcal{L}:\mathcal{M}_1 \to \mathcal{M}_2$ will mean that $\mathcal{L}$ is a single-valued mapping whose domain is $\mathcal{M}_1$ and whose range is contained in $\mathcal{M}_2$. For every operator $A \in \mathcal{M}_1$, the superoperator $\mathcal{L}$ assigns a uniquely determined operator $\mathcal{L}(A) \in \mathcal{M}_2$. Let $\mathcal{L}$ be a linear superoperator whose domain $D(\mathcal{L})$ and range $R(\mathcal{L})$ both lie in the same linear operator space $\mathcal{M}$.

DEFINITION. A *linear superoperator* is a mapping $\mathcal{L}$ from an operator space $\mathcal{M}$ into itself, such that the following requirements are satisfied:

(1) $\mathcal{L}(A+B) = \mathcal{L}(A) + \mathcal{L}(B)$ for all $A, B \in D(\mathcal{L}) \subset \mathcal{M}$.
(2) $\mathcal{L}(aA) = a\mathcal{L}(A)$ for all $A \in D(\mathcal{L}) \subset \mathcal{M}$ and $a \in \mathbb{C}$.

DEFINITION. Let $\mathcal{L}$ be a superoperator on $\mathcal{M}$. An *adjoint superoperator* of $\mathcal{L}$ is a superoperator $\bar{\mathcal{L}}$ on $\mathcal{M}^*$, such that

$$\big(\bar{\mathcal{L}}(A)|B\big) = \big(A|\mathcal{L}(B)\big)$$

for all $B \in D(\mathcal{L}) \subset \mathcal{M}$ and some $A \in D(\bar{\mathcal{L}}) \subset \mathcal{M}^*$.

An adjoint superoperator is also called the *dual* or *conjugate superoperator*. If we use the notation $\omega \in \mathcal{M}^*$, then

$$\bar{\mathcal{L}}\omega(A) = \omega\big(\mathcal{L}(A)\big), \qquad (\bar{\mathcal{L}}\omega|A) = (\omega|\mathcal{L}A).$$

Let $\mathcal{M}$ be a Liouville space and let $\mathcal{L}$ be a superoperator on $\mathcal{M}$. Then $(A|B) = Tr[A^*B]$, and a superoperator $\bar{\mathcal{L}}$ on $\mathcal{M}^*$ is adjoint of $\mathcal{L}$ if

$$Tr\big[\big(\bar{\mathcal{L}}(A)\big)^* B\big] = Tr\big[A^*\mathcal{L}(B)\big].$$

If there exists an isomorphism between $\mathcal{M}$ and $\mathcal{M}^*$, then we can define the symmetric and self-adjoint superoperators. Suppose $\mathcal{M}$ is an operator Hilbert space. Then by the Riesz–Fréchet theorem, $\mathcal{M}$ and $\mathcal{M}^*$ are isomorphic.

DEFINITION. Let $\mathcal{M}$ be an operator Hilbert space. A *symmetric superoperator* is a superoperator $\mathcal{L}$ on $\mathcal{M}$, such that

$$\big(\mathcal{L}(A)|B\big) = \big(A|\mathcal{L}(B)\big)$$

for all $A, B \in D(\mathcal{L}) \subset \mathcal{M}$.

DEFINITION. A *self-adjoint superoperator* is a superoperator $\mathcal{L}$ on a Hilbert operator space $\mathcal{M}$, such that the following requirements are satisfied:

(1) $\mathcal{L}$ is a symmetric superoperator.
(2) $D(\mathcal{L}) = D(\bar{\mathcal{L}})$.

Let $\mathcal{M}$ be a normed operator space. The most important is the class of bounded superoperators, which are naturally defined on the whole $\mathcal{M}$. The superoperator $\mathcal{L}$ is called bounded if $\|\mathcal{L}(A)\|_{\mathcal{M}} \leqslant c\|A\|_{\mathcal{M}}$ for some constant c and all $A \in \mathcal{M}$. Geometrically this means that $\mathcal{L}$ transforms norm bounded sets of $\mathcal{M}$ into the norm bounded sets. The least value of c, equal to

$$\|\mathcal{L}\| = \sup_{A \neq 0} \frac{\|\mathcal{L}(A)\|_{\mathcal{M}}}{\|A\|_{\mathcal{M}}}, \tag{5}$$

is called the *norm of the superoperator* $\mathcal{L}$. If $\mathcal{M}$ is a normed space, and $\mathcal{L}$ is a bounded superoperator, then $\|\bar{\mathcal{L}}\| = \|\mathcal{L}\|$.

In quantum theory, the most important is the class of real superoperators.

DEFINITION. Let $\mathcal{M}$ be an operator space, and let A^* be adjoint of $A \in \mathcal{M}$. A *real superoperator* is a superoperator $\mathcal{L}$ on $\mathcal{M}$, such that

$$\big[\mathcal{L}(A)\big]^* = \mathcal{L}(A^*)$$

for all $A \in D(\mathcal{L}) \subset \mathcal{M}$ and $A^* \in D(\mathcal{L})$.

If $\mathcal{L}$ is a real superoperator, then $\bar{\mathcal{L}}$ is real. If $\mathcal{L}$ is a real superoperator and A is a self-adjoint operator $A^* = A \in D(\mathcal{L})$, then the operator $B = \mathcal{L}(A)$ is self-adjoint, i.e., $B^* = [\mathcal{L}(A)]^* = \mathcal{L}(A) = B$. Let $\mathcal{M}$ be a set of observables. Then superoperators from $\mathcal{M}$ into itself should be real. All possible dynamics, i.e., temporal evolutions of quantum observables, must be described by a set of real superoperators.

In quantum mechanics, the class of positive (nonnegative) superoperators is very important.

DEFINITION. A *nonnegative superoperator* is a mapping $\mathcal{L}$ from $\mathcal{M}$ into $\mathcal{M}$, such that $\mathcal{L}(A^2) \geqslant 0$ for all $A^2 = A^*A \in D(\mathcal{L}) \subset \mathcal{M}$. A *positive superoperator* is a mapping $\mathcal{L}$ from $\mathcal{M}$ into itself, such that $\mathcal{L}$ is nonnegative and $\mathcal{L}(A) = 0$ if and only if $A = 0$.

A density operator is a positive (nonnegative) self-adjoint operator ρ with unit trace. The density operators represent quantum states. If $\mathcal{L}$ is a positive superoperator, then $\mathcal{L}(\rho)$ is a positive operator.

DEFINITION. A bounded linear superoperator $\mathcal{U}$ on a Hilbert operator space $\mathcal{M}$ is called (bounded) *isometric* if $\mathcal{U}$ leaves the scalar product invariant: $(\mathcal{U}A|\mathcal{U}B) = (A|B)$ for all $A, B \in \mathcal{M}$. If, in particular, $R(\mathcal{U}) = \mathcal{M}$, then a (bounded) isometric operator $\mathcal{U}$ is called a *unitary superoperator*.

It is conventional to describe symmetries of quantum systems by unitary superoperators on some kinematical set.

10.3. Left and right superoperators

Let $\mathcal{M}$ be an operator algebra. For $A \in \mathcal{M}$, let L_A be the mapping of $\mathcal{M}$ into $\mathcal{M}$ given by $L_A C = AC$ for $C \in \mathcal{M}$. We can think of L_A as meaning left multiplication by A.

DEFINITION. Suppose $\mathcal{M}$ is an operator algebra and A is in $\mathcal{M}$. A *left superoperator*, which is corresponded to $A \in \mathcal{M}$, is a superoperator L_A on $\mathcal{M}$ such that

$$L_A C = AC$$

for all $C \in D(L_A)$. Here $D(L_A) = \{C \in \mathcal{M}\colon\ AC \in \mathcal{M}\}$ is a domain of superoperators L_A. A *right superoperator*, which is corresponded to $A \in \mathcal{M}$, is a superoperator R_A on $\mathcal{M}$ such that

$$R_A C = CA$$

for all $C \in D(R_A)$, where $D(R_A) = \{C \in \mathcal{M}\colon\ CA \in \mathcal{M}\}$.

Superoperators L_A and R_B can be denoted by A^l and B^r. The following properties of L_A and R_A are satisfied.

(1) If $A \in \mathcal{M}$ is a linear operator, then L_A and R_A are linear superoperators.

(2) For $A, B \in \mathcal{M}$, we can define the products $L_A L_B$, $L_A R_B$, $R_A L_B$, $R_A R_B$ as the superoperators such that

$$\begin{aligned}
(L_A L_B)C &= L_A(L_B C) = A(BC),\\
(L_A R_B)C &= L_A(R_B C) = A(CB),\\
(R_A L_B)C &= R_A(L_B C) = (BC)A,\\
(R_A R_B)C &= R_A(R_B C) = (CB)A
\end{aligned}$$

for $C \in \mathcal{M}$. These multiplications are associative operations:

$$\begin{aligned}
(L_A L_B)L_C &= L_A(L_B L_C), \quad (R_A R_B)R_C = R_A(R_B R_C),\\
(L_A L_B)R_C &= L_A(L_B R_C), \quad (R_A R_B)L_C = R_A(R_B L_C),\\
(L_A R_B)R_C &= L_A(R_B R_C), \quad (R_A L_B)L_C = R_A(L_B L_C)
\end{aligned}$$

for $A, B, C \in \mathcal{M}$. Note that there equations are satisfied for each nonassociative algebra $\mathcal{M}$.

(3) If $A, B \in \mathcal{M}$ and $(A, C, B) = 0$ for all $C \in \mathcal{M}$, then the superoperators L_A and R_B are commutative

$$L_A R_B = R_B L_A.$$

In general, this statement is valid for each nonassociative operator algebra $\mathcal{M}$.

(4) If $A, B \in \mathcal{M}$ and $AB = BA$, then the superoperators L_A and L_B are commutative

$$L_A L_B = L_B L_A$$

on $D(L_A) \cap D(L_B)$, and $R_A R_B = R_B R_A$. In general, $\mathcal{M}$ need not be commutative. This statement is satisfied for noncommutative algebra $\mathcal{M}$. Suppose $\mathcal{M}$ is a commutative algebra. Then $AB = BA$ for all $A, B \in \mathcal{M}$, and

$$L_A = R_A \tag{6}$$

for all $A \in \mathcal{M}$.

If $\mathcal{M}$ is an anticommutative algebra, then $AB = -BA$ for all $A, B \in \mathcal{M}$, and $L_A = -R_A$ for all $A \in \mathcal{M}$.

(5) Let $\mathcal{M}$ be a nonassociative operator algebra. If $A, B \in \mathcal{M}$, and

$$(A, B, C) = 0, \quad (A, C, B) = 0, \quad (B, A, C) = 0,$$
$$(B, C, A) = 0, \quad (C, A, B) = 0, \quad (C, B, A) = 0$$

for all $C \in \mathcal{M}$, then these relations give

$$L_{AB} - L_A L_B = 0, \quad R_B L_A - L_A R_B = 0, \quad L_{BA} - L_B L_A = 0,$$
$$R_A L_B - L_B R_A = 0, \quad R_B R_A - R_{AB} = 0, \quad R_A R_B - R_{BA} = 0.$$

This statement is satisfied for all elements of an associative algebra $\mathcal{M}$.

(6) Let $\mathcal{M}$ be an associative operator algebra. Then

$$L_{AB} = L_A L_B, \quad R_{AB} = R_B R_A, \quad L_A R_B = R_B L_A$$

for all $A, B \in \mathcal{M}$.

(7) Let $\mathcal{M}$ be an involutive algebra. An involution on $\mathcal{M}$ is a map of $A \in \mathcal{M}$ into $A^* \in \mathcal{M}$ adjoint of A. We define the superoperator J on $\mathcal{M}$ by

$$JA = A^*$$

for all $A \in \mathcal{M}$. This superoperator is called the *involution superoperator*. The following conditions are satisfied:

$$J(aA + bB) = a^* J(A) + b^* J(B), \quad J\big(J(A)\big) = A,$$
$$J(AB) = J(B)J(A)$$

for all $A, B \in \mathcal{M}$ and $a, b \in \mathbb{C}$.

Let us define the superoperators L_A^* and R_A^* by setting

$$L_A^* = JL_AJ, \quad R_A^* = JR_AJ.$$

These equations give

$$L_A^*C = JL_AJC = JL_AC^* = JAC^* = (AC^*)^* = CA^* = R_{A^*}C,$$
$$R_A^*C = JR_AJC = JR_AC^* = JC^*A = (C^*A)^* = A^*C = L_{A^*}C$$

for all $C \in \mathcal{M}$. As a result, we obtain

$$L_A^* = JL_AJ = R_{A^*}, \qquad R_A^* = JR_AJ = L_{A^*}.$$

Let $\mathcal{M}$ be an associative algebra. For all $A, B \in \mathcal{M}$, we have the equation

$$(L_AL_B)^* = L_A^*L_B^*,$$

which can be proved by

$$(L_AL_B)^* = (L_{AB})^* = R_{(AB)^*} = R_{B^*A^*} = R_{A^*}R_{B^*} = L_A^*L_B^*.$$

Analogously, we obtain the equation $(R_AR_B)^* = R_A^*R_B^*$. Note, that we have $L_A^*L_B^*$ instead of $L_B^*L_A^*$ as for usual operators ($(AB)^* = B^*A^*$). In general, $L_A^*L_B^* \neq L_B^*L_A^*$. Also, we have $R_A^*R_B^*$ instead of $R_B^*R_A^*$.

(8) If $\mathcal{M}$ is a unital Banach algebra, then it is easy to prove that

$$\|L_A\| = \|R_A\| = \|A\|_{\mathcal{M}},$$

and

$$\sigma(L_A) = \sigma(R_A) = \sigma(A).$$

(9) Let $\mathcal{M}$ be a Liouville space. If $\mathcal{M}$ is also an operator algebra, then

$$(L_AB|C) = (B|L_{A^*}C) + Tr\big[(B^*, A^*, C)\big].$$

This equation can be proved by the following transformations

$$\begin{aligned}(L_AB|C) &= Tr\big[(L_AB)^*C\big] = Tr\big[(AB)^*C\big] = Tr\big[(B^*A^*)C\big] \\ &= Tr\big[B^*(A^*C) + (B^*A^*)C - B^*(A^*C)\big] \\ &= Tr\big[B^*(L_{A^*}C) + (B^*, A^*, C)\big] \\ &= (B|L_{A^*}C) + Tr\big[(B^*, A^*, C)\big].\end{aligned}$$

The following corollaries follow immediately from this equation.

(a) Let $\mathcal{M}$ be a Liouville space, and let $A \in \mathcal{M}$ be a self-adjoint operator. If $\mathcal{M}$ is an associative operator algebra, then the superoperators L_A and R_A on $\mathcal{M}$ are self-adjoint ($\bar{L}_A = L_A$, $\bar{R}_A = R_A$) on a dense set $D(L_A) \cap D(R_A)$:

$$(L_AB|C) = (B|L_AC), \qquad (R_AB|C) = (B|R_AC).$$

(b) Let $\mathcal{M}$ be a nonassociative operator algebra such that

$$Tr\big[(A, B, C)\big] = 0$$

for all $A, B, C \in \mathcal{M}$. If $A \in \mathcal{M}$ is a self-adjoint operator, then the superoperators L_A and R_A on $\mathcal{M}$ are self-adjoint ($\bar{L}_A = L_A$, $\bar{R}_A = R_A$), i.e.,

$$(L_A B|C) = (B|L_A C), \qquad (R_A B|C) = (B|R_A C).$$

As an example, we can consider a nonassociative Jordan algebra $\mathcal{M}^{(+)}$. Using

$$(A \circ B) \circ C - A \circ (B \circ C) = \frac{1}{4}\big[B, [A, C]\big],$$

we obtain

$$Tr\big[(A, B, C)\big] = Tr\big[(A \circ B) \circ C - A \circ (B \circ C)\big] = \frac{1}{4}\, Tr\big[B, [A, C]\big] = 0,$$

where $A \circ B = (1/2)(AB + BA)$, and $[A, B] = AB - BA$.

10.4. Superoperator kernel

Kernels of superoperators

Let $|x> = |e_x>$ be an orthonormal basis of a Hilbert space $\mathcal{H}$, such that

$$<x|y> = \delta(x - y), \qquad \int dx |x><x| = I.$$

Then the ket-bra operators $\hat{P}(x, y) = |x><y|$ on $\mathcal{H}$ form the orthonormal basis $|xy) = |\hat{P}(x, y))$ of the associated Hilbert space $\bar{\mathcal{H}}$, such that

$$(xy|x'y') = \delta(x, x')\delta(y', y), \qquad \int dx\, dy\, |xy><xy| = L_I, \tag{7}$$

where L_I is an identity superoperator. For each element $|A)$ of $\bar{\mathcal{H}}$, we have

$$|A) = \int dx\, dy\, |xy)(xy|A), \tag{8}$$

where $(xy|A) = <x|A|y> = a(x, y)$ is a kernel of A. This is the X-representation of the operator A.

A superoperator $\mathcal{L}$ on $\bar{\mathcal{H}}$ is a map that assigns to each operator $|A)$ of $D(\mathcal{L}) \subset \bar{\mathcal{H}}$ exactly one operator $|B) = |\mathcal{L}A)$. The classic notation to denote the operator B is $\mathcal{L}(A)$, and we have

$$\mathcal{L}|A) = |\mathcal{L}A)$$

for all $|A) \in \mathcal{D}(\mathcal{L}) \subset \bar{\mathcal{H}}$. Let us consider the kernel

$$b(x, y) = <x|B|y> = <x|\mathcal{L}(A)|y> = \big(xy|\mathcal{L}(A)\big) = (xy|\mathcal{L}|A)$$

of the operator $B = \mathcal{L}(A)$. If we substitute the identity superoperator L_I into $(xy|\mathcal{L}|A)$, we have

$$b(x, y) = (xy|\mathcal{L}|A) = (xy|\mathcal{L}L_I|A) = \int dx'\, dy'\, (xy|\mathcal{L}|x'y')(x'y'|A).$$

As a result, we obtain

$$b(x, y) = \int dx'\, dy'\, \mathcal{L}(x, y, x', y')a(x', y'),$$

where $a(x', y') = <x'|A|y'> = (xy|A)$ is a kernel of A, and $b(x, y) = <x|\mathcal{L}(A)|y> = (xy|\mathcal{L}A)$ is a kernel of $B = \mathcal{L}A$. The function $\mathcal{L}(x, y, x', y')$ can be considered as a kernel of superoperator $\mathcal{L}$ in X-representation.

DEFINITION. A *kernel of superoperator* $\mathcal{L}$ in X-representation is the function

$$\mathcal{L}(x, y, x', y') = (xy|\mathcal{L}|x'y') = \big(xy|\mathcal{L}\big(\hat{P}(x', y')\big)\big), \tag{9}$$

that is defined by the equation

$$\mathcal{L}(x, y, x', y') = \big(\hat{P}(x, y)|\mathcal{L}\big(\hat{P}(x', y')\big)\big) = Tr\big[\hat{P}(x, y)\mathcal{L}\big(\hat{P}(x', y')\big)\big].$$

As a result, the superoperator $\mathcal{L}$ can be presented as an integral operator with a kernel $\mathcal{L}(x, y, x', y')$, and $\mathcal{L}$ transforms a kernel $a(x, y)$ of A by the equation

$$(xy|\mathcal{L}|A) = \int dx'\, dy'\, \mathcal{L}(x, y, x', y')a(x', y').$$

Examples of superoperator kernels

We illustrate the superoperator kernels

$$\mathcal{L}(x, x', y, y') = (xx'|\mathcal{L}|yy') = Tr\big[\hat{P}(x, x')\mathcal{L}\big(\hat{P}(y, y')\big)\big] \tag{10}$$

with the following examples.

(1) Let $\mathcal{M}$ be an associative operator algebra, and let L_A be a left superoperator on $\mathcal{M}$, such that

$$L_A|C) = |AC).$$

The kernel $L_A(x, x', y, y')$ of the left superoperator L_A is

$$L_A(x, x', y, y') = a(x, y)\delta(y' - x'), \tag{11}$$

where $a(x, y)$ is a kernel of A. To prove this equation, we use (10).

$$\begin{aligned} L_A(x, x', y, y') &= (xx'|L_A|yy') = \big(\hat{P}(x, x')|A\hat{P}(y, y')\big) \\ &= Tr\big[\hat{P}(x', x)A\hat{P}(y, y')\big] = Tr\big[\hat{P}(y, y')\hat{P}(x', x)A\big] \\ &= \delta(y' - x')\, Tr\big[\hat{P}(y, x)A\big] \\ &= \delta(y' - x')(xy|A) = a(x, y)\delta(y' - x'). \end{aligned}$$

Here we use the relations $Tr[ABC] = Tr[CAB]$, and

$$\hat{P}(y, y')\hat{P}(x', x) = \delta(y' - x')\hat{P}(y, x).$$

(2) Let R_A be a right superoperator on $\mathcal{M}$. Using (10), we have

$$\begin{aligned} R_A(x, x', y, y') &= (xx'|R_A|yy') = \big(\hat{P}(x, x')|\hat{P}(y, y')A\big) \\ &= Tr\big[\hat{P}(x', x)\hat{P}(y, y')A\big] = \delta(x - y)\, Tr\big[\hat{P}(x', y')A\big] \\ &= \delta(x - y)(y'x'|A) = a(y', x')\delta(x - y). \end{aligned}$$

As a result, the kernel $R_A(x, x', y, y')$ of the superoperator R_A is

$$R_A(x, x', y, y') = a(y', x')\delta(x - y). \tag{12}$$

(3) Let us consider the superoperator

$$L_H^- = \frac{1}{i\hbar}(L_H - R_H).$$

The kernel $L_H^-(x, x', y, y')$ of L_H^- is

$$L_H^-(x, x', y, y') = (xx'|L_H^-|yy') = \frac{1}{i\hbar}\big[(xx'|L_H|yy') - (xx'|R_H|yy')\big].$$

Then

$$L_H^-(x, x', y, y') = \frac{1}{i\hbar}\big(L_H(x, x', y, y') - R_H(x, x', y, y')\big).$$

Using (11) and (12), we obtain

$$L_H^-(x, x', y, y') = \frac{1}{i\hbar}\big(h(x, y)\delta(y' - x') - h(y', x')\delta(x - y)\big),$$

where $h(x, y) = <x|H|y>$ is a kernel of H.

(4) Let us consider the superoperator

$$L_A^+ = \frac{1}{2}(L_A + R_A).$$

It is not hard to prove the following equation

$$L_H^-(x, x', y, y') = \frac{1}{2}\big(a(x, y)\delta(y' - x') + a(y', x')\delta(x - y)\big),$$

where $a(x, y) = <x|A|y>$ is a kernel of A.

(5) Let $\mathcal{L}$, $\mathcal{L}_1$ and $\mathcal{L}_2$ be superoperators on an associative operator algebra $\mathcal{M}$. If $\mathcal{L} = \mathcal{L}_1\mathcal{L}_2$, then

$$(xy|\mathcal{L}|x'y') = (xy|\mathcal{L}_1\mathcal{L}_2|x'y') = \int dx''\, dy''\, (xy|\mathcal{L}_1|x''y'')(x''y''|\mathcal{L}_2|x'y').$$

As an example, we consider the superoperator $\mathcal{L} = L_A R_B(L_C - R_C)$. The kernel $\mathcal{L}(x, x', y, y')$ of this superoperator is

$$\mathcal{L}(x, x', y, y') = \int dz \left(a(x, z)c(z, y)b(y', x') - a(x, y)c(y', z)b(z, x')\right),$$

where $a(x, y) = <x|A|y>$, $c(x, y) = <x|C|y>$, and $b(x, y) = <x|B|y>$.

10.5. Closed and resolvent superoperators

For the purposes of applications to quantum mechanics it is important to consider some linear superoperators that are not continuous. Many of the most important discontinuous superoperators have a property that in some respects compensates for the absence of the property of continuity.

DEFINITION. A *closed superoperator* is a superoperator $\mathcal{L}$ on a Banach operator space $\mathcal{M}$, such that the conditions

$$\lim_{k\to\infty} \|A_k x - Ax\|_{\mathcal{H}} = 0, \qquad \lim_{k\to\infty} \|\mathcal{L}A_k x - Bx\|_{\mathcal{H}} = 0,$$

where all $A_k \in D(\mathcal{L})$, imply $A \in D(\mathcal{L})$, $B = \mathcal{L}A$.

Thus the notion of a closed superoperator is an extension of the notion of a bounded superoperator. It is obvious that a bounded superoperator is closed.

THEOREM. *A self-adjoint superoperator is closed. The inverse $\mathcal{L}^{-1}$ of a closed linear superoperator $\mathcal{L}$ on $D(\mathcal{L})$, if it exists, is closed.*

Let $\mathcal{L}$ be a linear superoperator whose domain $D(\mathcal{L})$ and range $R(\mathcal{L})$ both lie in the same operator Banach space $\mathcal{M}$. We consider the linear superoperator $\mathcal{L}(z) = zL_I - \mathcal{L}$, where z is a complex number and L_I the identity superoperator. If z is such that the range $R(\mathcal{L}(z))$ is dense in $\mathcal{M}$ and $\mathcal{L}(z)$ has a continuous inverse $(zL_I - \mathcal{L})^{-1}$, we say that z is in the *resolvent set* $\rho(\mathcal{L})$ of $\mathcal{L}$. We denote this inverse by

$$R(z, \mathcal{L}) = (zL_I - \mathcal{L})^{-1},$$

and call it the *resolvent superoperator*, or *resolvent of* $\mathcal{L}$. All complex numbers z not in $\rho(\mathcal{L})$ form a set $\sigma(\mathcal{L})$ called the *spectrum* of $\mathcal{L}$. Note that $\sigma(L_A) = \sigma(R_A) = \sigma(A)$.

THEOREM. *Let $\mathcal{L}$ be a closed superoperator with its domain $D(\mathcal{L})$ and range $R(\mathcal{L})$ both lie in the same operator Banach space $\mathcal{M}$. Then the resolvent $R(z, \mathcal{L}) = (zL_I - \mathcal{L})^{-1}$ is a bounded superoperator for any $z \in \rho(\mathcal{L})$.*

As a result, the resolvent is an everywhere defined superoperator such that $\|R(z, \mathcal{L})\| \leqslant C(z)$, where $C(z)$ is a constant for each $z \in \rho(\mathcal{L})$. If $\mathcal{L}$ is a self-adjoint superoperator on a Hilbert operator space $\mathcal{M}$, then $C(z) = 1/\operatorname{Im}(z)$.

THEOREM. *Let $\mathcal{L}$ be a closed superoperator and z_k $(k = 1, 2)$ both belong to $\rho(\mathcal{L})$, then the resolvent superoperator equation holds*:

$$R(z_1, \mathcal{L}) - R(z_2, \mathcal{L}) = (z_2 - z_1)\, R(z_1, \mathcal{L})\, R(z_2, \mathcal{L}).$$

Using the bounded resolvents of closed and self-adjoint superoperators, we can define generalized (resolvent) norm convergence for a unbounded closed and self-adjoint superoperators.

DEFINITION. Let $\mathcal{L}_k$, $k = 1, 2, \ldots$, and $\mathcal{L}$ be self-adjoint superoperators. Then $\mathcal{L}_k$ is said to *converge to $\mathcal{L}$ in the norm resolvent sense* if

$$\lim_{k\to\infty} \big\| R(z, \mathcal{L}_k) - R(z, \mathcal{L}) \big\| = 0$$

for all z with $\operatorname{Im}(z) \neq 0$.

The notions of weak and strong resolvent convergences of self-adjoint (and closed) unbounded superoperators also can be defined.

10.6. Superoperator of derivation

DEFINITION. A *superoperator of derivation*, or *derivation*, is a superoperator $\mathcal{L}$ on an operator algebra $\mathcal{M}$, such that the following requirements are satisfied:

(1) $\mathcal{L}(aA + bB) = a\mathcal{L}(A) + b\mathcal{L}(B)$ for all $A, B \in \mathcal{D}(\mathcal{L}) \subset \mathcal{M}$, and $a, b \in \mathbb{C}$.
(2) $\mathcal{L}(AB) = (\mathcal{L}A)B + A(\mathcal{L}B)$ for all $A, B \in \mathcal{D}(\mathcal{L}) \subset \mathcal{M}$.

A derivation is a linear superoperator such that the Leibnitz rule $\mathcal{L}(AB) = (\mathcal{L}A)B + A(\mathcal{L}B)$ is satisfied for all operators A and B in $\mathcal{D}(\mathcal{L}) \subset \mathcal{M}$. The operator

$$Z_{\mathcal{L}}(A, B) = \mathcal{L}(AB) - \mathcal{L}(A)B - A\mathcal{L}(B)$$

is called the *Leibnitz defect* of $\mathcal{L}$ at A and B in $\mathcal{D}(\mathcal{L}) \subset \mathcal{M}$. The Leibnitz defect of a superoperator $\mathcal{L}$ shows how much the deviation of $\mathcal{L}$ from a derivation superoperator. If $\mathcal{M}$ is an involutive algebra, then $Z_{\mathcal{L}}(A^*, A)$ is called the *dissipative function*. It is not hard to prove the following statement.

STATEMENT. *The Leibnitz defect $Z_{\mathcal{L}}$ determines $\mathcal{L}$ up to a locally Hamiltonian superoperator.*

A derivation is a linear map $\mathcal{L}$ of an operator algebra $\mathcal{M}$ into itself such that $Z_{\mathcal{L}}$ are equal to zero on $\mathcal{D}(\mathcal{L}) \subset \mathcal{M}$. Let the set of all derivations on $\mathcal{M}$ be $Der(\mathcal{M})$. The following properties are satisfied:

(a) If $\mathcal{L}_1, \mathcal{L}_2 \in Der(\mathcal{M})$, then $\mathcal{L}_1 + \mathcal{L}_2 \in Der(\mathcal{M})$.
(b) If $\mathcal{L} \in Der(\mathcal{M})$ and $a \in \mathbb{R}$, then $a\mathcal{L} \in Der(\mathcal{M})$.
(c) The binary operation $(\mathcal{L}_1\mathcal{L}_2)A = \mathcal{L}_1(\mathcal{L}_2 A)$ is associative: $(\mathcal{L}_1\mathcal{L}_2)\mathcal{L}_3 = \mathcal{L}_1(\mathcal{L}_2\mathcal{L}_3)$ for all $\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3 \in Der(\mathcal{M})$.
(d) The Lie multiplication $\mathcal{L}_1 \cdot \mathcal{L}_2 = \mathcal{L}_1\mathcal{L}_2 - \mathcal{L}_2\mathcal{L}_1$ of $\mathcal{L}_1, \mathcal{L}_2 \in Der(\mathcal{M})$ is a derivation.

DEFINITION. Let $\mathcal{M}$ be an involutive algebra. A *symmetric derivation*, or *self-adjoint derivation*, is a linear superoperator $\mathcal{L}$ on $\mathcal{M}$, such that the following requirements are satisfied:

(1) $D(\mathcal{L})$ is an involutive subalgebra of $\mathcal{M}$.
(2) $\mathcal{L}(AB) = (\mathcal{L}A)B + A(\mathcal{L}B)$ for all $A, B \in D(\mathcal{L})$.
(3) $(\mathcal{L}A)^* = \mathcal{L}(A^*)$ for all $A \in \mathcal{D}(\mathcal{L})$.

Requirement (1) express the mathematical statement that the domain $D(\mathcal{L})$ is closed with respect to multiplication and involution. In short, if $A, B \in D(\mathcal{L})$, then $AB \in D(\mathcal{L})$ and $A^* \in D(\mathcal{L})$. Requirements (2) and (3) mean that a symmetric derivation is a real superoperator.

Associative operator algebra

Suppose $\mathcal{M}$ is an associative operator algebra, and A is in $\mathcal{M}$. Then we define the superoperator $\mathcal{L}_H = L_H - R_H$. This superoperator is a derivation. It is called the inner derivation of $\mathcal{M}$ determined by H.

DEFINITION. A derivation $\mathcal{L}$ of $\mathcal{M}$ is said to be *inner* if there exists H in $\mathcal{M}$ such that

$$\mathcal{L}A = HA - AH$$

for all A in $\mathcal{M}$, otherwise $\mathcal{L}$ is said to be *outer*.

Let $Inn(\mathcal{M})$ be a set of all inner derivations on $\mathcal{M}$. We shall denote the linear space of all outer derivations on $\mathcal{M}$ by $Out(\mathcal{M})$. Then $Out(\mathcal{M}) = Der(\mathcal{M})/Inn(\mathcal{M})$.

Consider now an associative algebra $\mathcal{P}$ generated by finite linear combinations and finite powers of the elements Q and P, where $QP - PQ = I$.

THEOREM. *All the derivations of $\mathcal{P}$ are inner.*

Though $\mathcal{P}$ itself does not admit outer derivations, there are a number of important subalgebras of $\mathcal{P}$ which do admit them. It is not hard to prove that the subalgebras of $\mathcal{P}$ formed by the linear span of the sets $\{I, Q, P, Q^2, P^2, QP\}$ and $\{I, Q^{k+1}, Q^k P\colon k \geqslant 0\}$ have outer derivation given by

$$\mathcal{L}\big(Q^k P^l\big) = \frac{a}{2}(2-k-l)Q^k P^l + \frac{a}{2}\big[Q^k, P^l\big]$$

with $l = 1, 2$. The subalgebras of $\mathcal{P}$ defined as the linear span of the set $\{I, Q^k P^l + P^l Q^k\colon k, l \in \mathbb{N}\}$ has outer derivation given by

$$\mathcal{L}\big(Q^k P^l + P^l Q^k\big) = \frac{a}{2}(2-k-l)\big(Q^k P^l + P^l Q^k\big).$$

Let $\mathcal{M}$ be an associative operator algebra. The set of all derivations $Der(\mathcal{M})$ of an associative algebra $\mathcal{M}$ form a Lie algebra under the multiplication $\mathcal{L}_1 \cdot \mathcal{L}_2 = \mathcal{L}_1\mathcal{L}_2 - \mathcal{L}_2\mathcal{L}_1$. The set of inner derivations forms an ideal in $Der(\mathcal{M})$. An ideal is a special kind of subalgebra. If $\mathcal{M}_0$ is an ideal, and $A \in \mathcal{M}_0$, then $A \cdot B \in \mathcal{M}_0$ for any $B \in \mathcal{M}$.

Jordan operator algebra

If $\mathcal{M}$ is a Jordan operator algebra and $H \in \mathcal{M}$, then $L_H^+ A = H \circ A$ for all $A \in \mathcal{M}$. The Jordan left multiplication L_H^+ is not a derivation. Using $L_H^+ = R_H^+$, we obtain $\mathcal{L}_H = L_H^+ - R_H^+ = 0$. Then $\mathcal{L}_H$ is not a derivation.

Let $\mathcal{M}$ be an associative algebra, and let $\mathcal{M}^{(+)}$ be a special Jordan algebra. A superoperator $\mathcal{L}$ on $\mathcal{M}^{(+)}$ is a derivation of a Jordan algebra $\mathcal{M}^{(+)}$ if

$$\mathcal{L}(A \circ B) - \mathcal{L}(A) \circ B - A \circ \mathcal{L}(B) = 0$$

for $A, B \in \mathcal{M}$. The superoperator $\mathcal{L}_H = L_H - R_H$ on $\mathcal{M}$ is a derivation for $\mathcal{M}^{(+)}$.

The next statement gives some features of special Jordan algebras $\mathcal{M}^{(+)}$.

STATEMENT. *All the derivation superoperators on an associative algebra $\mathcal{M}$ are derivations on the corresponding special Jordan algebra $\mathcal{M}^{(+)}$.*

This is easy to show by using $A \circ B = (1/2)(AB + BA)$.

Lie operator algebra

If $\mathcal{M}$ is a Lie operator algebra and $H \in \mathcal{M}$, then the left multiplication by H, i.e., the superoperator $\mathcal{L}_H = L_H^-$, is a derivation of $\mathcal{M}$. This is the *Lie left multiplication* L_H^-. If $A, B \in \mathcal{M}$, then by using the Jacobi identity and the anticommutative

law, we obtain

$$\mathcal{L}_H(A \cdot B) = A \cdot (\mathcal{L}_H B) - (\mathcal{L}_H A) \cdot B.$$

The derivation $\mathcal{L}_H$ is an inner derivation of the Lie algebra determined by H. As a result, Lie left multiplication is an inner derivation of Lie algebra.

Using $L_H^- = -R_H^-$, we see that $\mathcal{L}_H = L_H^-$ can be define by the relation

$$\mathcal{L}_H = \frac{1}{2}(L_H^- - R_H^-).$$

As a result, this superoperator is an inner derivation on Lie algebra $\mathcal{M}$.

The set of all derivations $Der(\mathcal{M})$ of a Lie algebra $\mathcal{M}$ form a Lie algebra under the Lie multiplication $\mathcal{L}_A \cdot \mathcal{L}_B = \mathcal{L}_A\mathcal{L}_B - \mathcal{L}_B\mathcal{L}_A$.

A mapping $H \to \mathcal{L}_H$, is a homomorphism from a Lie algebra $\mathcal{M}$ into a Lie algebra $Inn(\mathcal{M})$. It is not hard to prove the properties

$$\mathcal{L}_{(A+B)} = \mathcal{L}_A + \mathcal{L}_B, \qquad \mathcal{L}_{(A\cdot B)} = \mathcal{L}_A \cdot \mathcal{L}_B.$$

The set of inner derivations forms an ideal $Inn(\mathcal{M})$ in the Lie algebra $Der(\mathcal{M})$. If $A \in Inn(\mathcal{M})$, then $A \cdot B \in Inn(\mathcal{M})$ for any $B \in Der(\mathcal{M})$.

THEOREM *(Zassenhaus). If $\mathcal{M}$ is a semi-simple Lie algebra then every derivation $\mathcal{L}$ of $\mathcal{M}$ is inner.*

A Lie algebra which has no ideals (except the trivial ones comprising the full algebra itself or the ideal consisting only of zero) is called *simple*. A subalgebra in which all elements commute is called abelian or commutative. An algebra with no abelian ideals is called *semi-simple*.

If $\mathcal{M}$ is an associative algebra and $\mathcal{M}^{(-)}$ the Lie algebra corresponding to it in the sense $H \cdot A = (1/i\hbar)(HA - AH)$, then every derivation $\mathcal{L}$ of $\mathcal{M}$ is also a derivation of $\mathcal{M}^{(-)}$. The converse does not hold in general. However, inner derivation of $\mathcal{M}$ are inner derivation of $\mathcal{M}^{(-)}$, and vise versa.

As a result, we can give the basic theorem regarding Lie algebra corresponding to associative algebra.

THEOREM. *The inner derivations of an associative algebra $\mathcal{M}$ form an ideal $Inn(\mathcal{M})$ in the Lie algebra $Der(\mathcal{M})$ of all derivations of $\mathcal{M}$.*

An operator algebra $\mathcal{M}$ is called a *differential algebra* with the set $\mathcal{A}$ of derivation superoperators if the set $\mathcal{A}$ is given and there is assigned to every element $\mathcal{L} \in \mathcal{A}$ a certain derivation of $\mathcal{M}$. It is not assumed that distinct superoperators of $\mathcal{A}$ must correspond to distinct derivations.

Leibnitz defect

Let $\mathcal{M}$ be an operator algebra, and let $\mathcal{L}$ be a superoperator whose domain $D(\mathcal{L})$ is a subalgebra of $\mathcal{M}$.

DEFINITION. A *Leibnitz defect* of the superoperator $\mathcal{L}$ on $\mathcal{M}$ is a bilinear mapping $Z_{\mathcal{L}} : \mathcal{M} \times \mathcal{M} \to \mathcal{M}$, such that

$$Z_{\mathcal{L}}(A, B) = \mathcal{L}(AB) - \mathcal{L}(A)B - A\mathcal{L}(B)$$

for all $A, B \in D(\mathcal{L})$, such that $AB \in D(\mathcal{L})$.

A derivation on $\mathcal{M}$ is a linear superoperator $\mathcal{L}$, such that $Z_{\mathcal{L}}(A, B) = 0$ for all $A, B \in D(\mathcal{M})$. The Leibnitz defect of $\mathcal{L}$ shows how much the deviation of $\mathcal{L}$ from a derivation. The Leibnitz defect will be denoted by the following symbols. For an associative algebra $\mathcal{M}$, we use $Z_{\mathcal{L}}(A, B)$. For a Lie algebra $L(\mathcal{M}) = \mathcal{M}^{(-)}$, the Leibnitz defect will be denoted by

$$J_{\mathcal{L}}(A, B) = \mathcal{L}(A \cdot B) - (\mathcal{L}A) \cdot B - A \cdot (\mathcal{L}B).$$

For special Jordan algebra $\mathcal{M}^{(+)}$, we use the notation

$$K_{\mathcal{L}}(A, B) = \mathcal{L}(A \circ B) - (\mathcal{L}A) \circ B - A \circ (\mathcal{L}B).$$

10.7. Hamiltonian superoperator

DEFINITION. Let $\mathcal{M}$ be an involutive operator algebra. A *locally Hamiltonian superoperator* is a real superoperator of derivation on $\mathcal{M}$.

The locally Hamiltonian superoperator is also called the $*$-derivation, or *symmetric derivation*. A locally Hamiltonian superoperator is a superoperator $\mathcal{L}$ on $\mathcal{M}$, such that the following requirements are satisfied:

(1) $\mathcal{L}(AB) = (\mathcal{L}A)B + A(\mathcal{L}B)$ for all $A, B \in D(\mathcal{L})$.
(2) $(\mathcal{L}A)^* = \mathcal{L}(A^*)$ for all $A \in D(\mathcal{L})$.

Requirement (1) means that the Leibnitz defect is equal to zero $Z_{\mathcal{L}}(A, B) = 0$ for all $A, B \in D(\mathcal{L}) \subset \mathcal{M}$, such that $AB \in D(\mathcal{L})$. Requirement (2) means that $\mathcal{L}(A)$ is a self-adjoint operator if A is self-adjoint.

DEFINITION. Let $\mathcal{M}$ be an involutive operator algebra. A *globally Hamiltonian superoperator* is a real superoperator of inner derivation of $\mathcal{M}$.

If $\mathcal{L}$ is a globally Hamiltonian superoperator, then there exists a unique self-adjoint operator $H \in \mathcal{M}$ such that

$$\mathcal{L}(A) = \frac{1}{i\hbar}[H, A].$$

In this case, $Tr[\mathcal{L}(A)] = 0$ for all $A \in D(\mathcal{L}) \subset \mathcal{M}$.

Its is not hard to prove that a globally Hamiltonian superoperator $\mathcal{L}$ on $\mathcal{M}$ is a locally Hamiltonian. This proof uses the equation

$$\begin{aligned} Z_{\mathcal{L}}(A, B) &= \frac{1}{i\hbar}\big([H, AB] - [H, A]B - A[H, B]\big) \\ &= \frac{1}{i\hbar}\big(-(H, A, B) - (A, B, H) + (A, H, B)\big). \end{aligned}$$

If $\mathcal{M}$ is an associative algebra, then $(A, B, C) = 0$ for all $A, B, C \in \mathcal{M}$.

Let us give the important theorem regarding Hamiltonian superoperators.

THEOREM. *Let $\mathcal{M}$ be an operator W^*-algebra. A bounded locally Hamiltonian superoperator $\mathcal{L}$ on $\mathcal{M}$ is globally Hamiltonian.*

In other words, each derivation of a W^*-algebra is an inner derivation. As a result, we have the following set of equivalent conditions.

THEOREM. *Let $\mathcal{L}$ be a linear superoperator whose domain $D(\mathcal{L})$ is a subalgebra of an operator W^*-algebra $\mathcal{M}$. Then, the following conditions are equivalent*:

(1) *$\mathcal{L}$ is a locally Hamiltonian superoperator on $\mathcal{M}$.*
(2) *$\mathcal{L}$ is a globally Hamiltonian superoperator on $\mathcal{M}$.*
(3) *$\mathcal{L}$ is a superoperator on $\mathcal{M}$ such that $Z_{\mathcal{L}}(A, B) = 0$, and $\mathcal{L}^*(A) = \mathcal{L}(A^*)$ for all $A, B \in D(\mathcal{L})$.*
(4) *$\mathcal{L}$ is a real superoperator on $\mathcal{M}^{(-)}$ and $\mathcal{M}^{(+)}$ such that $J_{\mathcal{L}}(A, B) = 0$, $K_{\mathcal{L}}(A, B) = 0$ for all $A, B \in D(\mathcal{L})$.*
(5) *There exists a unique self-adjoin operator $H \in \mathcal{M}$ such that $\mathcal{L} = L_H^{(-)}$.*

In the conventional description of quantum Hamiltonian systems, equations of motion (1) is considered with the globally Hamiltonian superoperator $\mathcal{L} = L_H^{(-)}$. The following properties are satisfied:

(1) $Z_{\mathcal{L}}(A, B) = 0$ and $J_{\mathcal{L}}(A, B) = K_{\mathcal{L}}(A, B) = 0$ for all $A, B \in D(\mathcal{L})$.
(2) $\mathcal{L}$ is linear with respect to L_H^-.
(3) $\mathcal{L}$ is real.
(4) $Tr[\mathcal{L}(A)] = 0$ for all $A \in D(\mathcal{L})$.
(5) $\mathcal{L}(I) = 0$ and $\mathcal{L}(0) = 0$.

10.8. Integration of quantum observables

One-parameter operator and superoperator

Operators, defined on subset of the real line, are called one-parameter operator.

DEFINITION. Let $\mathcal{M}$ be an operator space. A *one-parameter operator* is a map that assigns to each t of $T \subset \mathbb{R}$ exactly one operator $A_t \in \mathcal{M}$.

Let $\mathcal{M}$ be a Banach operator space. A one-parameter operator $A_t \in \mathcal{M}$ is called the *continuous*, if

$$\lim_{t \to s} \|A_t - A_s\|_{\mathcal{M}} = 0$$

for all $s \in T$. We shall denote the linear space of all continuous one-parameter operators $A_t \in \mathcal{M}$ by $C(\mathcal{M}, T)$. The space $C(\mathcal{M}, T)$, together with the norm

$$\|A\|_{C(\mathcal{M},T)} = \max_{t \in T} \|A_t\|_{\mathcal{M}}$$

is a Banach space.

A one-parameter operator $A_t \in \mathcal{M}$ is *differentiable* at $t = t_0$, if there exists an element $A'(t_0) \in \mathcal{M}$ such that

$$\lim_{t \to t_0} \left\| \frac{A_t - A_{t_0}}{t - t_0} - A'(t_0) \right\|_{\mathcal{M}} = 0.$$

The operator $A'(t_0)$ is called the *derivative of operator* $A(t)$ at $t = t_0$. The classic notation to denote the derivative A' is $dA(t)/dt$. If $A_t \in \mathcal{M}$ is differentiable at all $t \in T$, then this one-parameter operator is *differentiable on the segment* $T \subset \mathbb{R}$. In this case, the derivative $dA(t)/dt$ is a one-parameter operator.

DEFINITION. Let $\mathcal{M}$ be an operator space. A *one-parameter superoperator* on $\mathcal{M}$ is a map Φ_t that assigns to each t of $T \subset \mathbb{R}$ exactly one superoperator Φ_t on $\mathcal{M}$.

A one-parameter superoperator Φ_t on $\mathcal{M}$ is called the continuous at $t = s$, if $\lim_{t \to s} \Phi_t = \Phi_s$ for $s \in T$. If the limit is considered with respect to the norm of the operator space $\mathcal{M}$, then the superoperator is *strongly continuous* at $t = s$. If the limit is considered in the sense of weak convergence in $\mathcal{M}$, then the superoperator is *weakly continuous* at $t = s$.

Riemann integral of one-parameter operator

Let $A(t)$ be a one-parameter operator $A(t) = A_t$ with values in a Banach operator space $\mathcal{M}$. The *Riemann integral* of $A(t)$, $t \in [a, b]$, is defined as the limit of

integral sums:

$$\lim_{\max(\Delta t_k)\to 0} \sum_{k=1}^{N} A(s_k)\Delta t_k = \int_a^b dt\ A(t),$$

where $\Delta t_k = t_k - t_{k-1}$, $t_{k-1} \leqslant s_k \leqslant t_k$ and $a = t_0 < t_1 < \cdots < t_N = b$. If this limit exists for an arbitrary sequences of decompositions of the interval $[a, b]$ and does not depend on the choice of this sequence and the choice of points s_k, then the one-parameter operator $A(t)$ is called *integrable according to Riemann*. The integral is called *strong* if the sum converge to it with respect to the operator norm of the space $\mathcal{M}$. If the sums are weakly convergent, then the integral is called *weak*.

THEOREM. *A strongly continuous one-parameter operator is strongly integrable according to Riemann.*

Note that the norm of a one-parameter operator, strongly integrable according to Riemann, can be a real-valued function, which is *not* integrable according to Riemann.

The usual properties of an integral hold for the integral of a one-parameter operator. In particular, if the one-parameter operator $A(t)$ has a continuous derivative $dA(t)/dt$ on $[a, b]$, then the Newton–Leibnitz formula is valid.

Bochner integral of one-parameter operator

The Pettis and Bochner integrals are generalizations of the Riemann integral.

DEFINITION. The one-parameter operator $A(t)$, $t \in [a, b]$, is called *integrable according to Bochner*, if it is strongly measurable and $\|A(t)\|_{\mathcal{M}}$ is a real-valued function summable according to Lebesgue.

In this connection, we give the following definitions.

DEFINITION. A one-parameter operator $A(t) \in \mathcal{M}$ is called *strongly measurable*, if it is a uniform limit of a sequence of finite-valued operators.

A linear operator $A(t) \in \mathcal{M}$ is a *finite-valued one-parameter operator* such that $A(t) = A_k \in \mathcal{M}$ for $t \in T_k$, where

$$\bigcup_{k=1}^{n} T_k = T = [a, b], \quad T_k \cap T_l = 0\ (k \neq l).$$

The Bochner integral for finite-valued one-parameter operator is defined by the sum

$$\int_a^b dt\, A(t) = \sum_{k=1}^{n} A_k \mu(T_k),$$

where $\mu(T_k)$ is Lebesgue measure of the interval T_k.

Let $A(t)$ be an arbitrary one-parameter operator, which is integrable according to Bochner, and let $A^{(n)}(t)$ be a sequence of finite-valued one-parameter operator converging to $A(t)$. The Bochner integral of the one-parameter operator $A(t)$ is defined by the limit

$$\int_a^b dt\, A(t) = \lim_{n\to\infty} \int_a^b dt\, A^{(n)}(t). \tag{13}$$

The limit is considered with respect to the strong operator topology. The limit does not depend on the choice of the sequence of finite-valued one-parameter operator $A^{(n)}(t)$ converging to $A(t)$.

Pettis integral of one-parameter operator

Let ω be a linear functional on a Banach space $\mathcal{M}$.

DEFINITION. The one-parameter operator $A(t)$, $t \in [a, b]$, is called *integrable according to Pettis*, if it is weakly measurable and $\omega(A(t))$ is a real-valued function summable according to Lebesgue.

DEFINITION. A one-parameter operator $A(t) \in \mathcal{M}$ is called *weakly measurable*, if the real-valued function $\omega(A(t))$ is Lebesgue measurable for every linear functional $\omega \in \mathcal{M}^*$.

Let us give the basic theorem regarding integrability according to Pettis and Bochner.

THEOREM. *If the Banach operator space $\mathcal{M}$ is separable, then the concept of strong measurability of a one-parameter operator $A(t) \in \mathcal{M}$ coincides with the concept of weak measurability.*

The Pettis integral of the one-parameter operator $A(t)$ is defined by the limit (13) that is considered with respect to the weak operator topology.

THEOREM. *If $A(t)$ is integrable according to Pettis, then $A(t)$ is integrable according to Bochner, and the Pettis integrals are equal to the Bochner integral.*

In general, a one-parameter operator $A(t) \in \mathcal{M}$, integrable according to Pettis, can be an operator, which is not integrable according to Bochner. If the Banach operator space $\mathcal{M}$ is separable, then the concept of Pettis integrability of a one-parameter operator $A(t) \in \mathcal{M}$ coincides with the concept of Bochner integrability.

If $A(t)$ is an integrable according to Bochner for almost all $t \in [a, b]$, then the one-parameter operator

$$B(t) = \int_a^t d\tau\, A(\tau)$$

is continuous and differentiable.

Suppose that the one-parameter superoperator $\mathcal{L}_t$ is integrable according to Bochner. Then instead of differential equation (1), we can take the equivalent integral equation

$$A(t) = A(0) + \int_0^t ds\, \mathcal{L}_s A(s).$$

This is the *Volterra integral equation* for the one-parameter operator $A(t)$.

Chapter 11

Superoperator Algebras and Spaces

11.1. Linear spaces and algebras of superoperators

The following are examples of some mathematical structures on a set of linear superoperators.

(1) Let $\mathcal{M}$ be a linear operator space. The set of all superoperators on $\mathcal{M}$ into $\mathcal{M}$ is a linear space if we define addition of superoperators and multiplication of superoperators by scalars in the natural way. We shall denote the linear space of all linear superoperators on $\mathcal{M}$ by $\mathcal{A}(\mathcal{M})$. Let $\mathcal{L}_1$ and $\mathcal{L}_2$ be linear superoperators of $\mathcal{A}(\mathcal{M})$. Then the sum $(\mathcal{L}_1 + \mathcal{L}_2) \in \mathcal{A}(\mathcal{M})$ is defined by

$$(\mathcal{L}_1 + \mathcal{L}_2)(A) = \mathcal{L}_1(A) + \mathcal{L}_2(A)$$

for all $A \in \mathcal{M}$. The scalar multiple $a\mathcal{L} \in \mathcal{A}(\mathcal{M})$ is $(a\mathcal{L})(A) = a\mathcal{L}(A)$ for all $A \in \mathcal{M}$. When $\mathcal{M}$ is a normed linear space, it is common practice to call the elements of $\mathcal{A}(\mathcal{M})$ bounded linear superoperators.

(2) For $\mathcal{L}_1, \mathcal{L}_2 \in \mathcal{A}(\mathcal{M})$, we define the product $\mathcal{L}_1\mathcal{L}_2$ as the linear superoperator such that

$$(\mathcal{L}_1\mathcal{L}_2)(A) = \mathcal{L}_1\big(\mathcal{L}_2(A)\big) \tag{1}$$

for all $A \in \mathcal{M}$. (If $\mathcal{L}_1, \mathcal{L}_2$ are unbounded superoperators, then equation (1) should be valid for all $A \in D(\mathcal{L}_2)$ such that $\mathcal{L}_2(A) \in D(\mathcal{L}_1)$.) With this definition of multiplication, $\mathcal{A}(\mathcal{M})$ becomes an algebra. That is, $\mathcal{A}(\mathcal{M})$ is a linear space, together with an operation of multiplication having the following properties.

(1) $(\mathcal{L}_1\mathcal{L}_2)\mathcal{L}_3 = \mathcal{L}_1(\mathcal{L}_2\mathcal{L}_3)$.
(2) $\mathcal{L}_1(\mathcal{L}_2 + \mathcal{L}_3) = \mathcal{L}_1\mathcal{L}_2 + \mathcal{L}_1\mathcal{L}_3$.
(3) $(\mathcal{L}_1 + \mathcal{L}_2)\mathcal{L}_3 = \mathcal{L}_1\mathcal{L}_3 + \mathcal{L}_2\mathcal{L}_3$.
(4) $(a\mathcal{L}_1)(b\mathcal{L}_2) = (ab)(\mathcal{L}_1\mathcal{L}_2)$.

As a result, $\mathcal{A}(\mathcal{M})$ is an associative superoperator algebra.

(3) For $\mathcal{L}_1, \mathcal{L}_2 \in \mathcal{A}(\mathcal{M})$, we can define the Lie product $\mathcal{L}_1 \cdot \mathcal{L}_2$ as the linear superoperator such that

$$(\mathcal{L}_1 \cdot \mathcal{L}_2)(A) = \mathcal{L}_1\big(\mathcal{L}_2(A)\big) - \mathcal{L}_2\big(\mathcal{L}_1(A)\big)$$

for $A \in \mathcal{M}$. With this definition of multiplication, $\mathcal{A}(\mathcal{M})$ becomes a Lie algebra $\mathcal{A}^{(-)}(\mathcal{M})$.

The Jordan product $\mathcal{L}_1 \circ \mathcal{L}_2$ can be defined as the linear superoperator such that

$$(\mathcal{L}_1 \circ \mathcal{L}_2)(A) = \mathcal{L}_1\big(\mathcal{L}_2(A)\big) + \mathcal{L}_2\big(\mathcal{L}_1(A)\big)$$

for $A \in \mathcal{M}$. Then $\mathcal{A}(\mathcal{M})$ becomes a Jordan algebra $\mathcal{A}^{(+)}(\mathcal{M})$.

(4) Let $\mathcal{M}$ be a Banach operator algebra. The set of all left superoperators on $\mathcal{M}$ is a linear space if we define addition and multiplication by scalars:

$$(L_A + L_B)C = L_A C + L_B C, \qquad (aL_A)C = aL_A C,$$

where $C \in \mathcal{M}$. We shall denote the linear space of all left superoperators on $\mathcal{M}$ by $\mathcal{A}_l(\mathcal{M})$, i.e.,

$$\mathcal{A}_l(\mathcal{M}) = \{L_A\colon\ A \in \mathcal{M}\}.$$

For $A \in \mathcal{M}$, we define

$$\|L_A\| = \|A\|_{\mathcal{M}}.$$

Then $\mathcal{A}_l(\mathcal{M})$ is a normed linear space. If $\mathcal{A}(\mathcal{M})$ is a Banach space of all bounded superoperators on $\mathcal{M}$, then it is easy to prove that $\mathcal{A}_l(\mathcal{M})$ is a closed subspace of $\mathcal{A}(\mathcal{M})$. We shall denote the linear space of all right superoperators on $\mathcal{M}$ by $\mathcal{A}_r(\mathcal{M})$.

(5) Let $\mathcal{M}$ be an associative Banach operator algebra. For $A \in \mathcal{M}$, let L_A be the left superoperator on $\mathcal{M}$ given by $L_A B = AB$ for $B \in \mathcal{M}$. Also, $R_A B = BA$. We define the *Lie left superoperator* on $\mathcal{M}$ by

$$L_A^- = \frac{1}{i\hbar}(L_A - R_A), \tag{2}$$

where $\hbar$ is a real number. For $A^* = A$, it is easy to prove that L_A^- is a real superoperator, i.e., $(L_A^- B)^* = L_A^- B^*$ for $B \in \mathcal{M}$. We shall denote the linear space of all Lie left superoperators on $\mathcal{M}$ by $\mathcal{A}_{l-}(\mathcal{M})$. It is easy to prove that $\mathcal{A}_{l-}(\mathcal{M})$ is an associative algebra, and $\mathcal{A}_{l-}(\mathcal{M})$ is isomorphic to $\mathcal{A}_l(\mathcal{M}^{(-)})$.

(6) Let $\mathcal{M}$ be an associative Banach operator algebra. We define the *Jordan left superoperator* on $\mathcal{M}$ by

$$L_A^+ = \frac{1}{2}(L_A + R_A). \tag{3}$$

For $A^* = A$, the superoperator L_A^+ is real, and $(L_A^+ B)^* = L_A^+ B^*$. We shall denote the linear space of all Jordan left superoperators on $\mathcal{M}$ by $\mathcal{A}_{l+}(\mathcal{M})$. It is easy to prove that $\mathcal{A}_{l+}(\mathcal{M})$ is an associative algebra, and $\mathcal{A}_{l+}(\mathcal{M})$ is isomorphic to $\mathcal{A}_l(\mathcal{M}^{(+)})$.

(7) It is easily seen that the correspondence $A \to L_A$ is a linear mapping that also preserves the operation of multiplication. These superoperators would

have formed an algebra of superoperators $\mathcal{A}_l(\mathcal{M}) = \{L_A\colon\ A \in \mathcal{M}\}$, isomorphic to $\mathcal{M}$. The mapping $A \to L_A$ is called the *left regular representation* of $\mathcal{M}$. The mapping $A \to R_A$ is called the *right regular representation* of $\mathcal{M}$. In general, $L_A \neq R_A$, and these representations are not equivalent. Using $L_A^- = -R_A^-$, $L_A^+ = R_A^+$, we obtain an equivalence of the left and right regular representations for commutative and anticommutative algebras.

(8) Let $\mathcal{M}$ be a Lie algebra and $A \in \mathcal{M}$. The mapping $A \to L_A$ associates with each element A in the Lie algebra $\mathcal{M}$ a linear transformation $L_A^-\colon L_A^- B = A \cdot B$. For classical systems, $A \cdot B$ is a Poisson bracket $\{A, B\}$. In quantum theory, $A \cdot B$ is a self-adjoint commutator $(1/i\hbar)[A, B]$. To prove that this is a representation, we must show it preserves the relations, that is, if $A \cdot B = C$ it must follows that

$$L_A^- L_B^- - L_B^- L_A^- = L_C^-.$$

Using the Jacobi identity, we obtain

$$\begin{aligned}\left[L_A^-, L_B^-\right]X &= A \cdot (B \cdot X) - B \cdot (A \cdot X) = A \cdot (B \cdot X) + B \cdot (X \cdot A)\\ &= -X \cdot (A \cdot B) = (A \cdot B) \cdot X = C \cdot X = L_C X.\end{aligned}$$

As a result, $\mathcal{A}_l(\mathcal{M})$ is a left regular representation of the Lie algebra $\mathcal{M}$.

(9) Let $\mathcal{M}$ be an associative Banach algebra of bounded operators, and for each $A \in \mathcal{M}$, define L_A by $L_A B = AB$, where $B \in \mathcal{M}$. Clearly L_A is a linear superoperator from $\mathcal{M}$ into itself. Also,

$$\|L_A B\|_{\mathcal{M}} = \|AB\|_{\mathcal{M}} \leqslant \|A\|_{\mathcal{M}} \|B\|_{\mathcal{M}},$$

which shows that L_A is a bounded superoperator with $\|L_A\| \leqslant \|A\|_{\mathcal{M}}$. It is easily seen that the correspondence $A \to L_A$ is a linear mapping that also preserves the operation of multiplication. For example, given $A, B, C \in \mathcal{M}$, we have

$$L_{AB} C = (AB)C = A(BC) = A(L_B C) = L_A L_B C.$$

Hence $L_{AB} = L_A L_B$. The mapping $A \to L_A$ is called the *left regular representation* of $\mathcal{M}$. Now suppose that $\mathcal{M}$ is a unital algebra, i.e., $\mathcal{M}$ has a unit I with $\|I\|_{\mathcal{M}} = 1$. Then

$$\|L_A\| = \sup_{\|B\|=1} \|L_A B\|_{\mathcal{M}} \geqslant \|L_A I\|_{\mathcal{M}} = \|A\|_{\mathcal{M}}.$$

Hence, by $\|L_A\| \leqslant \|A\|_{\mathcal{M}}$,

$$\|L_A\| = \|A\|_{\mathcal{M}}.$$

Thus the left regular representation of $\mathcal{M}$ is an isometric algebra isomorphism of $\mathcal{M}$ onto a subalgebra of $\mathcal{A}_l(\mathcal{M}) = \{L_A\colon\ A \in \mathcal{M}\}$.

(10) Let $\mathcal{M}$ be an associative Banach algebra of all bounded operators. The left regular representation of $\mathcal{M}$ preserves the property of invertibility. An operator A

in $\mathcal{M}$ is said to be *invertible* in $\mathcal{M}$, if there exists an inverse element A^{-1} in $\mathcal{M}$ such that $A^{-1}A = AA^{-1} = I$. If A is invertible, then the superoperator L_A is obviously invertible in the algebra $\mathcal{A}_l(\mathcal{M})$, because

$$L_A L_{A^{-1}} = L_{A^{-1}} L_A = L_I.$$

Thus $(L_A)^{-1} = L_{A^{-1}}$. This is the *inverse superoperator*.

11.2. Superoperator algebra for Lie operator algebra

A Lie algebra is defined by the identities:

$$A \cdot A = 0, \tag{4}$$

$$(A \cdot B) \cdot C + (B \cdot C) \cdot A + (C \cdot A) \cdot B = 0. \tag{5}$$

The algebra $\mathcal{M}^{(-)}$ obtained from an associative algebra $\mathcal{M}$ on replacing the product AB by $A \cdot B = (1/i\hbar)(AB - BA)$ is easily seen to be a Lie algebra.

In any Lie algebra $\mathcal{M}^{(-)}$, we denote by L_A^- the left multiplication (2). This is also called the regular representation of $\mathcal{M}^{(-)}$. In general, this is an admissible mapping of $\mathcal{M}^{(-)}$ into $\mathcal{A}(\mathcal{M}^{(-)})$, the algebra of linear superoperators on $\mathcal{M}^{(-)}$. There exist certain identities, which follows from equations (4) and (5).

Let us consider equation (4). In the first place, we have

$$L_{A \cdot A} = 0.$$

Secondly, denoting the left-hand side of (4) by $G(A) = A \cdot A$, consider the expression

$$G(A + B) - G(A) - G(B) = 0.$$

Its vanishing is expressed by the equation

$$A \cdot B + B \cdot A = 0. \tag{6}$$

The process by which (6) was obtained from (4) is called *linearization*. We shall also say that (6) was obtained by linearizing (4). Writing (6) as a superoperator equation for B, we obtain

$$L_A^- + R_A^- = 0. \tag{7}$$

Using equation (5) and expressing it as a superoperator equation acting on C, we find

$$L_{A \cdot B}^- + R_A^- L_B^- + R_B^- R_A^- = 0. \tag{8}$$

Equations (7) and (8) give

$$L_{A \cdot B}^- - L_A^- L_B^- + L_B^- L_A^- = 0. \tag{9}$$

Any linear mapping of a Lie operator algebra into an associative superoperator algebra satisfying the identities (7), (9) is called a *Lie representation* or *superoperator representation* of Lie algebra $\mathcal{M}^{(-)}$.

Consider a Lie algebra $\mathcal{M}^{(-)}$, contained in an associative algebra $\mathcal{M}$. If we denote right and left multiplication by $A \in \mathcal{M}$ by L_A and R_A, respectively, and the left regular representation in $\mathcal{M}^{(-)}$ by L_A^-, then, since $A \cdot B = (1/i\hbar)(AB - BA)$ it follows that we have (2). This is the *Lie left superoperator* on $\mathcal{M}$.

For L_A^- and L_B^-, we can define the Lie product $L_A^- \cdot L_B^-$ as the linear superoperator such that

$$L_A^- \cdot L_B^- = L_A^- L_B^- - L_B^- L_A^-.$$

With this definition of multiplication, a set $\{L_A^-\colon A \in \mathcal{M}\}$ becomes a Lie algebra. Using (9), it is not hard to prove that the condition $C = A \cdot B$ gives

$$L_A^- L_B^- - L_B^- L_A^- = L_C^-.$$

11.3. Superoperator algebra for Jordan operator algebra

A Jordan algebra is defined by the identities:

$$A \circ B = B \circ A, \tag{10}$$

$$(A \circ B) \circ B^2 - \left(A \circ B^2\right) \circ B = 0. \tag{11}$$

The algebra $\mathcal{M}^{(+)}$ obtained from an associative algebra $\mathcal{M}$ on replacing the product AB by $A \circ B = (1/2)(AB + BA)$ is easily seen to be a Jordan algebra. Any subalgebra of a Jordan algebra of this type is called special.

In any Jordan algebra $\mathcal{M}$, we denote by L_A the left multiplication

$$L_A B = A \circ B.$$

This is also called the left regular representation of $\mathcal{M}$. In contradiction to the Lie algebra, this is not in general an admissible mapping of $\mathcal{M}$ into $\mathcal{A}(\mathcal{M})$, the algebra of linear superoperators on $\mathcal{M}$. However, it does satisfy certain identities which follows from equations (10) and (11).

Expressing (10) as an operator equation acting on B, we obtain

$$L_A = R_A. \tag{12}$$

Let us consider equation (11). In the first place, we have from (11) the relation

$$R_{B^2} R_B = R_B R_{B^2}. \tag{13}$$

Using (12), this equation can be presented as

$$L_{A^2} L_A = L_A L_{A^2}.$$

Secondly, we can linearize (11) and express it as an operator equation acting on one of the variables replacing B. Thus denoting the left-hand side of (11) by

$$F(B) = (A \circ B) \circ B^2 - \big(A \circ B^2\big) \circ B,$$

consider the expression

$$\begin{aligned} &F(B + C + D) - F(B + C) - F(C + D) - F(B + D) \\ &\quad + F(B) + F(C) + F(D) = 0. \end{aligned}$$

Its vanishing is expressed by the equation

$$\begin{aligned} &(A \circ B) \circ (C \circ D) + (A \circ C) \circ (D \circ B) + (A \circ D) \circ (B \circ C) \\ &\quad = \big((B \circ C) \circ A\big) \circ D + \big((C \circ D) \circ A\big) \circ B + \big((D \circ B) \circ A\big) \circ C. \end{aligned}$$

Using (10), we have

$$\begin{aligned} &(A \circ B) \circ (C \circ D) + (A \circ C) \circ (B \circ D) + (B \circ C) \circ (A \circ D) \\ &\quad = \big((B \circ C) \circ A\big) \circ D + B \circ \big(A \circ (C \circ D)\big) + C \circ \big(A \circ (B \circ D)\big). \end{aligned} \tag{14}$$

Writing this as an operator equation for D, we obtain

$$\begin{aligned} &L_{A\circ B} L_C + L_{A\circ C} L_B + L_{B\circ C} L_A \\ &\quad = L_{((B\circ C)\circ A)} + L_B L_A L_C + L_C L_A L_B. \end{aligned} \tag{15}$$

In any special Jordan algebra $\mathcal{M}^{(+)}$, we denote by L_A^+ the left multiplication

$$L_A^+ B = A \circ B = \frac{1}{2}(AB + BA).$$

This can be called the special left regular representation of $\mathcal{M}^{(+)}$. The left superoperators L_A^+ satisfy the equations

$$\begin{aligned} &L_{A^2}^+ L_A^+ = L_A^+ L_{A^2}^+, \\ &L_{A\circ B}^+ L_C^+ + L_{A\circ C}^+ L_B^+ + L_{B\circ C}^+ L_A^+ = L_{((B\circ C)\circ A)}^+ + L_B^+ L_A^+ L_C^+ + L_C^+ L_A^+ L_B^+. \end{aligned}$$

Any linear mapping of a Jordan operator algebra into an associative superoperator algebra satisfying the identities (12), (13) and (15) is called a *Jordan representation* or *superoperator general representation* of Jordan algebra.

Consider a special Jordan algebra $\mathcal{M}^{(+)}$, contained in an associative algebra $\mathcal{M}$. If we denote right and left multiplication by $A \in \mathcal{M}$ by L_A and R_A, respectively, and the left regular representation in $\mathcal{M}^{(+)}$ by L_A^+, then, since $A \circ B = (1/2)(AB + BA)$ it follows that $L_A^+ = \frac{1}{2}(L_A + R_A)$. This is the *Jordan left superoperator* on $\mathcal{M}$.

In the general case, it is not hard to prove that $\frac{1}{2}(L_A^+ L_B^+ + L_B^- L_A^+) \neq L_{A\circ B}^+$.

11.4. Superoperator algebra for Lie–Jordan operator algebra

Consider a special Lie–Jordan algebra $\mathcal{M}^{(\pm)}$, contained in an associative algebra $\mathcal{M}$. The algebra $\mathcal{M}^{(\pm)}$ is defined by $<\mathcal{M}, \cdot, \circ>$, where

$$A \cdot B = \frac{1}{i\hbar}(AB - BA), \qquad A \circ B = \frac{1}{2}(AB + BA).$$

A special Lie–Jordan algebra can be considered as an associative algebra, together with two bilinear multiplication operations $\cdot$ and $\circ$ satisfying the conditions:

(1) $<\mathcal{M}, \cdot>$ is a Lie algebra $\mathcal{M}^{(-)}$:

$$A \cdot B = -B \cdot A, \qquad (A \cdot B) \cdot C + (B \cdot C) \cdot A + (C \cdot A) \cdot B = 0;$$

(2) $<\mathcal{M}, \circ>$ is a special Jordan algebra $\mathcal{M}^{(+)}$:

$$A \circ B = B \circ A, \qquad \big((A \circ A) \circ B\big) \circ A = (A \circ A) \circ (B \circ A);$$

(3) the Leibnitz rule

$$A \cdot (B \circ C) = (A \cdot B) \circ C + B \circ (A \cdot C);$$

(4) the equation for associators

$$(A \circ B) \circ C - A \circ (B \circ C) = \frac{\hbar^2}{4}\big((A \cdot B) \cdot C - A \cdot (B \cdot C)\big).$$

In this case, the special Lie–Jordan algebra is said to be defined. We shall also assume that $\mathcal{M}^{(\pm)}$ is a unital algebra with $I \in \mathcal{M}$, such that

$$A \circ I = A, \qquad A \cdot I = 0.$$

We denote right and left multiplications by $A \in \mathcal{M}$ by L_A and R_A, respectively. The left regular representation in $\mathcal{M}^{(\pm)}$ is presented by a pair (L_A^+, L_A^-). Using (2) and (3), we obtain

$$L_A = L_A^+ + \frac{i\hbar}{2}L_A^-, \qquad R_A = L_A^+ - \frac{i\hbar}{2}L_A^-.$$

Equations $L_A^+ = R_A^+$, and $L_A^- = -R_A^-$ give

$$L_A = R_A^+ - \frac{i\hbar}{2}R_A^-, \qquad R_A = R_A^+ + \frac{i\hbar}{2}R_A^-.$$

These equations express the superoperators (L_A, R_A) on an associative operator algebra $\mathcal{M}$ through the left and right superoperators on a special Lie–Jordan algebra $\mathcal{M}^{(\pm)}$.

The identities of a special Lie–Jordan algebra lead to the relations for $L_A^+ = R_A^+$ and $L_A^- = -R_A^-$. Using the linearization, we obtain the following identities:

(1) the Lie relations

$$L^-_{A\cdot B} = L^-_A L^-_B - L^-_B L^-_A, \tag{16}$$

(2) the Jordan relations

$$\begin{aligned} &L^+_{(A\circ B)\circ C} + L^+_B L^+_C L^+_A + L^+_A L^+_C L^+_B \\ &\quad = L^+_{A\circ B} L^+_C + L^+_{B\circ C} L^+_A + L^+_{A\circ C} L^+_B, \end{aligned} \tag{17}$$

$$\begin{aligned} &L^+_{(A\circ B)\circ C} + L^+_B L^+_C L^+_A + L^+_A L^+_C L^+_B \\ &\quad = L^+_C L^+_{A\circ B} + L^+_B L^+_{A\circ C} + L^+_A L^+_{B\circ C}, \end{aligned} \tag{18}$$

$$\begin{aligned} &L^+_C L^+_{A\circ B} + L^+_B L^+_{A\circ C} + L^+_A L^+_{B\circ C} \\ &\quad = L^+_{A\circ B} L^+_C + L^+_{B\circ C} L_A + L^+_{A\circ C} L^+_B, \end{aligned} \tag{19}$$

(3) the mixed relations

$$L^+_{A\cdot B} = L^-_A L^+_B - L^+_B L^-_A, \qquad L^-_{A\circ B} = L^+_A L^-_B + L^+_B L^-_A, \tag{20}$$

(4) the mixed relations with $\hbar$

$$L^+_{A\circ B} = L^+_A L^+_B - \frac{\hbar^2}{4} L^-_B L^-_A, \qquad L^+_B L^+_A - L^+_A L^+_B = -\frac{\hbar^2}{4} L^-_{A\cdot B}. \tag{21}$$

Note that $\hbar = 0$ in classical mechanics.

11.5. Superoperator C^*-algebra and double centralisers

We can associate to each C^*-algebra $\mathcal{M}$ a certain C^*-algebra $\mathcal{A}_2(\mathcal{M})$, which contains $\mathcal{M}$ as an ideal. We begin by considering a double centraliser and its properties.

DEFINITION. A *double centraliser* for an algebra $\mathcal{M}$ is a pair (L, R) of bounded linear maps on $\mathcal{M}$, such that for all $A, B \in \mathcal{M}$, the following conditions are satisfied:

$$L(AB) = L(A)B, \quad R(AB) = AR(B), \quad R(A)B = AL(B). \tag{22}$$

For example, if $C \in \mathcal{M}$ and L_C, R_C are the linear maps on $\mathcal{M}$ defined by

$$L_C A = CA, \qquad R_C A = AC,$$

then (L_C, R_C) is a double centraliser on $\mathcal{M}$.

If an algebra $\mathcal{M}$ has a unity I, then equations (22) give

$$L(AB) = L(A)B,\ A = I \quad \Rightarrow \quad L(B) = L(I)B,$$

$$R(AB) = AR(B),\ B = I \quad \Rightarrow \quad R(A) = AR(I),$$
$$R(A)B = AL(B),\ A = B = I \quad \Rightarrow \quad R(I) = L(I).$$

As a result, the maps L and R can be presented as the left and right superoperators

$$L(A) = L_C A, \qquad R(A) = R_C A,$$

where $C = L(I) = R(I)$. Then equations (22) are equivalent to the relations

$$L_{AB} = L_A L_B, \qquad R_{AB} = R_B R_A, \qquad L_A R_B = R_B L_A$$

for all $A, B \in \mathcal{M}$. These relations express the statement that the associator is equal to zero, $(A, B, C) = 0$ for all $A, B, C \in \mathcal{M}$.

Let $\mathcal{M}$ be a Banach algebra. If L and R are bounded maps on $\mathcal{M}$, then we can define the norms

$$\|L\| = \sup_{\|A\|_{\mathcal{M}}=1} \big\|L(A)\big\|_{\mathcal{M}}, \qquad \|R\| = \sup_{\|A\|_{\mathcal{M}}=1} \big\|R(A)\big\|_{\mathcal{M}}. \tag{23}$$

The following statement is satisfied.

STATEMENT. *If (L, R) is a double centraliser on a Banach algebra $\mathcal{M}$, then the norm $\|L\|$ is equal to $\|R\|$, i.e., $\|L\| = \|R\|$.*

PROOF. Since

$$\big\|AL(B)\big\|_{\mathcal{M}} = \big\|R(A)B\big\|_{\mathcal{M}} \leqslant \|R\|\,\|A\|_{\mathcal{M}}\|B\|_{\mathcal{M}},$$

we have

$$\big\|L(B)\big\|_{\mathcal{M}} = \sup_{\|A\|_{\mathcal{M}}=1} \big\|AL(B)\big\|_{\mathcal{M}} \leqslant \|R\|\,\|B\|_{\mathcal{M}},$$

and therefore $\|L\| \leqslant \|R\|$. The inequality

$$\big\|R(A)B\big\|_{\mathcal{M}} = \big\|AL(B)\big\|_{\mathcal{M}} \leqslant \|L\|\,\|A\|_{\mathcal{M}}\|B\|_{\mathcal{M}},$$

gives

$$\big\|R(A)\big\|_{\mathcal{M}} = \sup_{\|B\|_{\mathcal{M}}=1} \big\|R(A)B\big\|_{\mathcal{M}} \leqslant \|L\|\,\|A\|_{\mathcal{M}},$$

and therefore $\|R\| \leqslant \|L\|$. Thus, $\|L\| = \|R\|$. □

If $\mathcal{M}$ is a Banach algebra, we denote the set of its double centralisers by $\mathcal{A}_2(\mathcal{M})$. The set $\mathcal{A}_2(\mathcal{M})$ is a linear space with the following operations:

$$(L_1, R_1) + (L_2, R_2) = (L_1 + L_2, R_1 + R_2), \qquad a(L, R) = (aL, aR),$$

where $a \in \mathbb{C}$. We can define the norm of the double centraliser (L, R) by

$$\|(L, R)\|_{\mathcal{A}} = \|L\| = \|R\|.$$

As a result, $\mathcal{A}_2(\mathcal{M})$ is a normed linear space. It is easy to prove, that $\mathcal{A}_2(\mathcal{M})$ is a closed subspace of the direct sum $\mathcal{A}(\mathcal{M}) \oplus \mathcal{A}(\mathcal{M})$, where $\mathcal{A}(\mathcal{M})$ is the Banach space of all bounded superoperators on $\mathcal{M}$.

The space $\mathcal{A}_2(\mathcal{M})$ can be considered as an algebra. For (L_1, R_1) and (L_2, R_2), we define the product

$$(L_1, R_1)(L_2, R_2) = (L_1 L_2, R_2 R_1).$$

Direct computations show that this product is again a double centraliser (L_3, R_3) of $\mathcal{M}$. Note that the maps L_3 and R_3 are defined by $L_3 = L_1 L_2$ and $R_3 = R_2 R_1$. In general, R_3 is not equal to $R_1 R_2$. As a result, the space $\mathcal{A}_2(\mathcal{M})$ is an algebra under this multiplication.

Let $\mathcal{M}$ be an involutive algebra. We define the map J on $\mathcal{M}$ by $JA = A^*$ for all $A \in \mathcal{M}$. The map J is an involution superoperator, such that for all $A, B \in \mathcal{M}$, the following requirements are satisfied:

$$J(J(A)) = A, \qquad J(AB) = J(B)J(A),$$
$$J(A + B) = J(A) + J(B), \qquad J(aA) = a^* J(A).$$

Let us define the map L^* from $\mathcal{M}$ into itself by setting

$$L^* = JLJ,$$

i.e., $L^*(A) = [L(A^*)]^*$ for all $A \in \mathcal{M}$. The mapping $L \to L^*$ satisfies the following two properties

$$L^{**} = L, \qquad (L_1 L_2)^* = L_1^* L_2^*.$$

Using $JJ = L_I = R_I$, we obtain

$$L^{**} = (JLJ)^* = J(JLJ)J = JJ\,L\,JJ = L.$$

The second property can be proved by

$$(L_1^* L_2^*) = (JL_1J)(JL_2J) = JL_1JJL_2J = JL_1L_2J = (L_1L_2)^*.$$

Note, that we have $L_1^* L_2^*$ instead of $L_2^* L_1^*$ as for usual operators. In general, $L_1^* L_2^* \neq L_2^* L_1^*$.

The map $R^* : \mathcal{M} \to \mathcal{M}$ is defined by $R^* = JRJ$, i.e., $R^*(A) = [R(A^*)]^*$ for all $A \in \mathcal{M}$. The maps L^* and R^* are linear.

If (L, R) is a double centraliser, then we can define the mapping $(L, R) \to (L, R)^*$ by the equation

$$(L, R)^* = (R^*, L^*).$$

It is easily verified that this mapping is an involution on $\mathcal{A}_2(\mathcal{M})$. Then $\mathcal{A}_2(\mathcal{M})$ is an involutive algebra.

As a result, we can give the following definition.

DEFINITION. An *algebra of multiplicators*, or *multiplier algebra*, of $\mathcal{M}$ is a set $\mathcal{A}_2(\mathcal{M})$ of its double centralisers, such that $\mathcal{A}_2(\mathcal{M})$ is an involutive normed algebra under the following operations:

(1) Multiplication: $(L_1, R_1)(L_2, R_2) = (L_1L_2, R_2R_1)$.
(2) Norm: $\|(L, R)\|_{\mathcal{A}} = \|L\| = \|R\|$.
(3) Involution: $(L, R)^* = (JRJ, JLJ)$.

There is the following important theorem.

THEOREM. *If $\mathcal{M}$ is a C^*-algebra, then $\mathcal{A}_2(\mathcal{M})$ is a C^*-algebra of multiplicators under the multiplication, involution and norm defined above.*

PROOF. To prove the theorem, we check that if (L, R) is a double centraliser, then

$$\big\|(L, R)^*(L, R)\big\|_{\mathcal{A}} = \big\|(L, R)\big\|_{\mathcal{A}}^2. \tag{24}$$

If $\|A\|_{\mathcal{M}} \leqslant 1$, then

$$\begin{aligned}\big\|L(A)\big\|_{\mathcal{M}}^2 &= \big\|\big(L(A)\big)^*L(A)\big\|_{\mathcal{M}} = \big\|L^*(A^*)L(A)\big\|_{\mathcal{M}} \\ &= \big\|A^*R^*L(A)\big\|_{\mathcal{M}} \leqslant \|R^*L\|_{\mathcal{A}} = \big\|(L, R)^*(L, R)\big\|_{\mathcal{A}},\end{aligned}$$

so

$$\big\|(L, R)\big\|_{\mathcal{A}}^2 = \sup_{\|A\|_{\mathcal{M}}=1} \big\|L(A)\big\|_{\mathcal{M}}^2 \leqslant \big\|(L, R)^*(L, R)\big\|_{\mathcal{A}} \leqslant \big\|(L, R)\big\|_{\mathcal{A}}^2,$$

and therefore we have (24). □

The mapping $\mathcal{M} \to \mathcal{A}_2(\mathcal{M})$, such that $A \to (L_A, R_A)$ is an isometric $*$-homomorphism. Therefore we can identify $\mathcal{M}$ as a subalgebra of C^*-algebra $\mathcal{A}_2(\mathcal{M})$. In fact $\mathcal{M}$ is an ideal of $\mathcal{A}_2(\mathcal{M})$. The algebra $\mathcal{A}_2(\mathcal{M})$ is unital, such that the double centraliser (L_I, R_I) is the unit. Then $\mathcal{M} = \mathcal{A}_2(\mathcal{M})$ if and only if $\mathcal{M}$ is unital.

11.6. Superoperator W*-algebra

Let A be bounded operator on a Hilbert space $\mathcal{H}$. Then L_A can be considered as a left bounded superoperator on an associated Hilbert operator space $\bar{\mathcal{H}}$. These

superoperators form a set $\mathcal{A}_l(\bar{\mathcal{H}})$. If $\mathcal{M}$ is an operator algebra, then the map $A \to L_A$ is a left regular representation of $\mathcal{M}$. Using the equation

$$JL_AJ = R_{JA},$$

the left regular representation of $\mathcal{M}$ can be connected with a right regular representation of $\mathcal{M}$.

STATEMENT. *Let $\mathcal{A}_l(\mathcal{M})$ be a set of all left superoperators L_A on $\bar{\mathcal{H}}$. A weak closure of $\mathcal{A}_l(\bar{\mathcal{H}})$ is a W^*-algebra of superoperators.*

A weak closure of a set of all right superoperators on $\bar{\mathcal{H}}$ forms a W^*-algebra $\mathcal{A}_r(\bar{\mathcal{H}})$. There exist the relations

$$\mathcal{A}_r(\mathcal{M}) = \big(\mathcal{A}_l(\mathcal{M})\big)_c = \big\{J\mathcal{L}J\colon\ \mathcal{L} \in \mathcal{A}_l(\mathcal{M})\big\},$$
$$\mathcal{A}_l(\mathcal{M}) = \big(\mathcal{A}_r(\mathcal{M})\big)_c = \big\{J\mathcal{L}J\colon\ \mathcal{L} \in \mathcal{A}_r(\mathcal{M})\big\}.$$

The algebras $\mathcal{A}_l(\mathcal{M})$ and $\mathcal{A}_r(\mathcal{M})$ coincide with its bicommutants:

$$\big[(\mathcal{A}_l(\mathcal{M}))_c\big]_c = \mathcal{A}_l(\mathcal{M}), \qquad \big[(\mathcal{A}_r(\mathcal{M}))_c\big]_c = \mathcal{A}_r(\mathcal{M}).$$

The maps $A \to L_A$ and $A \to R_A$ are called the canonical maps from an algebra $\mathcal{M}$ into W^*-algebras $\mathcal{A}_l(\mathcal{M})$ and $\mathcal{A}_r(\mathcal{M})$.

Let $\mathcal{M}_0$ be a Hilbert operator algebra, and let $\mathcal{M}$ be the Hilbert space completion of $\mathcal{M}_0$. Then $\mathcal{M}$ is a Hilbert operator space. Suppose L_A and R_A are the bounded left and right superoperators on $\mathcal{M}$. These superoperators are elements of the algebra of bounded linear superoperators on $\mathcal{M}$, which are the continuous extensions of the left and right multiplications by A in $\mathcal{M}_0$. The mapping $A \to L_A$ is a nondegenerate representation of $\mathcal{M}_0$ on $\mathcal{M}$. The weak closure of the set of left superoperators L_A (respectively, R_A) is a W^*-algebra in $\mathcal{M}$. It is called the left (respectively, right) W^*-algebra of the given Hilbert operator algebra, and is denoted by $\mathcal{A}_l(\mathcal{M})$ (respectively, $\mathcal{A}_r(\mathcal{M})$). Note that $\mathcal{A}_l(\mathcal{M})$ and $\mathcal{A}_r(\mathcal{M})$ are mutual commutants. They are semi-finite W^*-algebras.

STATEMENT. *A trace on a C^*-algebra $\mathcal{M}$ is an additive functional ω_0 on the set $\mathcal{M}_+$ of positive elements of $\mathcal{M}$ that takes values in $[0, \infty]$, and satisfy the following conditions*:

(1) *ω_0 is homogeneous with respect to multiplication by positive numbers,*
(2) *$\omega_0(AA^*) = \omega_0(A^*A)$ for all $A \in \mathcal{M}$.*

A trace ω_0 is said to be *finite* if $\omega_0(A) < \infty$ for all $A \in \mathcal{M}_+$, and *semi-finite* if

$$\omega_0(A) = \sup\big\{\omega_0(B)\colon\ B \in \mathcal{M},\ B \leqslant A,\ \omega_0(B) < \infty\big\}$$

for all $A \in \mathcal{M}_+$. The finite traces on $\mathcal{M}$ are the restrictions to $\mathcal{M}_+$ of those positive linear functionals ω_1 on $\mathcal{M}$, such that $\omega_1(AB) = \omega_1(BA)$ for all $A, B \in \mathcal{M}$.

Each Hilbert algebra determines some normal semi-finite trace on the W^*-algebra $\mathcal{A}_l(\mathcal{M})$. Conversely, if an operator W^*-algebra $\mathcal{M}_N$ and a semi-finite trace on $\mathcal{M}_N$ are given, then it is possible to construct a Hilbert algebra $\mathcal{M}$ such that the left W^*-algebra $\mathcal{A}(\mathcal{M})$ of this Hilbert algebra is isomorphic to $\mathcal{M}_N$ and the trace determined by the Hilbert algebra coincides with the initial one. Thus, a Hilbert operator algebra is a method to study semi-finite W^*-algebras and traces on them. An extension of the concept of a Hilbert algebra makes it possible to study by similar methods W^*-algebras that are not necessarily semi-finite [151].

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Chapter 12

Superoperator Functions

12.1. Function of left and right superoperators

Let $\mathcal{M}$ be a Banach operator algebra, and $A, B \in \mathcal{M}$. Using the polynomial

$$F(x, y) = \sum_{i,j=0}^{n} l_{ij} x^i y^j,$$

where $l_{il} \in \mathbb{C}$, we define the superoperator polynomial

$$F[L_A, R_B] = \sum_{i,j=0}^{n} l_{ij} (L_A)^i (R_B)^j. \tag{1}$$

Note that $L_A R_B = R_B L_A$ if and only if $(A, C, B) = 0$ for all $C \in \mathcal{M}$.

When z belongs to the resolvent set $\rho(A)$ of A, the inverse of $L_{zI-A} = (zL_I - L_A)$ is called the *resolvent superoperator of* L_A and is denoted by

$$R(z, L_A) = (zL_I - L_A)^{-1} = L_{zI-A}^{-1} = L_{R(z,A)}.$$

If $\mathcal{M}$ is a complex Banach operator space and A is a closed operator with domain and range in $\mathcal{M}$, the fact that the resolvent superoperator $R(z, L_A)$ is an analytic function of z enables us to obtain some important results using contour integrals in the complex plane. The completeness of $\mathcal{M}$ (and hence of $\mathcal{A}_l(\mathcal{M})$) provides the existence of these integrals.

If $f(z)$ is a function, analytic in a region containing the spectrum $\sigma(A)$ of the operator A, then we can define the superoperator functions

$$f(L_A) = \frac{1}{2\pi i} \oint_{C_A} f(z) R(z, L_A)\, dz,$$

$$f(R_A) = \frac{1}{2\pi i} \oint_{C_A} f(z) R(z, R_A)\, dz, \tag{2}$$

where the contour C_A contains in its interior the spectrum of the operator A. Here we use

$$\sigma(A) = \sigma(L_A) = \sigma(R_A).$$

These integrals are generalizations of the Cauchy integral. It does not depend on the choice of the contour C_A.

Using equations (2), the correspondence $F(x, y) \leftrightarrow F[L_A, L_B]$ between the polynomials $F(x, y)$ and the superoperators $F[L_A, L_B]$ can be presented in the form

$$F[L_A, R_B] = \frac{1}{(2\pi i)^2} \oint_{C_A} \oint_{C_B} F(x, y)\,(xL_I - L_A)^{-1}(yR_I - R_B)^{-1}\,dx\,dy, \tag{3}$$

where $x \in \rho(A)$ and $y \in \rho(B)$. Note that $R_I = L_I$. It can be easy verified that in this way, we obtain the one-to-one correspondence between the polynomials $F(x, y)$ and the superoperator polynomials $F[L_A, R_B]$. Equation (3) allows us to extend this correspondence to functions (and superoperators) of a more general form.

Let $L(x, y)$ be an analytic function. We now propose to define a certain set of complex-valued analytic functions on $\mathbb{C}^2$ and to associate with each such function $L(x, y)$ an element of the superoperator space $\mathcal{A}(\mathcal{M})$. The superoperator associated with $L(x, y)$ will be denoted by $\mathcal{L}[L_A, L_B]$, and is called the *superoperator function*. To this purpose, we denote by $K_{A,B}$ the set of all single-valued functions $L(x, y)$, which are analytic in some neighborhood of the spectrum $\sigma(A) \times \sigma(B)$. Let $L(x, y) \in K_{A,B}$, and let sets $\sigma(A)$ and $\sigma(B)$ on the complex plane be contained inside of the curves C_A and C_B. Then the superoperator $\mathcal{L}[L_A, L_B]$ on a Banach operator space $\mathcal{M}$ will be defined by

$$\mathcal{L}[L_A, R_B] = \frac{1}{(2\pi i)^2} \oint_{C_A} \oint_{C_B} L(x, y)\,R(x, L_A)R(y, R_B)\,dx\,dy, \tag{4}$$

where $x, y \in \mathbb{C}$, and

$$R(x, L_A) = L^{-1}_{zI-A} = (xL_I - L_A)^{-1},$$
$$R(x, R_B) = R^{-1}_{zI-B} = (xR_I - R_B)^{-1}.$$

This formula gives a correspondence between functions from $K_{A,B}$ and superoperators on $\mathcal{M}$.

The feature of greatest importance in this association is that this correspondence between $L(x, y)$ and $\mathcal{L}[L_A, R_B]$ preserves the basic algebraic operations. The following properties are satisfied:

(1) If $L(x, y) \equiv 1$, then $\mathcal{L}[L_A, R_B] = L_I$.

(2) If $L(x, y) \equiv a_1 L_1(x, y) + a_2 L_2(x, y)$, where $a_1, a_2 \in \mathbb{C}$, then $\mathcal{L}[L_A, R_B] = a_1 \mathcal{L}_1[L_A, R_B] + a_2 \mathcal{L}_2[L_A, R_B]$.
(3) If $L(x, y) \equiv L_1(x, y) L_2(x, y)$, then

$$\mathcal{L}[L_A, R_B] = \mathcal{L}_1[L_A, R_B] \mathcal{L}_2[L_A, R_B]. \tag{5}$$

(4) If $L_k(x, y) \to L(x, y)$ for $(x, y) \in \sigma(A) \times \sigma(B)$, then $\mathcal{L}_k[L_A, R_B] \to \mathcal{L}[L_A, R_B]$.

The superoperator $\mathcal{L}[L_A, R_B]$ acts on $X \in \mathcal{M}$ by

$$\mathcal{L}[L_A, R_B]X = \frac{1}{(2\pi i)^2} \oint_{C_A} \oint_{C_B} L(x, y)\, R(x, A) X R(y, B)\, dx\, dy, \tag{6}$$

where $R(x, A) = (xI - A)^{-1}$, and $R(y, B) = (yI - B)^{-1}$.

It is possible to consider the association of $\mathcal{L}[L_A, R_B]$ with $L(x, y)$ as an algebraic homomorphism. But in order to be precise about this, it is first of all necessary to convert $K_{A,B}$ into an algebra by an appropriate equivalence relation. We define two functions $L_1(x, y)$, $L_2(x, y)$ as being equivalent if $L_1(x, y) = L_2(x, y)$ on some open set containing $\sigma(A) \times \sigma(B)$. Then $K_{A,B}$ is divided into equivalence classes, and these classes form a superoperator algebra with a unit element, if we define the algebraic operations in an obvious way.

THEOREM. *The mapping $L(x, y) \to \mathcal{L}[L_A, R_B]$ by the formula (4) is an algebraic homomorphism of the algebra of the equivalence classes of $K_{A,B}$ into the algebra $\mathcal{A}(\mathcal{M})$. This mapping carries the function $L(x, y) = 1$ into I_I, and the functions $L(x, y) = x$, $L(x, y) = y$ into L_A, R_B.*

As a result, we have an algebra $\mathcal{A}(\mathcal{M})$ of superoperator function. If $\mathcal{M}$ is an associative Banach operator algebra, then $L_A R_B = R_B L_A$ and the algebra $\mathcal{A}(\mathcal{M})$ is a commutative associative Banach algebra of superoperators.

12.2. Inverse superoperator function

Let $\mathcal{M}$ be an operator Banach space, and let A, B be bounded operators with domain and range in $\mathcal{M}$. A superoperator $F[L_A, R_B]$ on $\mathcal{M}$ is called an inverse of $\mathcal{L}[L_A, R_B]$ if

$$\mathcal{L}[L_A, R_B] F[L_A, R_B] X = X, \qquad F[L_A, R_B] \mathcal{L}[L_A, R_B] X = X$$

for all $X \in \mathcal{M}$.

THEOREM. *Suppose $A, B \in \mathcal{M}$ and $L(x, y) \in K_{A,B}$. Suppose $L(x, y) \neq 0$ when $(x, y) \in \sigma(A) \times \sigma(B)$. Then $\mathcal{L}[L_A, R_B]$ is a one-to-one mapping of $\mathcal{M}$*

onto all $\mathcal{M}$, with inverse $F[L_A, R_B]$, where $F(x, y)$ is any element of $K_{A,B}$ such that $F(x, y)L(x, y) = 1$.

In this case, the equation

$$\mathcal{L}[L_A, R_B]X = Y,$$

where $Y \in \mathcal{M}$, has the solution

$$X = \frac{1}{(2\pi i)^2} \oint_{C_A} \oint_{C_B} F(x, y)\, R(x, A) Y R(y, B)\, dx\, dy. \tag{7}$$

If $G(a, b)$ is a Fourier transform of $F(x, y) = 1/L(x, y)$, then

$$F(x, y) = \int da\, db\, e^{i(ax+by)} G(a, b).$$

Substituting of this equation into (7) and changing the order of integrations, we obtain

$$X = \frac{1}{(2\pi i)^2} \int da\, db\, G(a, b) \left(\oint_{C_A} e^{iax} R(x, A)\, dx \right) Y \left(\oint_{C_B} e^{iby} R(y, B)\, dy \right).$$

As a result, equation (7) has the form

$$X = \int da\, db\, G(a, b) e^{iaA} Y e^{ibB}.$$

Then this equation gives

$$F[L_A, R_B] = \int da\, db\, G(a, b)\, L_{\exp(iaA)} R_{\exp(ibB)}.$$

12.3. Superoperator function and Fourier transform

Using the one-to-one correspondence between the analytic functions $L(x, y)$ and the superoperators (4), we can derive another representation for the superoperator function $\mathcal{L}[L_A, R_B]$. To this purpose, we consider a Fourier transformation of $L(x, y) \in K_{A,B}$, where $(x, y) \in \sigma(A) \times \sigma(B)$. The Fourier transform of $L(x, y)$ gives

$$\tilde{L}(a, b) = \frac{1}{(2\pi)^2} \int da\, db\, e^{-i(ax+by)} L(x, y).$$

Then $L(x, y)$ is an inverse Fourier transform of $\tilde{L}(a, b)$, such that

$$L(x, y) = \int da\, db\, e^{i(ax+by)} \tilde{L}(a, b). \tag{8}$$

Substituting of (8) into (4) and changing the order of integration, we obtain

$$\mathcal{L}[L_A, R_B] = \frac{1}{(2\pi i)^2} \int da\, db\, \tilde{L}(a,b) \Bigg(\oint_{C_A} \oint_{C_B} e^{i(ax+by)} R(x, L_A) R(y, R_B)\, dx\, dy \Bigg).$$

As a result, this equation can be written in the form

$$\mathcal{L}[L_A, R_B] = \int da\, db\, \tilde{L}(a,b) e^{iaL_A} X e^{ibR_B},$$

where

$$\exp\{iaL_A\} = \frac{1}{2\pi i} \oint_{C_A} e^{iax} R(x, L_A)\, dx,$$

$$\exp\{ibR_B\} = \frac{1}{2\pi i} \oint_{C_B} e^{iby} R(x, R_B)\, dy.$$

12.4. Exponential superoperator function

To each pair L_A, R_B of elements of a superoperator linear space $\mathcal{A}(\mathcal{M})$, we can associate exponential superoperator functions $\exp\{iaL_A\}$ and $\exp\{ibR_B\}$ such that

$$e^{iaL_A} X = e^{iaA} X, \qquad e^{ibR_B} X = X e^{ibB}.$$

If L_A and R_A are bounded superoperators, we can define these exponentials of L_A and R_A by the relations

$$e^{iaL_A} = \sum_{k=0}^{\infty} \frac{(ia)^k}{k!} (L_A)^k, \qquad e^{ibR_B} = \sum_{k=0}^{\infty} \frac{(ib)^k}{k!} (R_B)^k$$

since each series converges in norm. If L_A and R_A are unbounded self-adjoint superoperators, we cannot use the power series directly, but we can use equation (4). The superoperator exponentials of L_A and R_A can be defined by

$$e^{iaL_A} = \frac{1}{2\pi i} \oint_{C_A} e^{iax} R(x, L_A)\, dx, \qquad e^{ibR_B} = \frac{1}{2\pi i} \oint_{C_B} e^{iby} R(y, R_B)\, dy.$$

If $\mathcal{M}$ is an associative algebra, then

$$\exp\{iaL_A\} = L_{\exp(iaA)}, \qquad \exp\{ibR_B\} = R_{\exp(ibB)}.$$

DEFINITION. A *one-parameter group* on $\mathcal{M}$ is a set of linear superoperators $\{U(a) | \, a \in \mathbb{R}\}$ on $\mathcal{M}$, such that the following requirements are satisfied:

(1) $U(a)U(a')A = U(a+a')A$ for all $A \in \mathcal{M}$ and $a, a' \in \mathbb{R}$.
(2) $U(0)A = A$ for all $A \in \mathcal{M}$.

Using

$$e^{ia_1x}e^{ia_2x} = e^{i(a_1+a_2)x}, \qquad \left[\exp\{iax\}\right]_{a=0} = 1,$$

equation (5) gives

$$e^{ia_1L_A}e^{ia_2L_A} = e^{i(a_1+a_2)L_A}, \qquad \left[\exp\{iaL_A\}\right]_{a=0} = L_I,$$
$$e^{ib_1R_B}e^{ib_2R_B} = e^{i(b_1+b_2)R_B}, \qquad \left[\exp\{ibR_B\}\right]_{b=0} = R_I.$$

These relations mean that the superoperator functions $\exp\{iaL_A\}$ and $\exp\{ibR_B\}$, $a, b \in \mathbb{R}$, form one-parameter groups of superoperators.

Let us consider the superoperator function

$$U(a,b) = e^{i(aL_A+bR_B)}.$$

The partial derivatives of $U(a,b)$ with respect to a and b at $a = b = 0$ give

$$\left(\frac{\partial}{\partial a}e^{i(aL_A+bR_B)}\right)_{a=b=0} = iL_A, \qquad \left(\frac{\partial}{\partial b}e^{i(aL_A+bR_B)}\right)_{a=b=0} = iR_B.$$

The superoperator functions $U(a,b)$, $a, b \in \mathbb{R}$, form a two-parameters group, since

$$U(a_1,b_1)U(a_2,b_2) = U(a_1+a_2, b_1+b_2), \quad U(0,0) = I.$$

Let us give the important definition regarding generators of subalgebra for the superoperator algebra.

DEFINITION. Let $\mathcal{A}(\mathcal{M})$ be a superoperator algebra and let $\mathcal{L}_k \in \mathcal{A}(\mathcal{M})$ for $k = 1, \ldots, n$. The smallest subalgebra of $\mathcal{A}(\mathcal{M})$ containing $\{\mathcal{L}_k | k = 1, \ldots, n\}$ is the *subalgebra generated by* $\{\mathcal{L}_k | k = 1, \ldots, n\}$. If this subalgebra is all of $\mathcal{A}(\mathcal{M})$, then $\{\mathcal{L}_k | k = 1, \ldots, n\}$ generates $\mathcal{A}(\mathcal{M})$ and the $\mathcal{L}_k$ are *generators of* $\mathcal{A}(\mathcal{M})$. The generators $\mathcal{L}_k$ can be called the *generating superoperators*.

If $\tilde{L}(a,b)$ is an integrable function of the real variables a and b, then

$$\mathcal{L}[L_A, R_B] = \int_{\mathbb{R}^2} \tilde{L}(a,b)e^{i(aL_A+bR_B)}da\,db \tag{9}$$

will be well-defined bounded superoperator. The superoperator $\mathcal{L}[L_A, R_B]$ is called the *symmetric ordered superoperator function*. It is clear that $\mathcal{L}[L_A, R_B]$ is constructed from L_A and R_B in a relatively explicit manner and so may be defined as an explicit superoperator function of L_A and R_B. The collection of all

such $\mathcal{L}[L_A, R_B]$, together with their uniform limits form a superoperator algebra. The superoperators L_A and R_B are generating superoperators of this algebra.

In general,

$$e^{i(aL_A+bR_B)} \neq e^{iaL_A}e^{ibR_B}.$$

If $\mathcal{M}$ is an associative operator algebra, and $A, B \in \mathcal{M}$, then

$$L_A R_B = R_B L_A, \qquad e^{i(aL_A+bR_B)} = e^{iaL_A}e^{ibR_B},$$

and we obtain

$$\mathcal{L}[L_A, R_B] = \int_{\mathbb{R}^2} \tilde{L}(a,b)e^{iaL_A}e^{ibR_B}\,da\,db.$$

In the general case, this superoperator function is not equal to the symmetric ordered superoperator (9).

12.5. Superoperator Heisenberg algebra

Let H_n be a Heisenberg algebra with generators Q_k, P_k, I $(k = 1, \ldots, n)$. The algebra H_n is defined by relations

$$\begin{aligned} &[Q_k, P_m] = i\hbar\delta_{km}I, \\ &[Q_k, Q_m] = [P_k, P_m] = [I, Q_k] = [I, P_k] = 0, \end{aligned} \tag{10}$$

where $k, m = 1, 2, \ldots, n$.

Let L_{Q_k}, R_{Q_k}, L_{P_k}, R_{P_k} be left and right superoperators. Equations (10) give the superoperator commutation relations

$$\begin{aligned} &L_{Q_k}L_{P_m} - L_{P_m}L_{Q_k} = i\hbar\delta_{km}L_I, \\ &R_{Q_k}R_{P_m} - R_{P_m}R_{Q_k} = -i\hbar\delta_{km}R_I, \end{aligned} \tag{11}$$

where $L_I = R_I$ is a unit superoperator. Using $L_A R_B = R_B L_A$, we obtain

$$L_{Q_k}R_{P_m} - R_{P_m}L_{Q_k} = 0, \qquad R_{Q_k}L_{P_m} - L_{P_m}R_{Q_k} = 0.$$

The other commutators are also equal to zero.

We have state that most of the observables in quantum mechanics are elements of enveloping algebras. Let us consider a linear superoperator space of all linear combinations of $L_{Q_k}, R_{Q_k}, L_{P_k}, R_{P_k}$. This linear space, together with the commutation relations for $L_{Q_k}, R_{Q_k}, L_{P_k}, R_{P_k}$, is a Lie algebra. This is the *superoperator Heisenberg algebra* H_n^s. A universal enveloping algebra U_n^s of H_n^s is an algebra of polynomials in $L_{Q_k}, R_{Q_k}, L_{P_k}, R_{P_k}$ $(k = 1, \ldots, n)$. For each polynomial

$$\mathcal{L}(x, y, z, s) = \sum_{|a|,|b|,|c|,|h|<m} L_{abch}x^a y^b z^c s^h,$$

there exists the superoperator polynomial

$$\mathcal{L}[L_Q, L_P, R_Q, R_P] = \sum_{|a|,|b|,|c|,|h|<m} L_{abch}(L_Q)^a (L_P)^b (R_Q)^c (R_P)^h,$$

where $a = (a_1, a_2, \ldots, a_n)$ are multi-indices such that $x^a = x_1^{a_1} x_2^{a_2} \cdots x_n^{a_n}$. It can be easily to verified that in this way we obtain the one-to-one correspondence between the polynomials and polynomial superoperators. We can extend this correspondence to functions and superoperators of a more general form. For this aim, the Weyl superoperators will be defined.

12.6. Superoperator Weyl system

In quantum mechanics the observables such as positions and momenta are represented by self-adjoint operators which are unbounded. Then L_{Q_k}, L_{P_k}, R_{Q_k}, R_{P_k} $(k = 1, \ldots, n)$ are unbounded superoperators. Let us consider bounded superoperator functions for L_{Q_k}, L_{P_k}, R_{Q_k}, R_{P_k}. These bounded superoperators will be defined by

$$\begin{aligned} U^l(a) &= \exp \frac{i}{\hbar} a L_Q, \qquad U^r(c) = \exp \frac{i}{\hbar} c R_Q, \\ V^l(b) &= \exp \frac{i}{\hbar} b L_P, \qquad V^r(h) = \exp \frac{i}{\hbar} h R_P, \end{aligned} \tag{12}$$

where $aL_Q \equiv \sum_{k=1}^n a_k L_{Q_k}$, and $bL_P \equiv \sum_{k=1}^n b_k L_{P_k}$. Using $L_A L_B = L_{AB}$ and $R_A R_B = R_{BA}$, it is not hard to prove that

$$\begin{aligned} U^l(a) &= L_{U(a)}, \qquad U^r(c) = R_{U(c)}, \\ V^l(b) &= L_{V(b)}, \qquad V^r(h) = R_{V(h)}, \end{aligned}$$

where $U(a)$ and $V(b)$ are bounded operators

$$U(a) = \exp \frac{i}{\hbar} a Q, \qquad V(b) = \exp \frac{i}{\hbar} a P.$$

As a result, we have four n-parameter abelian (commutative) groups of superoperators $\{U^l(a), V^l(b), U^r(c), V^r(h)\}$. These groups are continuous with respect to the parameters a, b, c, h.

The commutation relations for L_{Q_k}, L_{P_k}, R_{Q_k}, R_{P_k} can be considered as relations for a Lie algebra of the superoperators $U^l(a)$, $V^l(b)$, $U^r(c)$, $V^r(h)$, where $a, b, c, h \in \mathbb{R}^n$. To show this, we first bring the Heisenberg commutation relations into the so-called Weyl's form. We perform this using the Baker–Hausdorff formula

$$e^A e^B = e^B e^A e^{[A,B]}$$

valid for operators A and B whose commutator is a unity ($[A, B] = cI$, $c \in \mathbb{C}$). Equations (11) give

$$U^l(a)V^l(b) = V^l(b)U^l(a)e^{-\frac{i}{\hbar}ab}, \qquad U^r(c)V^r(h) = V^r(h)U^r(c)e^{+\frac{i}{\hbar}ch}.$$

It is not hard to obtain

$$\begin{aligned} U^l(a)U^l(a') &= U^l(a+a'), & U^r(c)U^r(c') &= U^r(c+c'),\\ V^l(b)V^l(b') &= V^l(b+b'), & V^r(h)V^r(h') &= V^r(h+h'),\\ U^l(a)U^r(c) &= U^r(c)U^l(a), & V^l(b)V^r(h) &= V^r(h)V^r(b). \end{aligned}$$

The representation of commutation relations in the exponential form is called the *superoperator Weyl system*. For any such system there exist by Stone's theorem a set of self-adjoint superoperators such that equations (12) are valid. If $U^l(a)$, $V^l(b)$, $U^r(c)$, $V^r(h)$ are strongly continuous with respect to a, b, c, h, then the generating superoperators Q^l_k, Q^r_k, P^l_k, P^r_k can be derived by

$$\begin{aligned} L_{Q_k} &= -i\frac{\partial U^l(a)}{\partial a_k}, & R_{Q_k} &= -i\frac{\partial U^r(c)}{\partial c_k},\\ L_{P_k} &= -i\frac{\partial V^l(b)}{\partial b_k}, & R_{P_k} &= -i\frac{\partial V^r(h)}{\partial h_k}. \end{aligned}$$

12.7. Algebra of Weyl superoperators

Using the Weyl operators

$$W(a, b) = \exp\frac{i}{\hbar}(aQ + bP),$$

we can define the superoperators $L_{W(a,b)}$ and $R_{W(c,h)}$. Using $L_A L_A = L_{A^2}$ and $R_A R_A = R_{A^2}$, we obtain

$$\begin{aligned} L_{W(a,b)} &= \exp\frac{i}{\hbar}L_{(aQ+bP)} = \exp\frac{i}{\hbar}(aL_Q + bL_P),\\ R_{W(c,h)} &= \exp\frac{i}{\hbar}R_{(cQ+hP)} = \exp\frac{i}{\hbar}(cR_Q + hR_P), \end{aligned}$$

where $a, b, c, h \in \mathbb{R}^n$. The superoperators

$$W(a, b, c, h) = \exp\frac{i}{\hbar}(aL_Q + bL_P + cR_Q + hR_P)$$

are called the *Weyl superoperators*. The relations

$$L_Q R_P = R_P L_Q, \qquad R_Q L_P = L_P R_Q$$

give

$$W(a,b,c,h) = L_{W(a,b)} R_{W(c,h)}.$$

Note that

$$L_{W(a,b)} R_{W(c,h)} = R_{W(c,h)} L_{W(a,b)}.$$

The Weyl superoperators satisfy the composition law

$$\begin{aligned} &W(a_1,b_1,c_1,h_1)W(a_2,b_2,c_2,h_2) \\ &\quad = W(a_1+a_2, b_1+b_2, c_1+c_2, h_1+h_2) \\ &\qquad \times \exp\frac{i}{2\hbar}\big(-[a_1b_2 - a_2b_1] + [c_1h_2 - c_2h_1]\big). \end{aligned} \tag{13}$$

We refer to (13) as the Weyl's form of the superoperator commutation relations. We notice that

$$\begin{aligned} &W(a,0,0,0) = U^l(a), \qquad &&W(0,b,0,0) = V^l(b), \\ &W(0,0,c,0) = U^r(c), \qquad &&W(0,0,0,h) = V^r(h), \end{aligned}$$

and

$$W(a,b,0,0) = L_{W(a,b)}, \qquad W(0,0,c,h) = R_{W(c,h)}.$$

Let $\mathcal{W}$ be a complex linear space of all finite linear combinations

$$\sum_{i=1}^{m} c_i W(a_i, b_i, c_i, h_i).$$

The composition of two elements of $\mathcal{W}$ is again such an element, if we define multiplication on $\mathcal{W}$ by (13). With this definition of multiplication, $\mathcal{W}$ becomes an algebra. We notice that the algebra $\mathcal{W}$ is moreover stable with respect to the conjugation. The adjoint of $W(a,b,c,h)$ is the superoperator $W^*(a,b,c,h)$ defined by

$$W^*(a,b,c,h) = JW(a,b,c,h)J.$$

Using

$$L_Q^* = R_Q, \qquad R_Q^* = L_Q, \qquad L_P^* = R_P, \qquad R_P^* = L_P,$$

and the composition law (13), we obtain

$$\begin{aligned} &W^*(a,b,c,h) = W(-a,-b,-c,-h), \\ &W^*(a,b,c,h)W(a,b,c,h) = L_I. \end{aligned}$$

Finally the superoperator norm provides the norm on $\mathcal{W}$ which then becomes a normed involutive algebra. The algebra $\mathcal{W}$ defined above is the *Weyl superoperator algebra*.

One may define an algebra of superoperators as a collection of bounded superoperators, including the identity superoperator $L_I = R_I$, which is closed under usual algebraic operations of addition, multiplication, and adjunction, and also closed in the weak topology. The algebra of superoperators generated by a set of bounded superoperators as defined above is the same as the smallest algebra of superoperators containing the set. As a result, the algebra of superoperator functions generated by L_Q, R_Q and L_P, R_P, may be defined as the set of all limits in the weak topology of the algebra of all finite linear combinations of the Weyl superoperators $W(a, b, c, h)$.

Let $\mathcal{A}(H_n)$ be a superoperator algebra, and let $\mathcal{L}_k \in \mathcal{A}(\mathcal{M})$ for $k = 1, \ldots, n$. If the smallest subalgebra of $\mathcal{A}(H_n)$ containing

$$\mathcal{G} = \{L_{Q_k}, R_{Q_k}, L_{P_k}, R_{P_k} | k = 1, \ldots, n\}$$

is all of $\mathcal{A}(H_n)$, then $\mathcal{G}$ generates $\mathcal{A}(H_n)$ and the elements of $\mathcal{G}$ are generators (generating superoperators) of $\mathcal{A}(H_n)$.

If $L(a, b, c, h)$ is an integrable function of the real variables a, b, c, h, then

$$\mathcal{L}[L_Q, R_Q, L_P, R_P] = \frac{1}{(2\pi\hbar)^{2n}} \int \tilde{L}(a, b, c, h)\, W(a, b, c, h)\, da\, db\, dc\, dh$$

will be well-defined bounded superoperator. It is clear that $\mathcal{L}[L_Q, R_Q, L_P, R_P]$ is constructed from L_Q, R_Q, L_P, R_P in a relatively explicit manner and so may be defined as an explicit superoperator function of L_Q, R_Q, L_P, R_P. The collection of all such $\mathcal{L}[L_Q, R_Q, L_P, R_P]$, together with their uniform limits form a superoperator algebra. The superoperators L_Q, R_Q, L_P, R_P are generating superoperators of this algebra.

12.8. Superoperator functions and ordering

Let us consider a rule that assigns to each function $L(x, y, z, s)$ exactly one superoperator function $\mathcal{L}[L_Q, L_P, R_Q, R_P]$. However, the rule is not uniquely defined procedure. For example, we may associate the product xy with the superoperators $L_{Q_k} L_{P_k}$ or $L_{P_k} L_{Q_k}$ or also $(1/2)(L_{Q_k} L_{P_k} + L_{P_k} L_{Q_k})$. These correspond to different ordering methods.

To describe the Weyl ordering, we first introduce the Fourier transformation. For $L(x, y, z, s)$ on $\mathbb{R}^{4n}$, define its Fourier transform $\tilde{L}(a, b, c, h)$ by

$$\tilde{L}(a, b, c, h) = \frac{1}{(2\pi\hbar)^{2n}} \int dx\, dy\, dz\, ds\, L(x, y, z, s) e^{-\frac{i}{\hbar}(ax+by+cz+hs)}, \tag{14}$$

where $x = (x_1, \ldots, x_n)$, and $dx = dx_1 \cdots dx_n$. We also define the inverse Fourier transform $L(x, y, z, s)$ of $\tilde{L}(a, b, c, h)$ by

$$L(x, y, z, s) = \frac{1}{(2\pi\hbar)^{2n}} \int da\, db\, dc\, dh\, \tilde{L}(a, b, c, h) e^{\frac{i}{\hbar}(ax+by+cz+hs)}.$$

The Weyl ordering defines $\mathcal{L}[L_Q, L_P, R_Q, R_P]$ for the function $L(x, y, z, s)$ by the equation

$$\begin{aligned}&\mathcal{L}[L_Q, L_P, R_Q, R_P]\\ &\quad = \frac{1}{(2\pi\hbar)^{2n}} \int da\, db\, dc\, dh\, \tilde{L}(a, b, c, h) e^{\frac{i}{\hbar}(aL_Q+bL_P+cR_Q+hR_P)}. \qquad (15)\end{aligned}$$

Using the Weyl superoperators $W(a, b, c, h)$, this equation has the form

$$\mathcal{L}[L_Q, L_P, R_Q, R_P] = \frac{1}{(2\pi\hbar)^{2n}} \int da\, db\, dc\, dh\, \tilde{L}(a, b, c, h) W(a, b, c, h).$$

Substitution of (14) into equation (15) gives

$$\begin{aligned}\mathcal{L}[L_Q, L_P, R_Q, R_P] = \frac{1}{(2\pi\hbar)^{4n}} \int da\, db\, dc\, dh\, dx\, dy\, dz\, ds\, L(x, y, z, s)\\ \cdot W(a, b, c, h) \exp -\frac{i}{\hbar}(ax + by + cz + hs).\end{aligned}$$

This formula can be rewritten in the form

$$\begin{aligned}\mathcal{L}[L_Q, L_P, R_Q, R_P] = \frac{1}{(2\pi\hbar)^{4n}} \int da\, db\, dc\, dh\, dx\, dy\, dz\, ds\, L(x, y, z, s)\\ \cdot \exp \frac{i}{\hbar}\big[a(L_Q - xL_I) + b(L_P - yL_I)\\ + c(R_Q - zR_I) + h(R_P - sR_I)\big].\end{aligned}$$

It can be easily verified that in this way we obtain the one-to-one correspondence between the functions $L(x, y, z, s)$ and the superoperators $\mathcal{L}[L_Q, L_P, R_Q, R_P]$.

These formulas make it possible to define the superoperator $\mathcal{L}[L_Q, L_P, R_Q, R_P]$ for a broad class of functions $L(x, y, z, s)$. For example, if a function $L(x, y, z, s)$ is in $C^\infty(\mathbb{R}^{4n})$ and

$$\left|\partial_x^a \partial_y^b \partial_z^c \partial_s^h L(x, y, z, s)\right| \leqslant C_{xyzs}\big(1 + |x| + |y| + |z| + |s|\big)^m$$

for certain fixed m and for all a, b, c, h, then the suggested formula allows us to define $\mathcal{L}[L_Q, L_P, R_Q, R_P]$ for all functions in $\mathcal{J}(\mathbb{R}^{4n})$. As a result, we consider the superoperator as a map from $\mathcal{J}(\mathbb{R}^{4n})$ into itself, such that it has a dense domain in $L^2(\mathbb{R}^{4n})$.

In general, a mapping from a set of functions $L(x, y, z, s)$ into a set of superoperator functions $\mathcal{L}[L_Q, L_P, R_Q, R_P]$ is not unique. There exist different orderings of generating superoperators L_Q, L_P, R_Q, R_P.

12.9. Weyl ordered superoperator

Weyl ordering for superoperators

Let $\mathcal{M}$ be a Lie–Jordan algebra with unity I that is generated by the set $\mathcal{G} = \{Q^k, P^k, I\colon\ k = 1, \dots, n\}$, such that

$$Q^k \cdot P^l = \delta_{kl} I, \qquad Q^k \cdot Q^l = 0, \qquad P^k \cdot P^l = 0, \tag{16}$$

where $A \cdot B = (1/i\hbar)(AB - BA)$. Then the corresponding multiplication algebra $\mathcal{A}(\mathcal{M})$ is generated by the set $\{L^{\pm}_{Q^k}, L^{\pm}_{P^k}, L^{\pm}_{I}\colon\ Q^k, P^k, I \in \mathcal{G}\}$, such that the following commutation relations are satisfied:

$$\begin{aligned}
&\left[L^{+}_{Q^k}, L^{-}_{P^l}\right] = \delta_{kl} L^{+}_{I}, \qquad \left[L^{-}_{Q^k}, L^{+}_{P^l}\right] = \delta_{kl} L^{+}_{I},\\
&\left[L^{\pm}_{Q^k}, L^{\pm}_{Q^l}\right] = \left[L^{\pm}_{Q^k}, L^{\pm}_{P^l}\right] = \left[L^{\pm}_{P^k}, L^{\pm}_{P^l}\right] = 0,\\
&\left[L^{\mp}_{Q^k}, L^{\pm}_{Q^l}\right] = \left[L^{\mp}_{P^k}, L^{\pm}_{P^l}\right] = \left[L^{\pm}_{Q^k}, L^{\pm}_{I}\right] = \left[L^{\pm}_{P^k}, L^{\pm}_{I}\right] = 0.
\end{aligned}$$

Using the relations

$$L_A = L^{+}_{A} + \frac{i\hbar}{2} L^{-}_{A}, \qquad R_A = L^{+}_{A} - \frac{i\hbar}{2} L^{-}_{A},$$

the Weyl superoperator $W(a, b, c, h)$ can be presented by

$$\mathcal{W}(a, b) = \exp \frac{i}{\hbar}\left(a_{\pm} L^{\pm}_{Q} + b_{\pm} L^{\pm}_{P}\right) \quad (a_{\pm}, b_{\pm} \in \mathbb{R}^n). \tag{17}$$

Here we introduce a new, more compact notation

$$a_{\pm} L^{\pm}_{Q} = a_{+} L^{+}_{Q} + a_{-} L^{-}_{Q}, \qquad b_{\pm} L^{\pm}_{P} = b_{+} L^{+}_{P} + b_{-} L^{-}_{P}.$$

The superoperators (17) satisfy the composition law

$$\mathcal{W}(a_1, b_1)\mathcal{W}(a_2, b_2) = C(a, b)\, \mathcal{W}(a_1 + a_2, b_1 + b_2),$$

where

$$C(a, b) = \exp \frac{-1}{2\hbar^2}\left\{(a_{1+} b_{2-} - a_{2+} b_{1-}) + (a_{1-} b_{2+} - a_{2-} b_{1+})\right\}.$$

We notice that as a consequence of this relation the linear space $\mathcal{A}_W(\mathcal{M})$ of all finite linear combinations

$$\sum_k C_k \mathcal{W}(a_k, b_k)$$

is stable under the product of any two of its elements. Hence it is a superoperator algebra that is moreover stable with respect to the involution

$$\mathcal{W}^* = J\mathcal{W}(a, b)J.$$

Finally the superoperator norm provides the norm on the algebra, which becomes a normed involutive algebra $\mathcal{A}_W(\mathcal{M})$.

If $L(a, b)$ is an integrable function of the variables $a_\pm$, $b_\pm$, then

$$\mathcal{L}[L_Q^\pm, L_P^\pm] = \frac{1}{(2\pi\hbar)^{2n}} \int\limits_{\mathbb{R}^{4n}} \tilde{L}(a, b)\, \mathcal{W}(a, b)\, da\, db$$

is well-defined bounded superoperator. It is clear that $\mathcal{L}[L_Q^\pm, L_P^\pm]$ is a superoperator function of $L_Q^\pm$, $L_P^\pm$. The collection of all such $\mathcal{L}[L_Q^\pm, L_P^\pm]$, together with their uniform limits form a superoperator algebra $\mathcal{A}_W(\mathcal{M})$. This is the *superoperator algebra of Weyl ordered superoperators*. The superoperators $L_Q^\pm$, $L_P^\pm$, R_P are generating superoperators of the algebra $\mathcal{A}_W(\mathcal{M})$.

For $L(x, y, z, s)$ on $\mathbb{R}^{4n}$, define its Fourier transform $\tilde{L}(a, b, c, h)$ by

$$\tilde{L}(a, b) = \frac{1}{(2\pi\hbar)^{2n}} \int dx\, dy\, L(x, y) e^{-\frac{i}{\hbar}(a_\pm x_\pm + b_\pm y_\pm)}, \tag{18}$$

where $x_\pm = (x_{1\pm}, \ldots, x_{n\pm})$, and $dx = dx_{1\pm} \cdots dx_{n\pm}$.

The Weyl ordering defines $\mathcal{L}[L_Q^\pm, L_P^\pm]$ for the function $L(x, y)$ by the equation

$$\mathcal{L}\big[L_Q^\pm, L_P^\pm\big] = \frac{1}{(2\pi\hbar)^{2n}} \int da\, db\, \tilde{L}(a, b) e^{\frac{i}{\hbar}(a_\pm L_Q^\pm + b_\pm L_P^\pm)}. \tag{19}$$

Using the Weyl superoperators $\mathcal{W}(a, b)$, this equation has the form

$$\mathcal{L}\big[L_Q^\pm, L_P^\pm\big] = \frac{1}{(2\pi\hbar)^{2n}} \int da\, db\, \tilde{L}(a, b) \mathcal{W}(a, b).$$

Substitution of (18) into equation (19) gives

$$\begin{aligned}\mathcal{L}\big[L_Q^\pm, L_P^\pm\big] = \frac{1}{(2\pi\hbar)^{4n}} \int da\, db\, dx\, dy\, L(x, y) \\ \times \exp \frac{i}{\hbar}\big(a_\pm\big(L_Q^\pm - x_\pm L_I\big) + b_\pm\big(L_P^\pm - y_\pm L_I\big)\big).\end{aligned} \tag{20}$$

It can be easily verified that in this way we obtain the one-to-one correspondence between the functions $L(x, y)$ and the superoperators $\mathcal{L}[L_Q^\pm, L_P^\pm]$. Then it possible to define the Weyl superoperator $\mathcal{L}[L_Q^\pm, L_P^\pm]$ for a broad class of functions $L(x, y)$. For example, if $L(x, y) \in C^\infty(\mathbb{R}^{4n})$ and

$$\big|\partial_x^\alpha \partial_y^\beta L(x, y)\big| \leqslant C_{xy}\big(1 + |x_+| + |x_-| + |y_+| + |y_-|\big)^m$$

for some m and for all $\alpha_\pm$, $\beta_\pm$, then equation (20) defines $\mathcal{L}[L_Q^\pm, L_P^\pm]$ on the space $\mathcal{J}(\mathbb{R}^{4n})$. As a result, we consider the superoperator as a map from $\mathcal{J}(\mathbb{R}^{4n})$ into itself, such that it has a dense domain in $L^2(\mathbb{R}^{4n})$.

Weyl ordered operators and superoperators

Let A be a quantum observable described by a Weyl ordered operator function $A(Q, P)$, and let $\mathcal{L}$ be a superoperator. The operator $B = \mathcal{L}A$ must be a Weyl ordered operator function $B(Q, P)$. Then $\mathcal{L}$ will be a Weyl ordered superoperator function $\mathcal{L}[L_Q^{\pm}, L_P^{\pm}]$.

Let us give the basic statement regarding Weyl ordered superoperators.

STATEMENT. *A Weyl ordered superoperator $\mathcal{L} = \mathcal{L}[L_Q^{\pm}, L_P^{\pm}]$ is a map that assigns to each Weyl ordered operator $A = A(Q, P)$ exactly one Weyl ordered operator $B(Q, P) = \mathcal{L}A$.*

In the conventional formulation of Hamiltonian quantum dynamics, this requirement is not used. The system is described by the Hamiltonian superoperator

$$\mathcal{L} = \frac{1}{i\hbar}(L_H - R_H) = L_H^-$$

with a Weyl ordered operator $H = H_W(Q, P)$. As a result, the dynamics is described by the operator

$$B = \mathcal{L}A = \frac{1}{i\hbar}[H, A]. \tag{21}$$

In general, this operator is not Weyl ordered.

The Weyl symbol $B_W(q, p)$ of (21) is the following infinite series

$$B_W(p, q) = -\frac{2}{\hbar} H_W(p, q)\left(\sin\frac{\hbar\mathcal{P}}{2}\right) A_W(p, q),$$

where $H_W(q, p)$ and $A_W(q, p)$ are Weyl symbols of the operators H and A. Note that

$$\sin\frac{\hbar\mathcal{P}}{2} = \sum_{k=0}^{\infty} \frac{(-1)^k \hbar^{2k+1}}{2^{2k+1}(2k+1)!}\, \mathcal{P}^{2k+1},$$

where $\mathcal{P} = \overleftarrow{\partial_p}\overrightarrow{\partial_q} - \overleftarrow{\partial_q}\overrightarrow{\partial_p}$ is the operator of Poisson bracket such that

$$H_W(p, q)\overleftarrow{\partial_p}\overrightarrow{\partial_q} A_W(p, q) = \partial_p H_W \partial_q A_W,$$

and $H_W \mathcal{P} A_W = -\{H_W, A_W\}$.

As a result, the equation of motion

$$\frac{d}{dt}A = L_H^- A$$

gives

$$\frac{d}{dt}A_W(q,\,p) = \sum_{kl}^{\infty} c_{kl}(q,\,p)\partial_q^k \partial_p^l A_W(q,\,p).$$

This is the infinite order differential equation. If $\mathcal{L}$ is a Weyl ordered superoperator, then we obtain a finite order differential equation for $A_W(q,\,p)$. The Weyl ordered superoperator $\mathcal{L} = \mathcal{L}[L_Q^{\pm}, L_P^{\pm}]$ gives an operator equation with Weyl ordered operators. As a result, the correspondent equation for the Weyl symbol is of finite order.

Note that the superoperator $L_H^- = L_{H(Q,P)}^-$ cannot be derived by the Weyl quantization of the operator $L_{H(q,p)}^- = \{H(q,\,p),\}$. The Weyl quantization of this operator and the Poisson bracket will be considered in chapter "Quantization of Dynamical Structure".

Chapter 13

Semi-Groups of Superoperators

13.1. Groups of superoperators

Let $\mathcal{M}$ be an operator Banach space.

DEFINITION. A *one-parameter superoperator group* is a set $\{\Phi_t | t \in \mathbb{R}\}$ of maps Φ_t from $\mathcal{M}$ into itself, such that the following requirements are satisfied:

(1) $\Phi_t(aA + bB) = a\Phi_t(A) + b\Phi_t(B)$ for all $A, B \in \mathcal{M}$, $a, b \in \mathbb{C}$, and $t \in \mathbb{R}$.
(2) $\Phi_t(\Phi_s(A)) = \Phi_{t+s}(A)$ for all $A \in \mathcal{M}$, $t, s \in \mathbb{R}$.
(3) $\Phi_{t=0}(A) = A$ for all $A \in \mathcal{M}$.

Requirement (1) expresses the mathematical statement that Φ_t is a linear superoperator on $\mathcal{M}$. Requirement (2) is a group law, and (3) means the existence of unity.

DEFINITION. A *strongly continuous one-parameter group* is a set $\{\Phi_t | t \in \mathbb{R}\}$ of maps from $\mathcal{M}$ into itself, such that the following requirements are satisfied:

(1) $\Phi_t(aA + bB) = a\Phi_t(A) + b\Phi_t(B)$ for all $A, B \in \mathcal{M}$, $a, b \in \mathbb{C}$, and $t \in \mathbb{R}$.
(2) $\Phi_t(\Phi_s(A)) = \Phi_{t+s}(A)$ for all $A \in \mathcal{M}$ and $t, s \in \mathbb{R}$.
(3) $\Phi_{t=0}(A) = A$ for all $A \in \mathcal{M}$.
(4) $\lim_{t\to 0} \|\Phi_t(A) - A\|_{\mathcal{M}} = 0$ for all $A \in \mathcal{M}$.

Requirement (4) define the strongly continuous condition for the one-parameter superoperator group. As a result, we obtain the following equivalent definition.

DEFINITION. A *strongly continuous one-parameter group* is a one-parameter group $\{\Phi_t | t \in \mathbb{R}\}$ on $\mathcal{M}$, such that the requirement

$$\lim_{t\to 0} \big\| \Phi_t(A) - A \big\|_{\mathcal{M}} = 0$$

is satisfied for all $A \in \mathcal{M}$.

DEFINITION. A *weakly continuous one-parameter group* is a one-parameter group $\{\Phi_t | t \in \mathbb{R}\}$ on $\mathcal{M}$, such that the requirement

$$\lim_{t \to 0} (\omega | \Phi_t A) = (\omega | A)$$

is satisfied for all $A \in \mathcal{M}$ and $\omega \in \mathcal{M}^*$.

Here we use the Dirac's notations $(\omega | A) = \omega(A)$. If $\mathcal{M}$ is an operator Hilbert space, then there is $B \in \mathcal{M}$ such that $\omega(A) = (B|A)$. A bounded superoperator Φ_t on an operator Hilbert space $\mathcal{M}$ is called unitary if Φ_t leaves the scalar product $(\ |\ )$ invariant.

DEFINITION. Let $\mathcal{M}$ be an operator Hilbert space. A *unitary one-parameter group* of superoperators is a one-parameter superoperator group $\{\Phi_t | t \in \mathbb{R}\}$ on $\mathcal{M}$, such that the condition

$$(\Phi_t A | \Phi_t B) = (A|B)$$

is satisfied for all $A, B \in \mathcal{M}$ and $t \in \mathbb{R}$.

Unitary superoperator groups play a very important role in quantum theory. It is conventional to describe symmetries of quantum systems by superoperator groups on the kinematical set. Let us give the basic theorem regarding unitary group. The Stone's theorem establishes the general form of a continuous unitary superoperator.

STONE'S THEOREM. *Let $\{\Phi_t | t \in \mathbb{R}\}$ be a strongly (or weakly) continuous unitary one-parameter group of superoperators on a Hilbert operator space $\mathcal{M}$. Then there exists a self-adjoint superoperator $\mathcal{L}$ on $\mathcal{M}$, such that*

$$\Phi_t = \exp it\mathcal{L}.$$

This theorem says that every continuous unitary group arises as the exponential of a self-adjoint superoperator $\mathcal{L}$. The superoperator $\mathcal{L}$ is called the *infinitesimal generator of the group* $\{\Phi_t | t \in \mathbb{R}\}$.

A superoperator of derivation is a linear superoperator $\mathcal{L}$ on $\mathcal{M}$, such that

$$\mathcal{L}(AB) - (\mathcal{L}A)B - A(\mathcal{L}B) = 0 \tag{1}$$

for all $A, B \in \mathcal{D}(\mathcal{L}) \subset \mathcal{M}$. The derivation arises as a generating superoperator of continuous one-parameter group $\{\Phi_t | t \in \mathbb{R}\}$ of automorphisms of C^*-algebra. Property (1) can be obtained by differentiation of the relation

$$\Phi_t(AB) = \Phi_t(A)\Phi_t(B)$$

with respect to t. If $\mathcal{L}$ is a real superoperator, i.e., $\mathcal{L}(A^*) = (\mathcal{L}A)^*$, then Φ_t is real and $\Phi_t(A^*) = (\Phi_t A)^*$.

13.2. Semi-groups of superoperators

Let $\mathcal{M}$ be an operator Banach space. A set of superoperators on $\mathcal{M}$, together with a single binary operation is called a superoperator groupoid. This is still rather to wide concept. The concept of a semi-group is somewhat narrowed. A groupoid satisfying the associative law is called a semi-group. We will consider unital semi-groups, which are semi-groups with an identity superoperator L_I. For the theory of one-parameter semi-groups see, for instance, the books [71,5].

DEFINITION. A *one-parameter semi-group of superoperators* is a set $\{\Phi_t | t \geqslant 0\}$ of all one-parameter superoperators Φ_t on $\mathcal{M}$, such that the following requirements are satisfied:

(1) $\Phi_t(aA + bB) = a\Phi_t(A) + b\Phi_t(B)$ for all $A, B \in \mathcal{M}$, $a, b \in \mathbb{C}$, and $t \geqslant 0$.
(2) $\Phi_t(\Phi_s(A)) = \Phi_{t+s}(A)$ for all $A \in \mathcal{M}$, and $t, s \geqslant 0$.
(3) $\Phi_{t=0}(A) = A$ for all $A \in \mathcal{M}$.

Requirement (1) expresses the statement that Φ_t is a linear superoperator on $\mathcal{M}$ for each $t \geqslant 0$. A one-parameter semi-group is very much like a one-parameter group except that the time interval cannot be negative.

STATEMENT. *All superoperators of a one-parameter semi-group commute.*

PROOF. It is not hard to prove this statement by

$$\Phi_t \Phi_s = \Phi_{t+s} = \Phi_{s+t} = \Phi_s \Phi_t$$

for all $t, s \geqslant 0$. □

A semi-group is said to be strongly continuous, if $t \to \Phi_t$ is a continuous mapping with respect to the norm $\| \ \|_{\mathcal{M}}$ for $t \in (0, \infty)$.

DEFINITION. A *strongly continuous one-parameter semi-group* of superoperators is a set $\{\Phi_t | t \geqslant 0\}$ of superoperators Φ_t on $\mathcal{M}$, such that the following requirements are satisfied:

(1) $\Phi_t(aA + bB) = a\Phi_t(A) + b\Phi_t(B)$ for all $A, B \in \mathcal{M}$, $a, b \in \mathbb{C}$, and $t \geqslant 0$.
(2) $\Phi_t(\Phi_s(A)) = \Phi_{t+s}(A)$ for all $A \in \mathcal{M}$ and $t, s \geqslant 0$.
(3) $\Phi_{t=0} A = A$ for all $A \in \mathcal{M}$.
(4) $\lim_{t \to s} \|\Phi_t(A) - \Phi_s(A)\|_{\mathcal{M}} = 0$ for all $A \in \mathcal{M}$ and $s \in (0, \infty)$.

The one-parameter semi-group $\{\Phi_t | t \geqslant 0\}$ on $\mathcal{M}$ is called the strongly continuous semi-group, if

$$\lim_{t \to s+0} \big\| \Phi_t(A) - \Phi_s(A) \big\|_{\mathcal{M}} = \lim_{t \to s-0} \big\| \Phi_t(A) - \Phi_s(A) \big\|_{\mathcal{M}} = 0 \tag{2}$$

for all $A \in \mathcal{M}$ and $s > 0$. Note that $s = 0$ is not included. As a result, we obtain the following equivalent definition.

DEFINITION. A *strongly continuous one-parameter semi-group* of superoperators is a one-parameter semi-group $\{\Phi_t | t \geqslant 0\}$ on $\mathcal{M}$, such that the requirement

$$\lim_{t \to s} \|\Phi_t A - \Phi_s A\|_{\mathcal{M}} = 0 \tag{3}$$

is satisfied for all $A \in \mathcal{M}$ and $s > 0$.

The notation

$$s\text{-}\lim_{t \to \tau} \Phi_t A = \Phi_\tau A$$

is also used for (3) in the literature.

DEFINITION. A *weakly continuous one-parameter semi-group* of superoperators is a one-parameter semi-group $\{\Phi_t |\ t \geqslant 0\}$ on $\mathcal{M}$, such that the requirement

$$\lim_{t \to s} \omega(\Phi_t A) = \omega(\Phi_s A) \tag{4}$$

is satisfied for all $A \in \mathcal{M}$, $s > 0$ and $\omega \in \mathcal{M}^*$.

In the Dirac's notations $\omega(A) = (\omega|A)$. Equation (4) is also written as

$$w\text{-}\lim_{t \to s} \Phi_t A = \Phi_s A.$$

We can consider a semi-group with the following requirement at $t = 0$:

$$\lim_{t \to 0+} \big\|\Phi_t(A) - A\big\|_{\mathcal{M}} = 0. \tag{5}$$

This is the right continuous at $t = 0$. The property $\Phi_t \Phi_s = \Phi_{t+s}$ and equation (5) gives the right continuous at each $t \geqslant 0$, i.e.,

$$\lim_{t \to s+0} \big\|\Phi_t(A) - \Phi_s A\big\|_{\mathcal{M}} = 0$$

for all $s \geqslant 0$. In general, this condition is not equivalent to (2).

We say that semi-group $\{\Phi_t | t \geqslant 0\}$ belongs to the class (C_0) if it is strongly continuous and satisfies condition (5) for arbitrary $A \in \mathcal{M}$. The semi-group of class (C_0) is strongly continuous on $[0, \infty)$.

DEFINITION. A *semi-group of class* (C_0) is a one-parameter semi-group $\{\Phi_t | t \geqslant 0\}$ of bounded superoperators on $\mathcal{M}$, such that

$$\lim_{t \to s} \|\Phi_t A - \Phi_s A\|_{\mathcal{M}} = 0 \tag{6}$$

for each $s \geqslant 0$ and each $A \in \mathcal{M}$.

A semi-group of class (C_0) is weakly continuous.

THEOREM. *If the semi-group* $\{\Phi_t | t \geqslant 0\}$ *on* $\mathcal{M}$ *belongs to the class* (C_0), *then condition* (6) *is equivalent to the weak continuity condition* (4) *for all* $t \geqslant 0$.

A *norm of superoperator* Φ_t on an operator Banach space $\mathcal{M}$ is the number

$$\|\Phi_t\| = \sup_{A \in \mathcal{M}} \frac{\|\Phi_t(A)\|_{\mathcal{M}}}{\|A\|_{\mathcal{M}}}.$$

DEFINITION. A *contractive semi-group* is a one-parameter semi-group of superoperators $\{\Phi_t | t \geqslant 0\}$ on $\mathcal{M}$, such that $\|\Phi_t\| \leqslant 1$ for all $t \geqslant 0$.

An *isometric semi-group* is a semi-group of bounded superoperators $\{\Phi_t |\ t \geqslant 0\}$ on a Hilbert operator space $\mathcal{M}$, such that Φ_t leaves the scalar product invariant:

$$(\Phi_t A | \Phi_t B) = (A|B) \tag{7}$$

for all $A, B \in \mathcal{M}$ and $t \geqslant 0$.

For a bounded linear superoperator Φ_t, condition (7) is equivalent to the condition of the isometry $\|\Phi_t A\|_{\mathcal{M}} = \|A\|_{\mathcal{M}}$ for all $A \in \mathcal{M}$, and $t \geqslant 0$.

DEFINITION. A *norm continuous one-parameter semi-group* of superoperators is a one-parameter semi-group $\{\Phi_t | t \geqslant 0\}$ on $\mathcal{M}$, such that

$$\lim_{t \to s} \|\Phi_t - \Phi_s\| = 0$$

for all $s \geqslant 0$ and $t > s$.

If $\{\Phi_t | t \geqslant 0\}$ is a semi-group, then the following conditions are equivalent:

(1) Φ_t is norm-continuous.
(2) $\lim_{t \to 0} \|\Phi_t - L_I\| = 0$.
(3) There exists a bounded superoperator $\mathcal{L}$ such that

$$\lim_{t \to 0} \|t^{-1}(\Phi_t - L_I) - \mathcal{L}\| = 0.$$

(4) $\Phi_t = \exp(t\mathcal{L}) = \sum_{k=0}^{\infty} (t^k/k!)\mathcal{L}^k$.

Note that $\|\Phi_t\| \leqslant \exp(t\|\mathcal{L}\|)$ for all $t \geqslant 0$.
We can define the function

$$f(t) = \ln \|\Phi_t\|.$$

Using $\Phi_{t_1+t_2} = \Phi_{t_1}\Phi_{t_2}$ and $\|AB\|_{\mathcal{M}} \leqslant \|A\|_{\mathcal{M}}\|B\|_{\mathcal{M}}$, we obtain

$$\|\Phi_{t_1+t_2}\| \leqslant \|\Phi_{t_1}\|\|\Phi_{t_2}\|.$$

Then $f(t_1 + t_2) \leqslant f(t_1) f(t_2)$. This condition is called the subadditivity. If $f(t)$ is a subadditive function, then there exists the limit

$$\lim_{t \to \infty} t^{-1} f(t) = \sigma_s < \infty.$$

As a result, we have

$$\lim_{t \to \infty} t^{-1} \ln \|\Phi_t\| = \sigma_s < \infty. \tag{8}$$

DEFINITION. Let $\{\Phi_t | t \geqslant 0\}$ be a one-parameter strongly continuous semi-group. The number

$$\sigma_s = \lim_{t \to \infty} t^{-1} \ln \|\Phi_t\|$$

is called the *leading index*.

For an arbitrary strongly continuous semi-group $\{\Phi_t | t \geqslant 0\}$, there exists the limit (8). If the semi-group belongs to the class (C_0), then we have the following estimate.

THEOREM. *A semi-group* $\{\Phi_t | t \geqslant 0\}$ *of class* (C_0) *satisfies the condition*

$$\|\Phi_t\| \leqslant M e^{\sigma_s t} \quad (t \geqslant 0)$$

with constants $M > 0$ *and* $\sigma_s < \infty$.

If $\sigma_s = 0$, then the semi-group $\{\Phi_t | t \geqslant 0\}$ of class (C_0) is bounded, i.e., $\|\Phi_t\| \leqslant M$. If $M \leqslant 1$, then $\{\Phi_t | \ t \geqslant 0\}$ is a contractive semi-group, i.e., $\|\Phi_t\| \leqslant 1$.

The following are examples of some semi-groups.

(1) For the superoperator

$$\mathcal{L} = \begin{pmatrix} 0 & L_I \\ 0 & 0 \end{pmatrix},$$

we obtain

$$\Phi_t = \exp(t\mathcal{L}) = L_I + t\mathcal{L}.$$

(2) The generating superoperator

$$\mathcal{L} = i \begin{pmatrix} 0 & L_I \\ L_I & 0 \end{pmatrix}$$

gives

$$\Phi_t = \exp(t\mathcal{L}) = (\cos t)\, L_I + (\sin t)\, \mathcal{L}.$$

13.3. Generating superoperators of semi-groups

Definition of generating superoperator

The theory of semi-groups of bounded superoperators on a Banach operator space deals with the exponential superoperator functions. It is connected with the problem of determining the most general bounded superoperators Φ_t, $t \geqslant 0$, which form a one-parameter semi-group. The problem for superoperator semi-group can be considered as a natural generalization of the well-known problem for the bounded operators on infinite-dimensional function space. This problem was investigated by E. Hille and K. Yosida. They introduced the infinitesimal generator $\mathcal{L}$ of Φ_t, and discussed the generation of Φ_t in terms of $\mathcal{L}$. A description of the infinitesimal generator $\mathcal{L}$ in terms of the spectral property of $\mathcal{L}$ is described by Hille–Yosida–Phillips theorem. The basic results of the superoperator semi-group theory may be considered as a generalization of the Stone's theorem for one-parameter superoperator group on a Hilbert operator space.

DEFINITION. Let $\{\Phi_t | t \geqslant 0\}$ be a strongly continuous semi-group on an operator Banach space $\mathcal{M}$. An *infinitesimal generator*, or *generating superoperator* of the semi-group $\{\Phi_t | t \geqslant 0\}$ is a linear superoperator $\mathcal{L}$ on $\mathcal{M}$, such that

$$\mathcal{L}(A) = s\text{-}\lim_{\varepsilon \to 0+} \frac{1}{\varepsilon}\big[\Phi_\varepsilon(A) - A\big]$$

for all $A \in \mathcal{M}$.

The linear superoperator $\mathcal{L}$ is defined on the elements $A \in \mathcal{M}$ for which $\Phi_t A$ is differentiable at $t = 0$. This is the domain $D(\mathcal{L}) \subset \mathcal{M}$ of $\mathcal{L}$. If the semi-group belongs to the class (C_0), then the domain $D(\mathcal{L})$ of the generating superoperator $\mathcal{L}$ is everywhere dense.

Let $\mathcal{L}$ be a bounded superoperator. By Dunford's theorem, we can define the one-parameter superoperator

$$e_t(\mathcal{L}) = \exp\{t\mathcal{L}\} = \frac{1}{2\pi i} \oint_{C_\mathcal{L}} e^{itx} R(x, \mathcal{L})\, dx.$$

The set of all superoperators $e_t(\mathcal{L})$ with $t \geqslant 0$ forms a semi-group. The semi-group $\{e_t(\mathcal{L}) | t \geqslant 0\}$ belongs to the class (C_0), and $\mathcal{L}$ is a generating superoperator of this semi-group.

Closed generating superoperator

In non-Hamiltonian quantum mechanics, it is important to consider some generating superoperators that are not continuous. Many of the most important discon-

tinuous superoperators have a property that in some respects compensates for the absence of the property of continuity.

DEFINITION. A *closed superoperator* is a superoperator $\mathcal{L}$ on an operator Banach space $\mathcal{M}$, such that the conditions

$$s\text{-}\lim_{k\to\infty} A_k = A, \qquad s\text{-}\lim_{k\to\infty} \mathcal{L}A_k = B,$$

where all $A_k \in D(\mathcal{L})$, implies $A \in D(\mathcal{L})$, and $B = \mathcal{L}A$.

Let us give the basic theorem regarding closed generating superoperators.

THEOREM. *If the semi-group* $\{\Phi_t | t \geqslant 0\}$ *belongs to the class* (C_0)*, then the infinitesimal generator* $\mathcal{L}$ *is closed and commutes with the superoperator* Φ_t *on its domain of definition*:

$$\mathcal{L}\Phi_t = \Phi_t \mathcal{L}.$$

Note that a bounded superoperator is closed, and a self-adjoint unbounded superoperator is also closed.

STATEMENT. *If* $\mathcal{L}$ *is a closed unbounded superoperator then the resolvent* $R(z, \mathcal{L}) = (zL_I - \mathcal{L})^{-1}$ *is a bounded superoperator for all* $z \in \rho(\mathcal{L})$.

As a result, the class of unbounded generating superoperators can be characterized by the behavior of the resolvents. Thus the notion of a closed superoperator is an extension of the notion of a bounded superoperator.

Resolvent of generating superoperator

THEOREM. *The spectrum of the generating superoperator* $\mathcal{L}$ *of a semi-group of class* (C_0) *lies always in the half-plane* $\mathrm{Re}(z) \leqslant \sigma_s$.

The generating superoperators $\mathcal{L}$ can be characterized by the behavior of the resolvents $R(z, \mathcal{L}) = (zL_I - \mathcal{L})^{-1}$.

THEOREM. *In order to the closed superoperator* $\mathcal{L}$ *to be the infinitesimal generator of a semi-group of class* (C_0)*, it is necessary and sufficient that there exist* $\sigma_s \in \mathbb{R}$ *and* $M > 0$ *such that*

$$\left\| R(z, \mathcal{L})^n \right\| \leqslant \frac{M}{(z - \sigma_s)^n} \quad (z > \sigma_s,\ n = 0, 1, 2, \ldots). \tag{9}$$

The estimate

$$\|\Phi_t\| \leqslant Me^{\sigma_s t}$$

is valid.

Note that the condition $z > \sigma_s$ means that $z \in \mathbb{R}$ and $z \in (\sigma_s, \infty)$. The verification of the necessary and sufficient conditions (9) is difficult since all the powers ($n \in \mathbb{N}$) of the resolvent superoperator appear in them. They will be satisfied if

$$\big\| R(z, \mathcal{L}) \big\| \leqslant \frac{1}{z - \sigma_s}, \tag{10}$$

where $z > \sigma_s$. If estimate (10) holds, then the inequality $\|\Phi_t\| \leqslant \exp\{\sigma_s t\}$ is valid. In particular, if $\sigma_s = 0$, then $\|\Phi_t\| \leqslant 1$ and the semi-group is contractive.

THEOREM. *The semi-group* $\{\Phi_t | t \geqslant 0\}$ *of class* (C_0) *can be represented by the equation*

$$\Phi_t = \frac{1}{2\pi i} \int\limits_{\sigma - i\infty}^{\sigma + i\infty} dz\, e^{zt} R(z, \mathcal{L}),$$

which is valid on $D(\mathcal{L})$, $t > 0$ *and some* $\sigma > 0$.

The resolvent superoperator $R(z, \mathcal{L})$ is the Laplace transform of the semi-group superoperator:

$$R(z, \mathcal{L}) = \int\limits_0^{+\infty} dt\, e^{-zt} \Phi_t. \tag{11}$$

The integral converges when $\mathrm{Re}(z) > \sigma_s$.

13.4. Contractive semi-groups and its generators

The basic results of the semi-groups theory can be considered as a natural generalization of the Stone's theorem. These results deal with the exponential form of semi-groups.

HILLE–YOSIDA THEOREM. *Let* $\mathcal{L}$ *be a closed superoperator on a Banach operator space* $\mathcal{M}$. *Then* $\mathcal{L}$ *is an infinitesimal generator of a contractive strongly continuous semi-groups if and only if the following requirements are satisfied*:

(1) $\|zI - \mathcal{L}\| \leqslant z^{-1}$ *for all* $\mathrm{Re}(z) > 0$.

(2) *All positive real numbers belong to the resolvent set* $\rho(\mathcal{L})$. *In other words, there exists the resolvent* $R(z, \mathcal{L}) = (zI - \mathcal{L})^{-1}$ *for all* z *such that* $\mathrm{Re}(z) > 0$.

Note that the right half plane $\mathrm{Re}(z) > 0$ of the complex z-plane is in the resolvent set $\rho(\mathcal{L})$, i.e., $\{z \in \mathbb{C}\colon \mathrm{Re}(z) > 0\} \subset \rho(\mathcal{L})$. If the requirements of the theorem are satisfied, then the resolvent $R(z, \mathcal{L})$ of $\mathcal{L}$ is the Laplace transformation (11) of Φ_t. This theorem can be presented in the form.

HILLE–YOSIDA THEOREM. *Let* $\mathcal{L}$ *be a closed superoperator whose domain* $D(\mathcal{L})$ *is dense in a Banach operator space* $\mathcal{M}$. *Then* $\mathcal{L}$ *is a generating superoperator of a contractive strongly continuous semi-group, if and only if the following requirements are satisfied*:

(1) *For any* $z > 0$, *the resolvent* $R(z, \mathcal{L})$ *is a bounded superoperator.*
(2) *For each integer* $n > 1$ *and* $z > 0$, $\|R(z, \mathcal{L})^n\| < 1/z^n$.

The Hille–Yosida theorem characterizes generators by properties of their resolvents. The application of the Hille–Yosida theorem is difficult since the resolvent $R(z, \mathcal{L}) = (zI - \mathcal{L})^{-1}$ should be constructed to verify the conditions. Therefore, we would like to have the description in terms connected with the superoperator itself and not with its resolvent. We would like to have requirements for the superoperator $\mathcal{L}$, which are analogs of self-conjugacy of the generating superoperator that is used in the Stone's theorem. For this purpose, we define a concept of dissipative superoperator. We will consider an alternative characterization of weakly continuous semi-group in which the notion of dissipative superoperator is used.

DEFINITION. Let A be an element of an operator Banach space $\mathcal{M}$. A *tangent functional* at A is an element $\omega \in \mathcal{M}^*$ such that $\omega(A) = \|\omega\|\|A\|_{\mathcal{M}}$.

The Hahn–Banach theorem states that for each $A \in \mathcal{M}$ there exists at least one nonzero tangent functional at A.

DEFINITION. Let A be an element of an operator Banach space $\mathcal{M}$. A *normalized tangent functional* at A is an element $\omega \in \mathcal{M}^*$ such that

$$\|\omega\| = 1, \qquad \omega(A) = \|A\|_{\mathcal{M}}.$$

Let us define dissipative, accretive, and conservative superoperators.

DEFINITION. A *dissipative superoperator* is a superoperator $\mathcal{L}$ with domain $D(\mathcal{L})$ in an operator Banach space $\mathcal{M}$, such that for each $A \in D(\mathcal{L})$ there exists a nonzero tangent functional ω at A, and $\mathrm{Re}[\omega(\mathcal{L}A)] \leqslant 0$.

A superoperator $\mathcal{L}$ is called *accretive* if $\mathrm{Re}[\omega(\mathcal{L}A)] \geqslant 0$ for each $A \in D(\mathcal{L})$.

A superoperator $\mathcal{L}$ is called *conservative* if $\mathrm{Re}[\omega(\mathcal{L}A)] = 0$ for all $A \in D(\mathcal{L})$.

The symbol $Dis(\mathcal{M})$ denotes the set of all dissipative superoperators. If $\mathcal{L}$ is a dissipative superoperator, then $-\mathcal{L}$ is accretive.

DEFINITION. Let $\mathcal{M}$ be a Hilbert operator space. A superoperator $\mathcal{L}$ on $\mathcal{M}$ with an everywhere dense domain $D(\mathcal{L})$ is called *dissipative* if $\operatorname{Re}(\mathcal{L}A|A) \leqslant 0$ for all $A \in D(\mathcal{L})$.

To explain the notation, we suppose that $\{\Phi_t | t \geqslant 0\}$ is a contractive semi-group of class (C_0) with generator $\mathcal{L}$ and that ω is a tangent functional at $A \in D(\mathcal{M})$. Then

$$\big|\omega(\Phi_t A)\big| = \|\omega\|\|\Phi_t A\|_{\mathcal{M}} \leqslant \|\omega\|\|A\|_{\mathcal{M}} = \big|\omega(\Phi_0 A)\big|$$

for all $t \geqslant 0$. This implies that

$$\operatorname{Re}\big[\omega(\Phi_t A)\big] \leqslant \operatorname{Re}\big[\omega(\Phi_0 A)\big],$$

and hence

$$\left(\frac{d}{dt}\operatorname{Re}\big[\omega(\Phi_t A)\big]\right)_{t=0} \leqslant 0.$$

Using $d\Phi_t/dt = \mathcal{L}$, we obtain the condition $\operatorname{Re}[\omega(\mathcal{L}A)] \leqslant 0$. As a result, we see that the generator $\mathcal{L}$ of a contractive semi-group of class (C_0) is dissipative.

THEOREM. *If $\mathcal{L}$ is a dissipative superoperator on a Banach operator space $\mathcal{M}$, then*

$$\big\|(L_I - z\mathcal{L})A\big\|_{\mathcal{M}} \geqslant \|A\|_{\mathcal{M}} \tag{12}$$

for all $z \geqslant 0$, and all $A \in D(\mathcal{L})$.

PROOF. Let ω be a nonzero tangent functional at $A \in D(\mathcal{L})$. If $\mathcal{L}$ is dissipative, then $-z\operatorname{Re}[\omega(\mathcal{L}A)] \geqslant 0$ for all $z \geqslant 0$, and hence

$$\|\omega\|\|A\|_{\mathcal{M}} = \operatorname{Re}\big[\omega(A)\big] \leqslant \operatorname{Re}\big[\omega\big((L_I - z\mathcal{L})A\big)\big] \leqslant \|\omega\|\big\|(L_I - z\mathcal{L})A\big\|_{\mathcal{M}}.$$

Division by $\|\omega\|$ gives the desired results. □

This theorem allows us to give the following definitions.

DEFINITION. A *dissipative superoperator* is a superoperator $\mathcal{L}$ with domain $D(\mathcal{L})$ in an operator Banach space $\mathcal{M}$, such that condition (12) is satisfied for all $A \in D(\mathcal{L})$ and $z > 0$.

The most interesting are the maximal dissipative extensions, i.e., the superoperators that cannot be extended further with preservation of dissipativeness.

DEFINITION. A superoperator $\mathcal{L}$ on a Banach operator space $\mathcal{M}$ is called *maximal dissipative*, or *m-dissipative*, if $L_I - z\mathcal{L}$ is a superoperator whose range is $\mathcal{M}$, i.e.,

$$R(L_I - z\mathcal{L}) = \mathcal{M}$$

for each $z > 0$.

THEOREM. *Let $\{\Phi_t | t \geqslant 0\}$ be a contractive semi-group of class (C_0). An infinitesimal generator of the semi-group is a superoperator $\mathcal{L}$ such that:*

(1) *$\mathcal{L}$ is maximal dissipative.*
(2) *$D(\mathcal{L})$ is dense in $\mathcal{M}$.*
(3) *The resolvent of $\mathcal{L}$ is the Laplace transform of the superoperator Φ_t:*

$$R(z, \mathcal{L}) = (zL_I - \mathcal{L})^{-1} = \int_0^\infty dt\, e^{-tz}\Phi_t \tag{13}$$

for all $z > 0$.

Let us give the basic theorem regarding characterization of generating superoperator $\mathcal{L}$ for the contractive semi-groups of class (C_0).

LUMER–PHILLIPS THEOREM. *Let $\mathcal{L}$ be a closed superoperator with domain $D(\mathcal{L})$ and range $R(\mathcal{L})$ both in a Banach operator space $\mathcal{M}$. Then $\mathcal{L}$ is a generating superoperator of a contractive semi-group of class (C_0) if and only if the following conditions are satisfied*:

(1) *$\mathcal{L}$ is a dissipative superoperator, i.e., $\mathcal{L} \in Dis(\mathcal{M})$.*
(2) *$D(\mathcal{L})$ is dense in $\mathcal{M}$.*
(3) *$\mathcal{L}$ is a m-dissipative superoperator, i.e., $R(L_I - z\mathcal{L}) = \mathcal{M}$.*

If $\mathcal{L}$ is a maximal dissipative superoperator, then $(L_I - z\mathcal{L})^{-1}$ is a bounded superoperator such that the estimate

$$\left\|(L_I - z\mathcal{L})^{-1}\right\| \leqslant 1$$

is valid of it.

Let Φ_t be a bounded superoperator for each t. If the semi-group $\{\Phi_t | t \geqslant 0\}$ belongs to the class (C_0), then the estimate

$$\|\Phi_t A\|_{\mathcal{M}} \leqslant Me^{\sigma t} \quad (t \geqslant 0)$$

is valid. For each $A \in \mathcal{M}$, the number

$$\sigma(A) = \lim_{t\to\infty} t^{-1} \ln \|\Phi_t A\|_{\mathcal{M}}$$

is called the *index of exponential growth of the orbit* $\Phi_t A$. Always

$$\sigma(A) \leqslant \sigma.$$

We have $\sigma(A) = \inf\{\sigma\colon \|\Phi_t A\|_{\mathcal{M}} \leqslant M e^{\sigma t}\}$.

We call the least upper bound of the numbers $\sigma(A)$, for all $A \in D(\mathcal{L})$, the *leading index* σ_s, i.e., $\sigma_s = \sup\{\sigma(A)\colon A \in D(\mathcal{L})\}$. It can be defined by the equation

$$\sigma_s = \lim_{t\to\infty} t^{-1} \ln \|\Phi_t\|.$$

The resolvent of the infinitesimal generator $\mathcal{L}$ is the Laplace transform (13) of Φ_t. The integral (13) converges when $\mathrm{Re}(z) > \sigma_s$. Moreover, the inequality

$$\left\| R(z, \mathcal{L})^n \right\| = \left\| (zL_I - \mathcal{L})^{-n} \right\| \leqslant \frac{M}{\mathrm{Re}(z) - \sigma_s}$$

is valid for $\mathrm{Re}(z) > \sigma_s$.

We call the least upper bound of the numbers $\sigma(A)$, for all $A \in \mathcal{M}$, the *index of exponential growth of the semi-group* Φ_t, or the *weakened leading index* σ_w: $\sigma_w = \sup\{\sigma(A)\colon A \in \mathcal{M}\}$. Here the element A does not have to belong to the domain $D(\mathcal{L})$ of the superoperator $\mathcal{L}$.

Let us give the basic theorem regarding noncontractive semi-groups with the leading index σ_s of exponential growth.

THEOREM *(Hille–Yosida–Fillips). Let $\mathcal{L}$ be a closed superoperator on $\mathcal{M}$ whose domain $D(\mathcal{L})$ is dense in $\mathcal{M}$. Then $\mathcal{L}$ is a generating superoperator of a strongly continuous semi-group, if and only if the following requirements are satisfied*:

(1) *All positive numbers $z > \sigma_s$ belong to the resolvent set $\rho(\mathcal{L})$.*
(2) *There exists a real positive M, such that*

$$\left\| R(z, \mathcal{L})^n \right\| \leqslant \frac{M}{(\mathrm{Re}(z) - \sigma_s)^n} \quad \big(\mathrm{Re}(z) > 0\big) \tag{14}$$

for all positive integer n.

Inequality (14) holds if $\|R(z, \mathcal{L})\| \leqslant M/(\mathrm{Re}(z) - \sigma_s)$ for $\mathrm{Re}(z) > \sigma_s$.

13.5. Positive semi-groups

Ordered Banach space and Banach lattice

The notion of "positivity" in an operator space is very important in quantum theory. A systematic abstract treatment of the "positivity" in linear spaces was

introduced by F. Riesz and further developed by many other authors. These results are called the theory of vector lattice.

Suppose there is a binary relation defined for every pair A, B of elements of a set $\mathcal{M}$, expressed by $A \leqslant B$, with the properties:

(a) $A \leqslant A$ for all $A \in \mathcal{M}$.
(b) If $A \leqslant B$, and $B \leqslant A$, then $A = B$, for $A, B \in \mathcal{M}$.
(c) If $A \leqslant B$, and $B \leqslant C$, then $A \leqslant C$ for all $A, B, C \in \mathcal{M}$.

Then $\mathcal{M}$ is said to be *partially ordered* by the relation $\leqslant$.

DEFINITION. An *ordered linear space* is a real linear space $\mathcal{M}$, together with a binary relation $\leqslant$, such that the following properties are satisfied:

(1) $\mathcal{M}$ is partially ordered by the relation $\leqslant$.
(2) If $A \leqslant B$, then $A + C \leqslant B + C$ for all $C \in \mathcal{M}$.
(3) If $A \leqslant B$, $z \in \mathbb{R}$, and $z \geqslant 0$, then $zA \leqslant zB$.

If $\mathcal{M}$ is an ordered linear space, then we can define the *positive cone* $\mathcal{M}_+ = \{A \in \mathcal{M}\colon\ A \geqslant 0\}$. A positive cone is a cone, i.e., $aA + bB \in \mathcal{M}_+$ for all $A, B \in \mathcal{M}_+$, and positive $a, b \in \mathbb{R}$.

An *ordered Banach space* is a real Banach space $\mathcal{M}$, such that the following properties are satisfied:

(1) $\mathcal{M}$ is an ordered linear space.
(2) $\mathcal{M}_+$ is closed with respect to the operator norm.

Suppose $\mathcal{M}$ is a partially ordered set $\mathcal{M}$, and A, B, C, D are in $\mathcal{M}$. If $A \leqslant C$ and $B \leqslant C$, we call C an *upper bound* for A and B. If furthermore $C \leqslant D$ whenever D is an upper bound for A and B, we call C the *least upper bound* or the *supremum* of A and B, and write $C = \sup(A, B)$. This element of $\mathcal{M}$ is unique if it exists. In a similar way, we define the *greatest lower bound* or the *infinimum* of A and B, and denote it by $\inf(A, B)$.

If $\sup(A, B)$ and $\inf(A, B)$ exist for every pair A, B in a partially ordered set $\mathcal{M}$, then $\mathcal{M}$ is called the *lattice*.

If $\sup(A, B)$ and $\inf(A, B)$ exist for every pair A, B in an ordered linear space $\mathcal{M}$, then $\mathcal{M}$ is called the *Riesz space*, or the *vector lattice*.

We define, in a Riesz space $\mathcal{M}$, the absolute value $|A| = \sup(A, -A)$. Then

$$|A| \geqslant 0, \qquad |A + B| \leqslant |A| + |B|, \qquad |zA| = |z|\,|A|,$$

and $|A| = 0$ if and only if $A = 0$.

DEFINITION. A real Banach space $\mathcal{M}$ is said to be a *Banach lattice* if it is a Riesz space such that $|A| \leqslant |B|$ implies $\|A\|_{\mathcal{M}} \leqslant \|B\|_{\mathcal{M}}$.

A positive superoperator is a superoperator Φ_t on $\mathcal{M}_+$ whose domain $D(\Phi_t)$ and range $R(\Phi_t)$ both lie in the same positive cone $\mathcal{M}_+$.

In quantum mechanics, positive semi-groups are very important to describe the time evolution of density operator.

DEFINITION. A *positive semi-group* is a semi-group $\{\Phi_t | t > 0\}$ on a Banach operator space $\mathcal{M}$, such that Φ_t are positive superoperators for all $t > 0$, i.e., $\Phi_t A^2 > 0$ for all $A^2 = A^* A \in \mathcal{M}$ and $t > 0$.

The next theorem gives some features of positive semi-groups.

STATEMENT. *A one-parameter semi-group* $\{\Phi_t | t \geqslant 0\}$ *of class* (C_0) *is a positive semi-group if and only if the resolvent superoperator* (13) *is positive for all* $z > \sigma_s$.

Dissipative and m-dissipative generating superoperators

Let $\mathcal{M}$ be a real Banach space, and let $\{\Phi_t | t \geqslant 0\}$ be a one-parameter semi-group of class (C_0) on $\mathcal{M}$. An infinitesimal generator of $\{\Phi_t | t \geqslant 0\}$ is a superoperator $\mathcal{L}$ with the domain

$$D(\mathcal{L}) = \left\{ A \in \mathcal{M} \colon \lim_{t \to 0+} t^{-1}(\Phi_t A - A) \text{ exists} \right\}$$

that is defined by

$$\mathcal{L} = \lim_{t \to 0+} t^{-1}(\Phi_t - L_I).$$

The Hille–Yosida theorem shows that $\mathcal{L}$ has the following properties:

(1) $D(\mathcal{L})$ is dense in $\mathcal{M}$.
(2) $\mathcal{L}$ is dissipative, i.e., $\|A - z\mathcal{L}A\|_{\mathcal{M}} \geqslant \|A\|_{\mathcal{M}}$.
(3) $\mathcal{L}$ is m-dissipative, i.e., $R(L_I - z\mathcal{L}) = \mathcal{M}$ for each $z > 0$.
(4) The resolvent of $\mathcal{L}$ is the Laplace transform (13) of the semi-group superoperator Φ_t.

THEOREM. *Let* $\mathcal{M}$ *be an operator Hilbert space, and let* $\mathcal{L}$ *be a symmetric dissipative superoperator on* $\mathcal{M}$. *Then* $\mathcal{L}$ *is a self-adjoint superoperator if and only if* $\mathcal{L}$ *is m-dissipative.* $\mathcal{L}$ *is a m-dissipative superoperator if and only if its adjoint superoperator* $\mathcal{L}$ *is dissipative.*

As a result, each symmetric dissipative superoperator is self-adjoint if it is a m-dissipative superoperator. The notion of a m-dissipative superoperator can be generalized.

p-dissipative generating superoperators

DEFINITION. A *sublinear functional* is a functional p on $\mathcal{M}$, such that

$$p(A+B) \leqslant p(A) + p(B), \qquad p(zA) = zp(A)$$

for all $A, B \in \mathcal{M}$ and $z \geqslant 0$.

The inequality $p(A) + p(-A) \geqslant p(0) = 0$ is valid for all $A \in \mathcal{M}$. Moreover, $\max(p(A), p(-A)) \geqslant 0$. If $p(A) + p(-A) > 0$ for $A \neq 0$, then p is called the *half-norm* on $\mathcal{M}$. If p is a half-norm, then $\|A\|_p = \max(p(A), p(-A))$ is a *norm induced by functional*.

DEFINITION. A *p-dissipative superoperator* is a superoperator $\mathcal{L}$ on $\mathcal{M}$ such that

$$p(A - z\mathcal{L}A) \geqslant p(A)$$

for all $A \in D(\mathcal{L})$ and $z > 0$.

Note that $\mathcal{L}$ is dissipative if and only if $\mathcal{L}$ is p-dissipative with respect to $p(A) = \|A\|_{\mathcal{M}}$. We can define

$$p'(A, B) = \lim_{\varepsilon \to 0+} \varepsilon^{-1}\big[p(A + \varepsilon B) - p(A)\big].$$

If $\mathcal{L}$ is p-dissipative, then $p'(A, -\mathcal{L}A) \geqslant 0$ for all $A \in D(\mathcal{L})$.

DEFINITION. A *strictly p-dissipative superoperator* is a superoperator $\mathcal{L}$ on $\mathcal{M}$, such that $p'(A, \mathcal{L}A) \leqslant 0$ for all $A \in D(\mathcal{L})$.

Using $-p'(A, -\mathcal{L}A) \leqslant p'(A, \mathcal{L}A)$, it is not hard to prove that $\mathcal{L}$ is p-dissipative if $\mathcal{L}$ is a strictly p-dissipative superoperator.

DEFINITION. A *p-contractive semi-group* is a one-parameter superoperator $\{\Phi_t | t \geqslant 0\}$ on $\mathcal{M}$, such that $p(\Phi_t A) \leqslant p(A)$ for all $A \in \mathcal{M}$.

Let us give the theorem regarding p-contractive semi-groups.

THEOREM. *Let $\{\Phi_t | t \geqslant 0\}$ be a one-parameter semi-group of class (C_0), and let $\mathcal{L}$ be a generating superoperator of the semi-group. Then $\{\Phi_t | t \geqslant 0\}$ is a p-contractive semi-group if and only if $\mathcal{L}$ is p-dissipative.*

Let $\mathcal{M}_+$ be a positive cone. If $\|A\|_{\mathcal{M}} \leqslant C\|B\|_{\mathcal{M}}$ for some $C > 0$, and all $0 \leqslant A \leqslant B$, then $\mathcal{M}_+$ is called the *normal positive cone*.

THEOREM. *Let $\mathcal{M}$ be a Banach space with normal positive cone $\mathcal{M}_+$, and let p be a canonical half-norm on $\mathcal{M}$. Then the following conditions are equivalent*:

(1) *$\mathcal{L}$ is a generating superoperator of contractive semi-group of class (C_0).*
(2) *$\mathcal{L}$ is p-dissipative, $D(\mathcal{L})$ is dense in $\mathcal{M}$ and $R(zL_I - \mathcal{L}) = \mathcal{M}$ for some $z > 0$.*

A *positive attained norm* is a norm of positive superoperator Φ_t, such that

$$\|\Phi_t\| = \sup\{\|\Phi_t A\|_{\mathcal{M}}\colon\ A \geqslant 0,\ \|A\|_{\mathcal{M}} \leqslant 1\}.$$

A *monotone norm* is an operator norm such that $\|A\|_{\mathcal{M}} \leqslant \|B\|_{\mathcal{M}}$ whenever $0 \leqslant A \leqslant B$.

THEOREM. *Let $\mathcal{M}$ be a Banach operator space with monotone norm. If Φ_t, $t \geqslant 0$, are positive superoperators with positive attained norms $\|\Phi_t\|$, then the following conditions are equivalent*:

(1) *$\mathcal{L}$ is a generator of positive contractive semi-group $\{\Phi_t | t \geqslant 0\}$ on $\mathcal{M}$.*
(2) *$\mathcal{L}$ is p-dissipative, $D(\mathcal{L})$ is dense in $\mathcal{M}$ and $R(zL_I - \mathcal{L}) = \mathcal{M}$ for some $z > 0$.*

As a result, generating superoperators of positive contractive semi-groups are p-dissipative.

Dispersive generating superoperator

A half-norm of an ordered Banach space is called the *canonical half-norm*, if

$$p(A) = \inf\{\|A + B\|_{\mathcal{M}}\colon\ B \in \mathcal{M}_+\}.$$

If $\mathcal{M}$ is a Banach lattice, then the canonical half-norm is of the form $p(A) = \|A_+\|$, where $A_+ = \sup(A, 0)$.

Let $\mathcal{M}$ be a Banach lattice, and let p be a canonical half-norm. A *dispersive superoperator* is a p-dissipative superoperator on $\mathcal{M}$.

A superoperator $\mathcal{L}$ is dispersive if and only if there exists $\varphi \in \mathcal{M}^*$ with the properties: $\varphi \geqslant 0$, $\|\varphi\| \leqslant 1$, $(\varphi|A) = \|A_+\|$, and $(\varphi|\mathcal{L}A) \leqslant 0$.

THEOREM. *Let $\mathcal{M}$ be a Banach lattice. If $\mathcal{L}$ is a linear superoperator on $\mathcal{M}$, then the following conditions are equivalent*:

(1) *$\mathcal{L}$ is a generating superoperator of positive contractive semi-group on $\mathcal{M}$.*
(2) *$\mathcal{L}$ is dispersive, $D(\mathcal{L})$ is dense in $\mathcal{M}$ and $R(zL_I - \mathcal{L}) = \mathcal{M}$ for some $z > 0$.*

Let us give the basic theorem regarding generating superoperators of positive semi-groups of class (C_0), which for the moment need not be contractive.

THEOREM. *Let $\mathcal{M}$ be an ordered Banach operator space with monotone norm, and let $\Phi_t, t \geqslant 0$, be superoperators with the positive attained norms $\|\Phi_t\| \leqslant M \exp(\sigma t)$. Then $\mathcal{L}$ is a generating superoperator of positive semi-group $\{\Phi_t | t \geqslant 0\}$ if and only if the following conditions are satisfied*:

(1) *$\mathcal{L}$ is a closed superoperator.*
(2) *$D(\mathcal{L})$ is dense in $\mathcal{M}$.*
(3) *$(\sigma, \infty) \subset \rho(\mathcal{L})$ and $p(R(z, \mathcal{L})^n A) \leqslant Mp(A)/(z - \sigma)^n$ for all $z > \sigma$ and $n \in \mathbb{N}$, where p is a canonical half-norm.*

This basic result can be considered as a natural generalization of the Hille–Yosida theorem.

Chapter 14

Differential Equations for Quantum Observables

14.1. Quantum dynamics and operator differential equations

Physical theories consist of two parts, a kinematical structure describing the instantaneous states and observables of the system, and a dynamical structure describing the change of these states and observables with time.

In the classical mechanics, the states are represented by distributions on a differentiable manifold (phase-space) and the observables by functions over the manifold. In the quantum mechanics, the states are given by density operators and the observables by functions on an operator space. We can identify the states with positive functionals over appropriate algebras of operators.

In quantum mechanics the dynamical description of system is given by superoperators, and dynamical semi-groups of maps of the underlying kinematical structure, which represent the motion of the system with time. In the conventional formulations of quantum theories the dynamical semi-group is introduced in an implicit manner. The natural description of the motion is in terms of the infinitesimal change of the system. The infinitesimal motion of a quantum system is directly described by some form of superoperator formalism, which allows the explicit definition of the system. In classical mechanics of non-Hamiltonian systems the infinitesimal change is defined by means of a vector field (or differential operator). In quantum mechanics the infinitesimal change is defined by real superoperator on some operator algebra. For Hamiltonian systems, this generating superoperator is defined by some form of derivation of the algebra.

The basic problem is the integration of these infinitesimal descriptions to give the dynamical semi-group. The integration problem (the Cauchy problem) involves the characterization of the dynamical structure which reflects the absence, or presence, of catastrophic behavior of the quantum system. The general problem is to study the operator differential equation

$$\frac{dA(t)}{dt} = \mathcal{L}A(t)$$

under a variety of conditions and assumptions. In each example, the operator $A = A(0)$ describes an observable, or state, of the quantum system and will be

represented by an element of some suitable operator space, or algebra, $\mathcal{M}$. The map $t \in \mathbb{R} \to A(t) \in \mathcal{M}$ describes the motion of A, and $\mathcal{L}$ is a superoperator on $\mathcal{M}$, which generates the infinitesimal change of A. The dynamics is given by solution of the operator differential equation. The existence of a "noncatastrophic" time development of the system is equivalent to the existence of global solutions of the equation of motion satisfying some boundary and initial conditions.

This is a chapter which reviews the basic facts of operator differential equations used in non-Hamiltonian dynamics. A consistent description of the theory of differential equations in abstract Banach spaces with accurate proofs can be found in the books [87,38,90].

14.2. Definition of operator differential equations

Let us consider the operator differential equation

$$\frac{d}{dt}A_t = \mathcal{L}A_t \tag{1}$$

with the linear superoperator $\mathcal{L}$ having an everywhere dense domain $D(\mathcal{L})$ in a Banach operator space $\mathcal{M}$. Here $A_t = A(t)$ is an unknown one-parameter operator with values in the space $\mathcal{M}$. The derivative $A'(t) = dA(t)/dt$ is as the following limit, in the operator norm of $\mathcal{M}$,

$$\lim_{\tau\to 0}\left\|\tau^{-1}\left[A(t+\tau) - A(t)\right] - A'(t)\right\|_{\mathcal{M}} = 0.$$

DEFINITION. A one-parameter operator $A(t)$ is called a *solution of differential equation* (1) on the segment $[0, t']$ if it satisfies the conditions:

(1) The values of $A(t)$ belong to the domain $D(\mathcal{L})$ of the superoperator $\mathcal{L}$ for all $t \in [0, t']$.
(2) The strong derivative $A'(t) = dA(t)/dt$ of the one-parameter operator $A(t)$ exists at every point t of the segment $[0, t']$.
(3) The equation $dA(t)/dt = \mathcal{L}A(t)$ is satisfied for all $t \in [0, t']$.

DEFINITION. An *initial value problem*, or *Cauchy problem*, on the segment $[0, t']$ is the problem of finding a solution $A(t)$ of equation (1) on $[0, t']$ satisfying the initial condition: $A(0) = A_0 \in \mathcal{M}$.

In this definition it was required that the solution of the equation satisfy the equation for $t = 0$ also. This requirement can be weakened.

DEFINITION. A one-parameter operator $A(t)$ is called a *weak solution* of the differential equation (1) on the segment $[0, t']$ if it satisfies the conditions:

(1) $A(t)$ for each $t \in (0, t']$ belongs to the domain $D(\mathcal{L})$ of the superoperator $\mathcal{L}$.
(2) $A(t)$ is strongly differentiable on $(0, t']$.
(3) $A(t)$ is continuous on $[0, t']$.
(4) The equation $dA(t)/dt = \mathcal{L}A(t)$ is satisfied for all $t \in (0, t']$.

We understand by the *weakened Cauchy problem* on $[0, t']$ the problem of finding a weak solution satisfying the initial condition $A(0) = A_0$. Here the operator A_0 does not have to belong to the domain of superoperator $\mathcal{L}$.

DEFINITION. A *correctly formulated Cauchy problem* is a Cauchy problem for equation (1) on the segment $[0, t']$, if the following conditions are satisfied.

(1) The unique solution of the Cauchy problem exists for arbitrary $A_0 \in D(\mathcal{L})$.
(2) This solution depends continuously on initial conditions in the sense that if $A_k(0) \in D(\mathcal{L})$ and

$$\lim_{k\to\infty} \|A_k(0)\|_{\mathcal{M}} = 0,$$

then

$$\lim_{k\to\infty} \|A_k(t)\|_{\mathcal{M}} = 0$$

for the corresponding solutions $A_k(t)$ of (1) and for all $t \in [0, t']$.

By virtue of the constancy of the superoperator $\mathcal{L}$, the correctness on $[0, \infty)$, follows from the correctness of the Cauchy problem on a single segment $[0, t']$.

THEOREM. *If the Cauchy problem for equation* (1)*, in which the initial condition is given by* $A(0) = A_0 \in D(\mathcal{L})$*, is correctly formulated, then its solution can be presented by the equation* $A(t) = \Phi_t A_0$*, where* Φ_t *is a strongly continuous semi-group of superoperators at* $t > 0$.

In general, Φ_t is not strongly continuous at $t = 0$. Moreover, the limit of $\Phi_t A_0$ at $t = 0$ may not be exist.

If the Cauchy problem is correctly formulated, then the superoperator Φ_t is defined on $D(\mathcal{L})$ and is bounded. Therefore it can be extended to a bounded superoperator, defined on the entire space $\mathcal{M}$, which we also denote by Φ_t. The superoperators Φ_t form a semi-group. A set of bounded superoperators Φ_t, depending on the parameter $t \in [0, \infty)$, is called a semi-group if $\Phi_t \Phi_s = \Phi_{t+s}$ for all $t \geqslant 0$ and $s \geqslant 0$.

If A_0 does not belong to the domain $D(\mathcal{L})$ of the superoperator $\mathcal{L}$, then the operator $A(t) = \Phi_t A_0$ may not be differentiable and its values may not belong to $D(\mathcal{L})$. In this case, we can call the operator $A(t) = \Phi_t A_0$ a *generalized solution* of equation (1).

14.3. Equations with constant bounded superoperators

Suppose $\mathcal{L}$ is a bounded superoperator. Under this condition, the properties of the solution of equation (1) are analogous to the properties of the solutions of a system of linear differential equations, which can be considered as a linear equation in a finite-dimensional Banach space.

A unique solution of the Cauchy problem exists for equation (1) with a constant bounded superoperator $\mathcal{L}$, and it can be written in the form

$$A(t) = \Phi_t A_0 = e^{t\mathcal{L}} A_0.$$

The superoperator $\Phi_t = \exp\{t\mathcal{L}\}$ is defined by the series

$$\exp\{t\mathcal{L}\} = \sum_{n=0}^{\infty} \frac{t^n}{n!} \mathcal{L}^n, \tag{2}$$

which converges in the superoperator norm. Note that $(\mathcal{L})^0 = L_I$. Using $\|\mathcal{L}_1\mathcal{L}_2\| \leqslant \|\mathcal{L}_1\|\|\mathcal{L}_2\|$, the bound of the norm of each term of (2) gives the inequality

$$\left\|\exp\{t\mathcal{L}\}\right\| \leqslant \exp\left\{t\|\mathcal{L}\|\right\}. \tag{3}$$

The superoperators $\Phi_t = \exp\{t\mathcal{L}\}$, $t \in [0, \infty)$, form a one-parameter semi-group of bounded superoperators, since

$$\Phi_{t_1}\Phi_{t_2} = e^{t_1\mathcal{L}} e^{t_2\mathcal{L}} = e^{(t_1+t_2)\mathcal{L}} = \Phi_{t_1+t_2} \quad (t_1, t_2 \geqslant 0),$$
$$\Phi_{t=0} = \left[e^{t\mathcal{L}}\right]_{t=0} = L_I.$$

Estimate (3) of the norm of the superoperator Φ_t is rough since it takes into account only the norm of the superoperator $\mathcal{L}$ and does not consider the distribution of its spectrum. A more precise estimate is given by the following statement.

STATEMENT. *If the real parts of all the points of the spectrum of the superoperator $\mathcal{L}$ are less than the number σ, then*

$$\left\|\exp\{t\mathcal{L}\}\right\| \leqslant Me^{\sigma_s t}. \tag{4}$$

Conversely, if (4) is satisfied, then the real parts of the points of the spectrum of $\mathcal{L}$ do not exceed σ_s, i.e., $\mathrm{Re}(z) \leqslant \sigma_s$.

It is necessary for the boundedness of all solutions of equation (1) on the half-axis $t \in [0, \infty)$, that the spectrum of the superoperator $\mathcal{L}$ lies in the closed left-hand half-plane. It is sufficiently that it lie in the open left-hand half-plane.

In a Hilbert operator space, a criterion can be given generalizing the well-known Lyapunov theorem.

THEOREM *(Lyapunov). The spectrum of the superoperator $\mathcal{L}$ on a Hilbert operator space lies in the open left-hand half-plane if and only if there exists a bounded self-adjoint positive superoperator $\mathcal{U}$ such that the superoperator $\mathcal{U}\mathcal{L} + \mathcal{L}^*\mathcal{U}$ is negative.*

In other words, it is necessary and sufficient that there exists a superoperator $\mathcal{U}$ such that $(A_t|\mathcal{U}A_t) \geqslant 0$, and

$$\frac{d}{dt}(A_t|\mathcal{U}A_t) \leqslant -\gamma(A_t|A_t) \quad (\gamma > 0)$$

for an arbitrary solution $A_t = A(t)$ of the operator differential equation.

Note that a bounded superoperator $\mathcal{U}$ on a Hilbert operator space is said to be self-adjoint if $(\mathcal{U}A|A) = (A|\mathcal{U}A)$.

14.4. Chronological multiplication

Let us consider the operator differential equation

$$\frac{d}{dt}A_t = \mathcal{L}_t\, A_t, \tag{5}$$

where $\mathcal{L}_t$ is a one-parameter bounded superoperator, which depends continuously on t. The solution of the Cauchy problem for equation (5) exists and is unique. It can be obtained by the method of successive approximations applied to the operator integral Volterra equation.

Instead of differential equation (5) with initial condition $A_t = A$ at the time $t = 0$, we can take the equivalent integral equation

$$A_t = A + \int_0^t dt_1\, \mathcal{L}_{t_1} A_{t_1}. \tag{6}$$

The operator A_t will be considered as $A(t) = \Phi_t A$, where Φ_t is a one-parameter bounded superoperator. Then equation (6) has the form

$$\Phi_t A = A + \int_0^t dt_1\, \mathcal{L}_{t_1} \Phi_{t_1} A. \tag{7}$$

Substitution of (7) in the form

$$\Phi_{t_{n+1}} A = A + \int_0^{t_{n+1}} dt_n\, \mathcal{L}_{t_n} \Phi_{t_n} A$$

into equation (7) gives the sum

$$\Phi_t A = A + \sum_{n=1}^{\infty} \int_0^t dt_1\, \mathcal{L}_{t_1} \int_0^{t_1} dt_2\, \mathcal{L}_{t_2} \cdots \int_0^{t_{n-1}} dt_n\, \mathcal{L}_{t_n} A,$$

which converges in the operator norm.

As a result, we obtain

$$\Phi_t = L_I + \sum_{n=1}^{\infty} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n\, \mathcal{L}_{t_1} \mathcal{L}_{t_2} \cdots \mathcal{L}_{t_n}. \tag{8}$$

This is the *Liouville decomposition formula* for (7). This series is converged in the superoperator norm.

In equation (8), each $t_k \in [0, t]$ satisfy $0 < t_k < t_{k+1} < t$, for all $k \in \mathbb{N}$. In each term of (8) the superoperators follow the chronological order. It is clear that the result will be the same if we rename the integration variables $t_1 \leftrightarrow t_2$. Changing the order of integration, we obtain

$$\int_0^t dt_1 \int_0^{t_1} dt_2\, \mathcal{L}_{t_1} \mathcal{L}_{t_2} = \int_0^t dt_1 \int_{t_1}^t dt_2\, \mathcal{L}_{t_2} \mathcal{L}_{t_1}.$$

The initial expression can be presented in the form

$$\int_0^t dt_1 \int_0^{t_1} dt_2\, \mathcal{L}_{t_1} \mathcal{L}_{t_2} = \frac{1}{2} \int_0^t dt_1 \left(\int_0^{t_1} dt_2\, \mathcal{L}_{t_1} \mathcal{L}_{t_2} + \int_{t_1}^t dt_2\, \mathcal{L}_{t_2} \mathcal{L}_{t_1} \right).$$

We introduce a new, more compact notation

$$\int_0^{t_1} dt_2\, \mathcal{L}_{t_1} \mathcal{L}_{t_2} + \int_{t_1}^t dt_2\, \mathcal{L}_{t_2} \mathcal{L}_{t_1} = \int_0^t dt_2\, T\{\mathcal{L}_{t_1} \mathcal{L}_{t_2}\},$$

where T is the *chronological multiplication*

$$T\{\mathcal{L}_{t_1} \mathcal{L}_{t_2}\} = \begin{cases} \mathcal{L}_{t_1} \mathcal{L}_{t_2}, & t_1 > t_2; \\ \mathcal{L}_{t_2} \mathcal{L}_{t_1}, & t_2 > t_1. \end{cases}$$

In general,

$$T\{\mathcal{L}_{t_1} \mathcal{L}_{t_2} \ldots \mathcal{L}_{t_n}\} = \mathcal{L}_{t_a} \mathcal{L}_{t_b} \ldots \mathcal{L}_{t_c}, \quad t_a \geqslant t_b \geqslant \cdots \geqslant t_c,$$

and $\mathcal{L}_{t_k} \neq \mathcal{L}_{t_l}$, $\mathcal{L}_{t_k}\mathcal{L}_{t_l} \neq \mathcal{L}_{t_l}\mathcal{L}_{t_k}$. Using the symmetry $T\{\mathcal{L}_{t_k}\mathcal{L}_{t_l}\} = T\{\mathcal{L}_{t_l}\mathcal{L}_{t_k}\}$, and the fact that the number of all permutations is equal to $n!$, we obtain

$$\Phi_t = L_I + \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^t dt_1 \int_0^t dt_2 \cdots \int_0^t dt_n \, T\{\mathcal{L}_{t_1}\mathcal{L}_{t_2}\cdots\mathcal{L}_{t_n}\}. \tag{9}$$

We introduce the following compact notation

$$\Phi_t = T\left\{\sum_{n=0}^{\infty} \frac{1}{n!}\left(\int_0^t d\tau \, \mathcal{L}_\tau\right)^n\right\} = T\left\{\exp \int_0^t d\tau \, \mathcal{L}_\tau\right\}. \tag{10}$$

Using this classic notation [27], we assume that the chronological ordering should be performed before the integration. For example,

$$T\left\{\left(\int_0^t d\tau \, \mathcal{L}_\tau\right)^2\right\} = \int_0^t dt_1 \int_0^t dt_2 \, T\{\mathcal{L}_{t_1}\mathcal{L}_{t_2}\}.$$

The temporal operations $T\{\ldots\}$ and $\int d\tau$ are noncommutative.

As a result, we obtain

$$\Phi_t = T\left\{\exp \int_0^t d\tau \, \mathcal{L}_\tau\right\}. \tag{11}$$

This is the *chronological exponential*, or *T-exponential*. In mathematics, it is usually called the *multiplicative Stieltjes integral*. Formal expression (11) presents explicit equation (9). This representation allows to write the solution of the Cauchy problem by $A_t = \Phi_t A$ with (11). If the superoperator $\mathcal{L}_t$ is constant, then $\Phi_t = \exp\{t\mathcal{L}\}$.

14.5. Equations with variable bounded superoperators

Let us consider the operator differential equation (5), where $\mathcal{L}_t$ is a one-parameter superoperator which depends continuously on t. We assume that for each fixed t this superoperator is the bounded superoperator on a Banach operator space $\mathcal{M}$. The solution of the Cauchy problem for this equation exists and is unique. This solution can be written in the form $A(t) = \Phi_t A_0$, where the superoperator Φ_t is defined by (11).

The superoperator Φ_t can be considered as the solution of the Cauchy problem for the superoperator differential equation

$$\frac{d}{dt}\Phi_t = \mathcal{L}_t\Phi_t, \quad \Phi_0 = L_I \tag{12}$$

in the space $\mathcal{A}(\mathcal{M})$ of all bounded superoperators acting on $\mathcal{M}$.

A bounded inverse superoperator Φ_t^{-1} exists for every t. This operator is the solution of the Cauchy problem for the superoperator differential equation

$$\frac{d}{dt}\Phi_t^{-1} = -\mathcal{L}_t\Phi_t^{-1}, \quad \Phi_0^{-1} = L_I,$$

which is called the *adjoint equation* to (12).

If we consider a Cauchy problem for equation (5) in which the initial condition is given not at the time $t = 0$, but at an arbitrary time t_0 by $A(t_0) = A_0$, then its solution can be written in the form

$$A(t) = \Phi_t\Phi_{t_0}^{-1}A_0 = \Phi_{t,t_0}A_0.$$

The superoperator

$$\Phi_{t,\tau} = \Phi_t\Phi_\tau^{-1}$$

is called an evolution superoperator. This superoperator is also called the resolving superoperator, or propagator. It has the properties

$$\Phi_{t,s}\Phi_{s,\tau} = \Phi_{t,\tau}, \qquad \Phi_{t,t} = L_I.$$

If $\mathcal{L}_t$ is constant, i.e., $\mathcal{L}_t = \mathcal{L}$, then $\Phi_{t,\tau} = \exp(t-\tau)\mathcal{L}$.

DEFINITION. An *evolution superoperator* is a two-parameter superoperator $\Phi_{t,s}$, $0 \leqslant s \leqslant t$, such that the following conditions are satisfied:

(1) $\Phi_{t,s}\Phi_{s,t_0} = \Phi_{t,t_0}$ for all $0 \leqslant t_0 \leqslant s \leqslant t$.
(2) $\Phi_{t_0,t_0} = I$ for all $t_0 \in [0, t]$.
(3) $\Phi_{t,s}$ is a strongly continuous superoperator with respect to t and s.

Let $\mathcal{L}_t$ $(t \geqslant 0)$ be uniformly bounded, i.e., $\|\mathcal{L}_t\| \leqslant M$, then the estimate

$$\big\|A(t)\big\|_{\mathcal{M}} \leqslant e^{t\sigma}\big\|A(0)\big\|$$

is valid for the solutions $A(t)$ of equation (5).

For each $A_0 = A(0)$, the number

$$\sigma(A_0) = \overline{\lim_{t\to\infty}}\, t^{-1}\ln\big\|A(t)\big\|_{\mathcal{M}} = \overline{\lim_{t\to\infty}}\, t^{-1}\ln\|\Phi_t A_0\|_{\mathcal{M}}$$

is called the *index of exponential growth* of the solution $A(t)$. Always $\sigma(A_0) \leqslant \sigma$. We call the least upper bound of the numbers σ, for *all* solutions of the equation, the *leading index* σ_s, i.e., $\sigma_s = \sup\{\sigma(A_0)\colon\ A_0 \in D(\mathcal{L})\}$. It can be defined by the equation

$$\sigma_s = \lim_{t\to\infty} t^{-1}\ln\|\Phi_t\|. \tag{13}$$

We call the least upper bound of the numbers σ, for *all* generalized solutions of the equation, the *weakened leading index* σ_w: $\sigma_w = \sup\{\sigma(A_0)\colon\ A_0 \in \mathcal{M}\}$. Here the element A does not have to belong to the domain $D(\mathcal{L})$. Then σ_w can be called the index of exponential growth of the weakened Cauchy problem. It can be defined by the equation

$$\sigma_w = \inf_{t>0}\bigl(t^{-1}\ln\|\Phi_t\|\bigr).$$

We define the *special index* of equation (5) by

$$\sigma^* = \lim_{t,(t-\tau)\to\infty}(t-\tau)^{-1}\ln\|\Phi_{t,\tau}\|.$$

If the superoperator $\mathcal{L}_t$ is constant, then the leading and special indices coincide. In the general case, the relation $\sigma_s \leqslant \sigma^*$ holds between the leading and special indices. For example, equation (5) with the superoperator

$$\mathcal{L}_t = (\sin\ln t + \cos\ln t)L_I$$

gives

$$\sigma_s = 1, \qquad \sigma^* = \sqrt{2}.$$

The value of the special index σ^* depends on the behavior of the superoperator $\mathcal{L}_t$ at infinity. If the limit

$$\mathcal{L}_\infty = \lim_{t\to\infty}\mathcal{L}_t$$

exists, and the spectrum of the superoperator $\mathcal{L}_\infty$ lies in the open left-hand half-plane, then the special index is negative.

In a Hilbert operator space, we can give the following criterion for negativeness of the special index.

THEOREM. *Let $\mathcal{M}$ be an operator Hilbert space. If there exists a superoperator $\mathcal{U}_t$ such that*

$$0 < a_1(A_t|A_t) \leqslant (A_t|\mathcal{U}_t A_t) \leqslant a_2(A_t|A_t),$$

and

$$\frac{d}{dt}(A_t|\mathcal{U}A_t) \leqslant -\gamma\,(A_t|A_t) \quad (\gamma > 0)$$

for all solutions $A_t = A(t)$ of equation (5), then the special index is negative, i.e., $\sigma^* < 0$.

Conversely, we can construct a superoperator $\mathcal{U}_t$ with the described properties for each equation (5) with a negative special index. For example, the superoperator

$\mathcal{U}_t$ can be obtained by

$$\mathcal{U}_t = \int_t^\infty d\tau \, \Phi^*_{\tau,t} \, \Phi_{\tau,t}.$$

14.6. Operator equations with constant unbounded superoperators

Suppose $\mathcal{H}$ is a Banach space and A_n are operators on $\mathcal{H}$ for every natural number n. We say that the sequence $\{A_n\}$ is *uniformly convergent* with limit A if for every $\varepsilon > 0$, there exists a natural number $N = N(\varepsilon)$ such that for all x in $\mathcal{H}$ and all $n \geqslant N$, we have $\|A_n x - Ax\|_{\mathcal{H}} < \varepsilon$.

Compare uniform convergence to the concept of pointwise convergence. The sequence $\{A_n\}$ *converges pointwise* with limit A if and only if for every x in $\mathcal{H}$ and every $\varepsilon > 0$, there exists a natural number $N = N(x, \varepsilon)$ such that for all $n \geqslant N$, we have $\|A_n x - Ax\|_{\mathcal{H}} < \varepsilon$. In the case of uniform convergence, N can only depend on ε, while in the case of pointwise convergence N may depend on ε and x. A sequence $\{A_n\}$ of operators converges uniformly to a limiting operator A if the speed of convergence of $A_n x$ to Ax does not depend on x. Therefore the uniform convergence implies a pointwise convergence. The uniform convergence is a type of convergence stronger than pointwise. The concept is important because several properties of the operators A_n, such as continuity, differentiability and Riemann integrability, are transferred to the limit A if the convergence is uniform.

DEFINITION. A correctly formulated Cauchy problem is called *uniformly corrected* if it follows from $A_k(0) \in D(\mathcal{L})$ and $\|A_k(0)\|_{\mathcal{M}} \to 0$ that the corresponding solutions $A_k(t)$ of (1) converge uniformly to 0 on every finite segment $[0, t']$.

If the superoperator $\mathcal{L}$ is closed, then there exists a bounded resolvent superoperator $R(z, \mathcal{L}) = (zL_I - \mathcal{L})^{-1}$. In this case, uniform correctness follows from the existence and uniqueness of a continuously differentiable solution of the Cauchy problem for arbitrary $A_0 \in D(\mathcal{L})$.

THEOREM. *If the Cauchy problem is uniformly correct, then the semi-group* $\{\Phi_t | t \geqslant 0\}$ *satisfies the condition*

$$\lim_{t \to 0+} \Phi_t A_0 = A_0 \tag{14}$$

for all $A_0 \in \mathcal{M}$.

For a uniformly correct Cauchy problem, the semi-group $\{\Phi_t | t \geqslant 0\}$ is *strongly continuous* that is the operator $\Phi_t A_0$ is continuous on $(0, \infty)$ for arbitrary $A_0 \in \mathcal{M}$. The semi-group $\{\Phi_t | t \geqslant 0\}$ belongs to the class (C_0) if it is strongly continuous at $t > 0$ and satisfies condition (14) for arbitrary $A_0 \in \mathcal{M}$.

THEOREM. *If the Cauchy problem is uniformly correct, then the semi-group* $\{\Phi_t | t \geqslant 0\}$ *belongs to the class* (C_0).

In other words, we can say that all generalized solutions are continuous on $[0, \infty)$ in this case. The limit (13) exists for an arbitrary strongly continuous semi-group $\{\Phi_t | t \geqslant 0\}$. If the semi-group belongs to the class (C_0), then the estimate $\|\Phi_t\| \leqslant M \exp\{\sigma_s t\}$ is valid. Thus, for a uniformly correct Cauchy problem, the orders of exponential growth of all solutions are bounded.

THEOREM. *If the Cauchy problem is uniformly correct, then* $\|\Phi_t\| \leqslant M \exp\{\sigma_s t\}$.

If $\sigma_s = 0$, then the semi-group is bounded, i.e., $\|\Phi_t\| \leqslant M$. In this case, we can introduced a new norm in the space $\mathcal{M}$, such that the superoperators Φ_t, $t \geqslant 0$, have a norm not greater than one. If $\|\Phi_t\| \leqslant 1$, then the semi-group is called *contractive*.

14.7. Generating superoperator and its resolvent

For the semi-group $\{\Phi_t | t \geqslant 0\}$ the one-parameter operator $A(t) = \Phi_t A$ must be differentiable. Differentiability of this operator for arbitrary t follows from its differentiability for $t = 0$. The linear superoperator

$$\Phi_0' A = \lim_{\varepsilon \to 0+} \varepsilon^{-1} [\Phi_\varepsilon A - A]$$

is defined on a set of operators A for which $A(t) = \Phi_t A$ is differentiable at zero. The superoperator Φ_0' is called the generating superoperator (or infinitesimal generator) of the semi-group $\{\Phi_t | t \geqslant 0\}$.

The theory of semi-groups of bounded linear superoperators on a Banach operator space deals with the exponential superoperator functions. It is concerned with the problem of determining the most general bounded linear superoperator Φ_t, $t \geqslant 0$, which satisfies the equations

$$\Phi_t \Phi_s = \Phi_{t+s} \ (t, s \geqslant 0), \quad \Phi_0 = L_I.$$

The problem for semi-group of superoperators can be considered as a natural generalization of the well-known problem for the bounded operators on infinite-dimensional function space. For function spaces, this problem was investigated by E. Hille and K. Yosida. They introduced the infinitesimal generator $\mathcal{L}$ of Φ_t,

and discussed the generation of Φ_t in terms of $\mathcal{L}$. A characterization of the infinitesimal generator $\mathcal{L}$ in terms of the spectral property of $\mathcal{L}$ is described by Hille–Yosida–Phillips theorem. The basic results of the superoperator semi-group theory may be considered as a natural generalization of the Stone's theorem for one-parameter superoperator group on a Hilbert operator space.

If the semi-group belongs to the class (C_0), then the domain $D(\mathcal{L})$ of the infinitesimal generator $\mathcal{L}$ is everywhere dense.

THEOREM. *Let $\mathcal{L}$ be a generating superoperator of a semi-group $\{\Phi_t | t \geqslant 0\}$ of class (C_0). Then $\mathcal{L}$ is closed and commutes with Φ_t on its domain $D(\mathcal{L})$:*

$$\mathcal{L}\Phi_t = \Phi_t \mathcal{L}.$$

Moreover, the Cauchy problem for equation (1) is uniformly correct.

Thus, if we restrict ourselves to equations with closed superoperators $\mathcal{L}$, then we have the following statement. Note that an unbounded self-adjoint superoperator is always closed.

STATEMENT. *Let $\mathcal{L}$ be a closed superoperator. Then the class of operator equations (1) for which the Cauchy problem is uniformly correct coincides with the class of equations for which $\mathcal{L}$ is a generating superoperator of a semi-group of class (C_0).*

This explains the role which the study of semi-groups of class (C_0) and their generating superoperators plays in the theory of operator differential equations.

The spectrum of the infinitesimal generator $\mathcal{L}$ of a semi-group of class (C_0) lies always in some half-plane $\mathrm{Re}(z) \leqslant \sigma_s$. The generating superoperators $\mathcal{L}$ can be characterized by the properties of the resolvents $R(z, \mathcal{L}) = (zL_I - \mathcal{L})^{-1}$.

THEOREM. *In order to the closed superoperator $\mathcal{L}$ to be the infinitesimal generator of a semi-group of class (C_0), it is necessary and sufficient that a real σ_s and a positive M exist such that*

$$\left\| R(z, \mathcal{L})^n \right\| \leqslant \frac{M}{(z - \sigma_s)^n} \quad (z > \sigma_s,\ n = 0, 1, 2, \ldots). \tag{15}$$

The estimate $\|\Phi_t\| \leqslant M \exp\{\sigma_s t\}$ is valid.

If the superoperator $\mathcal{L}$ in equation (1) is closed, then conditions (15) are necessary and sufficient for the uniform correctness of the Cauchy problem.

The test of the necessary and sufficient conditions (15) is difficult since all the powers ($n \in \mathbb{N}$) of the resolvent superoperator are used. Inequality (15) will be

satisfied if

$$\left\| R(z, \mathcal{L}) \right\| \leqslant \frac{1}{z - \sigma_s} \quad (z > \sigma_s). \tag{16}$$

Note that condition (15) with $n = 1$ and $M > 1$ is *not* sufficient for the correctness of the Cauchy problem. If estimate (16) holds, then the inequality $\|\Phi_t\| \leqslant \exp\{\sigma_s t\}$ is valid. In particular, if $\sigma_s = 0$, then $\|\Phi_t\| \leqslant 1$ and the semigroup is contractive.

Let us consider the operator differential equation

$$\frac{d}{dt} A(t) = \mathcal{L}_t A(t) \tag{17}$$

with a superoperator $\mathcal{L}_t$ which depends on t. The dependence of $\mathcal{L}_t$ on t is assumed to be smooth. In order to formulate conditions of smoothness for an unbounded one-parameter superoperator $\mathcal{L}_t$, it is natural to assume that $\mathcal{L}_t$ is defined for different $t \geqslant 0$ on the same subset of the operator space $\mathcal{M}$. In connection with this, the following assumption is made. The domain of the superoperator $\mathcal{L}_t$ is not dependent on t:

$$D(\mathcal{L}_t) = D.$$

We can now formulate a set of conditions, which provide the correctness of the Cauchy problem for an equation with a variable superoperator:

THEOREM. *The Cauchy problem for equation* (17) *is correctly formulated if the following conditions are satisfied*:

(1) *The superoperator $\mathcal{L}_t$ is the infinitesimal generator of a contractive semigroup for every $t \in [0, t']$ and the inequality*

$$\left\| R(z, \mathcal{L}_t) \right\| \leqslant \left[1 + \operatorname{Re}(z) \right]^{-1} \quad \left(\operatorname{Re}(z) \geqslant 0 \right)$$

is valid.

(2) *The bounded superoperator $\mathcal{L}_t \mathcal{L}_s^{-1}$ is strongly continuously differentiable with respect to t for arbitrary s.*

If these conditions are satisfied, then there exists a bounded evolution superoperator $\Phi_{t,s}$ $(t \geqslant s)$, which is strongly continuous with respect to the variables t and s, for $0 \leqslant s \leqslant t \leqslant t'$. For $t = s$, $\Phi_{s,s} = I$. The solution of the Cauchy problem for equation (17) with the initial condition $A(0) = A_0 \in D$ is unique and is given by the formula $A(t) = \Phi_{t,0} A_0$. If the initial condition is given for $t = s$ by $A(s) = A_0$, then the solution has the form $A(t) = \Phi_{t,s} A_0$. The superoperators $\Phi_{t,s}$ have the property $\Phi_{t,\tau} \Phi_{\tau,s} = \Phi_{t,s}$, where $0 \leqslant s \leqslant \tau \leqslant t \leqslant t'$. Generalized solutions $\Phi_t A_0$ of equation (17) for arbitrary $A_0 \in \mathcal{M}$ are continuous one-parameter operators for $t \in [0, t']$.

14.8. Equations in operator Hilbert spaces

In operator Hilbert spaces, the generating superoperators for several important classes of semi-groups can be completely described. The description can be realized in terms connected with the superoperators itself and not with its resolvent.

Let us give the basic statement regarding infinitesimal generators of a strongly continuous contractive semi-group. In order to the superoperator $\mathcal{L}$ be a generator of a strongly continuous contractive superoperator semi-group it is necessary and sufficient that it be a maximal dissipative superoperator with an everywhere dense domain o definition. We formulate this criterion again in the following theorem.

THEOREM. *Let $\mathcal{L}$ be a closed superoperator $\mathcal{L}$ with an everywhere dense domain $D(\mathcal{L})$ in a Hilbert operator space. Then $\mathcal{L}$ is a generating superoperator of a strongly continuous contractive semi-group of superoperators if and only if the following conditions are satisfied*

$$\mathrm{Re}(\mathcal{L}A|A) \leqslant 0, \quad A \in D(\mathcal{L}), \qquad \mathrm{Re}(\mathcal{L}^*B|B) \leqslant 0, \quad B \in D(\mathcal{L}^*).$$

This theorem describes strongly continuous semi-groups. Let us give the theorem regarding semi-groups of class (C_0).

THEOREM. *If the superoperators $\mathcal{L}$ and $\mathcal{L}^*$ have the same everywhere dense domain $D(\mathcal{L}^*) = D(\mathcal{L})$ in a Hilbert operator space, and the superoperator*

$$\mathrm{Re}\,\mathcal{L} = (1/2)[\mathcal{L} + \mathcal{L}^*]$$

is bounded, then $\mathcal{L}$ is the generating superoperator of a semi-group $\{\Phi_t | t \geqslant 0\}$ of class (C_0). The estimate $\|\Phi_t\| \leqslant \exp\{\sigma_s t\}$, is valid, where σ_s is an upper bound of the superoperator $\mathrm{Re}\,\mathcal{L}$.

In order to the superoperator $\mathcal{L}$ on an operator Hilbert space $\mathcal{M}$ to be the infinitesimal generator of a strongly continuous group of unitary superoperators, it is necessary and sufficient that $\mathcal{L} = i\Lambda$, where Λ is a self-adjoint superoperator. Note that Λ is self-adjoint if $(\Lambda A|B) = (A|\Lambda B)$ for all $A, B \in \mathcal{M}$.

Equations in an operator Hilbert space with basis

Let $\mathcal{M}$ be a separable operator Hilbert space. Then there is an operator basis $\{E_k\}$ for $\mathcal{M}$. The solution of operator differential equations can be presented in the form of expansion with respect to the basis.

Let us consider the linear differential operator equation

$$\frac{d}{dt}|A_t) = \mathcal{L}|A_t), \tag{18}$$

where $|A_t)$ is an unknown one-parameter operator with values in an operator Hilbert space $\mathcal{M}$. Now let an arbitrary denumerable basis $|E_k)$ be given in the space $\mathcal{M}$. Then $(E_k|$ can be considered as a basis for $\mathcal{M}^*$. Equation (18) gives

$$(E_k|\frac{d}{dt}|A_t) = (E_k|\mathcal{L}|A_t).$$

Using

$$\frac{d}{dt}|E_k) = 0, \qquad \sum_{l=1}^{\infty}|E_l)(E_l| = I,$$

we obtain

$$\frac{d}{dt}(E_k|A_t) = \sum_{l=1}^{\infty}(E_k|\mathcal{L}|E_l)(E_l|A_t).$$

As a result, we have

$$\frac{d}{dt}a_k(t) = \sum_{l=1}^{\infty}L_{kl}a_l(t), \tag{19}$$

where

$$a_k(t) = (E_k|A_t) = Tr[E_k^*A_t], \qquad L_{kl} = (E_k|\mathcal{L}|E_l).$$

If $a_k(t)$ is the probability that a quantum system of interest is in state $|E_k)$ at time t and

$$L_{kl} = -c\delta_{kl} + cM_{kl},$$

where cM_{kl} is the probability per unit time of a transition from $|E_l)$ to $|E_k)$, then (19) gives

$$\frac{d}{dt}a_k(t) = -ca_k(t) + c\sum_{l=1}^{\infty}M_{kl}a_l(t). \tag{20}$$

A standard starting point for the discussion of various random walks and other transport processes is this master equation. Equation (20) is equivalent to the "gain-loss" of the master equation

$$\frac{d}{dt}a_k(t) = c\sum_{l=1}^{\infty}\big[M_{kl}a_l(t) - M_{lk}a_k(t)\big], \tag{21}$$

since transition probabilities have the normalization $\sum_{l=1}^{\infty}M_{lk} = 1$. Equation (21) is known as the *Pauli master equation*.

If an operator basis $\{|E_k)\}$ consists of eigenelements of the superoperator $\mathcal{L}$, then

$$\mathcal{L}|E_k) = |E_k)z_k,$$

and the solution of equation (18) can be written in the form

$$|A_t) = \sum_{k=1}^{\infty} |E_k)c_k e^{z_k t},$$

where z_k are eigenvalues of the superoperator $\mathcal{L}$. The coefficients c_k can be found from the expansion

$$|A_0) = \sum_{k=1}^{\infty} |E_k)c_k. \tag{22}$$

The method of finding solutions in the form of their expansions with respect to a basis of eigenelements of the superoperator $\mathcal{L}$ is called the *Fourier method*.

Now let an arbitrary basis $\{E_k\}$ for $\mathcal{M}$. Suppose $A(t) = E_k(t)$ is the solution of Cauchy problem for equation (18) in which the initial condition is given by $|A_0) = |E_k)$. The system $\{|E_k(t))\}$ is called a fundamental system of solutions with respect to the basis $\{|E_k)\}$. The matrix-functions with the elements

$$p_{kl}(t) = \big(E_k|E_l(t)\big) = (E_k|\Phi_t E_k)$$

is called the *fundamental matrix* of the equation in the basis $\{|E_k)\}$.

If $|A_0)$ is defined by (22), then the solution of the Cauchy problem with the initial condition $A(0) = A_0$ can be written in the form

$$|A_t) = \sum_{k,l=1}^{\infty} |E_k)p_{kl}(t)c_l.$$

The functions $p_{kl}(t)$ satisfy the identity

$$\sum_{m=1}^{\infty} p_{km}(t)p_{ml}(s) = p_{kl}(t+s).$$

If the superoperator Φ_t is such that

$$p_{kl}(t) \geqslant 0, \qquad \sum_{l=1}^{\infty} p_{kl}(t) = 1,$$

then the numbers $p_{kl}(t)$ can be treated as the probabilities of the passage of quantum system from the state $|E_k)$ into the state $|E_l)$. In this case, the fundamental matrix describes the *Markov process with a denumerable number of states*.

14.9. Equations in coordinate representation

Let us consider the operator basis $|xy) = |\hat{P}(x, y))$. Equation (18) gives

$$(xy|\frac{d}{dt}|A_t) = (xy|\mathcal{L}|A_t).$$

Using

$$\frac{d}{dt}|xy) = \frac{d}{dt}\big|\hat{P}(x, y)\big) = 0, \qquad \int dx\, dy\, |xy)(xy| = I,$$

we obtain

$$\frac{d}{dt}(xy|A_t) = \int dx'\, dy'\, (xy|\mathcal{L}|x'y')(x'y'|A_t).$$

As a result, we have

$$\frac{d}{dt}a_t(x, y) = \int dx'\, dy'\, L(x, y, x', y')a_t(x', y'),$$

where $a_t(x, y) = (xy|A_t)$, and $L(x, y, x', y') = (xy|\mathcal{L}|x'y')$. If $(A|B) = Tr[A^*B]$, then

$$a_t(x, y) = (xy|A_t) = Tr\big[\hat{P}^*(x, y)A_t\big] = Tr\big[|y><x|A_t\big] = <x|A_t|y>,$$
$$L(x, y, x', y') = (xy|\mathcal{L}|x'y') = Tr\big[\hat{P}^*(x, y)\mathcal{L}\big(\hat{P}(x', y')\big)\big].$$

Let $\hat{P}(x, y)$ be a ket-bra operator. If $|x>$ is a basis of a Hilbert space $\mathcal{H}$, then $\hat{P}(x, y)$ is a basis of an associated operator Hilbert space $\bar{\mathcal{H}}$. Equation (18) for $A = \hat{P}(x, y)$ gives

$$\frac{d}{dt}\hat{P}_t(x, y) = \frac{\partial}{\partial t}\hat{P}_t(x, y) + \mathcal{L}\big(\hat{P}_t(x, y)\big),$$

where $\hat{P}_t(x, y) = \Phi_t(\hat{P}(x, y))$. The initial condition is $\hat{P}_{t=0}(x, y) = \hat{P}(x, y)$.

As a result, $|\hat{P}_t(x, y))$ is considered as a solution of equation (18) with the condition

$$|A_0) = \big|\hat{P}(x, y)\big) = |xy).$$

The operator $|\hat{P}_t(x, y))$ is a fundamental solutions with respect to the basis $\{|xy)\}$.

STATEMENT. *Let $\hat{P}(x, y)$ be a basis of an operator Hilbert space $\bar{\mathcal{H}}$. Then $\hat{P}_t(x, y) = \Phi_t(\hat{P}(x, y))$ is a basis if and only if the superoperator $\mathcal{L}$ is Hamiltonian.*

Differentiation of the relation $\hat{P}_t(x, y)\hat{P}_t(z, s) = \delta(y, z)\hat{P}_t(x, s)$ with respect to time t at $t = 0$ gives $Z_{\mathcal{L}}(\hat{P}(x, y), \hat{P}(z, s)) = 0$. This condition means that $\mathcal{L}$ is a Hamiltonian superoperator.

As a result, the evolution of a quantum system is a map from a set of basis operators into itself if and only if the system is Hamiltonian. In general, the evolution cannot be considered as a transformation of operator basis into basis.

If A_0 has the expansion

$$|A_0) = \int dx\, dy\, |xy) a_0(x, y),$$

then the solution of equation (18) with the initial condition $A(0) = A_0$ can be written in the form

$$|A_t) = \int dx\, dy\, dx'\, dy'\, |xy)\; p_t(x, y, x', y')\, a_0(x', y').$$

The functions $p_t(x, y, x', y')$ satisfy the identity

$$\int dx'\, dy'\; p_t(x, y, x', y') p_s(x', y', x'', y'') = p_{t+s}(x, y, x'', y'').$$

If the superoperator $\mathcal{L}$ is such that

$$p_t(x, y, x', y') \geqslant 0, \qquad \int dx'\, dy'\; p_t(x, y, x', y') = 1,$$

then $p_t(x, y, x', y') = (xy|\hat{P}_t(x', y'))$ can be treated as the probabilities of the passage of quantum system from the state $|xy)$ into the state $|x'y')$. In this case, the fundamental function describes the Markov process.

14.10. Example of operator differential equation

Let us consider the operator differential equation

$$\begin{aligned}\frac{d}{dt}A_t = &-H_0 \cdot A_t + (\lambda + \mu)P \circ (A_t \cdot Q) - (\lambda - \mu)Q \circ (A_t \cdot P)\\ &+ d_{pp}Q \cdot (Q \cdot A_t) + d_{qq}P \cdot (P \cdot A_t)\\ &- d_{pq}P \cdot (Q \cdot A_t) - d_{qp}Q \cdot (P \cdot A_t),\end{aligned}$$

where $H_0 = (1/2m)P^2 + (m\omega^2/2)Q^2$. The superoperator $\mathcal{L}$ has the form

$$\begin{aligned}\mathcal{L} = &-L^-_{H_0} - (\lambda + \mu)L^+_P L^-_Q + (\lambda - \mu)L^+_Q L^-_P\\ &+ d_{pp}L^-_Q L^-_Q + d_{qq}L^-_P L^-_P - d_{pq}L^-_P L^-_Q - d_{qp}L^-_Q L^-_P.\end{aligned}$$

It is not hard to prove that $\mathcal{L}$ is a non-Hamiltonian superoperator.

For Q and P, we obtain

$$\mathcal{L}Q = \frac{1}{m}P + \mu Q - \lambda Q, \qquad \mathcal{L}P = -m\omega^2 Q - \mu P - \lambda P.$$

Let us define the following matrices

$$A_0 = \begin{pmatrix} Q \\ P \end{pmatrix}, \qquad M = \begin{pmatrix} \mu - \lambda & \frac{1}{m} \\ -m\omega^2 & -\mu - \lambda \end{pmatrix}.$$

In this case, the operator differential equation for A_t becomes

$$\frac{d}{dt}A_t = MA_t, \tag{23}$$

where $\mathcal{L}A_t = MA_t$. The solution of (23) is

$$A_t = \Phi_t A_0 = \sum_{n=0}^{\infty} \frac{t^n}{n!}\mathcal{L}^n A_0 = \sum_{n=0}^{\infty} \frac{t^n}{n!}M^n A_0.$$

The superoperator Φ_t has the form

$$\Phi_t = e^{tM} = e^{-\lambda t}\begin{pmatrix} \cos(\omega_0 t) + \frac{\mu}{\omega_0}\sin(\omega_0 t) & \frac{1}{m\omega_0}\sin(\omega_0 t) \\ -\frac{m\omega^2}{\omega_0}\sin(\omega_0 t) & \cos(\omega_0 t) - \frac{\mu}{\omega_0}\sin(\omega_0 t) \end{pmatrix},$$

where $\omega_0^2 = \omega^2 - \mu^2$. As a result, we obtain

$$Q_t = e^{-\lambda t}\left[\cos(\omega_0 t) + \frac{\mu}{\omega_0}\sin(\omega_0 t)\right]Q_0 + \frac{1}{m\omega_0}e^{-\lambda t}\sin(\omega_0 t)P_0,$$

$$P_t = -\frac{m\omega^2}{\omega_0}e^{-\lambda t}\sin(\omega_0 t)Q_0 + e^{-\lambda t}\left[\cos(\omega_0 t) - \frac{\mu}{\omega_0}\sinh(\omega_0 t)\right]P_0.$$

These equations describe a solution of the operator differential equation (23).

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Chapter 15

Quantum Dynamical Semi-Group

15.1. Dynamical semi-groups

An axiomatic approach to quantum dynamics of non-Hamiltonian systems gives the most general dynamical laws for quantum systems. These laws describe the most general linear mapping of the set of states into itself. We can introduce the semi-group laws as the fundamental dynamical postulate for non-Hamiltonian systems. The axioms for a dynamical semi-group has been given by A. Kossakowski and R.S. Ingarden [88,74]. The dynamical semi-groups are special examples of strongly continuous contractive semi-groups.

The state of the quantum system can be identified with the density operator, i.e., with the self-adjoint, positive linear operator of unit trace. It is more natural for this purpose to take the real Banach space $\mathcal{K}_r^1(\mathcal{H})$ of trace-class operators. A set of states can be considered as a positive cone $\mathcal{K}_{r+}^1(\mathcal{H})$ of a Banach space $\mathcal{K}_r^1(\mathcal{H})$. We can also use a positive cone $\mathcal{K}_{r+}^2(\mathcal{H})$ of the Hilbert space $\mathcal{K}_r^2(\mathcal{H})$ of Hilbert–Schmidt operators.

DEFINITION. A *dynamical semi-group* is a one-parameter semi-group $\{S_t | t \geqslant 0\}$ of linear superoperators S_t on $\mathcal{K}_{r+}^1(\mathcal{H})$, such that the following requirements are satisfied:

(1) S_t maps $\mathcal{K}_{r+}^1(\mathcal{H})$ into itself for each $t \geqslant 0$.
(2) $\{S_t | t \geqslant 0\}$ is a one-parameter semi-group on $\mathcal{K}_{r+}^1(\mathcal{H})$.
(3) $\|S_t(\rho)\|_1 = \|\rho\|_1$ for all $\rho \in \mathcal{K}_{r+}^1(\mathcal{H})$ and $t \geqslant 0$.
(4) $w\text{-}\lim_{t\to+0} S_t(\rho) = \rho$ for all $\rho \in \mathcal{K}_r^1(\mathcal{H})$.

Requirement (2) express the mathematical statement that $\{S_t | t \geqslant 0\}$ is a positive semi-group. Requirement (4) means that

$$\lim_{t\to+0} (S_t \rho | A) = (\rho | A) \tag{1}$$

for any bounded linear operator A and $\rho \in \mathcal{K}_r^1(\mathcal{H})$. Here $(A|B) = Tr[A^*B]$. In this case, the weak limit in equation (1) is equivalent to the strong limit

$$\lim_{t\to+0} \big\| S_t(\rho) - \rho \big\|_1 = 0$$

for all $\rho \in \mathcal{K}_r^1(\mathcal{H})$.

THEOREM. *A set $\{S_t | t \geqslant 0\}$ of superoperators on $\mathcal{K}_r^1(\mathcal{H})$ is a dynamical semi-group if and only if the following requirements are satisfied*:

(1) $\{S_t|t \geqslant 0\}$ *is a one-parameter semi-group on* $\mathcal{K}_r^1(\mathcal{H})$.
(2) $(S_t\rho|I) = (\rho|I)$ *for all* $t \geqslant 0$, *and* $\rho \in \mathcal{K}_r^1(\mathcal{H})$.
(3) $\|S_t(\rho)\|_1 \leqslant \|\rho\|_1$ *for all* $t \geqslant 0$, *and* $\rho \in \mathcal{K}_r^1(\mathcal{H})$.
(4) $\lim_{t\to+0}(S_t\rho|A) = (\rho|A)$ *for any bounded linear operator* A *and* $\rho \in \mathcal{K}_r^1(\mathcal{H})$.

It is not hard to see that these requirements are written for the whole space $\mathcal{K}_r^1(\mathcal{H})$, not only in its positive cone $\mathcal{K}_{r+}^1(\mathcal{H})$. Requirement (2) expresses the statement that S_t is a *trace-preserving superoperator*, i.e.,

$$Tr\big[S_t(\rho)\big] = Tr[\rho]$$

for all $t \geqslant 0$, and $\rho \in \mathcal{K}_r^1(\mathcal{H})$. Requirement (3) means that $\{S_t|t \geqslant 0\}$ is a contractive semi-group, i.e., $\|S_t\| \leqslant 1$ for $t \in [0, \infty)$. This theorem gives us a complete description of dynamical semi-groups and it can be formulated in the following form.

STATEMENT. *A dynamical semi-group is a strongly continuous one-parameter contractive semi-group of trace-preserving bounded linear superoperators on* $\mathcal{K}_r^1(\mathcal{H})$.

Using the Hille–Yosida theorem to a dynamical semi-group $\{S_t|t \geqslant 0\}$, we obtain that there exists a generating superoperator Λ on $\mathcal{K}_r^1(\mathcal{H})$. The domain $D(\Lambda)$ of the superoperator Λ is dense in $\mathcal{K}_r^1(\mathcal{H})$, and $\Lambda S_t = S_t\Lambda$. Moreover, the superoperator differential equation

$$\frac{d}{dt}S_t = \Lambda S_t$$

holds for all $t \geqslant 0$. Using $\rho_s(t) = S_t(\rho)$, we see that $\rho_s(t)$ is the solution of the Cauchy problem for the operator equation

$$\frac{d}{dt}\rho_s(t) = \Lambda\rho_s(t) \tag{2}$$

in which the initial condition is given by $\rho_s(0) = \rho \in D(\Lambda)$. The generator Λ is called the *Liouville superoperator*, or *Liouvillian*. Equations of type (2) is called the *quantum Liouville equation*, or the *master equation*, for non-Hamiltonian systems.

It is not hard to see that non-Hamiltonian quantum dynamics should be formulated for density operators of mixed states, and cannot be reduced to pure states only. A non-Hamiltonian superoperator Λ can have a Hamiltonian part $\Lambda_H = L_H^-$ such that $\Lambda = \Lambda_H + \mathcal{D}$, where $\mathcal{D}$ is another non-Hamiltonian superoperator. Such a decomposition is not unique.

Using the Hille–Yosida theorem, we can describe the properties of the superoperator Λ.

THEOREM. *Let Λ be a linear superoperator whose domain $D(\Lambda)$ and rage $R(\Lambda)$ both lie in $\mathcal{K}_r^1(\mathcal{H})$. Then Λ is a generating superoperator of a dynamical semi-group if and only if the following requirements are satisfied*:

(1) *$D(\Lambda)$ is dense in $\mathcal{K}_r^1(\mathcal{H})$.*

(2) *$R(zL_I - \Lambda) = \mathcal{K}_r^1(\mathcal{H})$ for all $z > 0$.*

(3) *$\|(zL_I - \Lambda)\rho\|_1 \geqslant z\|\rho\|_1$ for all $\rho \in D(\Lambda)$ and $z > 0$.*

(4) *$Tr[\Lambda(\rho)] = 0$ for all $\rho \in D(\Lambda)$.*

Requirement (2) expresses the statement that Λ is a maximal dissipative superoperator for all $\rho \in D(\Lambda)$. Requirement (3) means that Λ is a dissipative superoperator for all $\rho \in D(\Lambda)$.

15.2. Semi-scalar product and dynamical semi-groups

The necessary and sufficient conditions for Λ to be the generating superoperator of a dynamical semi-group can also be formulated by semi-scalar product. G. Lumer and R.S. Phillips have described contractive semi-groups by virtue of the notion of semi-scalar product [101]. The infinitesimal generator of such a semi-group is dissipative with respect to this product.

DEFINITION. Let $\mathcal{M}$ be a real (or complex) Banach operator space. A *semi-scalar product* of elements A and B of $\mathcal{M}$ is a real (or complex) number $[A|B]$ with the following properties:

(1) $[A|aB + bC] = a[A|B] + b[A|C]$ for all $a, b \in \mathbb{R}$ (or $\mathbb{C}$) and $A, B, C \in \mathcal{M}$.

(2) $[A|A] = \|A\|_{\mathcal{M}}^2$ for all $A \in \mathcal{M}$.

(3) $|[A|B]| \leqslant \|A\|_{\mathcal{M}}\|B\|_{\mathcal{M}}$ for all $A, B \in \mathcal{M}$.

LUMER THEOREM. *To each pair A and B of a Banach space $\mathcal{M}$, we can associate a semi-scalar product* $[A|B]$.

Let $\mathcal{M}$ be a Banach operator space, and let A be an arbitrary element of $\mathcal{M}$. Then there exists a bounded linear functional $\omega_A \in \mathcal{M}^*$ such that

$$\|\omega_A\| = \|A\|_{\mathcal{M}}, \qquad \omega_A(A) = \|A\|^2_{\mathcal{M}}.$$

It is not hard to see that ω_A is a normalized tangent functional. Then the equation

$$[A|B] = \omega_B(A)$$

defines a semi-scalar product for all $A, B \in \mathcal{M}$.

DEFINITION. Let a Banach space $\mathcal{M}$ be endowed with a semi-scalar product $[A|B]$. A linear superoperator Λ with domain $D(\Lambda)$ and range $R(\Lambda)$ both in $\mathcal{M}$ is called *dissipative* with respect to $[A|B]$ if $\mathrm{Re}[\Lambda(A)|A] \leqslant 0$ for all $A \in D(\Lambda)$.

Let $\mathcal{M}$ be a Hilbert operator space. Then a symmetric superoperator Λ such that $\mathrm{Re}(\Lambda(A)|B) \leqslant 0$ is dissipative with respect to the semi-scalar product $[A|B] = (A|B)$, where $(A|B)$ is the scalar product of $\mathcal{M}$.

PHILLIPS–LUMER THEOREM. *Let Λ be a linear superoperator whose domain $D(\Lambda)$ and range $R(\Lambda)$ lie in the same Banach operator space $\mathcal{M}$. Then Λ is a generating superoperator of contractive semi-group of class (C_0) if and only if the following requirements are satisfied*:

(1) *$D(\Lambda)$ is dense in $\mathcal{M}$.*
(2) *$R(I - \Lambda) = \mathcal{M}$.*
(3) *Λ is a dissipative superoperator with respect to any semi-scalar product.*

COROLLARY. *Let Λ be a linear superoperator whose domain $D(\Lambda)$ and range $R(\Lambda)$ lie in the same Banach operator space $\mathcal{M}$, and let $\mathcal{L}$ be an adjoint superoperator. Then Λ is a generating superoperator of contractive semi-group of class (C_0) if and only if the following requirements are satisfied*:

(1) *$D(\Lambda)$ is dense in $\mathcal{M}$.*
(2) *Λ is closed.*
(3) *Λ and $\mathcal{L}$ are dissipative superoperators.*

The Phillips–Lumer theorem gives us complete information about generating superoperators of contractive semi-group of class (C_0). Let us give the basic theorem regarding necessary and sufficient conditions for Λ to be the generator of dynamical semi-group.

THEOREM. *Let Λ be a linear superoperator whose domain $D(\Lambda)$ and range $R(\Lambda)$ lie in the same Banach space $\mathcal{K}_r^1(\mathcal{H})$. Then Λ is a generating superoperator of dynamical semi-group if and only if the following conditions are satisfied*:

(1) *$D(\Lambda)$ is dense in $\mathcal{K}_r^1(\mathcal{H})$.*
(2) *$R(I-\Lambda)=\mathcal{K}_r^1(\mathcal{H})$.*
(3) *Λ is a dissipative superoperator with respect to semi-scalar product.*
(4) *$Tr[\Lambda(\rho)]=0$ for all $\rho\in D(\Lambda)$.*

It is not hard to see the following property.

STATEMENT. *Let Λ be a generating superoperator of contractive semi-group of class (C_0) on $\mathcal{K}_r^1(\mathcal{H})$. Then Λ be a generating superoperator of dynamical semi-group if and only if $Tr[\Lambda(\rho)]=0$ for all $\rho\in D(\Lambda)$.*

Differentiation of the equality $Tr[S_t\rho]=Tr[\rho]$ gives

$$Tr\left[\frac{d}{dt}(S_t\rho)\right]=Tr[\Lambda S_t\rho]=0.$$

For $t=0$, we obtain $Tr[\Lambda(\rho)]=0$.

STATEMENT. *A bounded linear superoperator Λ on $\mathcal{K}_r^1(\mathcal{H})$ is a generating superoperator of dynamical semi-group on $\mathcal{K}_r^1(\mathcal{H})$ if and only if the following conditions are satisfied*:

(1) *Λ is a dissipative superoperator.*
(2) *$Tr[\Lambda(\rho)]=0$ for all $\rho\in\mathcal{K}_r^1(\mathcal{H})$.*

As a result, each generating superoperator of dynamical semi-group on $\mathcal{K}_r^1(\mathcal{H})$ is a dissipative superoperator.

15.3. Dynamical semi-groups and orthogonal projections

The necessary and sufficient conditions for generating superoperators of a dynamical semi-group can be described by using a system of orthogonal projections [74]. Let $\{P_k\}$ be a complete set of orthogonal projection operators P_k on closed subspaces of a Hilbert space $\mathcal{H}$, such that

$$P_kP_l=\delta_{kl}P_l,\quad P_k^*=P_k,\quad Tr\,P_k<\infty,\quad \sum_{k=1}^{\infty}P_k=I \tag{3}$$

for $k,l\in\mathbb{N}$. This is the *discrete orthogonal resolution of identity*.

THEOREM *(Ingarden–Kossakowski). Let Λ be a bounded linear superoperator on $\mathcal{K}_r^1(\mathcal{H})$. Then Λ is a generating superoperator of a dynamical semi-groups on $\mathcal{K}_r^1(\mathcal{H})$ if and only if the conditions*

$$\Lambda_{kk} \leqslant 0, \quad \Lambda_{kl} \geqslant 0 \ (k \neq l), \quad \sum_{k=1}^{\infty} \Lambda_{kl} = 0, \tag{4}$$

are valid for any complete set $\{P_k\}$ of orthogonal projections (3), where

$$\Lambda_{kl} = (P_k|\Lambda|P_k) = Tr\big[P_k \Lambda(P_l)\big]. \tag{5}$$

Conditions (4) are quantum analogues of the Kolmogorov's conditions for a discrete Markov process. An observable with a discrete spectrum defines a complete set of orthogonal projections. Then the time evolution of quantum non-Hamiltonian system can be considered as an infinite set of classical discrete Markov processes corresponding to some observables with discrete spectrum. As a result, the quantum non-Hamiltonian dynamics describes quantum Markov processes.

Let us give the basic theorem regarding Hamiltonian quantum systems.

THEOREM. *Let $\{S_t|t \geqslant 0\}$ be a dynamical semi-group on $\mathcal{K}_r^1(\mathcal{H})$, such that the following requirements are satisfied*:

(1) *S_t is surjection, i.e., S_t is an epimorphism of $\mathcal{K}_r^1(\mathcal{H})$.*
(2) *$\|S_t(\rho)\|_1 = \|\rho\|_1$ for all $\rho \in \mathcal{K}_r^1(\mathcal{H})$ and $t \geqslant 0$.*

Then there exists a strongly continuous one-parameter group $\{U_t|\ t \in \mathbb{R}\}$ of unitary operators U_t on a Hilbert space $\mathcal{H}$, such that $S_t = L_{U_t} R_{U_t^*}$ for all $t \geqslant 0$.

Requirement (1) expresses the statement that the superoperator S_t is an epimorphism instead of endomorphism. Requirement (2) is expressed in the whole space $\mathcal{K}_r^1(\mathcal{H})$, not only in its positive cone $\mathcal{K}_{r+}^1(\mathcal{H})$.

This theorem describes the conditions for a quantum system to be Hamiltonian. By Stone's theorem, there exists a self-adjoint operator H such that

$$U_t = \exp \frac{1}{i\hbar} H, \qquad \frac{d}{dt} U_t = \frac{1}{i\hbar} H U_t.$$

For $\rho_s(t) = S_t \rho = U_t \rho U_t^*$, where $S_t = \exp t L_H^-$, we obtain

$$\begin{aligned} \frac{d}{dt}\rho_s(t) &= \frac{dU_t}{dt}\rho U_t^* + U_t \rho \frac{dU_t^*}{dt} \\ &= \frac{1}{i\hbar}\big(H U_t \rho U_t^* - U_t \rho U_t^* H\big) \end{aligned}$$

$$= \frac{1}{i\hbar}\big(H\rho_s(t) - \rho_s(t)H\big).$$

As a result, the Liouvillian Λ is a globally Hamiltonian superoperator, and equation (2) can be presented in the form

$$\frac{d}{dt}\rho_s(t) = L_H^-\rho_s(t).$$

This is the *von Neumann equation*.

15.4. Dynamical semi-groups for observables

We described the time evolution of the states of a system. The dynamical semi-groups have been discussed for density operators. This is the Schrödinger dynamical representation. We can define a dynamical semi-group for observables to describe the time evolution of the quantum observables. The axioms for a dynamical semi-group can be considered in the so-called Heisenberg dynamical representation.

To describe observables, we use the space $\mathcal{K}_r^{1*}(\mathcal{H})$ dual of $\mathcal{K}_r^1(\mathcal{H})$. For any bounded self-adjoint operator $\rho \in \mathcal{K}_r^1(\mathcal{H})$, the correspondence $\rho \to (\rho|A) = Tr[\rho A]$ defines a continuous linear functional on $\mathcal{K}_r^1(\mathcal{H})$. Conversely any continuous linear functional on $\mathcal{K}_r^1(\mathcal{H})$ has this form. If we denote by $\mathcal{B}(\mathcal{H})$ the Banach space of all bounded operators, then $\mathcal{K}_r^{1*}(\mathcal{H}) = [\mathcal{K}_r^1(\mathcal{H})]^* = \mathcal{B}(\mathcal{H})$. A state is considered as an element of $\mathcal{K}_r^1(\mathcal{H})$. The dual space $\mathcal{K}_r^{1*}(\mathcal{H})$ consists of all bounded observables.

DEFINITION. Let $\{S_t|t \geqslant 0\}$ be a dynamical semi-group on $\mathcal{K}_r^1(\mathcal{H})$. A *adjoint* (*conjugated*) *dynamical semi-group* of $\{S_t|t \geqslant 0\}$ is a set of all linear superoperators Φ_t, on $\mathcal{K}_r^{1*}(\mathcal{H}) = \mathcal{B}(\mathcal{H})$ adjoint of S_t, with respect to the scalar product $(A|B) = Tr[A^*B]$, i.e.,

$$\big(\Phi_t(A)|\rho\big) = \big(A|S_t(\rho)\big)$$

for all $A \in \mathcal{B}(\mathcal{H})$ and $\rho \in \mathcal{K}_r^1(\mathcal{H})$.

The classic notation to denote that Φ_t is adjoint of S_t is $\Phi_t = \bar{S}_t$. If A is a self-adjoint operator, then

$$(A|\rho) = Tr[A^*\rho] = Tr[\rho A] = (\rho|A).$$

As a result, S_t is an adjoint superoperator of Φ_t, such that $(S_t(\rho)|A) = (\rho|\Phi_t(A))$. We shall usually use the notation $S_t = \bar{\Phi}_t$.

STATEMENT. *Let S_t be a trace-preserving superoperator, and let Φ_t be an adjoint superoperator of S_t. Then Φ_t is unit preserving, i.e., $\Phi_t(I) = I$.*

PROOF. Let S_t be a trace-preserving superoperator. Then $Tr[S_t\rho] = Tr[\rho]$ for all $\rho \in \mathcal{K}_r^1(\mathcal{H})$. This equality can be rewritten in the form

$$(S_t\rho|I) = (\rho|I). \tag{6}$$

If Φ_t is adjoint of S_t, then equation (6) gives $(\rho|\Phi_t I) = (\rho|I)$ for all $\rho \in \mathcal{K}_r^1(\mathcal{H})$. As a result, Φ_t is unit preserving: $\Phi_t(I) = I$. □

The axioms for a dynamical semi-group will be repeated here in the Heisenberg dynamical representation.

STATEMENT. *Let* $\{S_t|t \geqslant 0\}$ *be a dynamical semi-group on* $\mathcal{K}_r^1(\mathcal{H})$. *Then the dynamical semi-group* $\{\Phi_t|t \geqslant 0\}$ *on* $\mathcal{M} = \mathcal{B}(\mathcal{H})$ *adjoint of* $\{S_t|t \geqslant 0\}$ *satisfies the following conditions*:

(1) Φ_t *maps* $\mathcal{B}_+(\mathcal{H})$ *into itself for each* $t \geqslant 0$.
(2) $\{\Phi_t|t \geqslant 0\}$ *is a one-parameter semi-group on* $\mathcal{B}_+(\mathcal{H})$.
(3) $\|\Phi_t A\|_{\mathcal{M}} \leqslant \|A\|_{\mathcal{M}}$ *for all* $A \in \mathcal{B}_+(\mathcal{H})$ *and* $t \geqslant 0$.
(4) $w\text{-}\lim_{t\to+0} \Phi_t A = A$ *for all* $A \in \mathcal{B}(\mathcal{H})$.

Requirement (4) means that

$$\lim_{t\to+0} (\rho|\Phi_t A) = (\rho|A)$$

for all $A \in \mathcal{B}(\mathcal{H})$ and $\rho \in \mathcal{K}_r^1(\mathcal{H})$, where $(A|B) = Tr[A^*B]$.

As a result, we can give the following definition.

DEFINITION. Let $\mathcal{M}$ be an algebra of bounded operators. A *dynamical semi-group* is a one-parameter semi-group $\{\Phi_t|t \geqslant 0\}$ on $\mathcal{M}$ such that the following conditions are satisfied:

(1) Φ_t is a positive superoperators for each $t \geqslant 0$.
(2) $\{\Phi_t|t \geqslant 0\}$ is a contractive semi-group.
(3) $\{\Phi_t|t \geqslant 0\}$ is a semi-group of class (C_0).

There exists a superoperator $\mathcal{L}$ on a domain $D(\mathcal{L}) \subset \mathcal{M}$ such that

$$\lim_{t\to0+} \left\|\mathcal{L}A - t^{-1}(\Phi_t - L_I)A\right\|_{\mathcal{M}} = 0.$$

This is the generating superoperator of the dynamical semi-group $\{\Phi_t|t \geqslant 0\}$. Moreover, $\mathcal{L}\Phi_t = \Phi_t\mathcal{L}$. The superoperator $\mathcal{L}$ will be called the *Heisenberg superoperator*. The Liouville superoperator Λ is adjoint of $\mathcal{L}$, i.e.,

$$\big(\rho|\mathcal{L}(A)\big) = \big(\Lambda(\rho)|A\big).$$

The classic notation to denote that Λ is adjoint of $\mathcal{L}$ is $\Lambda = \bar{\mathcal{L}}$.

Using $A(t) = \Phi_t A$, we see that $A(t)$ is the solution of the Cauchy problem for the operator differential equation

$$\frac{d}{dt}A(t) = \mathcal{L}A(t) \tag{7}$$

in which the initial condition is given by $A(0) = A \in D(\mathcal{L})$. Equation (7) describes the time evolution of the observable A. We may also say that (7) is a dual (conjugate) equation of the quantum Liouville equation.

If $\mathcal{L}$ is a globally Hamiltonian superoperator, then $\mathcal{L} = -L_H^-$ and equation (7) has the form

$$\frac{d}{dt}A(t) = -\frac{1}{i\hbar}\big[H, A(t)\big],$$

where $H \in \mathcal{M}$ is a self-adjoint operator. Note that the adjoint superoperator Λ of $\mathcal{L} = -L_H^-$ is $\Lambda = L_H^-$. This is easy to show:

$$\begin{aligned}(\Lambda A|B) &= Tr\left[\left(\frac{1}{i\hbar}[H, A]\right)^* B\right] = Tr\left[\left(\frac{1}{i\hbar}(HA - AH)\right)^* B\right] \\ &= Tr\left[\left(\frac{-1}{i\hbar}(A^*H - HA^*)\right)B\right] = Tr\left[\left(\frac{1}{i\hbar}(HA^*B - A^*HB)\right)\right] \\ &= Tr\left[A^*\left(\frac{1}{i\hbar}(BH - HB)\right)\right] = Tr\big[A^*\big(-L_H^- B\big)\big] = (A|\mathcal{L}B).\end{aligned}$$

15.5. Quantum dynamical semi-groups on W*-algebras

It is important to describe the explicit structure of a generating superoperator of a quantum dynamical semi-group. The structure is not known in general but important partial results are available.

We consider as an algebra $\mathcal{M}$ of quantum observables, an abstract C^*-algebra or W^*-algebra. The time evolution of an observable is described by a dynamical semi-group $\{\Phi_t, t \geqslant 0\}$ on $\mathcal{M}$.

If $\mathcal{M}$ is a C^*-algebra, then we always assume that $\{\Phi_t | t \geqslant 0\}$ is a strongly continuous semi-group for $t \geqslant 0$, i.e.,

$$\lim_{t \to s} \big\| \Phi_t(A) - \Phi_s(A) \big\|_{\mathcal{M}} = 0$$

for all $A \in \mathcal{M}$ and $t, s > 0$.

If $\mathcal{M}$ is a W^*-algebra, then we assume that the following conditions are satisfied:

(a) $A \to \Phi_t(A)$ is a ultraweakly (σ-weakly) continuous map for all $t \geqslant 0$, i.e.,

$$\lim_{k\to\infty} \|A_k - A\|_\sigma = 0 \quad \text{implies} \quad \lim_{k\to\infty} \big\|\Phi_t(A_k) - \Phi_t(A)\big\|_\sigma = 0$$

for all $t \geqslant 0$. If this requirement is satisfied, then the superoperator Φ_t is called *normal*, or ultraweakly continuous.

(b) $t \to \Phi_t(A)$ is a ultraweakly continuous map for all $A \in \mathcal{M}$, i.e.,

$$\lim_{t\to s} \big\|\Phi_t(A) - \Phi_s(A)\big\|_\sigma = 0$$

for all $A \in \mathcal{M}$ and $t, s \geqslant 0$.

Then we know that there exists a (bounded or unbounded) generating superoperator $\mathcal{L}$ defined on $\mathcal{M}$, such that

$$\lim_{t\to 0} \big\|\mathcal{L}(A) - t^{-1}(\Phi_t - L_I)A\big\| = 0$$

for all $A \in D(\mathcal{L})$. If $\mathcal{M}$ is a C^*-algebra, then $\| \ \| = \| \ \|_{\mathcal{M}}$ is an operator norm. If $\mathcal{M}$ is a W^*-algebra, then a ultraweak operator topology is used and $\| \ \| = \| \ \|_\sigma$. The set $D(\mathcal{L})$ is dense in $\mathcal{M}$.

The axioms for a dynamical semi-group on a W^*-algebra can be presented in the following form.

DEFINITION. A *dynamical semi-group* is a one-parameter semi-group $\{\Phi_t | t \geqslant 0\}$ of superoperators on a W^*-algebra $\mathcal{M}$, such that the following requirements are satisfied:

(1) Φ_t is a positive superoperator for each $t \geqslant 0$.
(2) $\Phi_t(I) = I$ for all $t \geqslant 0$.
(3) $\Phi_t A \to A$ ultraweakly for $t \to +0$.
(4) Φ_t is a ultraweakly continuous superoperator on $\mathcal{M}$.

The purpose of quantum theory is to derived an explicit form for the generating superoperator of a dynamical semi-group. It is concerned with the problem of determining the most general explicit form of this infinitesimal generator. The problem was investigated by V. Gorini, A. Kossakowski, E.C.G. Sudarshan and G. Lindblad around 1976. To describe this result, we have to introduce two restrictions in the class of dynamical semi-groups.

(1) We assume that the semi-group is norm continuous, that is the generator $\mathcal{L}$ is a *bounded superoperator*. This means that requirement (3) is replaced by

$$\lim_{t\to+0} \|\Phi_t - L_I\| = 0.$$

Then there exists a bounded superoperator $\mathcal{L}$ such that

$$\Phi_t = \exp t\mathcal{L}, \qquad \lim_{t\to+0} \left\| \mathcal{L} - t^{-1}(\Phi_t - L_I) \right\| = 0.$$

From the fact that the set of ultraweakly continuous superoperators on $\mathcal{M}$ is norm closed, we obtain that $\mathcal{L}$ is a ultraweakly continuous superoperator.

(2) We assume that the one-parameter semi-group $\{\Phi_t | t \geqslant 0\}$ is not merely positive but *completely positive* (CP), i.e., we replace requirement (1) by the condition $\Phi_t \in CP(\mathcal{M})$. The generating superoperator of completely positive semi-group is completely dissipative.

15.6. Completely positive superoperators

Let $\mathcal{M}$ be a C^*-algebra, and consider the set $M_n(\mathcal{M})$ of all $n \times n$ square arrays

$$[A_{ij}] = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \dots & \dots & \dots & \dots \\ A_{n1} & A_{n2} & \dots & A_{nn} \end{pmatrix},$$

where the A_{ij} are all in $\mathcal{M}$. Such a square arrays is a $n \times n$ matrix over $\mathcal{M}$. The set $M_n(\mathcal{M})$ of all $n \times n$ matrices with entries from $\mathcal{M}$ forms a C^*-algebra. $M_n(\mathcal{M})$ is called the $n \times n$ *matrix operator algebra* over a C^*-algebra $\mathcal{M}$.

If Φ_t is a one-parameter superoperator on $\mathcal{M}$, then there exists a superoperator Φ_{nt} on $M_n(\mathcal{M})$ defined by

$$\Phi_{nt}(A \otimes I_{ij}) \equiv \Phi_t(A) \otimes I_{ij},$$

where I_{ij} $(i, j = 1, \dots, n)$ are matrix units spanning $M_n(\mathbb{C})$. We write this as $\Phi_{nt} = \Phi_t \otimes I_n$.

DEFINITION. A *positive superoperator* is a superoperator Φ_t on $\mathcal{M}$, such that $\Phi_t(A^*A) \geqslant 0$ for all $A \in D(\Phi_t) \subset \mathcal{M}$.

If Φ_t is positive, then Φ_t is a map from a positive cone $\mathcal{M}_+$ of $\mathcal{M}$ into itself. We shall denote the set of all positive superoperators on $\mathcal{M}$ by $P(\mathcal{M})$. If Φ_t is a positive superoperator on $\mathcal{M}$, then Φ_{tn} is not necessary positive. We can restrict ourselves to maps Φ_t such that Φ_{tn} is always positive.

DEFINITION. A *completely positive superoperator* is a superoperator Φ_t from an operator algebra $\mathcal{M}$ into itself, such that the superoperators Φ_{nt} on $M_n(\mathcal{M})$ are positive for all $n \in \mathbb{N}$.

We shall denote the set of all completely positive superoperators on $\mathcal{M}$ by $CP(\mathcal{M})$. There are positive superoperators which are not completely positive. If Φ_t and Φ_s are completely positive superoperators on $\mathcal{M}$, then $\Phi_{t+s} = \Phi_t \Phi_s \in CP(\mathcal{M})$. Note that if $\Phi_t \in CP(\mathcal{M})$, then $\Phi_{tn} \in CP(M_n(\mathcal{M}))$ for each $n \in \mathbb{N}$.

There is another equivalent definition for completely positive superoperators that is often used.

DEFINITION. A *completely positive superoperator* is a superoperator Φ_t on a C^*-algebra $\mathcal{M}$, such that

$$\sum_{k=1}^{n}\sum_{l=1}^{n} B_k^* \Phi_t(A_k^* A_l) B_l \geqslant 0 \tag{8}$$

for all $A_k, B_k \in \mathcal{M}$, $k, l = 1, \ldots, n$, and all finite $n \in \mathbb{N}$.

We can illustrate this concept with an example. Let $\mathcal{M}$ be a C^*-algebra, and let Φ_t be an endomorphism of $\mathcal{M}$. Then

$$\Phi_t(AB) = \Phi_t(A)\Phi_t(B), \qquad \Phi_t(A^*) = (\Phi_t A)^*.$$

For $A_k, B_l \in \mathcal{M}$,

$$\begin{aligned}
\sum_{k=1}^{n}\sum_{l=1}^{n} B_k^* \Phi_t(A_k^* A_l) B_l &= \sum_{k=1}^{n}\sum_{l=1}^{n} B_k^* \Phi_t(A_k^*)\Phi_t(A_l) B_l \\
&= \sum_{k=1}^{n}\sum_{l=1}^{n} B_k^* (\Phi_t A_k)^* \Phi(A_l) B_l \\
&= \sum_{k=1}^{n}\sum_{l=1}^{n} \big((\Phi_t A_k) B_k\big)^* \big(\Phi(A_l) B_l\big) \\
&= \left(\sum_{k=1}^{n} (\Phi_t A_k) B_k\right)^* \left(\sum_{l=1}^{n} \Phi(A_l) B_l\right) \\
&= \left|\sum_{k=1}^{n} \Phi(A_k) B_k\right|^2 \geqslant 0.
\end{aligned}$$

As a result, we have the following statement.

STATEMENT. *If Φ_t is an endomorphism of a C^*-algebra $\mathcal{M}$, then Φ_t is a completely positive superoperator, i.e., $\Phi_t \in \mathrm{Hom}(\mathcal{M}, \mathcal{M}) \Rightarrow \Phi_t \in CP(\mathcal{M})$.*

Note that for classical systems where the algebra of observables is commutative, positive maps are always completely positive.

Let us give the basic theorem [148] regarding completely positive superoperators on a C^*-algebra. This theorem gives us the following canonical form of completely positive superoperators.

STINESPRING'S THEOREM. *Let $\mathcal{B}(\mathcal{H})$ be a unital C^*-algebra of all bounded operators on a Hilbert space $\mathcal{H}$, and let $\mathcal{M}$ be a C^*-subalgebra of $\mathcal{B}(\mathcal{H})$. Then Φ is a completely positive superoperator on $\mathcal{M}$ if and only if there exists a bounded linear operator V on $\mathcal{H}$ such that*

$$\Phi = L_{V^*} R_V. \tag{9}$$

It is not hard to prove half of this theorem: if the superoperator Φ has the form

$$\Phi A = L_{V^*} R_V A = V^* A V$$

for all $A \in \mathcal{M}$, then Φ is completely positive. For A_k, $B_l \in \mathcal{M}$,

$$\begin{aligned}
\sum_{k=1}^{n}\sum_{l=1}^{n} B_k^* \Phi(A_k^* A_l) B_l &= \sum_{k=1}^{n}\sum_{l=1}^{n} B_k^* V^* (A_k^* A_l) V B_l \\
&= \sum_{k=1}^{n}\sum_{l=1}^{n} (A_k V B_k)^* (A_l V B_l) \\
&= \left(\sum_{k=1}^{n} A_k V B_k\right)^* \left(\sum_{l=1}^{n} A_l V B_l\right) \\
&= \left|\sum_{k=1}^{n} A_k V B_k\right|^2 \geqslant 0.
\end{aligned}$$

Note that the representation (9) is not unique. This is the *Stinespring representation* of completely positive superoperator on a C^*-algebra $\mathcal{M}$. Let us give the basic theorem regarding completely positive superoperators on a W^*-algebra.

KRAUS THEOREM. *Let $\mathcal{B}(\mathcal{H})$ be a W^*-algebra of all bounded operators on a Hilbert space $\mathcal{H}$, and let $\mathcal{M}$ be a W^*-subalgebra of $\mathcal{B}(\mathcal{H})$. Then Φ is a completely positive superoperator on $\mathcal{M}$ if and only if the following conditions are satisfied*:

(1) *Φ is a ultraweakly continuous superoperator on $\mathcal{M}$.*
(2) *There exists a set of bounded linear operators $V_k \in \mathcal{M}$, such that the series $\sum_{k=1}^{\infty} V_k^* V_k \in \mathcal{M}$ strongly converges in $\mathcal{M}$.*
(3) *Φ can be represented in the form*

$$\Phi = \sum_{k=1}^{\infty} L_{V_k^*} R_{V_k}.$$

DEFINITION. Let $\mathcal{M}$ be an associative algebra of observables. A *quantum operation*, or *Kraus operation*, is a linear superoperator $\mathcal{E}$ on $\mathcal{M}$ that can be presented in the form

$$\mathcal{E}A = \sum_{k=1}^{\infty} L_{V_k} R_{V_k^*} A = \sum_{k=1}^{\infty} V_k A V_k^*$$

for all $A \in \mathcal{M}$, and some $V_k \in \mathcal{M}$.

The operators V_k, which satisfy

$$\sum_{k=1}^{\infty} V_k^* V_k = I$$

in order to $\mathcal{E}$ be trace-preserving, completely specify the quantum operation. We refer to the operators V_k as *Kraus operators*.

If $\mathcal{M}$ is an associative algebra and $\mathcal{M}^{(\pm)}$ the Lie–Jordan algebra corresponding to it, then we can obtain the following representation of the completely positive superoperator (9). Using

$$L_V = L_V^+ + \frac{i\hbar}{2} L_V^-,$$
$$R_V = L_V^+ - \frac{i\hbar}{2} L_V^-,$$

we obtain the superoperator (9) in the form

$$\Phi = L_{V^*}^+ L_V^+ + \frac{\hbar^2}{4} L_{V^*}^- L_V^- + \frac{i\hbar}{2}\left(L_{V^*}^- L_V^+ - L_{V^*}^+ L_V^-\right). \tag{10}$$

Another representations of Φ can be derived by using the mixed relations

$$L_A^- L_B^+ - L_B^+ L_A^- = L_{A\cdot B}^+, \qquad L_B^+ L_A^+ - L_A^+ L_B^+ = -\frac{\hbar^2}{4} L_{A\cdot B}^-,$$
$$L_A^+ L_B^- + L_B^+ L_A^- = L_{A\circ B}^-, \qquad L_A^+ L_B^+ - \frac{\hbar^2}{4} L_B^- L_A^- = L_{A\circ B}^+.$$

If $V = aQ + bP$, then the superoperator (10) is Weyl ordered. Then Φ is a map that assigns to each Weyl operator exactly one Weyl operator.

In general, the superoperator (10) with $V = V(Q, P)$ is not a Weyl ordered superoperator. Suppose $\mathcal{M}_W$ is an operator C^*-algebra of Weyl ordered operators $A(Q, P)$. This algebra is commutative with respect to the product $A(Q, P) * B(Q, P) = A(L_Q^+, L_P^+)A(L_Q^+, L_P^+)I$. Then positive superoperators on this operator algebra are always completely positive.

15.7. Bipositive superoperators

Let $\mathcal{M}$ is an involutive operator algebra.

DEFINITION. A *bipositive superoperator* is a superoperator Φ_t on $\mathcal{M}$, such that

$$\Phi_t(A^*A) \geqslant \Phi_t(A^*)\Phi_t(A) \tag{11}$$

for each $t \geqslant 0$, and $A \in \mathcal{M}$ where A^*, $A^*A \in \mathcal{M}$.

We shall denote the set of all bipositive superoperators on $\mathcal{M}$ by $CP_2(\mathcal{M})$.

THEOREM. *If Φ_t, $t \geqslant 0$, are completely positive superoperators on a C^*-algebra $\mathcal{M}$, then*

$$\Phi_t(A^*A) \geqslant \Phi_t(A^*)\big[\Phi_t(I)\big]^{-1}\Phi_t(A)$$

for all $A \in \mathcal{M}$.

The following corollary can be derived immediately from the theorem.

COROLLARY. *Let Φ_t, $t \geqslant 0$, be completely positive superoperators on a C^*-algebra $\mathcal{M}$, such that $\Phi_t(I) = I$. Then Φ_t are bipositive superoperators.*

Note that this property follows from equation (8) with $k, l = 1, 2$ and $A_1 = A$, $B_1 = I$, $A_2 = I$, $B_2 = -\Phi_t(A)$.

Let us give the properties of bipositive superoperators.

(1) Let Φ_t be a bipositive superoperator such that $\Phi_t J = J\Phi_t$, where J is an involution superoperator. Then Φ_t is positive. This is easily to show:

$$\Phi_t(A^2) = \Phi_t(A^*A) \geqslant \Phi_t(A^*)\Phi_t(A) = (\Phi_t A)^*(\Phi_t A) = |\Phi_t A|^2 \geqslant 0.$$

As a result, if $\Phi_t \in CP_2(\mathcal{M})$, then $\Phi_t \in P(\mathcal{M})$.

(2) If Φ_t is a bipositive superoperator on $\mathcal{M}$ and $\Phi_t J = J\Phi_t$, then

$$B^*\Phi_t(A^*A)B \geqslant 0$$

for all $A, B \in \mathcal{M}$. This is easy to show:

$$\begin{aligned} B^*\Phi_t(A^*A)B &\geqslant B^*\Phi_t(A^*)\Phi_t(A)B = B^*(\Phi_t A)^*\Phi_t(A)B \\ &= \big[\Phi_t(A)B\big]^*\Phi_t(A)B = \big|\Phi_t(A)B\big|^2 \geqslant 0. \end{aligned}$$

(3) If $\Phi_t \in CP_2(\mathcal{M})$ and $\Phi_t J = J\Phi_t$, then

$$\sum_{k=1}^{n} B_k^*\Phi_t(A_k^*A_k)B_k \geqslant 0$$

for all n.

(4) Let Φ_t be a bipositive superoperator. In general, Φ_t is *not* completely positive, since inequality (8) is not satisfied.

15.8. Completely dissipative superoperators

In this section, we consider completely positive and bipositive semi-groups, together with its infinitesimal generators.

Let $\mathcal{L}$ be a non-Hamiltonian superoperator on $\mathcal{M}$. Then there exist $A, B \in \mathcal{M}$ such that

$$Z_{\mathcal{L}}(A, B) \neq 0,$$

where

$$Z_{\mathcal{L}}(A, B) = \mathcal{L}(AB) - \mathcal{L}(A)B - A\mathcal{L}(B).$$

If $Z_{\mathcal{L}}(A, B) = 0$ for all $A, B \in D(\mathcal{L})$, then $\mathcal{L}$ is a locally Hamiltonian superoperator. If $\mathcal{L}$ is a locally Hamiltonian superoperator on a W^*-algebra, then $\mathcal{L}$ is globally Hamiltonian.

A superoperator $\mathcal{L}$ on $\mathcal{M}$ is dissipative, if for each $A \in D(\mathcal{L})$ there exists a nonzero tangent functional ω at A, such that $\mathrm{Re}[\omega(\mathcal{L}A)] \leqslant 0$. A superoperator $\mathcal{L}$ is called *accretive* if $\mathrm{Re}[\omega(\mathcal{L}A)] \geqslant 0$ for each $A \in D(\mathcal{L})$.

Let us give the basic theorem regarding dissipative and non-Hamiltonian superoperators for an operator algebra $\mathcal{M}$.

THEOREM. *Let $\mathcal{M}$ be a C^*-algebra with identity I, and let $\mathcal{L}$ be a superoperator from $D(\mathcal{L}) \subset \mathcal{M}$ into $\mathcal{M}$ such that*

(1) *$D(\mathcal{L})$ is an involutive subalgebra of $\mathcal{M}$.*
(2) *$I \in D(\mathcal{L})$.*
(3) *$\mathcal{L}(A^*) = (\mathcal{L}A)^*$.*
(4) *$\mathcal{L}(A^*A) - (\mathcal{L}A^*)A - A^*\mathcal{L}(A) \geqslant 0$.*

Then $\mathcal{L}$ is a dissipative superoperator.

There is again a terminology for a more general situation.

DEFINITION. A *dissipative superoperator* is a mapping $\mathcal{L}$ from an algebra $\mathcal{M}$ into itself, such that the following requirements are satisfied:

(1) $\mathcal{L}$ is a real superoperator on $D(\mathcal{L}) \subset \mathcal{M}$.
(2) The inequality $Z_{\mathcal{L}}(A^*, A) \geqslant 0$ is valid for all $A \in D(\mathcal{L})$ such that $A^*, A^*A \in D(\mathcal{L})$.

We shall denote the set of all dissipative superoperators on $\mathcal{M}$ by $Dis(\mathcal{M})$.

Let Φ_t be a bipositive superoperator. Then

$$\Phi_t(A^*A) - \Phi_t(A^*)\Phi_t(A) \geqslant 0.$$

Differentiation of this inequality at $t = 0$ gives

$$\mathcal{L}(A^*A) - \mathcal{L}(A^*)A - A^*\mathcal{L}(A) \geqslant 0$$

for all $A \in D(\mathcal{L}) \subset \mathcal{M}$. A bounded superoperator $\mathcal{L}$ on $\mathcal{M}$, which satisfies

$$\mathcal{L}(I) = 0, \quad \mathcal{L}(A^*) = (\mathcal{L}A)^*, \quad Z_{\mathcal{L}}(A^*, A) \geqslant 0,$$

is called dissipative. Hence the bipositivity of $\Phi_t = \exp\{t\mathcal{L}\}$ implies that $\mathcal{L}$ is dissipative.

If Φ_t is a completely positive superoperator on a C^*-algebra $\mathcal{M}$, then

$$\Phi_t(A^*A) \geqslant \Phi_t(A^*)\big[\Phi_t(I)\big]^{-1}\Phi_t(A)$$

for all $A \in \mathcal{M}$. Differentiation of this inequality at $t = 0$ gives

$$\mathcal{L}(A^*A) + A^*\mathcal{L}(I)A - \mathcal{L}(A^*)A - A^*\mathcal{L}(A) \geqslant 0.$$

For $\mathcal{L}(I) \neq 0$, we can define the superoperator $\mathcal{L}' = \mathcal{L} - L^+_{\mathcal{L}(I)}$ such that $\mathcal{L}'(I) = 0$, and

$$Z_{\mathcal{L}'}(A^*, A) = \mathcal{L}'(A^*A) - \mathcal{L}'(A^*)A - A^*\mathcal{L}'(A) \geqslant 0.$$

Let $\Phi_t = \exp t\mathcal{L}$ be a norm continuous semi-group on a W^*-algebra $\mathcal{M}$ such that $\Phi_t \in CP(\mathcal{M})$ and $\Phi_t(I) = I$. If $\mathcal{L}$ is a generating superoperator of Φ_t, then we can define the superoperator $\mathcal{L}_n = \mathcal{L} \otimes I_n$ on $M_n(\mathcal{M})$ by

$$\mathcal{L}_n(A \otimes I_{ij}) = \mathcal{L}(A) \otimes I_{ij}$$

for all $A \in \mathcal{M}$.

DEFINITION. A *completely dissipative superoperator* is a bounded superoperator $\mathcal{L}$ on $\mathcal{M}$, such that the following requirements are satisfied:

(1) $\mathcal{L}$ is a real superoperator on $\mathcal{M}$.
(2) $\mathcal{L}_n$ is a dissipative superoperator on $M_n(\mathcal{M})$ for all n.

Requirement (2) means that $Z_{\mathcal{L}_n}(A^*, A) \geqslant 0$ for all $A \in M_n(\mathcal{M})$ and all n. We shall denote the set of all completely dissipative superoperators on $\mathcal{M}$ by $CD(\mathcal{M})$. There exists the following equivalent definition of a completely dissipative superoperator.

DEFINITION. A *completely dissipative superoperator* is a superoperator $\mathcal{L}$ on $\mathcal{M}$, such that the following requirements are satisfied:

(1) $\mathcal{L}$ is a real superoperator.
(2) The inequality $Z_{\mathcal{L}}(A_k^*, A_l) \geqslant 0$ $(k, l = 1, \ldots, n)$ is valid for all n and $A_k \in D(\mathcal{L})$, $k = 1, \ldots, n$, where $A_k^* \in D(\mathcal{L})$ and $A_k^* A_l \in D(\mathcal{L})$.

We suppose that $\mathcal{L}$ is a superoperator from $D(\mathcal{L})$ into $\mathcal{M}$, such that the following conditions are satisfied.

(a) $\mathcal{L}$ is a generating superoperator of a dynamical semi-group.
(b) $\mathcal{L}$ is a real superoperator ($\mathcal{L}(A^*) = (\mathcal{L}A)^*$).
(c) $D(\mathcal{L})$ is closed with respect to involution: if $A \in D(\mathcal{L})$, then $A^* \in D(\mathcal{L})$.

In the general case, the domain $D(\mathcal{L})$ is not an involutive algebra.

Let us give the important theorem regarding bipositive superoperators.

THEOREM. *Let $\mathcal{L}$ be a bounded real superoperator, and let $\Phi_t = \exp t\mathcal{L}$ be a norm continuous semi-group on $\mathcal{M}$. The following conditions are equivalent*:

(1) $\Phi_t(A^*A) \geqslant \Phi_t(A^*)\Phi_t(A)$ *for all* $A \in \mathcal{M}$, *and* $\Phi_t(I) = I$.
(2) $Z_{\mathcal{L}}(A, B) \geqslant 0$ *for all* $A, B \in \mathcal{M}$, *and* $\mathcal{L}(I) = 0$.

PROOF. It is not hard to prove half of this theorem: (1) $\Rightarrow$ (2). Let $\mathcal{M}$ be a C^*-algebra. Differentiation of the inequality

$$\Phi_t(A^*A) - \Phi_t(A^*)\Phi_t(A) \geqslant 0$$

gives

$$\frac{d}{dt}\Phi_t(A^*A) - \left(\frac{d}{dt}\Phi_t(A^*)\right)\Phi_t(A) - \Phi_t(A^*)\left(\frac{d}{dt}\Phi_t(A)\right) \geqslant 0.$$

Using

$$\lim_{t\to+0}\left\|\Phi_t(A) - A\right\|_{\mathcal{M}} = 0, \qquad \lim_{t\to+0}\left\|\mathcal{L}(A) - t^{-1}(\Phi_t - L_I)A\right\|_{\mathcal{M}} = 0,$$

we obtain at $t \to +0$,

$$\mathcal{L}(A^*A) - \mathcal{L}(A^*)A - A^*\mathcal{L}(A) \geqslant 0.$$

Then $Z_{\mathcal{L}}(A^*, A) \geqslant 0$. □

This theorem shows that $\{\Phi_t | t \geqslant 0\}$ is a bipositive semi-group if and only if $\mathcal{L}$ is a dissipative superoperator. As a result, we can formulate this theorem in the following form.

THEOREM. *Let $\mathcal{L}$ be a bounded real superoperator on a W^*-algebra, and let $\Phi_t = \exp t\mathcal{L}$ be a norm continuous semi-group on $\mathcal{M}$. Then $\Phi_t \in CP_2(\mathcal{M})$, and $\Phi_t(I) = I$ if and only if $\mathcal{L} \in Dis(\mathcal{M})$, and $\mathcal{L}(I) = 0$.*

This is the basic theorem regarding generating superoperators of bipositive semi-group. Let us give the basic theorem regarding generating superoperators of completely positive semi-group.

THEOREM. *Let $\mathcal{L}$ be a bounded real superoperator on a W^*-algebra, and let $\Phi_t = \exp t\mathcal{L}$ be a norm continuous semi-group on $\mathcal{M}$. Then $\Phi_t \in CP(\mathcal{M})$, and $\Phi_t(I) = I$ if and only if $\mathcal{L} \in CD(\mathcal{M})$.*

This theorem shows that $\{\Phi_t | t \geqslant 0\}$ *is a completely positive semi-group if and only if $\mathcal{L}$ is a completely dissipative superoperator*, i.e., $\Phi_t \in CP(\mathcal{M})$ if and only if $\mathcal{L} \in CD(\mathcal{M})$.

COROLLARY. *A set $\{\Phi_t | t \geqslant 0\}$ is a norm continuous semi-group if and only if $\Phi_t = \exp t\mathcal{L}$, where $\mathcal{L}$ is a completely dissipative superoperator.*

As a result, necessary and sufficient conditions for $\mathcal{L}$ to be an infinitesimal generator of a completely positive dynamical semi-group on $\mathcal{M}$ are obtained. These conditions mean that $\mathcal{L}$ is completely dissipative. The purpose of the quantum dynamics is to derive an explicit form for this generating superoperator.

15.9. Lindblad equation

The natural description of the motion is in terms of the infinitesimal change of the system. The infinitesimal motion is described by some form of infinitesimal generator. The problem of the non-Hamiltonian dynamics is to derive an explicit form for this infinitesimal generator. It is concerned with the problem of determining the most general explicit form of this superoperator. The problem was investigated by V. Gorini, A. Kossakowski, E.C.G. Sudarshan and G. Lindblad for completely dissipative superoperators.

G. Lindblad has shown [95] that there exists a one-to-one correspondence between the completely positive norm continuous semi-groups and completely dissipative generating superoperators. The structural theorem of Lindblad gives the most general form of a completely dissipative superoperator.

THEOREM. *If $\mathcal{L}$ is a completely dissipative superoperator on a W^*-algebra $\mathcal{M}$, then there exist a completely positive superoperator $\mathcal{K}$, and a self-adjoint operator $H \in \mathcal{M}$ such that*

$$\mathcal{L} = -L_H^- + \mathcal{K} - L_{\mathcal{K}(I)}^+. \tag{12}$$

By Kraus theorem, completely positive superoperators $\mathcal{K}$ on a W^*-algebra $\mathcal{M}$ can be presented in the form

$$\mathcal{K}(A) = \sum_{k=1}^{\infty} V_k^* A V_k: \quad \mathcal{K}(I) = \sum_{k=1}^{\infty} V_k^* V_k,$$

where $\mathcal{K}(I) \in \mathcal{M}$.

THEOREM. *The superoperators* $\Phi_t = \exp(t\mathcal{L})$ *is completely positive if and only if* $\mathcal{L}$ *has the form* (12).

It is not hard to prove half of this theorem: if $\mathcal{L}$ has the form (12), then $\Phi_t = \exp(t\mathcal{L})$ is completely positive. The maps $\mathcal{K}$ and $-(L_H^- + L_{\mathcal{K}(I)}^+)$ on $\mathcal{M}$ can be considered as generating superoperators of the semi-groups

$$\exp(t\mathcal{K}), \quad \exp -t\big(L_H^- + L_{\mathcal{K}(I)}^+\big) \quad (t \geqslant 0).$$

These semi-groups are completely positive. Then, by the Trotter's product formula the semi-group

$$\Phi_t = \exp(t\mathcal{L}) = \lim_{n\to\infty}\big(e^{t\mathcal{K}/n}e^{-t(L_H^- + L_{\mathcal{K}(I)}^+)/n}\big)^n$$

is also completely positive. Moreover, $\mathcal{L}(I) = 0$ implies unity preservation $\Phi_t(I) = I$.

STATEMENT. *Let* $\mathcal{M}$ *be a* C^**-algebra. If* $\mathcal{K}$ *is a completely positive superoperator on* $\mathcal{M}$*, and* $H \in \mathcal{M}$ *is self-adjoint superoperator, then* $\mathcal{L}$ *defined by* (12) *is completely dissipative.*

From these statements and the Kraus theorem follow the structural theorem of Lindblad.

LINDBLAD THEOREM. *A ultraweakly continuous superoperator* $\mathcal{L}$ *on a* W^**-algebra* $\mathcal{M}$ *is completely dissipative if and only if it is of the form*

$$\mathcal{L}(A) = -\frac{1}{i\hbar}[H, A] + \frac{1}{2\hbar}\sum_{k=1}^{\infty}\big(V_k^*[A, V_k] + [V_k^*, A]V_k\big), \tag{13}$$

where $H, V_k, \sum_k V_k^*, V_k^*V_k \in \mathcal{M}$.

Equation (13) can be presented in the form

$$\mathcal{L}(A) = -\frac{1}{i\hbar}[H, A] + \frac{1}{\hbar}\sum_{k=1}^{\infty}\big(V_k^*AV_k - (V_k^*V_k)\circ A\big),$$

where $A \circ B = (1/2)(AB + BA)$. The form of $\mathcal{L}$ is not uniquely determined by (13). Indeed, the equation remains invariant under the changes

$$V_k \to V_k + a_k I, \qquad H \to H + \frac{1}{2i\hbar}\sum_{k=1}^{\infty}(a_k^*V_k - a_kV_k^*),$$

where a_k are arbitrary complex numbers.

COROLLARY. *A generating superoperator $\mathcal{L}$ of a completely positive unity-preserving semi-group $\{\Phi_t = \exp(t\mathcal{L}) | t \geqslant 0\}$ on $\mathcal{M}$ can be written by equation* (13).

Using $A_t = \Phi_t(A)$, we obtain the equation

$$\frac{d}{dt} A_t = \mathcal{L} A_t,$$

where $\mathcal{L}$ is defined by (13). This is the *Lindblad equation* for the quantum observable A, or the *quantum Markovian equation*.

Some generalizations

The Lindblad theorem gives the explicit form of the generators of norm continuous quantum dynamical semi-groups $\Phi_t = \exp(t\mathcal{L})$ on a W^*-algebra. There exists the following more general statement for C^*-algebras.

THEOREM. *Let $\mathcal{L}$ be a bounded real superoperator on a C^*-algebra $\mathcal{M}$ such that*

$$\mathcal{L} = L_H + R_{H^*} + \mathcal{K},$$

where $H \in \mathcal{M}$, H^* is adjoint of H, and $\mathcal{K}$ is completely positive superoperator on $\mathcal{M}$. Then $\Phi_t = \exp(t\mathcal{L})$ are completely positive superoperators on $\mathcal{M}$.

The Lindblad theorem gives the general explicit form of equations of motion, when we introduce the following restrictions in the class of quantum non-Hamiltonian systems:

(1) $\mathcal{L}$ and Λ are bounded superoperators.
(2) $\mathcal{L}$ and Λ are completely dissipative superoperators.

In the general case, the following condition can be realized.

(1) $D(\mathcal{L})$ and $D(\Lambda)$ are not involutive algebras.
(2) $\mathcal{L}$ and Λ are general non-Hamiltonian superoperators.

The Lindblad result has been extended by E.B. Davies [40] to a class of quantum dynamical semi-group with unbounded generating superoperators.

Dual Lindblad equation

LINDBLAD THEOREM. *Let $\mathcal{L}$ be a completely dissipative superoperator on a W^*-algebra $\mathcal{M}$. Then Λ is an adjoint superoperator of $\mathcal{L}$ if and only if Λ is of the*

form

$$\Lambda = L_H^- + \frac{i}{2}\sum_{k=1}^{\infty}\left(-L_{V_k^*}^- L_{V_k} + L_{V_k}^- R_{V_k^*}\right),$$

where $H, V_k, V_k^*, \sum_k V_k^* V_k \in \mathcal{M}$.

The Liouville superoperator Λ on the state ρ is

$$\Lambda\rho = \frac{1}{i\hbar}[H, \rho] + \frac{1}{2\hbar}\sum_{k=1}^{\infty}\left([V_k\rho, V_k^*] + [V_k, \rho V_k^*]\right).$$

This expression gives an explicit form of the most general time evolution equation with bounded completely dissipative Liouville superoperator

$$\frac{d}{dt}\rho_s(t) = \frac{1}{i\hbar}\left[H, \rho_s(t)\right] + \frac{1}{2\hbar}\sum_{k=1}^{\infty}\left(\left[V_k\rho_s(t), V_k^*\right] + \left[V_k, \rho_s(t)V_k^*\right]\right).$$

This equation describes a time evolution of density operators of non-Hamiltonian systems in the Schrödinger dynamical representation. In general,

$$\Lambda(I) = \frac{1}{\hbar}\sum_{k=1}^{\infty}[V_k,\ V_k^*] \neq 0,$$

and $Tr[\Lambda(\rho)] = 0$.

Formal derivation of Lindblad equation

The most general form for a completely positive map $\mathcal{E}$ is

$$\mathcal{E} = \sum_{k=0}^{\infty} L_{E_k} R_{E_k^*}.$$

The operators E_k, which must satisfy the condition

$$\sum_{k=0}^{\infty} E_k^* E_k = I \tag{14}$$

in order to $\mathcal{E}$ be trace-preserving, completely specify the quantum operation. We refer to the operators E_k as Kraus operators. Then the time evolution of quantum non-Hamiltonian system can be described by the quantum operations

$$\rho_s(t) = S_t\rho = \mathcal{E}_t\rho = \sum_{k=1}^{\infty} E_k\rho E_k^*. \tag{15}$$

Let us consider the description of the evolution in terms of the infinitesimal change of the density operator ρ. We define the Kraus operators by

$$E_0 = 1 + \left(\frac{1}{i\hbar}H - \frac{1}{2\hbar}K\right)\Delta t + \cdots, \quad E_k = V_k\sqrt{\frac{\Delta t}{\hbar}} + \cdots \quad (k > 1). \tag{16}$$

The normalization condition (14) for the Kraus operation requires

$$I + \left(-K + \sum_{k=1}^{\infty} V_k^* V_k\right)\frac{\Delta t}{\hbar} + \cdots = I.$$

Hence,

$$K = \sum_{k=1}^{\infty} V_k^* V_k.$$

Substitution of (16) into (15) gives

$$\begin{aligned}\rho_s(\Delta t) &= \left(I + \left(\frac{1}{i\hbar}H - \frac{1}{2\hbar}K\right)\Delta t\right)\rho\left(I + \left(-\frac{1}{i\hbar}H - \frac{1}{2\hbar}K\right)\Delta t\right) \\ &\quad + \frac{\Delta t}{\hbar}\sum_{k=1}^{\infty} V_k\rho V_k^* + \cdots \\ &= \rho + \Delta t\left(\frac{1}{i\hbar}[H,\rho] - \frac{1}{\hbar}\sum_{k=1}^{\infty}\big(V_k\rho V_k^* - \rho\circ(V_kV_k^*)\big)\right) + \cdots\end{aligned}$$

As a result, we obtain

$$\frac{d}{dt}\rho_s(t) = \frac{1}{i\hbar}\big[H,\rho_s(t)\big] + \frac{1}{\hbar}\sum_{k=1}^{\infty}\big(V_k\rho_s(t)V_k^* - (V_kV_k^*)\circ\rho_s(t)\big).$$

This is the Lindblad equation for the density operator $\rho_s(t)$.

Integral Lindblad equation

The operators $K = \mathcal{K}(I)$ and H generate a contractive semi-group of the operators

$$W_t = \exp\left(\frac{1}{i\hbar}t\,H - \frac{1}{2}t\,\mathcal{K}(I)\right)$$

on a Hilbert space $\mathcal{H}$. Instead of the Lindblad equation, we can take the equivalent integral equation

$$\Phi_t(A) = W_t^* A W_t + \int_0^t ds\; W_{t-s}^*\mathcal{K}\big(\Phi_s(A)\big)W_{t-s}, \tag{17}$$

where W_t^* is the adjoint operator

$$W_t^* = \exp\left(-\frac{1}{i\hbar}t\,H - \frac{1}{2}t\,\mathcal{K}(I)\right).$$

Equation (17) is the *integral Lindblad equation*.

Using the superoperator $\mathcal{N}_t = L_{W_t^*} R_{W_t}$, integral equation (17) can be rewritten as

$$\Phi_t(A) = \mathcal{N}_t(A) + \int_0^t ds\, N_{t-s}\mathcal{K}\Phi_s(A).$$

Successive iterations leads to the series:

$$\Phi_t(A) = \mathcal{N}_t(A) + \int_0^t ds\, \mathcal{N}_{t-s}\,\mathcal{K}\mathcal{N}_s(A) + \int_0^t ds \int_0^s d\tau\, \mathcal{N}_{t-s}\,\mathcal{K}\mathcal{N}_{s-\tau}\,\mathcal{K}\mathcal{N}_\tau(A) + \cdots, \tag{18}$$

where $t > s$. Using T-exponential and the superoperator $\tilde{\mathcal{K}}_s = \mathcal{N}_{-s}\mathcal{K}\mathcal{N}_s$, we can write equation (18) in the compact form

$$\Phi_t = \mathcal{N}_t\, T \exp\left\{\int_0^t \tilde{\mathcal{K}}_s\right\}.$$

Here T is the chronological multiplication such that

$$T\{\tilde{\mathcal{K}}_t\tilde{\mathcal{K}}_s\} = \begin{cases} \tilde{\mathcal{K}}_t\tilde{\mathcal{K}}_s, & t > s; \\ \tilde{\mathcal{K}}_s\tilde{\mathcal{K}}_t, & s > t. \end{cases} \tag{19}$$

Note that in each term of the series the superoperators $\tilde{\mathcal{K}}_s$ follow in chronological order. Let $|z) = |E(z))$ be a basis of an operator space $\mathcal{M}$. The matrix elements

$$(z|\Phi_t|z') = \big(E(z)|\Phi_t E(z')\big) = Tr\big[E^*(z)\Phi_t E(z')\big]$$

of the evolution superoperator Φ_t in the approximation (18), which is calculated between operator basis elements $E^*(z)$ and $E(z)$, are the transition amplitudes in the respective perturbation-theory order.

15.10. Example of Lindblad equation

The basic assumption is that the general form of a bounded completely dissipative superoperator $\mathcal{L}$ given by the Lindblad equation is also valid for an unbounded

completely dissipative superoperator $\mathcal{L}$. Another simple condition imposed to the operators H, V_k of the one-dimensional quantum system is that they are functions of the basic operators Q and P of such kind that the obtained model is exactly solvable [96,133]. This condition implies that $V_k = V_k(Q, P)$ are at most the first degree polynomials in Q and P, and $H = H(Q, P)$ is at most a second degree polynomial in Q and P. Then V_k and H are chosen in the forms:

$$V_k = a_k P + b_k Q, \quad H = \frac{1}{2m} P^2 + \frac{m\omega^2}{2} Q^2 + \frac{\mu}{2}(PQ + QP), \tag{20}$$

where a_k, b_k are complex numbers, $k = 1, 2$. It is easy to see, that

$$[Q, V_k] = i\hbar a_k, \quad [P, V_k] = -i\hbar b_k,$$
$$[V_k^*, Q] = -i\hbar a_k^*, \quad [V_k^*, P] = i\hbar b_k^*,$$
$$\mathcal{L}(Q) = \frac{1}{m} P + \mu Q + \frac{i}{2} Q \sum_{k=1}^{n=2} (a_k b_k^* - a_k^* b_k),$$
$$\mathcal{L}(P) = -m\omega^2 Q - \mu P + \frac{i}{2} P \sum_{k=1}^{n=2} (a_k b_k^* - a_k^* b_k).$$

Using

$$\lambda = \operatorname{Im}\left(\sum_{k=1}^{n=2} a_k b_k^* \right) = -\operatorname{Im}\left(\sum_{k=1}^{n=2} a_k^* b_k \right),$$

we obtain

$$\mathcal{L}(Q) = \frac{1}{m} P + \mu Q - \lambda Q, \qquad \mathcal{L}(P) = -m\omega^2 Q - \mu P - \lambda P.$$

Let us define the following matrices

$$A = \begin{pmatrix} Q \\ P \end{pmatrix}, \qquad M = \begin{pmatrix} \mu - \lambda & 1/m \\ -m\omega^2 & -\mu - \lambda \end{pmatrix}.$$

In this case, the Lindblad equation for A becomes

$$\frac{d}{dt} A_t = M A_t, \qquad \mathcal{L}(A) = MA,$$

where

$$A_t = \Phi_t A = \sum_{n=0}^{\infty} \frac{t^n}{n!} \mathcal{L}^n A = \sum_{n=0}^{\infty} \frac{t^n}{n!} M^n A.$$

The matrix M can be presented in the form

$$M = N^{-1} F N,$$

where F is a diagonal matrix. Using

$$\Phi_t = \sum_{n=0}^{\infty} \frac{t^n}{n!} M^n = N^{-1} \left(\sum_{n=0}^{\infty} \frac{t^n}{n!} F^n \right) N,$$

we obtain

$$\Phi_t = N^{-1} e^{tF} N.$$

Let ν be a complex parameter such that

$$\nu^2 = \mu^2 - \omega^2.$$

Then, we have

$$N = \begin{pmatrix} m\omega^2 & \mu + \nu \\ m\omega^2 & \mu - \nu \end{pmatrix}, \qquad N^{-1} = \frac{1}{2m\omega^2 \nu} \begin{pmatrix} -(\mu - \nu) & \mu + \nu \\ m\omega^2 & -m\omega^2 \end{pmatrix},$$

and

$$F = \begin{pmatrix} -(\lambda + \nu) & 0 \\ 0 & -(\lambda - \nu) \end{pmatrix}.$$

The superoperator Φ_t can be presented as

$$\begin{aligned} \Phi_t &= e^{tM} = N^{-1} e^{tF} N \\ &= e^{-\lambda t} \begin{pmatrix} \cosh(\nu t) + (\mu/\nu) \sinh(\nu t) & (1/m\nu) \sinh(\nu t) \\ -(m\omega^2/\nu) \sinh(\nu t) & \cosh(\nu t) - (\mu/\nu) \sinh(\nu t) \end{pmatrix}. \end{aligned}$$

Here sinh and cosh are hyperbolic sine and cosine. Then the equation $A_t = \Phi_t A$ has the form

$$\begin{pmatrix} Q_t \\ P_t \end{pmatrix} = e^{-\lambda t} \begin{pmatrix} \cosh(\nu t) + (\mu/\nu) \sinh(\nu t) & (1/m\nu) \sinh(\nu t) \\ -(m\omega^2/\nu) \sinh(\nu t) & \cosh(\nu t) - (\mu/\nu) \sinh(\nu t) \end{pmatrix} \begin{pmatrix} Q \\ P \end{pmatrix}.$$

As a result, we obtain

$$\begin{aligned} Q_t &= e^{-\lambda t} \left(\cosh(\nu t) + \frac{\mu}{\nu} \sinh(\nu t) \right) Q + \frac{1}{m\nu} e^{-\lambda t} \sinh(\nu t) P, \\ P_t &= -\frac{m\omega^2}{\nu} e^{-\lambda t} \sinh(\nu t) Q + e^{-\lambda t} \left(\cosh(\nu t) - \frac{\mu}{\nu} \sinh(\nu t) \right) P. \end{aligned} \tag{21}$$

Let us consider Jacobian $J_{\mathcal{L}}(Q_t, P_t)$ for the operators $Q_t = \Phi_t(Q)$ and $P_t = \Phi_t(P)$. If equations (21) are presented in the form

$$Q_t = a_1(t) Q + b_1(t) P, \qquad P_t = a_2(t) Q + b_2(t) P,$$

then

$$J_{\mathcal{L}}(Q_t, P_t) = a_1(t)b_2(t)J_{\mathcal{L}}(Q, P) + a_2(t)b_1(t)J_{\mathcal{L}}(P, Q)$$
$$= \big[a_1(t)b_2(t) - a_2(t)b_1(t)\big]J_{\mathcal{L}}(Q, P).$$

For equations (21),

$$a_1(t)b_2(t) - a_2(t)b_1(t) = \det\big(N^{-1}e^{F}N\big)$$
$$= e^{-\lambda t}\left[\cosh^2(\nu t) - \frac{\mu^2}{\nu^2}\sinh^2(\nu t) + \frac{\omega^2}{\nu^2}\sinh^2(\nu t)\right] = e^{-\lambda t}.$$

As a result, we obtain

$$J_{\mathcal{L}}(Q_t, P_t) = \det\big(N^{-1}e^{F}N\big)\, J_{\mathcal{L}}(Q, P) = e^{-\lambda t}J_{\mathcal{L}}(Q, P).$$

15.11. Gorini–Kossakowski–Sudarshan equation

Let $\mathcal{K}_r^1(\mathcal{H})$ be a Banach space of trace-class operators on a Hilbert space $\mathcal{H}$. The superoperator Λ in the quantum Liouville equation can be considered as the infinitesimal generator of a strongly continuous one-parameter semi-group of positive trace-preserving superoperators S_t on $\mathcal{K}^1(\mathcal{H})$. The adjoint superoperator Φ_s is a completely positive (and automatically ultraweakly continuous and identity preserving) map of $\mathcal{B}(\mathcal{H})$. These semi-groups are called the dynamical semi-groups. A general form of the bounded generating superoperator $\mathcal{L}$ of norm continuous dynamical semi-group on $\mathcal{K}_r^1(\mathcal{H})$ with a separable Hilbert space $\mathcal{H}$ has been given by the Lindblad theorem [95]. In the case of an N-level quantum non-Hamiltonian system, the problem was investigated by V. Gorini, A. Kossakowski, and E.C.G. Sudarshan [67]. The general form of the generating superoperator of a completely positive dynamical semi-group of this systems has been established [67]. In the case of N-level quantum system, $\dim\mathcal{H} = N$, and we have the identification $\mathcal{K}^1(\mathcal{H}) = \mathcal{B}(\mathcal{H}) = \mathcal{M}$.

THEOREM. *Let $\mathcal{K}$ be a completely positive superoperator on $\mathcal{M}$, and let $\{E_k,\ k = 1, \ldots, N^2\}$ be a complete orthonormal set on $\mathcal{M}$ such that*

$$(E_k|E_l) = Tr[E_k^* E_l] = \delta_{kl}.$$

Then $\mathcal{K}$ can be uniquely written in the form

$$\mathcal{K}A = \sum_{k,l=1}^{N^2} c_{kl}E_k A E_l^*$$

for all $A \in \mathcal{M}$.

Note that this important theorem comes from the Kraus theorem.
If $A \in \mathcal{M}$, then

$$|A) = \sum_{k}^{N^2} |E_k) a_k, \quad a_k = (E_k|A).$$

Using

$$\sum_{k=1}^{N^2} |E_k)(E_k| = I,$$

the trace $Tr[A]$ can be presented in the form

$$Tr[A] = Tr[IA] = \sum_{k=1}^{N^2} Tr\big[|E_k)(E_k|A\big] = \sum_{k=1}^{N^2} (E_k|A|E_k)$$
$$= \sum_{k=1}^{N^2} Tr[E_k^* A E_k].$$

THEOREM. *A linear superoperator $\mathcal{L}$ on $\mathcal{M}$ is an infinitesimal generator of a completely positive dynamical semi-group on $\mathcal{M}$ if it can be written in the form*

$$\mathcal{L}A = -\frac{1}{i\hbar}[H, A] + \frac{1}{2\hbar} \sum_{k,l=1}^{N^2-1} c_{kl}\big([E_k^*, A]E_l + E_k^*[A, E_l]\big),$$

where $H^* = H$ is a self-adjoint operator with $Tr[H] = 0$, c_{kl} is a complex positive matrix, and $(E_k|E_l) = \delta_{kl}$, $Tr[E_k] = 0$, $E_{N^2} = \sqrt{1/N}I$.

For a given $\mathcal{L}$, the operator H is uniquely determined by the condition $Tr[H] = 0$, and c_{kl} is uniquely determined by the choice of the operators $\{E_k\}$. The conditions $Tr[H] = 0$ and $Tr[E_k] = 0$ provide a canonical separation of the generator into a Hamiltonian plus a non-Hamiltonian part.

THEOREM. *A linear map Λ from $\mathcal{M}$ into itself is a generating superoperator of a dynamical semi-group on $\mathcal{M}$ if it can be written in the form*

$$\Lambda\rho = \frac{1}{i\hbar}[H, \rho] + \frac{1}{2\hbar} \sum_{k,l=1}^{N^2-1} c_{kl}\big([E_k, \rho E_l^*] + [E_k\rho, E_l^*]\big), \tag{22}$$

where $H^* = H$ is a self-adjoint operator with $Tr[H] = 0$, c_{kl} is a complex positive matrix, and $(E_k|E_l) = \delta_{kl}$, $Tr[E_k] = 0$, $E_{N^2} = \sqrt{1/N}I$.

The superoperator (22) is the Liouville superoperator for the N-level quantum system. Equation (2) with the superoperator (22) is called the Gorini–Kossakowski–Sudarshan equation.

15.12. Two-level non-Hamiltonian quantum system

One can represent an arbitrary density operator $\rho(t)$ for a two-level quantum system in terms of Pauli matrices σ_μ:

$$\rho(t) = \frac{1}{2}\sum_{\mu=0}^{3} \sigma_\mu P_\mu(t),$$

where $P_\mu(t) = Tr[\sigma_\mu \rho(t)]$ and $P_0(t) = 1$. Here σ_μ are the *Pauli matrices*

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{23}$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \sigma_0 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{24}$$

The pure state can be identified with the *Bloch sphere*

$$P_1^2(t) + P_2^2(t) + P_3^2(t) = 1.$$

The mixed state is identified with the *closed Bloch ball*

$$P_1^2(t) + P_2^2(t) + P_3^2(t) \leqslant 1.$$

Let us consider this two-level quantum system for a positive trace-preserving semi-group. Suppose $\{E_k\}$, where $k \in \{0, 1, 2, 3\}$, is a complete orthonormal set of the self-adjoint matrices:

$$E_0 = \frac{1}{\sqrt{2}} I, \quad E_1 = \frac{1}{2}\sigma_1, \quad E_2 = \frac{1}{\sqrt{2}}\sigma_2, \quad E_3 = \frac{1}{\sqrt{2}}\sigma_3.$$

The basic assumption imposed to the operators H and $\rho(t)$ is that they are functions of the Pauli matrices:

$$H = \sum_{k=1}^{3} H_k \sigma_k, \qquad \rho(t) = \frac{1}{2}\left(P_0 I + \sum_{k=1}^{3} P_k(t)\sigma_k\right),$$

where $P_0 = 1$. Using the relations

$$\sigma_k \sigma_l = I\delta_{kl} + i\sum_{m=1}^{3} \varepsilon_{klm}\sigma_m, \quad [\sigma_k, \sigma_l] = 2i\sum_{m=1}^{3} \varepsilon_{klm}\sigma_m,$$

and $\varepsilon_{klm}\varepsilon_{ijm} = \delta_{ki}\delta_{lj} - \delta_{kj}\delta_{li}$, we obtain

$$\frac{d}{dt}P_k(t) = \sum_{l=1}^{3}\left(2H_m\varepsilon_{kml} + \frac{1}{8}(C_{kl} + C_{lk}) - \frac{1}{4}C\delta_{kl}\right)P_l(t) - \frac{1}{4}\varepsilon_{ijk}(\operatorname{Im} C_{ij})P_0,$$

where $C = \sum_{m=1}^{3} C_{mm}$ and $k, l \in \{1, 2, 3\}$. This is the Gorini–Kossakowski–Sudarshan equation for two-level system. We can rewrite this equation in the form

$$\frac{d}{dt}P_\mu(t) = \sum_{\nu=0}^{3} \Lambda_{\mu\nu}P_\nu(t), \tag{25}$$

where $\mu, \nu \in \{0, 1, 2, 3\}$ and the matrix $\Lambda_{\mu\nu}$ is

$$[\Lambda_{\mu\nu}] = \begin{pmatrix} 0 & 0 & 0 & 0 \\ B_1 & -C_{(22)} - C_{(33)} & C_{(12)} - 2H_3 & C_{(13)} + 2H_2 \\ B_2 & C_{(12)} + 2H_3 & -C_{(11)} - C_{(33)} & C_{(23)} - 2H_1 \\ B_3 & C_{(13)} - 2H_2 & C_{(23)} + 2H_1 & -C_{(11)} - C_{(22)} \end{pmatrix},$$

where

$$B_k = -\frac{1}{4}\varepsilon_{ijk}(\operatorname{Im} C_{ij}), \qquad C_{(kl)} = \frac{1}{8}(C_{kl} + C_{lk}).$$

If the matrix C_{kl} and the operator H are not time-dependent, then equation (25) has the solution

$$P_\mu(t) = \sum_{\nu=0}^{3} \mathcal{E}_{\mu\nu}(t - t_0)P_\nu(t_0),$$

where the matrix $[\mathcal{E}_{\mu\nu}]$ has the form

$$[\mathcal{E}_{\mu\nu}] = \begin{pmatrix} 1 & 0 & 0 & 0 \\ T_1 & R_{11} & R_{12} & R_{13} \\ T_2 & R_{21} & R_{22} & R_{23} \\ T_3 & R_{31} & R_{32} & R_{33} \end{pmatrix}.$$

The matrices $T = [T_k(\tau)]$ and $R = [R_{kl}(\tau)]$ of the matrix $\mathcal{E}_{\mu\nu}(\tau)$ are defined by

$$T = \left(e^{\tau A} - I\right)(\tau A)^{-1}B = \sum_{n=0}^{\infty} \frac{\tau^{n-1}}{n!}A^{n-1},$$

$$R = e^{\tau A} = \sum_{n=0}^{\infty} \frac{\tau^n}{n!}A^n,$$

where $\tau = t - t_0$ and the matrix $A = [A_{kl}]$ is

$$A_{kl} = 2H_m\varepsilon_{kml} + \frac{1}{8}(C_{kl} + C_{lk}) - \frac{1}{4}C\delta_{kl}.$$

If C_{kl} is a real matrix, then all $T_k = 0$, where $k = 1, 2, 3$.

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Chapter 16

Classical Non-Hamiltonian Dynamics

16.1. Introduction to classical dynamics

To motivate the basic concepts of the quantization of classical non-Hamiltonian systems, we begin with an introduction of classical dynamics.

Classical system in Euclidean space $\mathbb{R}^n$

Suppose that a classical system, whose position is determined by a point x in a region $\mathcal{M}$ of $\mathbb{R}^n$, moves in a field $F(t, x)$. The motion of the system is described by the equation

$$\frac{dx}{dt} = F(t, x). \tag{1}$$

The points $x \in \mathcal{M}$ represent pure states in classical mechanics. A classical observable is a function on $\mathcal{M}$.

Let $\mathcal{M}$ be a real linear space. The elements in a subset $\{e_k, k \in \mathbb{N}\}$ of $\mathcal{M}$ generate (or span) $\mathcal{M}$ if for every $x \in \mathcal{M}$, we have $x = \sum_{k=1}^{n} e_k x^k$ for some $x^k \in \mathbb{R}$. If $\mathcal{M}$ is a linear space, the elements in a subset $\{e_k, k \in \mathbb{N}\}$ of $\mathcal{M}$ form a basis for $\mathcal{M}$ if they generate $\mathcal{M}$ and are linearly independent. The number of elements in a basis is the dimension of $\mathcal{M}$.

Let $\{e_k,\ k = 1, \ldots, n\}$ be a basis of $\mathcal{M}$. Then

$$x = e_k x^k, \qquad F(t, x) = e_k F^k(t, x).$$

Here and subsequently we use the usual summation convention for repeated indices $e_k x^k = \sum_{k=1}^{n} e_k x^k$. Since $F(t, x)$ is uniquely determined by its components F^k, we can represent $F(t, x)$ by the symbol F^k. If $de_k/dt = 0$, then equation (1) can be presented in the form

$$\frac{dx^k}{dt} = F^k(t, x). \tag{2}$$

If $\mathcal{M}$ is a set, we denote by $\mathcal{M} \times \mathcal{M}$ the set of all ordered pairs x, y, where $x, y \in \mathcal{M}$, and $\mathcal{M} \times \mathcal{M}$ will be called the direct product. A set $\mathcal{M}$ is called a

metric space if there is defined a function d with domain $\mathcal{M} \times \mathcal{M}$ and range in the real field $\mathbb{R}$ such that

(1) $d(x, y) \geqslant 0$ and $d(x, y) = 0$ if and only if $x = y$,
(2) $d(x, y) = d(y, x)$,
(3) $d(x, z) \leqslant d(x, y) + d(y, z)$ (the triangle inequality).

The function g is called the metric. We can represent the metric d by the numbers $g_{kl} = d(e_k, e_l)$. There exists the following scalar product $(F, G) = g_{kl} F^k G^l$, where F^k, G^l are vector fields on $\mathcal{M}$.

The points x determine the pure states of the classical system. The set of such points constitutes the phase-space of the system, $\mathcal{M}$, which in our case is the n-dimensional Euclidean space with the metric $g_{kl} = \delta_{kl}$ and the standard scalar product.

Classical system on a manifold

The phase-space of the classical system discussed before is Euclidean space $\mathbb{R}^n$. However, this is not always the case. Some problems involve phase-space which are more complicated manifolds.

A manifold is a topological space that is locally Euclidean. Every point $x \in \mathcal{M}$ has a neighborhood that is topologically the same as an open set in $\mathbb{R}^n$. A manifold is a topological space in which every point has a neighborhood which resembles Euclidean space, but in which the global structure may be more complicated. The spherical Earth is described using flat charts, collected in an atlas. Similarly, a smooth manifold can be described using coordinate charts collected in a mathematical atlas. It is not generally possible to describe a manifold with just one chart, because the global structure of the manifold is different from the simple structure of the charts. For example, no single flat chart can properly represent the entire Earth.

Let $\mathcal{M}$ be a smooth manifold which is endowed with a metric structure. The metric tensor $g_{kl}(x)$ allows us to define the scalar product $(F, G) = g_{kl}(x) F^k(x) G^k(x)$, where $F^k(x)$ and $G^k(x)$ are vector fields. We can define the covariant vector field

$$F_k(x) = g_{kl}(x) F^l(x).$$

The field $F^l(x)$ is called contravariant. In general, the metric tensor $g_{kl}(x)$ is not symmetric. If the metric tensor $g_{kl}(x)$ is nondegenerate ($\det[g_{kl}(x)] \neq 0$), then there exists $g^{kl}(x)$ such that $g^{kl}(x) g_{lm}(x) = \delta^k_m$.

Let F be a vector field, and let H be a differentiable function. It is known that the vector operators *grad*, *div*, *curl* can be presented by

$$grad\ H = e_k g^{kl} \partial_l H,$$

$$div\, F = \partial_k F_k,$$
$$curl\, F = e_i \varepsilon^{ikl} \partial_k F_l,$$

where $\partial_k = \partial/\partial x^k$, and ε^{ikl} is Levi-Civita symbol. The condition $curl\, F = 0$ is satisfied if and only if

$$\partial_k F_l - \partial_l F_k = 0.$$

Let us consider a classical system on a manifold $\mathcal{M}$ endowed with a metric. The motion of the system will be described by equations (2).

DEFINITION. A *locally potential system* is a classical system described by equation (2), such that the following conditions are satisfied

$$\partial_l F_k(t, x) - \partial_k F_l(t, x) = 0 \tag{3}$$

for all $x \in \mathcal{M}$, and $t \geqslant 0$.

These conditions mean that the vector field $F_k(t, x) = g_{kl}(x) F^l(t, x)$ is irrotational. A system is nonpotential if there are $x \in \mathcal{M}$ such that conditions (3) are not satisfied. A bosonic string on affine-metric manifold is an example of nonpotential system [152].

DEFINITION. A *dissipative system* is a classical system described by equation (2) such that the field $F^k(t, x)$ is solenoidal, i.e.,

$$div\, F(t, x) = 0$$

for all $x \in \mathcal{M}$, and $t \geqslant 0$.

DEFINITION. A *globally potential system* is a classical system described by equation (2), such that there exists a unique single-valued function $H = H(t, x)$, and

$$F(t, x) = grad\, H(t, x)$$

for all $x \in \mathcal{M}$, and $t \geqslant 0$.

The globally potential system is locally potential. The converse statement does not hold in general. If $\mathcal{M}$ is simply connected, then a locally potential system is globally potential. A region is simply connected if it is path-connected and every path between two points can be continuously transformed into every other. A region where any two points can be joined by a path is called path-connected.

A functional derivative is a generalization of the usual derivative. In a functional derivative, instead of differentiating a function with respect to a variable, one

differentiates a functional $S[x(t)]$ with respect to a function $x^k(t)$:

$$\frac{\delta S[x(t)]}{\delta x^k(t)} = \lim_{\varepsilon\to 0} \varepsilon^{-1}\big(S\big[x(t)+\varepsilon y(t)\big] - S\big[x(t)\big]\big) = 0.$$

It is well known that some differential equations are the result of functional differentiation of the functional. A system of equations is called potential if there exists a functional $S[x(t)]$ such that the conditions $\delta S[x(t)]/\delta x^k(t) = 0$ give these equations.

Let us consider the differential equations

$$g_{kl}(x)\frac{d}{dt}x^k - F_k(x) = 0.$$

These equations are potential if and only if the following conditions are satisfied

$$g_{kl}(x) + g_{lk}(x) = 0, \tag{4}$$

$$\frac{\partial g_{kl}(x)}{\partial x^s} + \frac{\partial g_{ls}(x)}{\partial x^k} + \frac{\partial g_{sk}(x)}{\partial x^l} = 0, \tag{5}$$

$$\frac{\partial F_k(x)}{\partial x^l} - \frac{\partial F_l(x)}{\partial x^k} = 0. \tag{6}$$

Equation (4) expresses the statement that the metric $g_{kl}(x)$ is skew-symmetric (antisymmetric). Requirement (5) is called the Jacobi identity for the metric $g_{kl}(x)$. A manifold $\mathcal{M}$ is called a symplectic manifold, if for every $x \in \mathcal{M}$, there is a skew-symmetric metric such that the Jacobi identities are satisfied. Requirement (6) is a statement that the vector field $F_k(x)$ is irrotational, and the system is locally potential.

16.2. Systems on symplectic manifold

Symplectic manifold

We shall consider here an important class of manifolds in which the metric tensor $g_{kl}(x) = \omega_{kl}(x)$, $k, l = 1, \ldots, 2n$, is antisymmetric. These manifolds are called symplectic [60].

DEFINITION. A *symplectic manifold* $(\mathcal{M}, \omega)$ is a smooth manifold $\mathcal{M}$ endowed with a closed nondegenerate differential 2-form ω.

In local coordinates, the form ω is defined by the equation

$$\omega = \omega_{kl}(x)\, dx^k \wedge dx^l. \tag{7}$$

The nondegeneracy condition means that $\det[\omega_{kl}(x)] \neq 0$ at every point of $\mathcal{M}$, so that there exists an inverse (skew-symmetric) matrix $\Psi^{kl}(x) = \omega^{kl}(x)$. It follows that the dimension of $\mathcal{M}$ is even.

The condition for ω to be closed, $d\omega = 0$, is expressed in local coordinates as

$$\partial_k \omega_{lm} + \partial_l \omega_{mk} + \partial_m \omega_{kl} = 0.$$

This is the Jacobi identity for ω_{kl}.

All symplectic manifolds have locally the same structure. A precise formulation of this statement is given by the Darboux's theorem: For any point x of a symplectic manifold $(\mathcal{M}, \omega)$ there exists a local coordinate system $(q, p) = (q^1, \ldots, q^n, p^1, \ldots, p^n)$ in a neighbourhood of x such that the symplectic form ω has the canonical expression $\omega = dq^k \wedge dp^k$. By this theorem, any statement, which is invariant under symplectic transformations and has been proved for the canonical coordinates, can be extended to all symplectic manifolds.

Symplectic manifolds have some specific topological properties. We shall note here only one of them. Suppose $(\mathcal{M}, \omega)$ is a compact symplectic manifold of dimension $2n$. Then the nth power ω^n of the symplectic form ω is a volume form on $\mathcal{M}$. Moreover, it should be noted that all the powers of ω up to ω^n must be nonzero.

Let $(\mathcal{M}, \omega)$ be a symplectic manifold with symplectic form (7). The tensors $\omega_{kl}(x)$ and $\Psi^{kl}(x) = \omega^{kl}(x)$ give rise to a correspondence between 1-forms $\omega(F) = F_k(x)dx^k$ and vector fields $F = e_k F^k(x)$ on $\mathcal{M}$. A vector field F can be considered as a first-order differential operator on $\mathcal{M}$:

$$\mathcal{L} = F^k \partial_k,$$

where $\partial_k = \partial/\partial x^k$. Note that $F^k(x) = \mathcal{L}(x^k)$.

The Hilbert space approach to classical dynamics

Let us consider a classical system on a symplectic manifold $(\mathcal{M}, \omega)$. The motion of the system will be described by the equations

$$\frac{dx^k}{dt} = F^k(x) \quad (k = 1, \ldots, 2n). \tag{8}$$

In general, these equations are nonlinear ordinary differential equations in a finite-dimensional manifold. There is a standard method for rewriting such a system as a linear equation on an infinite-dimensional space.

A classical observable is a function on $\mathcal{M}$. We shall denote the linear space of all smooth square-integrable functions on $\mathcal{M}$ by $\mathcal{F}(\mathcal{M})$. The scalar product

$$(A, B) = \int dx \big(A(x)\big)^* B(x) \tag{9}$$

is defined for all $A, B \in \mathcal{F}(\mathcal{M})$. Note that $(A, A) \leqslant \infty$, since $A \in \mathcal{F}(\mathcal{M})$ is square-integrable.

If we consider a Cauchy problem for equation (8) in which the initial condition is given by x_0 at the time $t = 0$, then its solution can be written in the form $x(t) = \varphi(t, x_0)$. We can define the operator φ_t^* such that

$$\varphi_t^* A(x_0) = A\big(\varphi(t, x_0)\big).$$

Note that $\{\varphi_t^* | t \geqslant 0\}$ is a one-parameter semi-group, i.e., $\varphi_t^* \varphi_s^* = \varphi_{t+s}^*$, for $t, s \geqslant 0$ and $\varphi_0^* = I$. The differentiation of the composite function $A(\varphi(t, x_0))$ with respect to t gives

$$\frac{d}{dt} A\big(\varphi(t, x_0)\big) = \frac{d\varphi(t, x_0)}{dt} \frac{\partial A(\varphi(t, x_0))}{\partial \varphi(t, x_0)} = F^k(x) \partial_k A\big(\varphi(t, x_0)\big),$$

where we use equations (8). As a result, we obtain the equation

$$\frac{d}{dt} \varphi_t^* A(x_0) = \mathcal{L} \varphi_t^* A(x_0), \tag{10}$$

where $\mathcal{L} = F^k(x) \partial_k$ is a first order differential operator. If $A = x^k$, then this equation gives (8). As a result, equations (8) are special cases of (10). For $A = x^k x^l$, equation (10) gives

$$\frac{d(x^k x^l)}{dt} = F^k(x) x^l + x^k F^l(x).$$

In general, we can consider equation (10), where $\mathcal{L}$ is a linear operator on $\mathcal{F}(\mathcal{M})$. In this case, $\mathcal{L}$ is not necessary a first order differential operator. If $A = x^k$, and

$$\mathcal{L} = F^k(x) \partial_k + N^{kl}(x) \partial_k \partial_l,$$

then equation (10) gives (8). For $A = x^k x^l$, equation (10) gives

$$\frac{d(x^k x^l)}{dt} = F^k(x) x^l + x^k F^l(x) + N^{kl}(x).$$

Then (10) is not equivalent to (8). As a result, equation (10) allows us to describe wider class of classical systems than equation (8).

Let $\mathcal{L}$ be an operator on $\mathcal{F}(\mathcal{M})$. We define the superoperator δ_A, such that

$$\delta_A \mathcal{L} = [L_A, \mathcal{L}] = L_A \mathcal{L} - \mathcal{L} L_A,$$

where L_A is an operator of multiplication by the function $A(x) \in \mathcal{F}(\mathcal{M})$, i.e., $L_A B = A(x) B(x)$. Here δ_A is a Lie left multiplication by the operator L_A. In classical dynamics, the superoperator δ_A allows us to define a differential operator of order $\leqslant k$ [83,84].

DEFINITION. A *differential operator of order* $\leqslant k$ on a commutative associative algebra $\mathcal{F}(\mathcal{M})$ is an operator $\mathcal{L}$ such that

$$\delta_{A_0}\delta_{A_1}\dots\delta_{A_k}\mathcal{L} = 0$$

for all $A_0, A_1, \dots, A_k \in \mathcal{F}(\mathcal{M})$.

A differential operator of order $\leqslant 1$ is defined by the condition

$$\big[L_A, [L_B, \mathcal{L}]\big]X = 0.$$

For $X = 1$, this equation gives the Leibnitz rule

$$\mathcal{L}(AB) - \mathcal{L}(A)B - A\mathcal{L}(B) + AB\mathcal{L}(1) = 0.$$

A differential operator of order $\leqslant 2$ satisfies the equation

$$\big[L_A, \big[L_B, [L_C, \mathcal{L}]\big]\big]X = 0.$$

For $X = 1$, we obtain

$$\begin{aligned}&\mathcal{L}(ABC) - \mathcal{L}(AB)C - A\mathcal{L}(BC) - B\mathcal{L}(AC)\\ &\quad + \mathcal{L}(A)BC + A\mathcal{L}(B)C + AB\mathcal{L}(C) - ABC\mathcal{L}(1) = 0.\end{aligned}$$

This definition can be used for a commutative associative algebra. In the general case, this definition cannot be used.

STATEMENT. *The operator* $i\mathcal{L} = iF^k(x)\partial_k$ *is self-adjoint with respect to* (9) *if and only if the classical system is nondissipative. In general, the operator*

$$\Lambda = -\mathcal{L} - \Omega \tag{11}$$

is adjoint of $\mathcal{L} = F^k(x)\partial_k$, *where* Ω *is a left multiplication by the function* $\Omega(x) = \partial_k F^k(x)$.

PROOF. Let Λ be an adjoint operator of $\mathcal{L}$ with respect to the scalar product (9). Then $(\Lambda A, B) = (A, \mathcal{L}B)$. If $i\mathcal{L} = iF^k(x)\partial_k$, then an integration by parts proves that

$$i\int dx\, A^* F^k(\partial_k B) = \int dx\, (iF^k\partial_k A)^* B - i\int dx\, A^*(\partial_k F^k)B.$$

Then

$$(A, i\mathcal{L}B) = (i\mathcal{L}A, B) + (i\Omega A, B).$$

Using $(zA, B) = z^*(A, B)$, and $(A, zB) = z(A, B)$, we obtain (11). □

Locally Hamiltonian systems on symplectic manifold

Let us consider a classical system on a symplectic manifold $(\mathcal{M}, \omega)$. The motion of the system will be described by the equations

$$\frac{dx^k}{dt} = F^k(x) \quad (k = 1, \ldots, 2n). \tag{12}$$

A classical observable is a function on $\mathcal{M}$. Let A be a smooth function on $\mathcal{M}$. We then have the equation

$$\frac{d}{dt}A = \mathcal{L}A,$$

where $\mathcal{L} = F^k(t, x)\partial_k$ is a first order differential operator. A classical system (12) on a symplectic manifold $(\mathcal{M}, \omega)$ is said to be locally Hamiltonian if the corresponding 1-form $\omega(F) = \omega_{kl}F^l(x)\,dx^k$ is closed, i.e., $d\omega(F) = 0$. In local coordinates, this condition gives

$$\partial_k\big(\omega_{lm}(x)F^m(x)\big) - \partial_l\big(\omega_{km}(x)F^m(x)\big) = 0. \tag{13}$$

DEFINITION. A *locally Hamiltonian system* is a classical system (12) on a symplectic manifold (M^{2n}, ω), such that equations (13) are satisfied for all $x \in \mathcal{M}$.

Globally Hamiltonian systems on symplectic manifold

A classical system (12) on a symplectic manifold $(\mathcal{M}, \omega)$ is said to be globally Hamiltonian, if the corresponding 1-form $\omega(F) = \omega_{kl}F^l(x)dx^k$ is exact, i.e., $\omega(F) = dH$, where H is a function on $\mathcal{M}$ called the Hamiltonian function of the system, or simply the Hamiltonian. Conversely, if H is a function on $\mathcal{M}$, then the system with the operator

$$\mathcal{L} = \partial_l H\omega^{kl}\partial_k$$

associated with the 1-form dH is globally Hamiltonian.

DEFINITION. A *globally Hamiltonian system* is a classical system (12) on a symplectic manifold (M^{2n}, ω), such that

$$\omega_{kl}F^l(x) = \partial_k H$$

for all $x \in \mathcal{M}$.

Let us give a simple example of a locally Hamiltonian system which is not globally Hamiltonian. Let $\mathcal{M}$ be a two-dimensional torus, $\omega = dq \wedge dp$, where $0 \leqslant q \leqslant 2\pi$, and $0 \leqslant p \leqslant 2\pi$. The classical system with $\mathcal{L} = a\partial_q + b\partial_p$, where

$a, b \in \mathbb{R}$, is a locally Hamiltonian system, but not globally Hamiltonian. It is easy to see that this effect reflects on the topological properties of $\mathcal{M}$, namely, on the nonvanishing of the first cohomology group $H^1(\mathcal{M}, \mathbb{R})$.

Since operators $\mathcal{L} = F^k \partial_k$ are first order differential operators on $\mathcal{M}$, one can define their commutator, which makes them into a Lie algebra. The commutator of two locally Hamiltonian operators is globally Hamiltonian, so that the globally Hamiltonian operators form an ideal in the Lie algebra of locally Hamiltonian operators.

In the conventional formulation of classical dynamics, it mostly deals with globally Hamiltonian systems, so that the dynamics on $\mathcal{M}$ is determined by a Hamiltonian $H(x)$, and the equations of motion are written in local coordinates as

$$\omega_{kl}(x)\frac{d}{dt}x^l = \partial_k H \quad \text{or} \quad \frac{d}{dt}x^k = \Psi^{lk}(x)\partial_l H.$$

Let $\mathcal{M} = \mathbb{R}^n$, $\omega = dq^k \wedge dp^k$, and $H = H(q, p)$. The equations of motion are then the usual Hamilton's equations

$$\frac{d}{dt}q^k = -\frac{\partial H}{\partial p^k}, \qquad \frac{d}{dt}p^k = \frac{\partial H}{\partial q^k}.$$

These equations are induced by the Hamiltonian H.

Let A be a smooth function on $\mathcal{M}$. We then have the equation

$$\frac{d}{dt}A = \frac{\partial H}{\partial x^k}\Psi^{kl}(x)\frac{\partial A}{\partial x^l}. \tag{14}$$

In local coordinates (q, p), equation (14) has the form

$$\frac{d}{dt}A = \sum_{k=1}^{n}\left(\frac{\partial H}{\partial q^k}\frac{\partial A}{\partial p^k} - \frac{\partial H}{\partial p^k}\frac{\partial A}{\partial q^l}\right).$$

Non-Hamiltonian systems on symplectic manifold

A classical system (12) on a symplectic manifold $(\mathcal{M}, \omega)$ is said to be non-Hamiltonian if the corresponding 1-form $\omega(F) = \omega_{kl}F^l(x)\,dx^k$ is nonclosed

$$d\omega(F) \neq 0.$$

In local coordinates, this condition for the system to be a non-Hamiltonian system means that there exists $x \in \mathcal{M}$ and k, l such that

$$\partial_k\big(\omega_{lm}(x)F^m(x)\big) - \partial_l\big(\omega_{km}(x)F^m(x)\big) \neq 0. \tag{15}$$

DEFINITION. A *non-Hamiltonian system* is a classical system (12) on a symplectic manifold (M^{2n}, ω), such that inequality (15) is satisfied for some $x \in \mathcal{M}$, and some k, l.

The important non-Hamiltonian systems are dissipative, accretive and generalized dissipative systems.

DEFINITION. A *generalized dissipative system* on a symplectic manifold (M^{2n}, ω) is a classical system such that

$$\Omega(t, x) = \partial_k F^k(t, x) \neq 0.$$

If $\Omega(t, x) < 0$ for all $x \in \mathcal{M}$ and $t \geqslant 0$, then the system is *dissipative*. If $\Omega > 0$ for all $x \in \mathcal{M}$ and $t \geqslant 0$, then the system is called *accretive*.

It is not hard to prove the following important theorem.

THEOREM. *A generalized dissipative system on a symplectic manifold* (M^{2n}, ω) *is a non-Hamiltonian system on* (M^{2n}, ω).

If we consider the Euclidean space $\mathbb{R}^n$, $n \geqslant 2$, instead of a symplectic manifold (M^{2n}, ω), then there exist a field F such that $div\, F \neq 0$, and $curl\, F = 0$. For example, the vector field $F = x_k e_k$ in $\mathbb{R}^n$ has $curl\, F = 0$ and $div\, F = n$. A classical system on a symplectic manifold (M^{2n}, ω) cannot be a dissipative Hamiltonian system.

16.3. Systems on Poisson manifold

Poisson manifold and Lie–Jordan algebra

In the classical mechanics an observable is represented by a function. A mathematical structure is obtained by taking a set of observables and equipping this set with a structure by defining relations between these observables. The dynamical structure can be given by operators on the set.

Let $\mathcal{M}$ be a manifold. A classical observable is a function on $\mathcal{M}$. We shall denote the linear space of all smooth functions on $\mathcal{M}$ by $\mathcal{F}(\mathcal{M})$. We say that $\mathcal{M}$ is endowed with a Poisson structure if we are given an operation assigning to every pair of functions $A, B \in \mathcal{F}(\mathcal{M})$ a new function $\{A, B\} \in \mathcal{F}(\mathcal{M})$, which is linear in A and B, and satisfies the following requirements:

(1) the skew-symmetry condition $\{A, B\} = -\{B, A\}$,
(2) the Jacobi identity $\{\{A, B\}, C\} + \{\{B, C\}, A\} + \{\{C, A\}, B\} = 0$,
(3) the Leibnitz rule $\{A, BC\} = \{A, B\}C + B\{A, C\}$.

Requirements (1) and (2) are the axioms of a Lie algebra. In this way, the space $\mathcal{F}(\mathcal{M})$, together with the Poisson bracket becomes a Lie algebra. We can define the Jordan multiplication $A \circ B = A(x)B(x)$, where AB is the usual pointwise

product. Then requirement (3) expresses that the Lie operation $\{\ ,\ \}$ is connected with the Jordan multiplication.

As a result, we define two bilinear multiplications on $\mathcal{F}(\mathcal{M})$ denoted by symbols $\{\ ,\ \}$ and $\circ$, and satisfying the conditions:

(1) $<\mathcal{F}(\mathcal{M}), \{\ ,\ \}>$ is a Lie algebra:

$$\{A, B\} = -\{B, A\},$$
$$\big\{\{A, B\}, C\big\} + \big\{\{B, C\}, A\big\} + \big\{\{C, A\}, B\big\} = 0.$$

(2) $<\mathcal{F}(\mathcal{M}), \circ>$ is a special Jordan algebra:

$$A \circ B = B \circ A,$$
$$\big((A \circ A) \circ B\big) \circ A = (A \circ A) \circ (B \circ A).$$

(3) $<\mathcal{F}(\mathcal{M}), \circ>$ is an associative Jordan algebra:

$$(A \circ B) \circ C - A \circ (B \circ C) = 0.$$

(4) $\{\ ,\ \}$ is a derivation on $<\mathcal{F}(\mathcal{M}), \circ>$:

$$\big\{A, (B \circ C)\big\} = \{A, B\} \circ C + B \circ \{A, C\}.$$

In this case, the Lie–Jordan algebra on $\mathcal{F}(\mathcal{M})$ is said to be defined. We shall also assume that there exists a unity I in $\mathcal{F}(\mathcal{M})$ such that $A \circ I = A$ and $\{A, I\} = 0$.

DEFINITION. A *Poisson manifold* is a manifold $\mathcal{M}$ equipped with two bilinear operations $\{\ ,\ \}$ and $\circ$ from $\mathcal{F}(\mathcal{M}) \times \mathcal{F}(\mathcal{M})$ into $\mathcal{F}(\mathcal{M})$ with the property that $<\mathcal{F}(\mathcal{M}), \circ, \{\ ,\ \}>$ is a Lie–Jordan algebra.

Let us consider the Poisson bracket of the form

$$\{A, B\} = \Psi^{kl}(x)\partial_k A(x)\partial_l B(x). \tag{16}$$

The skew-symmetry condition and the Jacobi identity give

$$\Psi^{kl}(x) = -\Psi^{lk}(x), \qquad \Psi^{ki}\partial_i\Psi^{lm} + \Psi^{li}\partial_i\Psi^{mk} + \Psi^{mi}\partial_i\Psi^{kl} = 0.$$

We note that Poisson brackets obey the Leibnitz rule and so is completely determined by the Poisson brackets of the coordinates $\{x^k, x^l\} = \Psi^{kl}(x)$.

If $\det[\Psi^{kl}(x)] = 0$, then the Poisson structure is called *degenerate*. Note that a general Poisson manifold with a degenerate Poisson structure is stratified into symplectic submanifolds on which the tensor $\Psi^{kl}(x)$ is nondegenerate. For each Poisson manifold there exists a family of symplectic manifolds. The fact that an arbitrary Poisson manifold is stratified into symplectic submanifolds is somewhat analogous to the decomposition of a finite-dimensional C^*-algebra as a direct sum of matrix algebras.

Derivations of Lie–Jordan algebra of classical observables

DEFINITION. A *derivation of a Lie–Jordan algebra* $<\mathcal{F}(\mathcal{M}), \circ, \{\ ,\ \}>$ is a linear operator $\mathcal{L}$ on $\mathcal{F}(\mathcal{M})$ satisfying

$$\mathcal{L}\big(\{A, B\}\big) = \big\{\mathcal{L}(A), B\big\} + \big\{A, \mathcal{L}(B)\big\},$$
$$\mathcal{L}(A \circ B) = \mathcal{L}(A) \circ B + A \circ \mathcal{L}(B)$$

for all A, B in $\mathcal{F}(\mathcal{M})$. A derivation $\mathcal{L}$ is said to be *inner* if there exists $H \in \mathcal{F}(\mathcal{M})$ such that

$$\mathcal{L}(A) = \{H, A\}$$

for all $A \in \mathcal{F}(\mathcal{M})$. It is said to be *outer* if it is not of this form.

The set of all derivations of $<\mathcal{F}(\mathcal{M}), \circ, \{\ ,\ \}>$ forms a Lie–Jordan algebra under the commutator

$$\mathcal{L}_1 \cdot \mathcal{L}_2 = (\mathcal{L}_1\mathcal{L}_2 - \mathcal{L}_2\mathcal{L}_1),$$

and anticommutator

$$\mathcal{L}_1 \circ \mathcal{L}_2 = \frac{1}{2}(\mathcal{L}_1\mathcal{L}_2 + \mathcal{L}_2\mathcal{L}_1).$$

Let $\mathcal{P}$ be a set of all complex polynomials in the real variables q_k and p_k, $k = 1, \ldots, n$. This set forms a Lie–Jordan algebra $<\mathcal{P}, \circ, \{\ ,\ \}>$ under the Poisson bracket $\{\ ,\ \}$ and the pointwise multiplication $\circ$. We can give the basic theorem regarding derivations of this Lie–Jordan algebra [190].

THEOREM *(Wollenberg). Every derivation $\mathcal{L}$ of the algebra $<\mathcal{P}, \circ, \{\ ,\ \}>$ is of the form*

$$\mathcal{L}A = \{H, A\} + b\left(A - \sum_{k=1}^{n} a_k p_k \circ \{q_k, A\} + \sum_{k=1}^{n}(1 - a_k) q_k \circ \{p_k, A\}\right),$$

where A in $\mathcal{P}$, and a_k, b in $\mathbb{C}$.

As a result, an arbitrary derivation of $<\mathcal{P}, \circ, \{\ ,\ \}>$ is a linear combination of an inner derivation $L_H^- = \{H,\ .\ \}$ and the explicitly determined outer derivation

$$\mathcal{L}_{outer} = L_1^+ - \sum_{k=1}^{n} a_k L_{p_k}^+ L_{q_k}^- + \sum_{k=1}^{n}(1 - a_k) L_{q_k}^+ L_{p_k}^-.$$

However this decomposition is not unique. If $\mathcal{L}_1$ and $\mathcal{L}_1$ are any two outer derivations

$$\mathcal{L}_s A = A - \sum_{k=1}^{n} a_k^{(s)} p^k \circ \frac{\partial A}{\partial p^k} - \sum_{k=1}^{n} \bigl(1 - a_k^{(s)}\bigr) q^k \circ \frac{\partial A}{\partial q^k} \quad (s = 1, 2),$$

then we have

$$(\mathcal{L}_1 - \mathcal{L}_2)A = \left\{ \sum_{k=1}^{n} \bigl(a_k^{(2)} - a_k^{(1)}\bigr) q^k p^k, A \right\}$$

for all $A \in \mathcal{P}$. Therefore we can replace the outer derivation in the decomposition by any other by redefining H.

COROLLARY. *Every derivation $\mathcal{L}$ of $<\mathcal{P}, \circ, \{\ ,\ \}>$ can be presented in the form*

$$\mathcal{L} = \sum_{k=1}^{n} \Biggl(\bigl(\mathcal{L}(q^k) - q^k \circ \mathcal{L}(1)\bigr) \circ \frac{\partial A}{\partial q^k} + \bigl(\mathcal{L}(p^k) - p^k \circ \mathcal{L}(1)\bigr) \circ \frac{\partial A}{\partial p^k} + \mathcal{L}(1) \circ A \Biggr)$$

for all A in $\mathcal{P}$.

Note that

$$\frac{\partial \mathcal{L}(q^k)}{\partial q^k} + \frac{\partial \mathcal{L}(p^k)}{\partial p^k} = \bigl\{\mathcal{L}(q^k), p^k\bigr\} + \bigl\{q^k, \mathcal{L}(p^k)\bigr\} = \mathcal{L}\bigl(\{q^k, p^k\}\bigr) = \mathcal{L}(1).$$

This corollary shows that $\mathcal{L}$ is completely determined by its values on the canonical variables q and p.

COROLLARY. *If $\mathcal{L}$ is a derivation of $<\mathcal{P}, \circ, \{\ ,\ \}>$, and $\mathcal{L}(1) = 0$, then $\mathcal{L}$ is inner.*

As a result, each derivation $\mathcal{L}$ of $<\mathcal{P}, \circ, \{\ ,\ \}>$ is inner if $\mathcal{L}(1) = 0$.

16.4. Properties of locally Hamiltonian systems

In general, we can consider the equation

$$\frac{d}{dt} A = \mathcal{L} A, \tag{17}$$

where $\mathcal{L}$ is a linear operator. If $\mathcal{L}$ is a first-order differential operator, then $\mathcal{L} = F^k(x)\partial_k$.

THEOREM. *Let $\mathcal{L}$ be a linear first-order differential operator. Then the equations*

$$\partial_k\big(\omega_{lm}(x)F^m(x)\big) - \partial_l\big(\omega_{km}(x)F^m(x)\big) = 0 \tag{18}$$

are equivalent to the relations

$$\mathcal{L}\big(\{x^j, x^i\}\big) + \big\{x^i, \mathcal{L}(x^j)\big\} - \big\{x^j, \mathcal{L}(x^i)\big\} = 0$$

for all $x \in \mathcal{M}$.

PROOF. If condition (18) is valid for all $x \in \mathcal{M}$, then $\mathcal{L}$ is locally Hamiltonian. Equations (18) can be written as

$$\big(\partial_k\omega_{lm}(x) - \partial_l\omega_{km}(x)\big)F^m(x) + \omega_{lm}(x)\partial_k F^m(x) - \omega_{km}(x)\partial_l F^m(x) = 0.$$

Equation

$$\partial_k\omega_{lm} + \partial_l\omega_{mk} + \partial_m\omega_{kl} = 0$$

gives

$$\big(-\partial_m\omega_{kl}(x)\big)F^m(x) + \omega_{lm}(x)\partial_k F^m(x) - \omega_{km}(x)\partial_l F^m(x) = 0.$$

Then the tensor $\Psi^{kl} = \Psi^{kl}(x)$ such that $\Psi^{kl}\omega_{km} = \Psi^{lk}\omega_{mk} = \delta^l_m$ gives

$$-\Psi^{ki}\Psi^{jl}\big(\partial_m\omega_{kl}(x)\big)F^m(x) + \Psi^{ki}\partial_k F^j(x) - \Psi^{jl}\partial_l F^i(x) = 0.$$

Using

$$\Psi^{jl}\partial_m\omega_{kl}(x) = -\omega_{kl}(x)\partial_m\Psi^{jl},$$

we obtain

$$\big(\partial_m\Psi^{ji}\big)F^m(x) + \Psi^{ki}\partial_k F^j(x) - \Psi^{jl}\partial_l F^i(x) = 0.$$

For the Poisson bracket (16), we have

$$\{x^i, A\} = \Psi^{il}(x)\partial_l A(x), \qquad \{x^i, x^j\} = \Psi^{ij}(x),$$

and

$$F^m\big(\partial_m\{x^j, x^i\}\big) + \big\{x^i, F^j\big\} - \big\{x^j, F^i\big\} = 0.$$

Substitution $F^k = \mathcal{L}(x^k)$ gives

$$\mathcal{L}\big(\{x^j, x^i\}\big) + \big\{x^i, \mathcal{L}(x^j)\big\} - \big\{x^j, \mathcal{L}(x^i)\big\} = 0. \qquad \square$$

THEOREM. *Let $\mathcal{L}$ be a linear first-order differential operator. Then the following conditions are equivalent.*

(1) *$\mathcal{L}$ is locally Hamiltonian.*

(2) *The equations*

$$\mathcal{L}\big(\{x^j, x^i\}\big) + \big\{x^i, \mathcal{L}(x^j)\big\} - \big\{x^j, \mathcal{L}(x^i)\big\} = 0$$

are valid for all $x \in \mathcal{M}$.

(3) *The condition*

$$J_{\mathcal{L}}\{A, B\} = \mathcal{L}\big(\{A, B\}\big) - \big\{\mathcal{L}(A), B\big\} - \big\{A, \mathcal{L}(B)\big\} = 0$$

is valid for all $A, B \in \mathcal{F}(\mathcal{M})$.

PROOF. The previous theorem proves (1) $\Rightarrow$ (2). Using $A = x^j$, $B = x^i$ and $\{A, B\} = -\{B, A\}$, we prove (3) $\Rightarrow$ (2). Using the equality

$$J_{\mathcal{L}}\{A, B\} = J_{\mathcal{L}}\{x^k, x^l\}\partial_k A \partial_l B$$

it is not hard to prove that (3) $\Rightarrow$ (2) and (2) $\Rightarrow$ (1). □

Note that these important theorems come from the simple form of the operator $\mathcal{L}$. In the general case, $\mathcal{L}$ is not necessary a first order differential operator. If we drop the condition that $\mathcal{L}$ be a first order differential operator, just retaining $J_{\mathcal{L}}\{A, B\} = 0$, then we obtain the following general definitions.

DEFINITION. A *locally Hamiltonian system* is a classical system on a Poisson manifold described by the equation

$$\frac{d}{dt}A = \mathcal{L}A,$$

such that the condition

$$J_{\mathcal{L}}\{A, B\} = \mathcal{L}\big(\{A, B\}\big) - \big\{\mathcal{L}(A), B\big\} - \big\{A, \mathcal{L}(B)\big\} = 0$$

is valid for all $A, B \in \mathcal{F}(\mathcal{M})$.

DEFINITION. A *globally Hamiltonian system* is a classical system on a Poisson manifold, such that $\mathcal{L}$ is a first order operator of inner differentiation on a Lie–Jordan algebra of classical observables.

DEFINITION. A classical system on a Poisson manifold is called a *non-Hamiltonian system*, if there exist observables A and B, such that the inequality

$$J_{\mathcal{L}}\{A, B\} \neq 0$$

is valid.

In general, a classical system can be either Hamiltonian or non-Hamiltonian. In order to determine a type of the system, it is not necessary to have the explicit solution $x_t^k = \varphi^k(x, t)$ of equations of motion. For this purpose, we can consider the properties of the operator $\mathcal{L}$.

16.5. Quantum Hamiltonian and non-Hamiltonian systems

Using definitions of Hamiltonian and non-Hamiltonians systems, we can define corresponding quantum analogs.

We consider the operator differential equation

$$\frac{dA_t}{dt} = \mathcal{L}A_t \tag{19}$$

with the real superoperator $\mathcal{L}$ having an everywhere dense domain $D(\mathcal{L})$ in an operator algebra $\mathcal{M}$ such that $D(\mathcal{L})$ is a subalgebra of $\mathcal{M}$. In each example the operator A corresponds to an observable of the quantum system and will be represented by an element of the operator algebra $\mathcal{M}$.

DEFINITION. A quantum system is said to be *locally Hamiltonian* if the superoperator $\mathcal{L}$ in equation (19) satisfies the conditions

$$J_{\mathcal{L}}(A, B) = \mathcal{L}(A \cdot B) - (\mathcal{L}A) \cdot B - A \cdot (\mathcal{L}B) = 0,$$
$$K_{\mathcal{L}}(A, B) = \mathcal{L}(A \circ B) - (\mathcal{L}A) \circ B - A \circ (\mathcal{L}B) = 0$$

for all A and B in $D(\mathcal{L})$.

Using $A \cdot B = (1/i\hbar)[A, B]$, $A \circ B = (1/2)[A, B]_+$, these conditions give

$$\mathcal{L}\big([A, B]\big) - \big[\mathcal{L}(A), B\big] - \big[A, \mathcal{L}(B)\big] = 0,$$
$$\mathcal{L}\big([A, B]_+\big) - \big[\mathcal{L}(A), B\big]_+ - \big[A, \mathcal{L}(B)\big]_+ = 0.$$

STATEMENT. *A quantum system is locally Hamiltonian if the superoperator $\mathcal{L}$ in equation* (19) *satisfies the conditions*

$$J_{\mathcal{L}}\big(X^k, X^l\big) = 0, \qquad K_{\mathcal{L}}\big(X^k, X^l\big) = 0 \tag{20}$$

for all $k, l = 1, \ldots, n$.

Here X^k, $k = 1, \ldots, 2n$, are operators that correspond to the coordinates x^k in $\mathbb{R}^{2n}$:

$$\pi(x^k) = X^k,$$

where $X^k = P_k = \pi(p_k)$ $(k = 1, \ldots, n)$, and $X^{n+k} = Q_k = \pi(q_k)$ $(k = 1, \ldots, n)$.

DEFINITION. A quantum system is said to be *non-Hamiltonian*, if there exist A and B in $D(\mathcal{L})$ such that

$$J_{\mathcal{L}}(A, B) \neq 0.$$

Suppose $A = A(X) = A(Q, P)$ and $B = B(X) = B(Q, P)$ are some operator functions. We note that the commutator obeys the Leibnitz rule and so is completely determined by the commutators of the coordinate operators

$$\left[X^k, X^l\right] = \Psi^{kl}(X).$$

STATEMENT. *A quantum system is non-Hamiltonian, if there exist X^k and X^l, such that*

$$J_{\mathcal{L}}\left(X^k, X^l\right) \neq 0.$$

Note that $J_{\mathcal{L}}(X^k, X^l)$ can be considered as a quantum analog of $J_{\mathcal{L}}\{x^k, x^l\}$, i.e., $J_{\mathcal{L}}(X^k, X^l) = \pi(J_{\mathcal{L}}\{x^k, x^l\})$.

DEFINITION. A *quantum dissipative system* is a quantum system, such that the superoperator $\mathcal{L}$ in equation (19) satisfies the requirement

$$\Omega(Q, P) = -\sum_{k=1}^{n} J_{\mathcal{L}}(Q_k, P_k) \neq 0.$$

All quantum dissipative systems are non-Hamiltonian.

STATEMENT. *If equation* (19) *describes a quantum non-Hamiltonian system, then there exist A and B such that*

$$Z_{\mathcal{L}}(A, B) = \mathcal{L}(AB) - \mathcal{L}(A)B - A\mathcal{L}(B) \neq 0.$$

It is not hard to prove this statement by using the relation

$$Z_{\mathcal{L}}(A, B) = K_{\mathcal{L}}(A, B) + \frac{i\hbar}{2} J_{\mathcal{L}}(A, B).$$

In general, there exists a special class of quantum systems, such that $K_{\mathcal{L}}(A, B) \neq 0$ and $J_{\mathcal{L}}(A, B) = 0$. These systems will be called the *exotic non-Hamiltonian systems*.

Note that

$$J_{\mathcal{L}}(A, B) = \frac{1}{i\hbar}\left(Z_{\mathcal{L}}(A, B) - Z_{\mathcal{L}}(B, A)\right),$$

$$K_{\mathcal{L}}(A, B) = \frac{1}{2}\left(Z_{\mathcal{L}}(A, B) + Z_{\mathcal{L}}(B, A)\right).$$

Therefore, if $Z_{\mathcal{L}}(A, B) = 0$ for all A and B, then $J_{\mathcal{L}}(A, B) = K_{\mathcal{L}}(A, B) = 0$.

16.6. Hamiltonian and Liouvillian pictures

Classical statistical ensemble

Let us consider a set of independent classical systems identical in equations of motion, but differing in their initial conditions with respect to coordinates and momenta. The forces are supposed to be determined for every system by the same law, being functions of the coordinates $(q, p) = \{q_1, \ldots, q_n, p_1, \ldots, p_n\}$ in a phase-space of the system, either alone or with the external parameters $a = \{a_1, \ldots, a_m\}$. It is not necessary that these systems should be Hamiltonian. The coordinates $x = (q, p)$, which have different values in the different classical systems, are considered. We can suppose that the systems are continuously distributed in the phase-space. An ensemble is a set of classical systems identical in nature and subject to forces determined by identical laws [66], but distributed in phase-space in any continuous way.

Let us consider the differential equation

$$\frac{d}{dt}A(t, x) = \mathcal{L}A(t, x) \tag{21}$$

with the linear differential operator $\mathcal{L}$ having an everywhere dense domain of definition $D(\mathcal{L})$ in a function space $\mathcal{M}$. Here $A(t, x)$ is an unknown classical observable such that $A(t, x) \in \mathcal{M}$ for $t \geqslant 0$. A Cauchy problem is the problem of finding a solution $A(t, x)$ of equation (21) satisfying the initial condition: $A(0, x) = A_0(x) \in \mathcal{M}$.

DEFINITION. A *classical statistical ensemble* is a set of classical systems identical in equations of motion (21), i.e., identical in the operator $\mathcal{L}$, but differing in their initial conditions $A(0, x) = A_0(x) \in \mathcal{M}$.

Let us consider a statistical ensemble distributed in phase-space with the density $\varrho(t, x) \geqslant 0$. We can define the normalized density function

$$\rho(t, x) = N^{-1}(t)\varrho(t, x), \quad N(t) = \int dx\, \varrho(t, x), \quad \int dx\, \rho(t, x) = 1.$$

The $\rho(t, x)$ can be interpreted as the probability distribution for finding the system at the point x in phase-space.

The average quantity $<A>$ is identified with the usual expectation value of the observable $A(t, x)$, corresponding to the given probability distribution

$$<A>(t, a) = \int dx\, A(t, x, a)\rho(t, x). \tag{22}$$

The concept of an ensemble is considered as a postulate not needing further justification. Let us note the reasonableness of the postulate. The main argument is

the violent instability of motion. If we can determine exactly the initial condition of a classical system, we make some prediction of its behavior at time t. But if we make a tiny error, picking up a slightly different initial condition, very close to the former, we would very quickly be off by an appreciable amount. This is a result of the property that seems to be usual for most classical systems. In rough (structurally stable) classical systems, on the other hand, we do not generally find such violent sensitivity on the choice of initial conditions. An observation can involve some kind of smoothing. Hence we cannot make a definite prediction about the system, as we do not know its initial condition. We can predict only the features that are common to all, or at least to most systems whose initial condition is compatible. Hence we cannot predict definitely the outcome of a given experiment. We may, however, predict the most probable or the average (expectation) result of this experiment if we repeat it a large number of times under the same conditions.

The introduction of statistical ensemble is necessary not only by our ignorance of the exact initial conditions for a large number of particles. A statement like "$x = \sqrt{2} = 1.4142135623729866\ldots$" would have a physical meaning only if one could distinguish between it and the approximation of $\sqrt{2}$ by the first n decimals for all n. This, however, is impossible, since n can always be chosen so large that experimental distinction is not possible. Concepts that correspond to impossible observations can be eliminated from theory. This is possible in this case. Then, classical mechanics must be formulated statistically.

In classical mechanics, the statistical method should be used not only for systems of very many individual particles. It is necessary to use it in every case, even that of a single particle in the simplest possible conditions [28]. This does not require any new mathematics. We can use the law where the probability density satisfies the classical Liouville equation.

We may now formulate the following basic postulate of classical mechanics. The state of a classical system is completely specified at a given time by a certain distribution function $\rho(t, x)$, satisfying the normalization condition. The expectation value $<A>(a, t)$ of a classical observable $A(t, x, a)$ in such a system is calculated by equation (22).

Quantum statistical ensemble

Let us consider the operator differential equation

$$\frac{d}{dt}A_t = \mathcal{L}A_t \tag{23}$$

with the linear superoperator $\mathcal{L}$ having an everywhere dense domain of definition $D(\mathcal{L})$ in an operator space $\mathcal{M}$. Here $A_t = A(t)$ is an unknown one-parameter operator such that $A(t) \in \mathcal{M}$ for all $t \geqslant 0$. A Cauchy problem is the problem of

finding a solution $A(t)$ of equation (23) satisfying the initial condition: $A(0) = A_0 \in \mathcal{M}$.

DEFINITION. A *quantum statistical ensemble* is a set of quantum (non-Hamiltonian) systems identical in equations of motion (23), i.e., identical in the superoperator $\mathcal{L}$, but differing in their initial condition $A(0) = A_0 \in \mathcal{M}$.

This notion is a quantum (operator) generalization of the concept of the classical statistical ensemble.

Dynamical pictures in physics

There are two modes of description of a continuous medium, the *Lagrangian* and *Eulerian*. In dynamics of continuous media the Lagrangian reference frame is a way of looking at medium motion where the observer follows individual medium particles as they move through space and time. The Eulerian reference frame is a way of looking at medium motion that focuses on specific points in the space through which the medium moves. Eulerian coordinates are a system of coordinates in which properties of a medium are assigned to points in space at each given time, without attempt to identify individual medium particles. Lagrangian coordinates are a system of coordinates by which medium particles are identified for all time by assigning them coordinates that do not vary in time.

A statistical ensemble can be considered as a special medium. The *Liouvillian picture* is the Eulerian description of statistical ensemble. The *Hamiltonian picture* is the Lagrangian description of statistical ensemble. In the quantum mechanics, the Liouvillian picture corresponds to Schrödinger picture, and the Hamiltonian description corresponds to Heisenberg picture.

Mechanics of Continuous Media	Classical Mechanics	Quantum Mechanics
Lagrangian	Hamiltonian	Heisenberg
Eulerian	Liouvillian	Schrödinger

Hamiltonian picture

The Hamiltonian description employs the coordinates x_0 of a particle in the initial state as the independent variables. In classical dynamics the Hamiltonian picture is a way of looking at motion where the observer follows individual system as they move through phase-space and time. The Hamiltonian picture is a description by

which ensemble systems are identified for all time by assigning them initial coordinates that do not vary in time. Plotting the phase-space position of an individual system through time gives the phase-space trajectory of the system.

Suppose that a classical system, whose phase-space is determined by a point $x = (q, p)$ in a region $\mathcal{M}$ of $2n$-dimensional phase-space $\mathbb{R}^{2n}$, moves in a vector field $F(x)$. The motion of the system is described by the equations

$$\frac{dx_t}{dt} = F(t, x_t). \tag{24}$$

The solution of a Cauchy problem in which the initial condition is given by x_0 at the time $t = 0$ can be presented in the form $x_t = x(t) = \varphi_t(x_0)$, where φ_t is the semi-group of operators. A classical observable is a function on the phase-space $\mathcal{M}$. Now we shall consider the differentiation of an observable as a composite function. In the Hamiltonian picture, $A(t, x_t)$ is a composition of two functions $A(t, x_t)$ and $x_t = x(t)$. The time derivative of this composition function is

$$\frac{d}{dt}A(t, x_t) = \frac{\partial A(t, x_t)}{\partial t} + \frac{\partial A(t, x_t)}{\partial x_t^k}\frac{dx_t^k}{dt}.$$

Using equation (24), we obtain

$$\frac{d}{dt}A(t, x_t) = \frac{\partial A(t, x_t)}{\partial t} + F^k(t, x_t)\frac{\partial A(t, x_t)}{\partial x_t^k}. \tag{25}$$

This is the equation of motion for the classical observable A. The solution of a Cauchy problem in which the initial condition is given by $A = A(0, x_0)$ at the time $t = 0$ can be presented in the form $A_t = \Phi_t A$, where Φ_t is the semi-group of operators. Note that Φ_t is an adjoint (dual) operator of φ_t, i.e., $\Phi_t = \varphi_t^*$ and

$$\Phi_t A(x_0) = \varphi_t^* A(x_0) = A(\varphi_t x_0) = A(x_t).$$

A distribution function for each ensemble is a nonnegative real-valued function $\rho(t, x)$ with unit integral:

$$\rho(t, x) \geqslant 0, \qquad \rho(t, x)^* = \rho(t, x), \qquad \int dx\, \rho(t, x) = 1$$

for all $t \geqslant 0$ and $x \in \mathcal{M}$. The distribution functions represent states in classical mechanics. In the Hamiltonian picture, the distribution $\rho(t, x_t)$ can be considered as an observable. Then

$$\frac{d}{dt}\rho(t, x_t) = \frac{\partial \rho(t, x_t)}{\partial t} + F^k(x_t)\frac{\partial \rho(t, x_t)}{\partial x_t^k}.$$

Moreover,

$$\int dx_t\, \rho(t, x_t) = 1 \tag{26}$$

for all $t \geqslant 0$. Differentiation of equation (26) with respect to t gives

$$\int dx_t \left(\Omega(t, x_t)\rho(t, x_t) + \frac{d\rho(t, x_t)}{dt} \right) = 0,$$

where

$$\Omega(t, x) = \sum_{k=1}^{n} \frac{\partial F^k(t, x)}{\partial x^k}. \tag{27}$$

As a result, we obtain

$$\frac{d\rho(t, x_t)}{dt} + \Omega(t, x_t)\rho(t, x_t) = 0. \tag{28}$$

This is the *Liouville equation* in the Hamiltonian picture. If there exist points $x_t \in \mathcal{M}$ such that $\Omega(t, x_t) < 0$, then the system is called dissipative. If $\Omega(t, x_t) < 0$, the system is accretive. If there exist points x_t such that $\Omega(t, x_t) \neq 0$, then the classical system is called the generalized dissipative system.

For Hamiltonian systems, $\Omega(t, x_t) = 0$, and

$$\frac{d\rho(t, x_t)}{dt} = 0$$

for all $t \geqslant 0$. Then the distribution is constant in time

$$\rho(t, x_t) = \rho(0, x_0) = const.$$

As a result, the distribution functions of Hamiltonian systems are integrals of motion. This is the principle of conservation of distribution for Hamiltonian systems.

In the general case, there exists an evolution of state in the Hamiltonian picture. The distribution of non-Hamiltonian system can be nonconstant in time.

The expectation value is

$$<A> = \int dx_t \, \rho(t, x_t)A(t, x_t).$$

Differentiation of this equation with respect to t gives

$$\frac{d<A>}{dt} = \int dx_t \left(\Omega(t, x_t)\rho(t, x_t)A(t, x_t) + \frac{d\rho(t, x_t)}{dt}A(t, x_t) + \rho(t, x_t)\frac{dA(t, x_t)}{dt} \right).$$

Using the Liouville equation, we obtain

$$\frac{d}{dt}<A> = <\frac{dA}{dt}>.$$

Let $\mathcal{F}(\mathcal{M})$ be a space of smooth functions on $\mathcal{M}$. To each pair A, B of the space $\mathcal{F}(\mathcal{M})$, we can associate a real number (A, B) defined by (9). Using the scalar product, we can define the adjoint operator S_t by $(\rho, \Phi_t A) = (S_t\rho, A)$. Then

$$\int dx \left(\rho(t,x)\right)^* \Phi_t A(x) = \int dx \left(S_t\rho(t,x)\right)^* A(x).$$

In the Hamiltonian picture, we can define

$$(A_t, B_t)_t = \int dx_t \left(A(t,x_t)\right)^* B(t,x_t).$$

In general, $dx_t \neq dx_0$ and $(A, B)_t \neq (A, B)$. Using $dx_t\rho(t,x_t) = dx_0\,\rho(t,x_0)$ we obtain $(\rho_t, A_t)_t = (\rho_0, A_t)_0$. Then $A_t = A(x_t) = \Phi_t A(x_0)$ gives

$$\begin{aligned}(\rho_t, A_t)_t &= \int dx_t \left(\rho(t,x_t)\right)^* A(x_t) = \int dx_t\,\rho(t,x_t)A(x_t)\\ &= \int dx_0\,\rho(t,x_0)\Phi_t A(x_0) = \int dx_0 \left[S_t\rho(t,x_0)\right]A(x_0)\\ &= (S_t\rho, A_0)_0.\end{aligned}$$

Liouvillian picture

In the Liouvillian picture the independent variables are the coordinates x of a point in the ensemble. The Liouvillian picture is a way of looking at ensemble motion that focuses on some points in the phase-space through which the ensemble systems move. In the Liouvillian picture, properties of an ensemble are assigned to points in phase-space at each given time, without attempt to identify individual system of the ensemble.

Let $A(t,x)$ be a classical observable. In the Liouvillian picture, the evolution equation of this observable is

$$\frac{d}{dt}A(t,x) = \frac{\partial}{\partial t}A(t,x).$$

Here x is a fixed point of the phase-space, and $dx/dt = 0$.

Let $\rho(t,x)$ be a distribution function. Then

$$\frac{d\rho(t,x)}{dt} = \frac{\partial\rho(t,x)}{\partial t},$$

since x is a fixed point.

If the number of systems in the ensemble is constant, then we can write the continuity equation for density $\rho(t,x)$ in phase-space

$$\frac{\partial}{\partial t}\rho(t,x) + div\big(F(t,x)\rho(t,x)\big) = 0.$$

Applying chain rule, we obtain:

$$\frac{\partial}{\partial t}\rho(t,x) + F^k(t,x)\frac{\partial}{\partial x^k}\rho(t,x) = -\Omega(t,x)\rho(t,x), \tag{29}$$

where $\Omega(t,x)$ is defined by (27). The left-hand side of equation (29) is the full (total time) derivative of the distribution function $\rho(t,x)$. Equation (29) is the *Liouville equation* in the Liouvillian picture. This is the continuity phase-space equation in the Eulerian variables.

This Liouville equation can be presented in the form

$$i\frac{\partial}{\partial t}\rho(t,x) = \Lambda_t\rho(t,x), \tag{30}$$

where Λ_t is the Liouville operator

$$\Lambda_t = -i\left(F^k(t,x)\frac{\partial}{\partial x^k} + \Omega(t,x)\right).$$

Note that the Liouville operator can be a starting point for non-Hamiltonian statistical mechanics. One can describe a system for which a Hamiltonian does not exist, but for which a Liouville operator can be constructed. In other words, equation (30) can be taken as the basis of a theory even when Λ is not defined by $\Lambda\rho = \{H, \rho\}$, where $\{\ ,\ \}$ is the Poisson bracket.

Chapter 17

Quantization of Dynamical Structure

17.1. Quantization in kinematics and dynamics

Classical and quantum theories consist of two parts, a kinematical structure, describing the initial observables and states of the system, and a dynamical structure describing the evolution of these observables and states with time. Therefore main requirement imposed on the quantization π is that it should satisfy the two following conditions:

(1) For a given kinematical structure, there are operations g_q on the set of quantum observables corresponding to the operations g_c on the set of classical observables.
(2) For a given dynamical structure, there are linear superoperators $\mathcal{L}_q$, Λ_q on the set of quantum observables corresponding to the linear operators $\mathcal{L}_c$, Λ_c on the set of classical observables.

Setting quantization in kinematics means establishing a map π assigning a quantum observable $A(X)$ to each classical observable $A(x)$:

$$\pi\big(A(x)\big) = A(X).$$

In the case of a system with n degrees of freedom, we consider the phase space $\mathbb{R}^{2n}$ such that $x = (q, p)$. We can make correspond to the function x^k, the operator X^k:

$$\pi(x^k) = X^k.$$

There exist natural requirements that must be satisfied by the quantization in kinematics. First of all, if

$$\{x^k, x^l\} = \Psi^{kl},$$

where Ψ^{kl} are constants such that

$$\{q^k, q^l\} = \{p^k, p^l\} = 0, \qquad \{q^k, p^l\} = \delta^k_l,$$

with corresponding sets of indices, then

$$\frac{1}{i\hbar}\big[X^k, X^l\big] = \Psi^{kl} I,$$

and we have

$$\big[Q^k, Q^l\big] = \big[P^k, P^l\big] = 0, \qquad \big[Q^k, P^l\big] = i\hbar\delta^k_l I.$$

Setting quantization in dynamics means establishing a map π assigning a superoperator $\mathcal{L}[L^+_X, L^-_X]$ to each operator $\mathcal{L}[L^+_x, L^-_x]$. As a result, we have

$$\pi\big(\mathcal{L}\big[L^+_x, L^-_x\big]\big) = \mathcal{L}\big[L^+_X, L^-_X\big].$$

Here L^+_x, L^-_x are operators on a set of classical observables, where $L^+_{x^k}$ is a multiplication by x^k, and $L^-_{x^k}$ is a differentiation, such that

$$L^+_{x^k} A(x) = x^k \circ A(x), \qquad L^-_{x^k} = \big\{x^k, A(x)\big\}.$$

In local coordinates (q, p), we have

$$\begin{aligned}
&L^+_{q^k} A(q, p) = q^k A(q, p),\\
&L^-_{q^k} A(q, p) = \big\{q^k, A(q, p)\big\} = \frac{\partial}{\partial p^k} A(q, p),\\
&L^+_{p^k} A(q, p) = p^k A(q, p),\\
&L^-_{p^k} A(q, p) = \big\{p^k, A(q, p)\big\} = -\frac{\partial}{\partial q^k} A(q, p).
\end{aligned}$$

Note that L^+_X, L^-_X are superoperators on a set of quantum observables, where $L^+_{X^k}$ is a Jordan left multiplication by X^k, and $L^-_{X^k}$ is a Lie left multiplication by X^k, such that

$$\begin{aligned}
&L^+_{X^k} A(X) = X^k \circ A(X) = \frac{1}{2}\big(X^k A + A X^k\big),\\
&L^-_{X^k} A(X) = X^k \cdot A(X) = \frac{1}{i\hbar}\big(X^k A - A X^k\big).
\end{aligned}$$

There exist natural requirements that must be satisfied by the quantization in dynamics:

$$\pi\big(L^+_{x^k}\big) = L^+_{X^k}, \qquad \pi\big(L^-_{x^k}\big) = L^-_{X^k}.$$

17.2. Quantization map for equations of motion

Let a classical system has n degrees of freedom, and its phase space be the real linear space $\mathbb{R}^{2n}$. Classical observables are real-valued functions $A(q, p)$, where $(q, p) \in \mathbb{R}^{2n}$. Setting quantization means establishing a procedure assigning a quantum observable $A(Q, P)$ to each classical observable $A(q, p)$. Here a quantum observable is a self-adjoint element of some operator algebra. In this case, the function $A(q, p)$ itself is called the symbol of the operator $A(Q, P)$. We shall denote the linear space of all smooth functions on $\mathbb{R}^{2n}$ by $C^\infty(\mathbb{R}^{2n})$. We assume that evolution of the classical system is described by the differential equation

$$\frac{d}{dt}A(q, p) = \mathcal{L}\left(q, p, \frac{\partial}{\partial q}, \frac{\partial}{\partial p}\right)A(q, p), \tag{1}$$

where $\mathcal{L}(q, p, \partial_q, \partial_p)$ is a linear differential operator on $C^\infty(\mathbb{R}^{2n})$.

In order to obtain equations of motion for quantum systems, one should specify the rules making it possible to quantize classical equations of motion (1) and the corresponding differential operators $\mathcal{L}(q, p, \partial_q, \partial_p)$. In defining these rules, one often tries to write the equations of motion in a Hamiltonian form, i.e., in terms of the Poisson bracket with a certain Hamilton function. However, in the general case, it is difficult to determine whether the Hamilton function exists, and, if it does, whether it is unique, and to find its explicit form if it exists and is unique. Therefore, quantization is more conveniently carried out starting from equations of motion.

Lie–Jordan algebras

Let the set of observables form a linear space $\mathcal{M}_0$ over the field of real numbers $\mathbb{R}$. For the observables from $\mathcal{M}_0$, we define two bilinear multiplication operations denoted by symbols $\cdot$ and $\circ$, and satisfying the conditions:

(1) $<\mathcal{M}_0, \cdot>$ is a Lie algebra:

$$A \cdot B = -B \cdot A, \qquad (A \cdot B) \cdot C + (B \cdot C) \cdot A + (C \cdot A) \cdot B = 0;$$

(2) $<\mathcal{M}_0, \circ>$ is a special Jordan algebra:

$$A \circ B = B \circ A, \qquad \big((A \circ A) \circ B\big) \circ A = (A \circ A) \circ (B \circ A);$$

(3) the Leibnitz rule:

$$A \cdot (B \circ C) = (A \cdot B) \circ C + B \circ (A \cdot C);$$

(4) the equation for associators:

$$(A \circ B) \circ C - A \circ (B \circ C) = \frac{\hbar^2}{4}\big((A \cdot B) \cdot C - A \cdot (B \cdot C)\big).$$

In this case, the Lie–Jordan algebra is said to be defined. We shall also assume that there exists a unity I in $\mathcal{M}_0$ such that $A \circ I = A$ and $A \cdot I = 0$.

We denote as $\mathcal{M}_c$ a free Lie–Jordan algebra over the field $\mathbb{R}$ with unity 1 and generators q_k and p_k, where $k = 1, \ldots, n$ and

$$q_k \cdot p_l = \delta_{kl} 1, \qquad q_k \cdot q_l = 0, \qquad p_k \cdot p_l = 0. \tag{2}$$

This is the Lie–Jordan algebra of classical observables. Note that a free algebra is an algebra generated by finite linear combinations and finite powers of the elements $\{q_k, p_k\colon k = 1, \ldots, n\}$ and the identity 1.

For the classical observables $A(q, p)$ and $B(q, p)$, these operations can be defined in terms of the Poisson bracket in $\mathbb{R}^{2n}$ and the usual pointwise multiplication

$$\begin{aligned} &A(q, p) \cdot B(q, p) = \big\{A(q, p), B(q, p)\big\}, \\ &A(q, p) \circ B(q, p) = A(q, p)B(q, p). \end{aligned} \tag{3}$$

We denote as $\mathcal{M}_q$ a free Lie–Jordan algebra over the field $\mathbb{R}$ with unity I and generators Q_k and P_k, where $k = 1, \ldots, n$ and

$$Q_k \cdot P_l = \delta_{kl} I, \qquad Q_k \cdot Q_l = 0, \qquad P_k \cdot P_l = 0. \tag{4}$$

This is the Lie–Jordan algebra of quantum observables. For the quantum observables $A = A(Q, P)$ and $B = B(Q, P)$, the operations of Lie and Jordan multiplication are defined in the form

$$\begin{aligned} &A(Q, P) \cdot B(Q, P) = \frac{1}{i\hbar}(AB - BA), \\ &A(Q, P) \circ B(Q, P) = \frac{1}{2}(AB + BA). \end{aligned} \tag{5}$$

Multiplication algebra for the Lie–Jordan algebra

For any element $A \in \mathcal{M}$, we define two operations of left ($L_A^{\pm}$) and two operations of right ($R_A^{\pm}$) multiplications by A, which map $\mathcal{M}$ into itself by the following rules:

$$L_A^+ C = A \circ C, \quad L_A^- C = A \cdot C, \quad R_A^+ C = C \circ A, \quad R_A^- C = C \cdot A$$

for all $C \in \mathcal{M}$. These maps are endomorphisms of the algebra $\mathcal{M}$. A subalgebra of the algebra of endomorphisms of $\mathcal{M}$, generated by various $L_A^{\pm}$ and $R_A^{\pm}$, is called the multiplication algebra of the Lie–Jordan algebra $\mathcal{M}$ and is denoted by $\mathcal{A}(\mathcal{M})$. Algebras generated by all operations of left and right multiplications of the Lie–Jordan algebra coincide with $\mathcal{A}(\mathcal{M})$ since $L_A^{\pm} = \pm R_A^{\pm}$.

The identities of a Lie–Jordan algebra lead to the relations for the multiplication operations. To obtain them, one should use the linearization of these identities.

THEOREM. *Multiplication algebra $\mathcal{A}(\mathcal{M})$ for the Lie–Jordan algebra $\mathcal{M}$ is defined by the following conditions*

(1) *the Lie relations*

$$L^-_{A\cdot B} = L^-_A L^-_B - L^-_B L^-_A, \tag{6}$$

(2) *the Jordan relations*

$$\begin{aligned} &L^+_{(A\circ B)\circ C} + L^+_B L^+_C L^+_A + L^+_A L^+_C L^+_B \\ &\quad = L^+_{A\circ B} L^+_C + L^+_{B\circ C} L^+_A + L^+_{A\circ C} L^+_B, \end{aligned} \tag{7}$$

$$\begin{aligned} &L^+_{(A\circ B)\circ C} + L^+_B L^+_C L^+_A + L^+_A L^+_C L^+_B \\ &\quad = L^+_C L^+_{A\circ B} + L^+_B L^+_{A\circ C} + L^+_A L^+_{B\circ C}, \end{aligned} \tag{8}$$

$$\begin{aligned} &L^+_C L^+_{A\circ B} + L^+_B L^+_{A\circ C} + L^+_A L^+_{B\circ C} \\ &\quad = L^+_{A\circ B} L^+_C + L^+_{B\circ C} L_A + L^+_{A\circ C} L^+_B, \end{aligned} \tag{9}$$

(3) *the mixed relations*

$$L^+_{A\cdot B} = L^-_A L^+_B - L^+_B L^-_A, \qquad L^-_{A\circ B} = L^+_A L^-_B + L^+_B L^-_A, \tag{10}$$

$$L^+_{A\circ B} = L^+_A L^+_B - \frac{\hbar^2}{4} L^-_B L^-_A, \qquad L^+_B L^+_A - L^+_A L^+_B = -\frac{\hbar^2}{4} L^-_{A\cdot B}. \tag{11}$$

For the algebra $\mathcal{M}_c$ of classical observables $\hbar = 0$. If $\mathcal{M} = \mathcal{M}_q$, then $\hbar \neq 0$.

The following corollaries follow from the relations.

COROLLARY 1. *If the Jordan algebra $<\mathcal{M}, \circ>$ is generated by the set $\mathcal{G} = \{x_k\}$, then the corresponding multiplication algebra is generated by the set $\{L^+_{x_k}, L^+_{x_k\circ x_m}\colon x_k, x_m \in \mathcal{G}\}$.*

COROLLARY 2. *If the Lie algebra $<\mathcal{M}, \cdot>$ is generated by the set $\mathcal{G} = \{x_k\}$, then the corresponding multiplication algebra is generated by the set $\{L^-_{x_k}\colon x_k \in \mathcal{G}\}$.*

COROLLARY 3. *If the Lie–Jordan algebra $\mathcal{M}$ is generated by the set $\mathcal{G} = \{x_k\}$, then the corresponding multiplication algebra $\mathcal{A}(\mathcal{M})$ is generated by the set of operators $\{L^+_{x_k}, L^-_{x_k}\colon x_k \in \mathcal{G}\}$.*

Note that, in the latter statement, we use the set of operators $\{L^+_{x_k}, L^-_{x_k}\colon x_k \in X\}$, and not the set $\{L^+_{x_k}, L^+_{x_k\circ x_l}, L^-_{x_k}\colon x_k, x_l \in X\}$, and this is due to first relation of (11). These corollaries are valid for $\mathcal{M}_c$ and $\mathcal{M}_q$.

Using the properties of generators (2) and relations (10), it is easy to prove the following theorem.

THEOREM. *Let $\mathcal{M}_c$ be a Lie–Jordan algebra with unity* 1 *that is generated by the set $\mathcal{G}_c = \{q_k, p_k, 1\colon\ k = 1, \dots, n\}$, such that relations* (2) *are valid. Then the corresponding multiplication algebra $\mathcal{A}(\mathcal{M})$ is generated by the set $\{L^{\pm}_{q_k}, L^{\pm}_{p_k}, L^{\pm}_{1}\colon\ q_k, p_k, 1 \in \mathcal{G}_c\}$, such that the following commutation relations are satisfied*:

$$\left[L^{\pm}_{q_k}, L^{\mp}_{p_l}\right] = \delta_{kl} L^{+}_{1}, \tag{12}$$

$$\left[L^{\pm}_{q_k}, L^{\pm}_{q_l}\right] = \left[L^{\pm}_{q_k}, L^{\pm}_{p_l}\right] = \left[L^{\pm}_{p_k}, L^{\pm}_{p_l}\right] = 0, \tag{13}$$

$$\left[L^{\mp}_{q_k}, L^{\pm}_{q_l}\right] = \left[L^{\mp}_{p_k}, L^{\pm}_{p_l}\right] = \left[L^{\pm}_{q_k}, L^{\pm}_{1}\right] = \left[L^{\pm}_{p_k}, L^{\pm}_{1}\right] = 0. \tag{14}$$

These relations define the Lie algebra generated by $L^{\pm}_{q_k}, L^{\pm}_{p_k}, L^{\pm}_{1}$.

THEOREM. *Let $\mathcal{M}_q$ be a Lie–Jordan algebra with unity I that is generated by the set $\mathcal{G}_q = \{Q_k, P_k, I\colon\ k = 1, \dots, n\}$, such that relations* (4) *are valid. Then the corresponding multiplication algebra $\mathcal{A}(\mathcal{M})$ is generated by the set $\{L^{\pm}_{Q_k}, L^{\pm}_{P_k}, L^{\pm}_{I}\colon\ Q_k, P_k, I \in \mathcal{G}_q\}$, such that the following commutation relations are satisfied*:

$$\left[L^{\pm}_{Q_k}, L^{\mp}_{P_l}\right] = \delta_{kl} L^{+}_{I}, \tag{15}$$

$$\left[L^{\pm}_{Q_k}, L^{\pm}_{Q_l}\right] = \left[L^{\pm}_{Q_k}, L^{\pm}_{P_l}\right] = \left[L^{\pm}_{P_k}, L^{\pm}_{P_l}\right] = 0, \tag{16}$$

$$\left[L^{\mp}_{Q_k}, L^{\pm}_{Q_l}\right] = \left[L^{\mp}_{P_k}, L^{\pm}_{P_l}\right] = \left[L^{\pm}_{Q_k}, L^{\pm}_{I}\right] = \left[L^{\pm}_{P_k}, L^{\pm}_{I}\right] = 0. \tag{17}$$

Note that the given commutation relations for the generators of $\mathcal{A}(\mathcal{M}_c)$ and $\mathcal{A}(\mathcal{M}_q)$ are the same.

Consider now an associative algebra $\mathcal{P}(\mathcal{M}_c)$ and $\mathcal{P}(\mathcal{M}_q)$ generated by finite linear combinations and finite powers of the elements $\{L^{\pm}_{q_k}, L^{\pm}_{p_k}, L^{\pm}_{1}\colon\ q_k, p_k, 1 \in \mathcal{G}_c\}$ and $\{L^{\pm}_{Q_k}, L^{\pm}_{P_k}, L^{\pm}_{1}\colon\ Q_k, P_k, l \in \mathcal{G}_q\}$, where equations (12)–(17) are valid. The algebra $\mathcal{P}(\mathcal{M})$ is an associative algebra with respect to multiplication $(\mathcal{L}_1\mathcal{L}_2)A = \mathcal{L}_1(\mathcal{L}_2 A)$ for all $A \in \mathcal{M}$ and $\mathcal{L}_1, \mathcal{L}_2 \in \mathcal{P}(\mathcal{M})$. Moreover, $\mathcal{P}(\mathcal{M})$ is a Lie–Jordan algebra with respect to the multiplications

$$\mathcal{L}_1 \cdot \mathcal{L}_2 = \mathcal{L}_1\mathcal{L}_2 - \mathcal{L}_2\mathcal{L}_1, \qquad \mathcal{L}_1 \circ \mathcal{L}_2 = \mathcal{L}_1\mathcal{L}_2 + \mathcal{L}_2\mathcal{L}_1. \tag{18}$$

The following statement follows immediately from the theorems.

STATEMENT. *Any element $\mathcal{L}$ of the multiplication algebra $\mathcal{P}(\mathcal{M}_c)$ of the Lie–Jordan algebra $\mathcal{M}_c$ can be written as a polynomial $\mathcal{L}[L^{\pm}_{q_k}, L^{\pm}_{p_k}, L^{\pm}_{1}]$ in the operators $\{L^{\pm}_{q_k}, L^{\pm}_{p_k}, L^{\pm}_{1}\}$.*

There is analogous statement for quantum observables.

STATEMENT. *Any element $\mathcal{L}$ of the multiplication algebra $\mathcal{P}(\mathcal{M}_q)$ of the Lie–Jordan algebra $\mathcal{M}_q$ can be written as a polynomial $\mathcal{L}[L^{\pm}_{Q_k}, L^{\pm}_{P_k}, L^{\pm}_I]$ in the superoperators $\{L^{\pm}_{Q_k}, L^{\pm}_{P_k}, L^{\pm}_I\}$.*

These statements allow us to formulate the Weyl quantization of classical equations of motion as a map from $\mathcal{P}(\mathcal{M}_c)$ into $\mathcal{P}(\mathcal{M}_q)$.

Weyl quantization

The correspondence between operators $\hat{A} = A(Q, P)$ and symbols $A(q, p)$ is completely defined by the formulas that express the symbols of operators $Q_k\hat{A}$, $\hat{A}Q_k$, $P_k\hat{A}$, $\hat{A}P_k$ in terms of the symbols of the operator $\hat{A}$. Weyl quantization π_W is said to be defined if these formulas have the form

$$\pi_W\left(\left(q_k + \frac{i\hbar}{2}\frac{\partial}{\partial p_k}\right)A(q, p)\right) = Q_k\hat{A}, \tag{19}$$

$$\pi_W\left(\left(q_k - \frac{i\hbar}{2}\frac{\partial}{\partial p_k}\right)A(q, p)\right) = \hat{A}Q_k, \tag{20}$$

$$\pi_W\left(\left(p_k - \frac{i\hbar}{2}\frac{\partial}{\partial q_k}\right)A(q, p)\right) = P_k\hat{A}, \tag{21}$$

$$\pi_W\left(\left(p_k + \frac{i\hbar}{2}\frac{\partial}{\partial q_k}\right)A(q, p)\right) = \hat{A}P_k \tag{22}$$

for any $\hat{A} = \pi_W(A(q, p))$.

These formulas can be rewritten in the form

$$\begin{aligned}
&\pi_W\left(\frac{\partial}{\partial q_k}A(q, p)\right) = -\frac{1}{i\hbar}\big(P_k\hat{A} - \hat{A}P_k\big),\\
&\pi_W\left(\frac{\partial}{\partial p_k}A(q, p)\right) = \frac{1}{i\hbar}\big(Q_k\hat{A} - \hat{A}Q_k\big),\\
&\pi_W\big(q_kA(q, p)\big) = \frac{1}{2}\big(Q_k\hat{A} + \hat{A}Q_k\big),\\
&\pi_W\big(p_kA(q, p)\big) = \frac{1}{2}\big(P_k\hat{A} + \hat{A}P_k\big).
\end{aligned} \tag{23}$$

Equations (3) imply that the operators L^-_A and L^+_A acting on classical observables are defined by the formulas

$$\begin{aligned}
&L^-_AB(q, p) = \big\{A(q, p), B(q, p)\big\},\\
&L^+_AB(q, p) = A(q, p)B(q, p).
\end{aligned} \tag{24}$$

By virtue of definition (5), the superoperators L_A^- and L_A^+ are expressed as

$$L_Q^-\hat{A} = \frac{1}{i\hbar}\big(Q\hat{A} - \hat{A}Q\big), \qquad L_P^-\hat{A} = \frac{1}{i\hbar}\big(P\hat{A} - \hat{A}P\big),$$
$$L_Q^+\hat{A} = \frac{1}{2}\big(Q\hat{A} + \hat{A}Q\big), \qquad L_P^+\hat{A} = \frac{1}{2}\big(P\hat{A} + \hat{A}P\big).$$

Using $L_q^\pm$, $L_p^\pm$ and $L_Q^\pm$, $L_P^\pm$, we rewrite formulas (23) in the form

$$\pi_W\big(L_{q_k}^\pm A\big) = L_{Q_k}^\pm \hat{A}, \qquad \pi_W\big(L_{p_k}^\pm A\big) = L_{P_k}^\pm \hat{A}.$$

Since these relations are valid for all $\hat{A} = \pi_W(A)$, we can define the Weyl quantization of the operators $L_{q_k}^\pm$ and $L_{p_k}^\pm$ in the following manner:

$$\pi_W\big(L_{q_k}^\pm\big) = L_{Q_k}^\pm, \qquad \pi_W\big(L_{p_k}^\pm\big) = L_{P_k}^\pm. \tag{25}$$

These relations define the Weyl quantization of the generators of the multiplication algebra $\mathcal{P}(\mathcal{M}_c)$, where $\mathcal{M}_c$ is a Lie–Jordan algebra of classical observables.

From definition (24) for classical observables, we obtain

$$L_{q_k}^+ A(q, p) = q_k A(q, p), \qquad L_{p_k}^+ A(q, p) = p_k A(q, p), \tag{26}$$

and

$$L_{q_k}^- A(q, p) = \frac{\partial A(q, p)}{\partial p_k}, \qquad L_{p_k}^- A(q, p) = -\frac{\partial A(q, p)}{\partial q_k}. \tag{27}$$

The operators (26) and (27) allow us to consider a linear polynomial differentiation operator as an element of the multiplication algebra $\mathcal{P}(\mathcal{M}_c)$. As a result, we have the following theorem.

THEOREM. *The linear polynomial differentiation operator $\mathcal{L}(q, p, \partial_q, \partial_p)$, acting on the classical observables $A(q, p) \in \mathcal{M}_c$ is an element of the multiplication algebra $\mathcal{P}(\mathcal{M}_c)$, and*

$$\mathcal{L}\left(q, p, \frac{\partial}{\partial q}, \frac{\partial}{\partial p}\right) = \mathcal{L}\big[L_q^+, L_p^+, -L_p^-, L_q^-\big].$$

The proof evidently follows from the definition of the operators $L_{q_k}^\pm$ and $L_{p_k}^\pm$ specified in (26) and (27).

COROLLARY. *A classical observable $A(q, p) \in \mathcal{M}_c$ can be represented as an element $A(L_q^+, L_p^+)$ of $\mathcal{P}(\mathcal{M}_c)$.*

By virtue of (25) and commutation relations (16), (17), the Weyl quantization π_W associates the differential operator $\mathcal{L}(q, p, \partial_q, \partial_p)$ on the function space and

the operator $\mathcal{L}[L_Q^+, L_P^+, -L_P^-, L_Q^-]$, acting on the operator space. Thus, the Weyl quantization of differential equation (1) with polynomial operators is defined by the formula

$$\pi_W\left(\mathcal{L}\left(q, p, \frac{\partial}{\partial q}, \frac{\partial}{\partial p}\right)\right) = \mathcal{L}\big[L_Q^+, L_P^+, -L_P^-, L_Q^-\big]. \tag{28}$$

Since the commutation relations for the operators $L_{q_k}^{\pm}$, $L_{p_k}^{\pm}$ and the superoperators $L_{Q_k}^{\pm}$, $L_{P_k}^{\pm}$ coincide, the following theorem takes place.

THEOREM. *In the Weyl quantization, ordering of generators $L_Q^{\pm}$, $L_P^{\pm}$ in the superoperator $\mathcal{L}[L_Q^+, L_P^+, -L_P^-, L_Q^-]$ is uniquely determined by ordering of $L_q^{\pm}$, $L_p^{\pm}$ in the operator $\mathcal{L}[L_q^+, L_p^+, -L_p^-, L_q^-]$.*

As a result, the quantization of equations of motion and differential operators is a rule that assigns to each element $\mathcal{L}(q, p, \partial_q, \partial_p)$ of $\mathcal{P}(\mathcal{M}_c)$ exactly one element (superoperator) $\mathcal{L}[L_Q^+, L_P^+, -L_P^-, L_Q^-]$ of $\mathcal{P}(\mathcal{M}_q)$. If we use the Weyl quantization for classical observables, then it is reasonable to use the Weyl quantization of differential operators.

It can be easy verified that in this way we obtain the one-to-one correspondence between the polynomial operators and $\mathcal{L}(q, p, \partial_q, \partial_p)$ and the superoperator $\mathcal{L}[L_Q^+, L_P^+, -L_P^-, L_Q^-]$ on $\mathcal{M}_q$. We can extend this correspondence to differential operators (and superoperators) of a more general form. Let $L(x, y)$ be a Weyl symbol of operator $\mathcal{L}(q, p, \partial_q, \partial_p)$, i.e.,

$$\mathcal{L}\big[L_q^{\pm}, L_p^{\pm}\big] = \frac{1}{(2\pi\hbar)^{2n}} \int da_+\, da_-\, db_+\, db_-\, \tilde{L}(a, b) W_c(a, b),$$

where

$$W_c(a, b) = \exp\frac{i}{\hbar}\big(a_{\pm}L_q^{\pm} + b_{\pm}L_p^{\pm}\big) \quad \big(a_{\pm}, b_{\pm} \in \mathbb{R}^n\big).$$

Here $\tilde{L}(a, b)$ is a Fourier transform of $L(x, y)$:

$$L\big(x^{\pm}, y^{\pm}\big) = \frac{1}{(2\pi\hbar)^{2n}} \int da_+\, da_-\, db_+\, db_-\, \tilde{L}(a, b) \exp\frac{-i}{\hbar}\big(a_{\pm}x^{\pm} + b_{\pm}y^{\pm}\big).$$

Then the superoperator $\mathcal{L}[L_Q^{\pm}, L_P^{\pm}]$ will be defined by

$$\mathcal{L}\big[L_q^{\pm}, L_p^{\pm}\big] = \frac{1}{(2\pi\hbar)^{2n}} \int da_+\, da_-\, db_+\, db_-\, \tilde{L}(a, b) W_q(a, b),$$

where

$$W_q(a, b) = \exp\frac{i}{\hbar}\big(a_{\pm}L_Q^{\pm} + b_{\pm}L_P^{\pm}\big).$$

17.3. Quantization of Lorenz-type systems

Consider an evolution equation for classical observable $A_t(q, p)$ for a classical dissipative Lorenz-type system of the form

$$\frac{d}{dt}A_t(q,p) = (-\sigma q_1 + \sigma p_1)\frac{\partial A_t(q,p)}{\partial q_1} + (rq_1 - p_1 - q_1 p_2)\frac{\partial A_t(q,p)}{\partial p_1} + (\sigma p_2)\frac{\partial A_t(q,p)}{\partial q_2} + (-bp_2 + q_1 p_1)\frac{\partial A_t(q,p)}{\partial p_2}. \tag{29}$$

This equation written for the observables $x = q_1$, $y = p_1$ and $z = p_2$, describes the dissipative Lorenz model

$$x' = -\sigma x + \sigma y, \qquad y' = rx - y - xz, \qquad z' = -bz + xy,$$

where $x' = dx(t)/dt$. This model was proposed by E.N. Lorenz in [100], and it is the most known classical dissipative system with a strange attractor. This system demonstrates a chaotic behavior when parameters are chosen to be closed to the value $\sigma = 10$, $r = 28$, $b = 8/3$.

The differential operator $\mathcal{L}$ for system (29) has the form

$$\mathcal{L}(q,p,\partial_q,\partial_p) = (-\sigma q_1 + \sigma p_1)\frac{\partial}{\partial q_1} + (rq_1 - p_1 - q_1 p_2)\frac{\partial}{\partial p_1} + (\sigma p_2)\frac{\partial}{\partial q_2} + (-bp_2 + q_1 p_1)\frac{\partial}{\partial p_2}. \tag{30}$$

Rewriting this operator in terms of $L^{\pm}_{q^k}$ and $L^{\pm}_{p^k}$, we obtain

$$\begin{aligned}\mathcal{L}\big[L^+_q, L^+_p, -L^-_p, L^-_q\big] &= -\big(-\sigma L^+_{q_1} + \sigma L^+_{p_1}\big)L^-_{p_1} + \big(rL^+_{q_1} - L^+_{p_1} - L^+_{q_1}L^+_{p_2}\big)L^-_{q_1} \\ &\quad - \big(\sigma L^+_{p_2}\big)L^-_{p_2} + \big(-bL^+_{p_2} + L^+_{q_1}L^+_{p_1}\big)L^-_{q_2}.\end{aligned}$$

The Weyl quantization of this operator gives the superoperator

$$\begin{aligned}\mathcal{L}\big[L^+_Q, L^+_P, -L^-_P, L^-_Q\big] &= -\big(-\sigma L^+_{Q_1} + \sigma L^+_{P_1}\big)L^-_{P_1} + \big(rL^+_{Q_1} - L^+_{P_1} - L^+_{Q_1}L^+_{P_2}\big)L^-_{Q_1} \\ &\quad - \big(\sigma L^+_{P_2}\big)L^-_{P_2} + \big(-bL^+_{P_2} + L^+_{Q_1}L^+_{P_1}\big)L^-_{Q_2}.\end{aligned}$$

Using the definition of the operators L^+_A, L^-_A, we obtain the quantum Lorenz-type equation [161–163]:

$$\frac{d}{dt}\hat{A}_t = \frac{i}{\hbar}\left[\frac{\sigma(P_1^2 + P_2^2)}{2} - \frac{rQ_1^2}{2}, \hat{A}_t\right] - \frac{i\sigma}{\hbar}Q_1 \circ \big[P_1, \hat{A}_t\big] + \frac{i}{\hbar}P_1 \circ \big[Q_1, \hat{A}_t\big] + \frac{i}{\hbar}bP_2 \circ \big[Q_2, \hat{A}_t\big]$$

$$+\frac{i}{\hbar}Q_1\circ\big(P_2\circ\big[Q_1,\hat{A}_t\big]\big)-\frac{i}{\hbar}Q_1\circ\big(P_1\circ\big[Q_2,\hat{A}_t\big]\big).$$

We notice that the Weyl quantization leads just to the following form of the last two terms: $Q_k\circ(P_l\circ[Q_m,\hat{A}])$, each of which is equal to $P_l\circ(Q_k\circ[Q_m,\hat{A}])$. However, they are not equal to $(Q_k\circ P_l)\circ[Q_m,\hat{A}]$, which follows from (11).

17.4. Quantization of Poisson bracket

Quantization and isomorphism of Lie–Jordan algebras

Let us consider a linear map π from $<\mathcal{P}_c,\circ,\{\ ,\ \}>$ into $<\mathcal{P}_q,\circ,\cdot>$ such that

$$\pi\big(\{A,B\}\big)=\frac{1}{i\hbar}\big[\pi(A),\pi(B)\big],\qquad \pi(A\circ B)=\pi(A)\circ\pi(B)$$

for all $A,B\in\mathcal{P}_c$. This map provides a possible canonical quantization procedure for classical systems. Such a map π defines a homomorphism of the Lie–Jordan algebra $<\mathcal{P}_c,\circ,\{\ ,\ \}>$ into the algebra $<\mathcal{P}_q,\circ,\cdot>$. The algebras are isomorphic if and only if the map π is a one-to-one mapping. To show that π is one-to-one, you show that $\pi(A)=\pi(B)$ implies $A=B$. An isomorphism maps the identity onto the identity. Therefore, the condition $\pi(1)=I$ can be used.

However, if two Lie algebras are isomorphic then so are their derivation algebras. And if one Lie algebra has outer derivations and the other not, then they cannot be isomorphic. We see that π *cannot form an isomorphism* of the Lie–Jordan algebra $\mathcal{P}_c$ and the Lie–Jordan algebra $\mathcal{P}_q$, since one algebra admits outer derivations while the other does not.

STATEMENT. *The quantization map π is not an isomorphism of the Lie–Jordan algebra $\mathcal{P}_c$ and the Lie–Jordan algebra $\mathcal{P}_q$.*

Let us give the basic definitions and theorems regarding this statement.

Suppose $\mathcal{P}_c$ is a set of all complex polynomials in the real variables q_k and p_k, $k=1,\dots,n$. This set forms a Lie–Jordan algebra $<\mathcal{P}_c,\circ,\{\ ,\ \}>$ under the Poisson bracket and the pointwise multiplication $\circ$.

DEFINITION. A *derivation of a Lie–Jordan algebra* $<\mathcal{P}_c,\circ,\{\ ,\ \}>$ is a linear operator $\mathcal{L}$ on $\mathcal{P}_c$ satisfying the equation

$$\mathcal{L}\big(\{A,B\}\big)=\big\{\mathcal{L}(A),B\big\}+\big\{A,\mathcal{L}(B)\big\},$$
$$\mathcal{L}(A\circ B)=\mathcal{L}(A)\circ B+A\circ\mathcal{L}(B)$$

for all A, B in $\mathcal{P}_c$. A derivation $\mathcal{L}$ is said to be *inner* if there exists $H \in \mathcal{P}_c$ such that

$$\mathcal{L}(A) = \{H, A\}$$

for all $A \in \mathcal{P}_c$. It is said to be *outer* if it is not of this form.

The set of all derivations $Der(\mathcal{P}_c)$ of $\mathcal{P}_c$ forms a Lie–Jordan algebra under the multiplications (18). We can give the basic theorem regarding derivations of this Lie–Jordan algebra.

THEOREM *(Wollenberg). Every derivation $\mathcal{L}$ of $\mathcal{P}_c$ is of the form*

$$\mathcal{L}A = \{H, A\} + b\left(A - \sum_{k=1}^{n} a_k p_k \circ \{q_k, A\} + \sum_{k=1}^{n}(1 - a_k) q_k \circ \{p_k, A\}\right),$$

where A in $\mathcal{P}$, and a_k, b in $\mathbb{C}$.

As a result, an arbitrary derivation of $\mathcal{P}_c$ is a linear combination of an inner derivation $\{H, \cdot\}$ and an explicitly determined outer derivation

$$\mathcal{L}_{outer} = L_1^+ - \sum_{k=1}^{n} a_k L_{p_k}^+ L_{q_k}^- + \sum_{k=1}^{n}(1 - a_k) L_{q_k}^+ L_{p_k}^-.$$

As a result, the Lie–Jordan algebra $\mathcal{P}_c$ admits outer derivations. Note that

$$\pi(\mathcal{L}_{outer}) = L_I^+ - \sum_{k=1}^{n} a_k L_{P_k}^+ L_{Q_k}^- + \sum_{k=1}^{n}(1 - a_k) L_{Q_k}^+ L_{P_k}^-,$$

but $\pi(\{H, A\}) \neq (1/i\hbar)[\pi(H), \pi(A)]$.

Consider now an associative algebra $\mathcal{P}_q$ over $\mathbb{C}$ generated by finite linear combinations and finite powers of elements Q, P where $QP - PQ = i\hbar I$. Then $\mathcal{P}_q$ is a Lie–Jordan algebra with respect to the commutator $A \cdot B = (1/i\hbar)[A, B]$ and anticommutator $A \circ B = (1/2)(AB + BA)$ for A, B in $\mathcal{P}_q$.

DEFINITION. A *derivation of a Lie–Jordan algebra* $<\mathcal{P}_q, \circ, \cdot>$ is a linear operator $\mathcal{L}$ on $\mathcal{P}_q$ satisfying

$$\mathcal{L}(A \cdot B) = (\mathcal{L}A) \cdot B + A \cdot (\mathcal{L}B),$$

$$\mathcal{L}(A \circ B) = \mathcal{L}(A) \circ B + A \circ \mathcal{L}(B)$$

for all A, B in $\mathcal{P}_q$. A derivation $\mathcal{L}$ is said to be *inner* if there exists an $H \in \mathcal{P}_q$ such that

$$\mathcal{L}(A) = H \cdot A = \frac{1}{i\hbar}[H, A]$$

for all $A \in \mathcal{P}_q$. It is said to be *outer* if it is not of this form.

We can give the basic theorem regarding derivations of this algebra.

THEOREM. *Each derivation of the Lie–Jordan algebra $\mathcal{P}_q$ is inner.*

As a result, the Lie–Jordan algebra $\mathcal{P}_q$ does not admit outer derivations.

Weyl quantization of Poisson bracket and commutator

The following statement is well known.

STATEMENT. *If π is a Weyl quantization, then the inequality*

$$\pi\big(\{A, B\}\big) \neq \frac{1}{i\hbar}\big[\pi(A), \pi(B)\big]$$

is valid for a wide class of smooth square-integrable functions $A(q, p)$ and $B(q, p)$.

As a result, the Weyl quantization π is not a map that assigns to a Poisson bracket exactly one commutator. The same is true for the inverse operation.

The Weyl symbol of the commutator $[A, B]$ has the form

$$\big([A, B]\big)_W(p, q) = -2i\, A_W(p, q)\left(\sin\frac{\hbar\mathcal{P}}{2}\right)B_W(p, q).$$

Here $\mathcal{P}$ is the operator

$$\mathcal{P} = \overleftarrow{\partial_p}\overrightarrow{\partial_q} - \overleftarrow{\partial_q}\overrightarrow{\partial_p} = \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q} - \frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p},$$

such that $A_W\mathcal{P}B_W = -\{A_W, B_W\}$.

Weyl quantization can not be considered as a map of a Poisson bracket into a commutator. Therefore, it is interesting to obtain a quantum analog of Poisson bracket on $\mathbb{R}^{2n}$.

A classical observable is a function on $\mathbb{R}^{2n}$. We shall denote the linear space of all smooth functions on $\mathbb{R}^{2n}$ by $C^\infty(\mathbb{R}^{2n})$. We say that $\mathbb{R}^{2n}$ is endowed with a Poisson structure if we are given an operation assigning to every pair of functions $A, B \in C^\infty(\mathbb{R}^{2n})$ a new function $\{A, B\} \in C^\infty(\mathbb{R}^{2n})$, which is linear in A and B and satisfies the following conditions:

(1) the skew-symmetry, $\{A, B\} = -\{B, A\}$,
(2) the Jacobi identity, $\{\{A, B\}, C\} + \{\{B, C\}, A\} + \{\{C, A\}, B\} = 0$,
(3) the Leibnitz rule, $\{A, BC\} = \{A, B\}C + B\{A, C\}$.

Requirements (1) and (2) are the axioms of a Lie algebra. In this way, the space $C^\infty(\mathbb{R}^{2n})$, together with the Poisson bracket becomes a Lie algebra. We can define

the Jordan multiplication

$$A \circ B = A(x)B(x),$$

where AB is the usual pointwise multiplication. Then requirement (3) expresses that the Lie operation $\{\ ,\ \}$ is connected with the Jordan multiplication. As a result, we define two bilinear multiplications on $C^\infty(\mathbb{R}^{2n})$ denoted by symbols $\{\ ,\ \}$ and $\circ$. In this case, the Lie–Jordan algebra $<C^\infty(\mathbb{R}^{2n}), \circ, \{\ ,\ \}>$ on $C^\infty(\mathbb{R}^{2n})$ is said to be defined.

In local coordinates $(q, p) = (q_1, \ldots, q_n, p_1, \ldots, p_n)$, the expression

$$\{A, B\} = \sum_{k=1}^{n}\left(\frac{\partial A}{\partial q_k}\frac{\partial B}{\partial p_k} - \frac{\partial A}{\partial p_k}\frac{\partial B}{\partial q_k}\right) \tag{31}$$

determines the standard Poisson bracket for $A, B \in C^\infty(\mathbb{R}^{2m})$.

In order to derive a quantum analog of this bracket, we should rewrite equation (31) by using the multiplication operators $L^{\pm}_{q_k}$ and $L^{\pm}_{p_k}$. To realize this representation, we consider the following equivalent form of (31). Using the relations

$$\frac{\partial A}{\partial q_k}\frac{\partial B}{\partial p_k} = \frac{\partial}{\partial q_k}\left(A\frac{\partial B}{\partial p_k}\right) - A\frac{\partial}{\partial q_k}\frac{\partial B}{\partial p_k},$$
$$\frac{\partial A}{\partial p_k}\frac{\partial B}{\partial q_k} = \frac{\partial}{\partial p_k}\left(A\frac{\partial B}{\partial q_k}\right) - A\frac{\partial}{\partial p_k}\frac{\partial B}{\partial q_k},$$

we obtain

$$\{A, B\} = \sum_{k=1}^{n}\left(\frac{\partial}{\partial q_k}\left(A\frac{\partial}{\partial p_k}B\right) - \frac{\partial}{\partial p_k}\left(A\frac{\partial}{\partial q_k}B\right)\right)$$
$$- \sum_{k=1}^{n} A\left(\frac{\partial}{\partial q_k}\frac{\partial}{\partial p_k} - \frac{\partial}{\partial p_k}\frac{\partial}{\partial q_k}\right)B. \tag{32}$$

If $B = B(q, p)$ is a smooth function, then

$$\frac{\partial}{\partial q_k}\frac{\partial B}{\partial p_k} - \frac{\partial}{\partial p_k}\frac{\partial B}{\partial q_k} = 0 \quad (k = 1, \ldots, n)$$

and the Poisson bracket can be defined by

$$\{A, B\} = \sum_{k=1}^{n}\left(\frac{\partial}{\partial q_k}\left(A\frac{\partial}{\partial p_k}B\right) - \frac{\partial}{\partial p_k}\left(A\frac{\partial}{\partial q_k}B\right)\right). \tag{33}$$

Let us consider the operator L^+_A such that

$$L^+_{A(q,p)}B(q, p) = A(q, p) \circ B(q, p) = A(q, p)B(q, p)$$

for all A, B in $C^\infty(\mathbb{R}^{2n})$. It is not hard to prove the following theorem.

THEOREM. *Let $A(q, p)$ be an element of $C^\infty(\mathbb{R}^{2n})$. Then every operator $L^+_{A(q,p)}$ on $C^\infty(\mathbb{R}^{2n})$ is of the form*

$$L^+_{A(q,p)} = A\big(L^+_q, L^+_p\big). \tag{34}$$

This theorem is proved by using the equation

$$L^+_{A\circ B} = L^+_A L^+_B - \frac{\hbar}{4} L^-_B L^-_A \tag{35}$$

with $\hbar = 0$.

The following corollary follows immediately from this theorem.

COROLLARY. *Every pointwise multiplication $C^\infty(\mathbb{R}^{2n})$ is of the form*

$$A(q, p)B(q, p) = A\big(L^+_q, L^+_p\big)B(q, p) \tag{36}$$

for all $A, B \in C^\infty(\mathbb{R}^{2n})$.

PROOF. Using the theorem, we have

$$A(q, p)B(q, p) = L^+_{A(q,p)}B(q, p) = A\big(L^+_q, L^+_p\big)B(q, p). \qquad \square$$

As a result, we obtain the following important statement.

STATEMENT. *Let $A(q, p)$ be an element of $C^\infty(\mathbb{R}^{2n})$. Then $A(q, p)$ can be represented in the form*

$$A(q, p) = A\big(L^+_q, L^+_p\big)1. \tag{37}$$

PROOF. If $B(q, p) = 1$, then (36) gives (37). $\square$

Substitution of equation (37) in the form

$$B(q, p) = B\big(L^+_q, L^+_p\big)1$$

into equation (36) gives

$$A(q, p)B(q, p) = A\big(L^+_q, L^+_p\big)B\big(L^+_q, L^+_p\big)1. \tag{38}$$

As a result, the pointwise multiplication of $A, B \in C^\infty(\mathbb{R}^{2n})$ is represented as a multiplication of operators $A(L^+_q, L^+_p)$ and $B(L^+_q, L^+_p)$.

In quantum mechanics, a quantum analog of equation (37) is valid in the form

$$A(Q, P) = A\big(L^+_Q, L^+_P\big)I,$$

where $A(Q, P)$ is a Weyl-ordered operator. Let us consider a quantum analog of (38). In general, we have

$$A(Q, P)B(Q, P) \neq A\big(L_Q^+, L_P^+\big)B\big(L_Q^+, L_P^+\big)I$$

for usual multiplication AB of operators. Therefore we define the following new multiplicative binary operation for a set of operators. The multiplication $*$ defined by the formula

$$A(Q, P) * B(Q, P) = A\big(L_Q^+, L_P^+\big)B\big(L_Q^+, L_P^+\big)I$$

is called the *Weyl product*. This binary operation assigns to the Weyl-ordered operators $A(Q, P)$ and $B(Q, P)$ exactly one Weyl-ordered operator.

Equation (33) has differential operators. The operators L_q^- and L_p^- are first order differential operators such that

$$L_{q_k}^- B(q, p) = \{q_k, B\} = \frac{\partial B}{\partial p_k}, \qquad L_{p_k}^- B(q, p) = \{p_k, B\} = -\frac{\partial B}{\partial p_k}.$$

Let us give the basic theorem regarding Poisson bracket.

THEOREM. *Let $A(q, p)$ be an element of $C^\infty(\mathbb{R}^{2n})$. Then every operator $L_{A(q,p)}^-$ on $C^\infty(\mathbb{R}^{2n})$ is of the form*

$$L_{A(q,p)}^- = \sum_{k=1}^{n}\big(L_{q_k}^- A\big(L_q^+, L_p^+\big)L_{p_k}^- - L_{p_k}^- A\big(L_q^+, L_p^+\big)L_{q_k}^-\big). \tag{39}$$

PROOF. Using (36) and the operators L_q^- and L_p^-, we obtain the relations

$$A(q, p)\frac{\partial}{\partial p_k}B(q, p) = A\big(L_q^+, L_p^+\big)L_{q_k}^- B(q, p), \tag{40}$$

$$A(q, p)\frac{\partial}{\partial q_k}B(q, p) = -A\big(L_q^+, L_p^+\big)L_{p_k}^- B(q, p). \tag{41}$$

Substitution of (40) and (41) into (33) gives

$$\begin{aligned}\{A, B\} = \sum_{k=1}^{n}\big(&-L_{p_k}^- A\big(L_q^+, L_p^+\big)L_{q_k}^- B(q, p)\\ &+ L_{q_k}^- A\big(L_q^+, L_p^+\big)L_{p_k}^- B(q, p)\big).\end{aligned} \tag{42}$$

The Poisson brackets can be presented in the form

$$\{A, B\} = L_{A(q,p)}^- B(q, p). \tag{43}$$

As a result, equations (42) and (43) give (39). □

We can present the Poisson bracket by the equation

$$\{A, B\} = L^-_{A(q,p)} L^+_{B(q,p)} 1,$$

where $L^-_{A(q,p)}$ is determined by (39) and $L^+_{B(q,p)}$ by equation (34). As a result, we obtain the following theorem.

THEOREM. *Let $A(q, p)$ and $B(q, p)$ be elements of $C^\infty(\mathbb{R}^{2n})$. Then each Poisson bracket $\{A(q, p), B(q, p)\}$ on $C^\infty(\mathbb{R}^{2n})$ is of the form*

$$L^-_{A(q,p)} L^+_{B(q,p)} 1 = \sum_{k=1}^{n} \big(L^-_{q_k} A\big(L^+_q, L^+_p\big) L^-_{p_k} B\big(L^+_q, L^+_p\big) - L^-_{p_k} A\big(L^+_q, L^+_p\big) L^-_{q_k} B\big(L^+_q, L^+_p\big)\big) 1.$$

The Weyl quantization is realized by the rules

$$\pi_W\big(L^\pm_{q_k}\big) = L^\pm_{Q_k}, \qquad \pi_W\big(L^\pm_{p_k}\big) = L^\pm_{P_k},$$
$$\pi_W\big(\mathcal{L}\big[L^\pm_q, L^\pm_p\big]\big) = \mathcal{L}\big[L^\pm_Q, L^\pm_P\big],$$

where $\hat{A} = \pi_W(A)$, $\pi_W(1) = I$, and

$$L^-_Q \hat{A} = \frac{1}{i\hbar}\big[Q, \hat{A}\big] = \frac{1}{i\hbar}\big(Q\hat{A} - \hat{A}Q\big), \qquad L^+_Q \hat{A} = \frac{1}{2}\big(Q\hat{A} + \hat{A}Q\big).$$

As a result, the Weyl quantization maps the Poisson bracket into the relation

$$\pi_W\big(\{A(q, p), B(q, p)\}\big) = \sum_{k=1}^{n} \big(L^-_{Q_k} A\big(L^+_Q, L^+_P\big) L^-_{P_k} B\big(L^+_Q, L^+_P\big) - L^-_{P_k} A\big(L^+_Q, L^+_P\big) L^-_{Q_k} B\big(L^+_q, L^+_P\big)\big) I. \tag{44}$$

This is the quantum analog of the Poisson bracket.

In the general case, the right hand side of equation (44) cannot be presented as a commutator, and

$$\pi\big(\{A(q, p), B(q, p)\}\big) = \pi\big(L^-_{A(q,p)} B(q, p)\big) \neq L^-_{A(Q,P)} B(Q, P),$$

where $A(Q, P) = \pi_W(A(q, p))$ and $B(Q, P) = \pi_W(B(q, p))$, since $\hbar \neq 0$ in relation (35).

17.5. Discontinuous functions and nonassociative operators

For discontinuous functions $B(q, p)$ such that

$$\frac{\partial}{\partial q_k}\frac{\partial B(q, p)}{\partial p_k} \neq \frac{\partial}{\partial p_k}\frac{\partial B(q, p)}{\partial q_k}, \tag{45}$$

we should take into account the second sum of (32). Using

$$\left(\frac{\partial}{\partial q_k}\frac{\partial}{\partial p_k} - \frac{\partial}{\partial p_k}\frac{\partial}{\partial q_k}\right)B(q,p) = -\big(L^-_{p_k}L^-_{q_k} - L^-_{q_k}L^-_{p_k}\big)B(q,p),$$

inequality (45) can be presented in the form

$$\big(L^-_{p_k}L^-_{q_k} - L^-_{q_k}L^-_{p_k}\big)B(q,p) \neq 0. \tag{46}$$

In this case, the Poisson bracket (32) is defined by the equation

$$\{A,B\} = L^-_{A(q,p)}B(q,p),$$

where

$$\begin{aligned} L^-_{A(q,p)} = \{A,\cdot\} = \sum_{k=1}^{n}\big(L^-_{q_k}A\big(L^+_q,L^+_p\big)L^-_{p_k} - L^-_{p_k}A\big(L^+_q,L^+_p\big)L^-_{q_k}\big) \\ + \sum_{k=1}^{n}A\big(L^+_q,L^+_p\big)\big(L^-_{p_k}L^-_{q_k} - L^-_{q_k}L^-_{p_k}\big). \end{aligned} \tag{47}$$

Let $B(q,p)$ be a discontinuous function on $\mathbb{R}^{2n}$. If $\hat{B} = B(Q,P)$ is an operator that corresponds to $B(q,p)$, then the Weyl quantization of inequality (46) gives

$$\big(L^-_{P_k}L^-_{Q_k} - L^-_{Q_k}L^-_{P_k}\big)B(Q,P) \neq 0. \tag{48}$$

This relation can be represented through associators.

THEOREM. *Let $B(q,p)$ be a discontinuous function on $\mathbb{R}^{2n}$, and let $\hat{B} = B(Q,P)$ be an operator that corresponds to $B(q,p)$. Then the inequality*

$$-\big(P,Q,\hat{B}\big) + \big(P,\hat{B},Q\big) - \big(Q,\hat{B},P\big) + \big(Q,P,\hat{B}\big) \neq 0$$

should be valid for the operator $\hat{B}$.

PROOF.

$$\begin{aligned} \big(L^-_{P_k}L^-_{Q_k} - L^-_{Q_k}L^-_{P_k}\big)\hat{B} &= -\frac{1}{\hbar^2}\big(\big[P,\big[Q,\hat{B}\big]\big] - \big[Q,\big[P,\hat{B}\big]\big]\big) \\ &= -\frac{1}{\hbar^2}\big(P\big(Q\hat{B}\big) - P\big(\hat{B}Q\big) - \big(Q\hat{B}\big)P + \big(\hat{B}Q\big)P \\ &\quad - Q\big(P\hat{B}\big) + Q\big(\hat{B}P\big) + \big(P\hat{B}\big)Q - \big(\hat{B}P\big)Q\big) \\ &= -\frac{1}{\hbar^2}\big(-\big(P,Q,\hat{B}\big) + \big(P,\hat{B},Q\big) - \big(Q,\hat{B},P\big) \\ &\quad + \big(Q,P,\hat{B}\big)\big). \end{aligned}$$

□

If $\hat{B}$ is an associative operator, then

$$-\big(P, Q, \hat{B}\big) + \big(P, \hat{B}, Q\big) - \big(Q, \hat{B}, P\big) + \big(Q, P, \hat{B}\big) = 0,$$

and

$$\big(L^{-}_{P_k} L^{-}_{Q_k} - L^{-}_{Q_k} L^{-}_{P_k}\big)\hat{B} = 0.$$

As a result, we obtain that an associative operator cannot describe a discontinuous function. Then the quantization should be a rule that assigns to each discontinuous function exactly one nonassociative operator. A consistent formulation of the rule is an open question. We illustrate this problem by the following remarks. It is well known that the function

$$B(q, p) = \begin{cases} \frac{q^2-p^2}{q^2+p^2}, & q^2 + p^2 \neq 0, \\ 0, & q^2 + p^2 = 0 \end{cases}$$

has the following derivatives at $(q, p) = (0, 0)$:

$$\frac{\partial}{\partial q_k}\frac{\partial B(q, p)}{\partial p_k} = 1, \qquad \frac{\partial}{\partial p_k}\frac{\partial B(q, p)}{\partial q_k} = -1.$$

Let $\hat{B} = B(Q, P)$ be an operator that corresponds to this function. In the matrix representation, the operator $\hat{B}$ is described by the matrix

$$b_{kl} = <k|\hat{B}|l>.$$

In the general case, the multiplication of infinite matrices is not associative

$$(AB)C \neq A(BC),$$

or

$$\sum_{l=1}^{\infty}\left(\sum_{k=1}^{\infty} a_{ik}b_{kl}\right)c_{lj} \neq \sum_{k=1}^{\infty} a_{ik}\left(\sum_{l=1}^{\infty} b_{kl}c_{lj}\right). \tag{49}$$

This can be easy demonstrated by the following example. If $a_{kl} = c_{kl} = 1$ for all k and l, then inequality (49) gives

$$\sum_{l=1}^{\infty}\left(\sum_{k=1}^{\infty} b_{kl}\right) \neq \sum_{k=1}^{\infty}\left(\sum_{l=1}^{\infty} b_{kl}\right).$$

As an example of a matrix satisfying this condition, we can take

$$b_{kl} = \begin{cases} \frac{(k-l)}{2^{k+l-2}}\frac{(k+l-3)!}{(k-1)(l-1)}, & k, l > 1, \\ 2^{-(k-1)}, & k > 1,\ l = 1, \\ -2^{-(l-1)}, & l > 1,\ k = 1, \\ 0, & k = l = 1. \end{cases}$$

In this case, we have

$$\sum_{l=1}^{\infty}\left(\sum_{k=1}^{\infty} b_{kl}\right) = 1, \qquad \sum_{k=1}^{\infty}\left(\sum_{l=1}^{\infty} b_{kl}\right) = -1.$$

As a result, the operator $\hat{B}$ can be nonassociative.

Let $B(q, p)$ be a discontinuous function. If the functions

$$\frac{\partial B(q, p)}{\partial q_k} = -\{p_k, B(q, p)\}, \qquad \frac{\partial B(q, p)}{\partial p_k} = \{q_k, B(q, p)\}$$

are continuous, then $\{A(q, p), B(q, p)\}$ is a continuous function for all $A(q, p) \in C^{\infty}(\mathbb{R}^{2n})$. In this case, the operator $B(Q, P) = \pi(B(q, p))$ can be considered as an element of an operator commutant-associative algebra and a Valya algebra. We say that $\mathcal{M}$ is a commutant-associative algebra if the commutant of this algebra is an associative subalgebra. A commutant of $\mathcal{M}$ is a subalgebra of $\mathcal{M}$ generated by all commutators $[A, B]$, where $A, B \in \mathcal{M}$. If $\mathcal{M}$ is a commutant-associative algebra, then $\mathcal{M}^{(-)}$ is a Valya algebra. We say that $\mathcal{M}$ is a Valya algebra if the commutant $\mathcal{M}'$ of this algebra is a Lie subalgebra. A Valya algebra is a generalization of a Lie algebra. Let us give the important examples regarding Valya algebras.

(1) Every finite Valya algebra is the tangent algebra of an analytic local commutant-associative loop (Valya loop) as each finite Lie algebra is the tangent algebra of an analytic local group (Lie group).

(2) A bilinear operation for the differential 1-forms

$$\alpha = \alpha_k(x)\, dx^k, \qquad \beta = \beta_k(x)\, dx^k$$

on a symplectic manifold $(\mathcal{M}, \omega)$ can be introduced by the rule

$$(\alpha, \beta) = d\Psi(\alpha, \beta) + \Psi(d\alpha, \beta) + \Psi(\alpha, d\beta),$$

where (α, β) is 1-form, and $\Psi(\alpha, \beta) = \Psi^{kl}\alpha_k\beta_l$. A set of all nonclosed 1-forms, together with this operation, is a Lie algebra. If α and β are closed 1-forms, then $d\alpha = d\beta = 0$ and

$$(\alpha, \beta) = d\Psi(\alpha, \beta). \tag{50}$$

A set of all closed 1-forms, together with the bracket (50), form a Lie algebra. A set of all nonclosed 1-forms together with the bilinear operation (50) is a Valya algebra, and it is not a Lie algebra.

For other examples of Valya algebra and loop see [157].

Chapter 18

Quantum Dynamics of States

18.1. Evolution equation for normalized operator

Trace equation

Let A be an operator, and let $Tr[A] < \infty$ be a trace of A. Using

$$Tr[A] = \int dx <x|A|x>, \qquad \frac{d|x>}{dt} = 0,$$

we obtain

$$\frac{d}{dt} Tr[A_t] = Tr\left[\frac{d}{dt} A_t\right].$$

Using $dA_t/dt = \mathcal{L}A_t$, we have

$$\frac{d}{dt} Tr[A_t] = Tr[\mathcal{L}A_t],$$

and $Tr[A_t] = const$ if $Tr[\mathcal{L}A_t] = 0$.

Trace-preserving equation

The observables of a quantum system are identified with self-adjoint linear operators. The state of the quantum system is identified with the density operator, i.e., with the self-adjoint, nonnegative, linear operator of unit trace. Then the state can be considered as an observable with unit trace.

Let $A_t = \Phi_t(A)$ be an operator that satisfy the equation

$$\frac{d}{dt} A_t = \frac{\partial}{\partial t} A_t + \mathcal{L}(A_t). \tag{1}$$

In general, the operator A_t is not an observable of unit trace for all $t > 0$, and $Tr[A_t] \neq 1$ for some $t > 0$. We can define the operator

$$\bar{A}_t = \frac{1}{Tr[A_t]} A_t. \tag{2}$$

It is not hard to prove that $\bar{A}_t$ is an operator with unit trace $Tr[\bar{A}_t] = 1$ for all $t \geqslant 0$. Differentiation of (2) with respect to t gives

$$\frac{d}{dt}\bar{A}_t = \frac{\partial}{\partial t}\bar{A}_t + \mathcal{L}\big(\bar{A}_t\big) - \bar{A}_t\, Tr\big[\mathcal{L}\big(\bar{A}_t\big)\big], \tag{3}$$

This equation will be rewritten in the form

$$\frac{d}{dt}\bar{A}_t = \frac{\partial}{\partial t}\bar{A}_t + \tilde{\mathcal{L}}\big(\bar{A}_t\big),$$

where

$$\tilde{\mathcal{L}}(A) = \mathcal{L}(A) - A\, Tr\big[\mathcal{L}(A)\big].$$

Equation (3) is called the *trace-preserving evolution equation* in the Heisenberg picture. If $Tr[\mathcal{L}(A)] = 0$ for all $A \in D(\mathcal{L})$, then $\tilde{\mathcal{L}}(A) = \mathcal{L}(A)$. For example, $\mathcal{L} = (1/i\hbar)[H, A]$ gives $\tilde{\mathcal{L}} = \mathcal{L}$. Note, that

$$Tr\big[\tilde{\mathcal{L}}\big(\bar{A}_t\big)\big] = 0$$

for all $t \geqslant 0$.

In general, $\bar{A}_t \neq \Phi_t(\bar{A})$. Using $A_t = \Phi_t A$, we obtain $\bar{A}_t = \hat{\Phi}_t \bar{A}$, where $\hat{\Phi}_t$ is a nonlinear superoperator such that

$$\hat{\Phi}_t \bar{A} = \big(Tr[\Phi_t \bar{A}]\big)^{-1} \Phi_t \bar{A} = \big(Tr[\Phi_t A]\big)^{-1} \Phi_t A,$$

where $\bar{A} = A/\,Tr[A]$.

Density operator in the Heisenberg picture

Suppose ρ is a density operator. In general, $Tr[\Phi_t \rho] \neq 1$. Then $\Phi_t \rho$ cannot be considered as a density operator at $t > 0$. Let us define the operator

$$\rho_H(t) = \bar{\rho}_t = \frac{1}{Tr[\Phi_t \rho]} \Phi_t \rho.$$

If $\rho_H(t)$ is nonnegative for all $t \geqslant 0$ and $\mathcal{L}$ is a real superoperator, then $\rho_H(t)$ is a density operator in the Heisenberg picture. The operator $\rho_H(t)$ can be considered as an observable. The equation determining the evolution of any such operator $\rho_H(t)$ is

$$\frac{d}{dt}\rho_H(t) = \frac{\partial}{\partial t}\rho_H(t) + \tilde{\mathcal{L}}\big(\rho_H(t)\big),$$

or

$$\frac{d}{dt}\rho_H(t) = \frac{\partial}{\partial t}\rho_H(t) + \mathcal{L}\big(\rho_H(t)\big) - \rho_H(t)\, Tr\big[\mathcal{L}\big(\rho_H(t)\big)\big].$$

In general, $d\rho_H(t)/dt \neq 0$.

18.2. Quantization for Hamiltonian picture

Suppose that a classical system, whose pure state is determined by a point (q, p) in $2n$-dimensional phase-space $\mathbb{R}^{2n}$, is described by the equation

$$\frac{d}{dt}\varrho(t, q_t, p_t) = -\Omega(q_t, p_t)\varrho(t, q_t, p_t), \tag{4}$$

where

$$\Omega(q, p) = -\sum_{k=1}^{n} J_{\mathcal{L}}\big[q^k, p^k\big],$$
$$J_{\mathcal{L}}\big[q^k, p^k\big] = \mathcal{L}\big(\{q^k, p^k\}\big) - \{\mathcal{L}(q^k), p^k\} - \{q^k, \mathcal{L}(p^k)\}.$$

Equation (4) is the classical Liouville equation in the Hamiltonian picture. Note that this equation can be presented in the form

$$\frac{d}{dt}\varrho(t, q_t, p_t) = -\Omega\big[L^+_{q_t}, L^+_{p_t}\big]\varrho(t, q_t, p_t), \tag{5}$$

If the classical system is Hamiltonian, then $\Omega(q, p) = 0$ and $\varrho(t, q_t, p_t)$ is an integral of motion.

The Weyl quantization of equation (5) gives

$$\frac{d}{dt}\varrho_t = -\Omega\big[L^+_Q, L^+_P\big]\varrho_t, \tag{6}$$

where $\varrho_t = \pi(\varrho(t, q_t, p_t))$, and

$$\Omega\big[L^+_Q, L^+_P\big] = \pi\big(\Omega\big[L^+_q, L^+_p\big]\big).$$

Note that

$$\Omega\big[L^+_Q, L^+_P\big]I = \Omega(Q, P) = \pi\big(\Omega(q, p)\big) = -\sum_{k=1}^{n} J_{\mathcal{L}}(Q_k, P_k).$$

Equation (6) is the quantum Liouville equation in the Heisenberg picture. The quantum system is dissipative if the right hand side of (6) is not equal to zero.

In general, $Tr[\varrho_t] \neq 1$. Let us define the following operator of unit trace:

$$\rho_t = \bar{\varrho}_t = \frac{\varrho_t}{Tr[\varrho_t]}.$$

Then equation (6) gives

$$\frac{d}{dt}\rho_t = -\Omega\big[L^+_Q, L^+_P\big]\rho_t + \rho_t\, Tr\big[\Omega\big[L^+_Q, L^+_P\big]\rho_t\big].$$

This nonlinear equation can be presented in the form

$$\frac{d}{dt}\rho_t = -\tilde{\Omega}\big[L^+_Q, L^+_P\big]\rho_t,$$

where

$$\tilde{\Omega}\big[L_Q^+, L_P^+\big] = \Omega\big[L_Q^+, L_P^+\big] - Tr\big[\Omega\big[L_Q^+, L_P^+\big]\rho_t\big]L_I.$$

This equation is the trace-preserving quantum Liouville equation in the Heisenberg picture.

If $\mathcal{L}_t$ is a constant superoperator ($\mathcal{L}_t = \mathcal{L}$), then the formal solution of this equation can be written in the form

$$\rho_t = \frac{1}{Tr[\mathcal{E}_t\rho_0]}\mathcal{E}_t\rho_0.$$

For quantum Hamiltonian systems,

$$J_{\mathcal{L}}(Q_k, P_k) = 0, \qquad \Omega\big[L_Q^+, L_P^+\big] = 0, \qquad \mathcal{E}_t = L_I,$$

and equation (6) gives

$$\frac{d}{dt}\rho_t = 0.$$

As a result, ρ_t is not changed in time, $\rho_t = \rho_0$. Then the density operators of Hamiltonian systems are integrals of motion.

18.3. Expectation values for non-Hamiltonian systems

Expectation values and evolution of density operator

The state of a quantum system is identified with the density operator. The expectation value of an observable A on a state ρ is then computed with the formula

$$<A> = (\rho|A) = Tr[\rho A].$$

Here we have not mentioned time and have completely ignored the time evolution of the state. If the system is Hamiltonian, then the density operator is an integral of motion, and the time evolution of ρ can be ignored. For dissipative quantum systems,

$$\frac{d}{dt}\rho_H(t) \neq 0,$$

where $\rho_H(t)$ be a density operator in the Heisenberg picture. Then the expectation value of an observable A_t on a state $\rho_t = \rho_H(t)$ can be defined by the formula

$$<A_t>_t = (\rho_t|A_t) = Tr[\rho_t A_t]. \tag{7}$$

In the conventional formulations of quantum theories, the expectation value of an observable A_t at $t \neq 0$ is computed on a state ρ_0 at $t = 0$ by the formula

$$<A_t> = (\rho_0|A_t) = Tr[\rho_0 A_t].$$

If the systems is Hamiltonian, then $\rho_t = \rho_0$. In the general case, $\rho_t \neq \rho_0$. As a result, *the expectation value at $t \neq 0$ must be defined by an observable A_t at the instant t and by a state ρ_t at the same instant $t \neq 0$.*

STATEMENT. *If A_t is an observable of a dissipative quantum system, then*

$$\frac{d}{dt}<A_t>_t = <A_t \frac{d \ln \rho_t}{dt}>_t + <\frac{dA_t}{dt}>_t.$$

PROOF. Differentiation of (7) with respect to t gives

$$\frac{d}{dt}<A_t>_t = \frac{d}{dt} Tr[\rho_t A_t] = Tr\left[\frac{d}{dt}(\rho_t A_t)\right]$$
$$= Tr\left[\left(\frac{d}{dt}\rho_t\right)A_t + \rho_t\left(\frac{d}{dt}A_t\right)\right] = <A_t \frac{d \ln \rho_t}{dt}>_t + <\frac{dA_t}{dt}>_t.$$

□

The following corollary follows immediately from the statement.

COROLLARY. *If A_t is an observable of a quantum Hamiltonian system, then*

$$\frac{d}{dt}<A_t>_t = <\frac{d}{dt}A_t>_t.$$

The following properties of the expectation value (7) are satisfied:

(1) $<aA_t + bB_t>_t = a<A_t>_t + b<B_t>_t$.
(2) $<A_t>_t^* = <A_t^*>_t$.
(3) $<I>_t = 1$.
(4) $<0>_t = 0$.

These properties of the expectation value $<A_t>_t$ for $A_t = \Phi_t(A)$ give the following properties of the superoperator Φ_t:

(1) $\Phi_t(aA + bB) = a\Phi_t(A) + b\Phi_t(B)$.
(2) $\Phi_t(A)^* = \Phi_t(A^*)$.
(3) $\Phi_t(I) = 1$.
(4) $\Phi_t(0) = 0$.

Let $\mathcal{L}$ be a generating superoperator for Φ_t. The properties of Φ_t give the following conditions for $\mathcal{L}$:

(1) $\mathcal{L}(aA_t + bB_t) = a\mathcal{L}(A_t) + b\mathcal{L}(B_t)$.
(2) $\mathcal{L}(A_t)^* = \mathcal{L}(A_t^*)$.
(3) $\mathcal{L}(I) = 0$.
(4) $\mathcal{L}(0) = 0$.

Using $\mathcal{L}\Phi_t = \Phi_t\mathcal{L}$, we can consider these properties for $t = 0$.

Dual equation for density operator

The expectation value (7) can be presented in the form

$$<A_t>_t = (\rho_t|A_t) = (\mathcal{E}_t\rho|\Phi_t A) = (\bar{\Phi}_t\mathcal{E}_t\rho|A),$$

where $\bar{\Phi}_t$ is adjoint of Φ_t. If $\Omega(Q, P) = 0$, then $\mathcal{E}_t = L_I$ for all $t \geqslant 0$ and $<A_t>_t = Tr[\bar{\Phi}_t\rho A]$.

Let us define the following density operator

$$\rho_s(t) = \bar{\Phi}_t\rho_t = \bar{\Phi}_t\mathcal{E}_t\rho_0. \tag{8}$$

Differentiation of (8) gives

$$\frac{d}{dt}\rho_s(t) = \frac{d}{dt}\left(\bar{\Phi}_t\rho_t\right) = \frac{d\bar{\Phi}_t}{dt}\rho_t + \bar{\Phi}_t\frac{d}{dt}\rho_t.$$

We can use the equations

$$\frac{d\bar{\Phi}_t}{dt} = \bar{\Phi}_t\bar{\mathcal{L}}, \qquad \frac{d}{dt}\rho_t = -\tilde{\Omega}\rho_t.$$

As a result, we obtain

$$\frac{d}{dt}\rho_s(t) = \bar{\Phi}_t\bar{\mathcal{L}}\rho_t - \bar{\Phi}_t\tilde{\Omega}\rho_t. \tag{9}$$

If $\bar{\Phi}_t^{-1}$ is left inverse of $\bar{\Phi}_t$, then equation (9) has the form

$$\frac{d}{dt}\rho_s(t) = \bar{\mathcal{L}}_s\rho_s(t) - \bar{\Omega}_s\rho_s(t), \tag{10}$$

where $\mathcal{L}_s = \bar{\Phi}_t\bar{\mathcal{L}}\bar{\Phi}_t^{-1}$, and $\bar{\Omega}_s = \bar{\Phi}_t\tilde{\Omega}\bar{\Phi}_t^{-1}$. Using $\bar{\Phi}_t\bar{\mathcal{L}} = \bar{\mathcal{L}}\bar{\Phi}_t$, we obtain $\bar{\mathcal{L}}_s = \bar{\mathcal{L}}$. If $\tilde{\Omega} = 0$, then equation (10) gives

$$\frac{d}{dt}\rho_s(t) = \bar{\mathcal{L}}\rho_s(t), \tag{11}$$

where $\bar{\mathcal{L}}$ is an adjoint superoperator of $\mathcal{L}$. As a result, we obtain that equation (11) is a special case of (10) for nondissipative quantum systems. In the conventional formulation of quantum mechanics, equation (11) is used for quantum dissipative systems. Note that this is connected with some problems in quantum theory.

Alpha-pi problem

In the quantum theory of non-Hamiltonian systems, there exists the following problem. Let α_q be a map from a set of superoperators into a set of adjoint superoperators, and let α_c be a map from a set of operators into a set of adjoint

operators. In general, we have the inequality

$$\pi\alpha_c \neq \alpha_q\pi,$$

where π is a quantization map. In order to have the equality $\pi\alpha_c = \alpha_q\pi$, it should be used as an additional requirement for quantization procedure.

We illustrate this problem in the following remarks. If a classical observable $A(q, p)$ in the Hamiltonian picture is described by the equation

$$\frac{d}{dt}A(q, p) = \mathcal{L}_c A(q, p),$$

then the quantization π gives

$$\frac{d}{dt}A(Q, P) = \mathcal{L}_q A(Q, P),$$

where

$$\pi(\mathcal{L}_c) = \mathcal{L}_q, \qquad \pi\big(A(q, p)\big) = A(Q, P).$$

We suppose that a classical state $\rho(t, q, p)$ in the Liouville picture is described by

$$\frac{d}{dt}\rho(t, q, p) = \Lambda_c\rho(t, q, p),$$

and the quantization π gives

$$\frac{d}{dt}\rho(t, Q, P) = \Lambda_q\rho(t, Q, P),$$

where

$$\pi(\Lambda_c) = \Lambda_q, \qquad \pi\big(\rho(t, q, p)\big) = \rho(t, Q, P).$$

If Λ_c is an adjoint operator of $\mathcal{L}_c$,

$$\Lambda_c = \alpha_c(\mathcal{L}_c) = \bar{\mathcal{L}}_c,$$

then in general we have

$$\Lambda_q \neq \bar{\mathcal{L}}_q,$$

where $\bar{\mathcal{L}}_q = \alpha_q(\mathcal{L}_q)$, i.e.,

$$\pi\big(\alpha_c(\mathcal{L}_c)\big) \neq \alpha_q\big(\pi(\mathcal{L}_c)\big).$$

As a result, we can have two quantum Liouville equation that are not equivalent. This appearance of two nonequivalent equations for one quantum non-Hamiltonian system we call the $\alpha\pi$-problem.

Let us explain the used notations. Here Λ_c is adjoint of $\mathcal{L}_c$ if

$$(\Lambda_c A|B) = (A|\mathcal{L}_c B) \tag{12}$$

for all $A, B \in \mathcal{M}_c$. For $\mathcal{M}_c = L_2(\mathbb{R}^{2n})$,

$$(A|B) = \int dq\, dp \left(A(q,p)\right)^* B(q,p).$$

If $\mathcal{M}_q$ is a Liouville space, then $(A|B) = Tr[A^* B]$. If condition (12) is valid, then we write

$$\Lambda_c = \alpha_c(\mathcal{L}_c), \qquad \Lambda_q = \alpha_q(\mathcal{L}_q).$$

DEFINITION. If the Liouville picture (LP) is adjoint to Hamiltonian, and the Heisenberg picture (HS) is obtained by quantization of the Hamiltonian picture, then there exist two following Schrödinger pictures:

(1) the "QL"-Schrödinger picture that is obtained by the quantization of the LP;
(2) the "AH"-Schrödinger picture that is adjoint of HP.

In general, these Schrödinger pictures are not equivalent. The problem of the non-equivalence of these pictures is called the *$\alpha\pi$-problem*.

The $\alpha\pi$-problem can be solved if we use the "Weyl representation" of quantum dynamics. In particular, *all equation in quantum theory must be ordered by the same ordering rule that is used for observables*.

In the "Weyl representation" of quantum kinematics, a set of quantum observables is considered as a Lie–Jordan algebra of Weyl ordered operators. In order to all operators be Weyl ordered, the Weyl multiplication must be used instead of usual multiplication. Each algebraic operation on a set of quantum observables must assign to Weyl ordered operators exactly one Weyl ordered operator.

In the "Weyl representation" of quantum dynamics, all evolution superoperators must be real Weyl ordered superoperators. The time evolution of quantum systems must be described by superoperators that assign to each Weyl ordered operator exactly one Weyl ordered operator.

Dual equation for observable

Let us define the operator

$$A_s(t) = \bar{\Phi}_t A_t = \bar{\Phi}_t \Phi_t A.$$

Differentiation of $A_s(t)$ gives

$$\frac{d}{dt} A_s(t) = \frac{d}{dt}\left(\bar{\Phi}_t A_t\right) = \frac{d\bar{\Phi}_t}{dt} A_t + \bar{\Phi}_t \frac{dA_t}{dt}.$$

If

$$\frac{d\bar{\Phi}_t}{dt} = \frac{\partial}{\partial t}\bar{\Phi}_t + \bar{\Phi}_t\bar{\mathcal{L}},$$

then

$$\frac{d}{dt}A_s(t) = \frac{\partial}{\partial t}A_s(t) + \bar{\Phi}_t\big(\bar{\mathcal{L}}(A_t)\big) + \bar{\Phi}_t\big(\mathcal{L}(A_t)\big).$$

Let $\bar{\Phi}_t^{-1}$ be a left inverse superoperator of $\bar{\Phi}_t$, i.e., $\bar{\Phi}_t^{-1}(\bar{\Phi}_t(A)) = A$ for all $A \in \bar{\mathcal{H}}$. Then we can define the superoperators

$$\mathcal{L}_s = \bar{\Phi}_t\mathcal{L}\bar{\Phi}_t^{-1}, \qquad \bar{\mathcal{L}}_s = \bar{\Phi}_t\bar{\mathcal{L}}\bar{\Phi}_t^{-1} = \bar{\mathcal{L}}.$$

In this case,

$$\frac{d}{dt}A_s(t) = \frac{\partial}{\partial t}A_s(t) + \bar{\mathcal{L}}_s(A_s) + \mathcal{L}_s(A_s). \tag{13}$$

This is the Heisenberg equation in the Schrödinger picture. If $\mathcal{L}$ is a Hamiltonian superoperator, then $\bar{\mathcal{L}} = -\mathcal{L}$, $\mathcal{L}_s = \mathcal{L}$, and equation (13) give

$$\frac{d}{dt}A_s(t) = \frac{\partial}{\partial t}A_s(t).$$

This equation describes the time evolution of quantum observable of Hamiltonian system in the Schrödinger picture.

18.4. Adjoint and inverse superoperators

Adjoint superoperator

Let $\mathcal{L}$ be a bounded superoperator on $\mathcal{M}$. The adjoint of $\mathcal{L}$ is the superoperator $\bar{\mathcal{L}}$ defined by $(\bar{\mathcal{L}}A|B) = (A|\mathcal{L}B)$. The scalar product $(A|B) = Tr[A^*B]$ gives the condition

$$Tr\big[(\bar{\mathcal{L}}A)^*B\big] = Tr\big[A^*\mathcal{L}(B)\big]$$

for all $A, B \in \mathcal{M}$. If $\mathcal{L}$ is a real superoperator, then $(\mathcal{L}A)^* = \mathcal{L}(A^*)$. Using the Leibnitz defect

$$Z_{\mathcal{L}}(A^*, B) = \mathcal{L}(A^*B) - \mathcal{L}(A^*)B - A^*\mathcal{L}(B),$$

we obtain

$$Tr\big[A^*\mathcal{L}(B)\big] = Tr\big[-\mathcal{L}(A^*)B + \mathcal{L}(A^*B) - Z_{\mathcal{L}}(A^*, B)\big].$$

It is not hard to see that $\bar{\mathcal{L}} \neq -\mathcal{L}$.

STATEMENT. *Let $\mathcal{L}$ be a bounded locally Hamiltonian superoperator* ($Z_{\mathcal{L}}(A, B) = 0$). *If the condition*

$$Tr\big[\mathcal{L}(A)\big] = 0$$

is valid for all $A \in \mathcal{M}$, then $\bar{\mathcal{L}} = -\mathcal{L}$.

If Φ_t is a norm continuous superoperator, i.e.,

$$\lim_{t\to 0+} \|\Phi_t - L_I\| = 0,$$

then there exists a bounded generating superoperator $\mathcal{L}$ such that

$$\Phi_t = \exp(t\mathcal{L}), \qquad \lim_{t\to 0+} \big\|t^{-1}(\Phi_t - L_I) - \mathcal{L}\big\| = 0.$$

The superoperator $\bar{\Phi}_t$ is adjoint of Φ_t if

$$(\bar{\Phi}_t A|B) = (A|\Phi_t B).$$

If $\mathcal{L}$ is Hamiltonian, then $\bar{\mathcal{L}} = -\mathcal{L}$, and the superoperator $\bar{\Phi}_t = \exp(t\bar{\mathcal{L}})$, is inverse of Φ_t such that

$$\bar{\Phi}_t = \Phi_t^{-1} = \exp(-t\mathcal{L}).$$

In the general case, we have the inequalities

$$\bar{\Phi}_t \neq \Phi_t^{-1}, \qquad \bar{\mathcal{L}} \neq -\mathcal{L}.$$

An adjoint superoperator $\bar{\Phi}_t$ of Φ_t is not inverse of Φ_t.

Inverse superoperator

Let us consider the linear operator differential equation

$$\frac{d}{dt} A_t = \mathcal{L}_t A_t,$$

where $\mathcal{L}_t$ is a one-parameter superoperator which depends continuously on t. We assume that for each fixed t this superoperator is the bounded superoperator on a Banach space $\mathcal{M}$. The solution of the Cauchy problem for this equation exists and is unique. This solution can be written in the form $A_t = \Phi_t A$, where the superoperator Φ_t is the sum of the series

$$\Phi_t = T\left\{\exp \int_0^t d\tau \mathcal{L}_\tau\right\}.$$

If $\mathcal{L}_t$ is a constant superoperator ($\mathcal{L}_t = \mathcal{L}$), then $\Phi_t = \exp(t\mathcal{L})$. The superoperator Φ_t can be considered as the solution of the Cauchy problem

$$\frac{d}{dt}\Phi_t = \mathcal{L}\Phi_t, \quad \Phi_0 = L_I \tag{14}$$

for this differential equation in the space $\mathcal{A}(\mathcal{M})$ of all bounded superoperators acting on $\mathcal{M}$.

A bounded inverse superoperator Φ_t^{-1} exists for every t. This superoperator is the solution of the Cauchy problem for the superoperator differential equation

$$\frac{d}{dt}\Phi_t^{-1} = -\mathcal{L}\Phi_t^{-1}, \quad \Phi_0^{-1} = L_I,$$

which is called the adjoint equation of (14).

As a result, for non-Hamiltonian superoperator $\mathcal{L}$, we can define the superoperator

$$\Phi_t^{-1} = \exp(-t\mathcal{L}).$$

The superoperator Φ_t^{-1} is a bounded norm continuous superoperator. It is not hard to prove that Φ_t^{-1} is inverse of Φ_t, and

$$\Phi_t^{-1}\Phi_t = \Phi_t\Phi_t^{-1} = L_I. \tag{15}$$

In general,

$$\Phi_t^{-1} \neq \bar{\Phi}_t.$$

Using $(\bar{\Phi}_t A|\bar{\Phi}_t B) = (A|\Phi_t\bar{\Phi}_t B)$, it is not hard to prove that

$$(\bar{\Phi}_t A|\bar{\Phi}_t B) \neq (A|B), \tag{16}$$

where $(\bar{\Phi}_t A|B) = (A|\Phi_t B)$ for all $A, B \in \mathcal{M}$. Equations (15) and (16) give

$$\Phi_t\bar{\Phi}_t \neq L_I, \qquad \Phi_t\Phi_t^{-1} = L_I.$$

The Stone's theorem states that, if $\bar{\Phi}_t$ is a superoperator such that $\Phi_t\bar{\Phi}_t = L_I$, then $\mathcal{L}$ is Hamiltonian.

As a result, an adjoint superoperator $\bar{\Phi}_t$ of $\Phi_t = \exp(t\mathcal{L})$ is inverse if and only if the generating superoperator $\mathcal{L}$ is Hamiltonian. An inverse superoperator Φ_t^{-1} of $\Phi_t = \exp(t\mathcal{L})$ is adjoint if and only if the generating superoperator $\mathcal{L}$ is Hamiltonian.

18.5. Adjoint Lie–Jordan superoperator functions

Lie superoperator functions

Let $\mathcal{M}$ be an operator algebra. We define the Lie left superoperators L_A^- on $\mathcal{M}$ by

$$L_A^- B = A \cdot B = \frac{1}{i\hbar}(AB - BA).$$

STATEMENT. *If Q and P are self-adjoint operators such that*

$$Q \cdot P = I, \qquad Q \cdot Q = P \cdot P = 0, \tag{17}$$

then L_Q^- and L_P^- are commutative superoperators, i.e.,

$$L_Q^- L_P^- = L_P^- L_Q^-. \tag{18}$$

PROOF. Using

$$L_A^- L_B^- = L_B^- L_A^- + L_{A\cdot B}^-,$$

and $Q \cdot P = I$, we obtain

$$L_Q^- L_P^- = L_P^- L_Q^- + L_I^-.$$

The relation $L_I^- A = (1/i\hbar)(A - A) = 0$ gives (18). □

It is not hard to prove that

$$L_{Q_k}^- L_{Q_l}^- = L_{Q_l}^- L_{Q_k}^-, \qquad L_{P_k}^- L_{P_l}^- = L_{P_l}^- L_{P_k}^-,$$

if $Q_k \cdot Q_l = P_k \cdot P_l = 0$.

STATEMENT. *Let $\mathcal{L}[L_Q^-, L_P^-]$ be a superoperator function. Then $\mathcal{L}[L_Q^-, L_P^-]$ is a function of the commutative variables L_Q^-, and L_P^-. In particular, we have $\mathcal{L}[L_Q^-, L_P^-] = \mathcal{L}[L_P^-, L_Q^-]$.*

Let $\mathcal{M}$ be an operator algebra. We shall denote the linear space of all superoperator functions $\mathcal{L}[L_Q^-, L_P^-]$ on $\mathcal{M}$ by $\mathcal{A}_-(\mathcal{M})$. The element of $\mathcal{A}_-(\mathcal{M})$ will be called the *Lie superoperator function*. For $\mathcal{L}_1, \mathcal{L}_2 \in \mathcal{A}_-(\mathcal{M})$ we define the product $\mathcal{L}_1\mathcal{L}_2$ as the superoperator functions $(\mathcal{L}_1\mathcal{L}_2)A = \mathcal{L}_1(\mathcal{L}_2 A)$ for $A \in \mathcal{M}$. With this definition of multiplication, $\mathcal{A}_-(\mathcal{M})$ becomes a *commutative algebra* of Lie superoperator functions.

STATEMENT. *Let A be a self-adjoint operator. If $\bar{L}_A^- = \alpha_q(L_A^-)$ is adjoint of L_A^-, then*

$$\bar{L}_A^- = -L_A^-.$$

PROOF. Let $\mathcal{M}$ be an operator algebra, together with the scalar product $(A|B) = Tr[A^*B]$. If $A^* = A \in \mathcal{M}$, then

$$\begin{aligned}\big(\bar{L}_A^- B|C\big) &= Tr\big[\big(\bar{L}_A^- B\big)^* C\big] = -\,Tr\big[\big(L_A^- B\big)^* C\big] \\ &= -\,Tr\big[(A\cdot B)^* C\big] = \frac{1}{i\hbar}\,Tr\big[(AB - BA)^* C\big] \\ &= \frac{1}{i\hbar}\,Tr[B^*AC - AB^*C] \\ &= \frac{1}{i\hbar}\,Tr[B^*AC - B^*CA] = Tr\big[B^*(A\cdot C)\big] = (B|L_A^- C).\end{aligned}$$

□

This statement gives

$$\bar{L}_Q^- = -L_Q^-, \qquad \bar{L}_P^- = -L_P^-.$$

Let $\mathcal{L} = \mathcal{L}[L_Q^-, L_P^-]$ be a superoperator polynomial. If there is a positive integer n such that

$$\mathcal{L}\big[zL_Q^-, zL_P^-\big] = z^n \mathcal{L}\big[L_Q^-, L_P^-\big],$$

then $\mathcal{L}[L_Q^-, L_P^-]$ is called the *homogeneous polynomial of the order n*.

COROLLARY. *Let $\mathcal{L} = \mathcal{L}[L_Q^-, L_P^-]$ be a homogeneous superoperator polynomial of the order n. Then the superoperator*

$$\bar{\mathcal{L}} = \alpha_q(\mathcal{L}) = (-1)^{n+1}\mathcal{L}\big[L_Q^-, L_P^-\big]$$

is adjoint of $\mathcal{L}[L_Q^-, L_P^-]$.

Jordan superoperator functions

Let $\mathcal{M}$ be an operator algebra. We define the Jordan left superoperators L_A^+ on $\mathcal{M}$ by

$$L_A^+ B = A \circ B = \frac{1}{2}(AB + BA).$$

STATEMENT. *If Q and P are self-adjoint operators and relations (17) are valid, then L_Q^+ and L_P^+ are commutative superoperators, i.e.,*

$$L_Q^+ L_P^+ = L_P^+ L_Q^+. \tag{19}$$

PROOF. Using

$$L_A^+ L_B^+ = L_B^+ L_A^+ + \frac{\hbar^2}{4} L_{A\cdot B}^-,$$

and $Q \cdot P = I$, we obtain

$$L_Q^+ L_P^+ = L_P^+ L_Q^+ + \frac{\hbar^2}{4} L_I^-,$$

then the relation $L_I^- = 0$ gives (19). □

It is not hard to prove that

$$L_{Q_k}^+ L_{Q_l}^+ = L_{Q_l}^+ L_{Q_k}^+, \qquad L_{P_k}^+ L_{P_l}^+ = L_{P_l}^+ L_{P_k}^+,$$

if $Q_k \cdot Q_l = P_k \cdot P_l = 0$.

STATEMENT. *Let $\mathcal{L}[L_Q^+, L_P^+]$ be a superoperator function. Then $\mathcal{L}[L_Q^+, L_P^+]$ is a function of the commutative variables L_Q^+, and L_P^+. In particular, we have $\mathcal{L}[L_Q^+, L_P^+] = \mathcal{L}[L_P^+, L_Q^+]$.*

Let $\mathcal{M}$ be an operator algebra. We shall denote the linear space of all superoperator functions $\mathcal{L}[L_Q^+, L_P^+]$ on $\mathcal{M}$ by $\mathcal{A}_+(\mathcal{M})$. The element of $\mathcal{A}_+(\mathcal{M})$ will be called the *Jordan superoperator function*. For $\mathcal{L}_1, \mathcal{L}_2 \in \mathcal{A}_+(\mathcal{M})$ we define the product $\mathcal{L}_1\mathcal{L}_2$ as the superoperator functions $(\mathcal{L}_1\mathcal{L}_2)A = \mathcal{L}_1(\mathcal{L}_2 A)$ for $A \in \mathcal{M}$. With this definition of multiplication, $\mathcal{A}_+(\mathcal{M})$ becomes a *commutative algebra* of Jordan superoperator functions.

STATEMENT. *Let $A \in \mathcal{M}$ be a self-adjoint operator. If $\bar{L}_A^+ = \alpha_q(L_A^+)$ is adjoint of L_A^+, then*

$$\bar{L}_A^+ = L_A^+.$$

PROOF. Let $\mathcal{M}$ be an operator algebra, together with the scalar product $(A|B) = Tr[A^* B]$. Then

$$\begin{aligned}
\big(\bar{L}_A^+ B|C\big) &= Tr\big[\big(\bar{L}_A^+ B\big)^* C\big] = Tr\big[\big(L_A^+ B\big)^* C\big] \\
&= Tr\big[(A \circ B)^* C\big] = \frac{1}{2}\, Tr[B^* AC + AB^* C] \\
&= \frac{1}{2}\, Tr[B^* AC + B^* CA] \\
&= Tr\big[B^*(A \circ C)\big] = (B|L_A^+ C).
\end{aligned}$$

□

This statement gives

$$\bar{L}_Q^+ = L_Q^+, \qquad \bar{L}_P^+ = L_P^+.$$

COROLLARY. *Let $\mathcal{L} = \mathcal{L}[L_Q^+, L_P^+]$ be a superoperator polynomial. Then the superoperator*

$$\bar{\mathcal{L}} = \mathcal{L}\big[L_Q^+, L_P^+\big]$$

is adjoint of $\mathcal{L}[L_Q^+, L_P^+]$.

This corollary gives that all elements of $\mathcal{A}_+(\mathcal{M})$ are self-adjoint.

Adjoint superoperator functions

Let us give the basic theorem regarding adjoint superoperators.

THEOREM. *Let $\mathcal{J} = \mathcal{J}[L_Q^+, L_P^+]$ be a Jordan superoperator function, and let $\mathcal{P}_n = \mathcal{P}_n[L_Q^-, L_P^-]$ be a homogeneous Lie superoperator polynomial of the order n. Then*

$$\bar{\mathcal{L}} = \alpha_q(\mathcal{L}) = (-1)^n \mathcal{P}_n\big[L_Q^-, L_P^-\big]\mathcal{J}\big[L_Q^+, L_P^+\big]$$

is an adjoint superoperator of the superoperator

$$\mathcal{L} = \mathcal{J}\big[L_Q^+, L_P^+\big]\mathcal{P}_n\big[L_Q^-, L_P^-\big].$$

PROOF. If $\bar{\mathcal{L}} = (-1)^n \mathcal{P}_n \mathcal{J}$, then

$$(\bar{\mathcal{L}}B|C) = (-1)^n (\mathcal{P}_n \mathcal{J} B|C).$$

Using $(-1)^n(\mathcal{P}_n B_J|C) = (B_J, \mathcal{P}_n C)$, where $B_J = \mathcal{J}B$, we obtain

$$(\bar{\mathcal{L}}B|C) = (\mathcal{J}B|\mathcal{P}_n C).$$

The equation $(\mathcal{J}B|C_n) = (B, \mathcal{J}C_n)$, where $C_n = \mathcal{P}_n C$, gives

$$(\bar{\mathcal{L}}B|C) = (B|\mathcal{L}C).$$

This ends the proof. □

The following corollary follows immediately from the theorem.

COROLLARY. *Let $\mathcal{L}$ be a superoperator function of the form*

$$\mathcal{L}\big[L_Q^+, L_P^+, L_Q^-, L_P^-\big] = \sum_{n=0} \mathcal{J}_n\big[L_Q^+, L_P^+\big]\mathcal{P}_n\big[L_Q^-, L_P^-\big], \tag{20}$$

where $\mathcal{J}_n[L_Q^+, L_P^+]$ are Jordan superoperator functions, and $\mathcal{P}_n[L_Q^-, L_P^-]$ are homogeneous Lie superoperator polynomial of the order n. If $\bar{\mathcal{L}}$ is an adjoint of the superoperator (20), then

$$\bar{\mathcal{L}} = \sum_{n=0} (-1)^n \mathcal{P}_n\big[L_Q^-, L_P^-\big]\mathcal{J}_n\big[L_Q^+, L_P^+\big].$$

Example of adjoint superoperator function

Let us consider a classical system. If

$$\frac{dq}{dt} = G(q, p), \qquad \frac{dp}{dt} = F(q, p),$$

then

$$\frac{d}{dt}A(q, p) = \left(G(q, p)\frac{\partial}{\partial q} + F(q, p)\frac{\partial}{\partial p}\right)A(q, p). \tag{21}$$

Using the operators

$$L_B^- A(q, p) = \big\{B(q, p), A(q, p)\big\},$$
$$L_B^+ A = B(q, p)A(q, p),$$

equation (21) can be presented in the form

$$\frac{d}{dt}A(q, p) = \mathcal{L}\big[L_q^+, L_p^+, L_q^-, L_p^-\big]A(q, p),$$

where

$$\mathcal{L}\big[L_q^+, L_p^+, L_q^-, L_p^-\big] = -G\big[L_q^+, L_p^+\big]L_p^- + F\big[L_q^+, L_p^+\big]L_q^-.$$

The Weyl quantization of this equation gives

$$\frac{d}{dt}A(Q, P) = \mathcal{L}\big[L_Q^+, L_P^+, L_Q^-, L_P^-\big]A(Q, P),$$

where

$$\mathcal{L}\big[L_Q^+, L_P^+, L_Q^-, L_P^-\big] = -G\big[L_Q^+, L_P^+\big]L_P^- + F\big[L_Q^+, L_P^+\big]L_Q^-, \tag{22}$$

and $L_B^- A = (1/i\hbar)(BA - AB)$, $L_B^+ A = (1/2)(BA + AB)$. The superoperator (22) is homogeneous with respect to L_Q^- and L_P^- of the order $n = 1$. It is not hard to prove that the superoperator

$$\bar{\mathcal{L}} = L_P^- G\big[L_Q^+, L_P^+\big] - L_Q^- F\big[L_Q^+, L_P^+\big] \tag{23}$$

is adjoint of (22).

Note that $\bar{\mathcal{L}}$ can be presented as $-\mathcal{L} - \Omega$. To prove this, we use the relation

$$L_A^- L_B^+ = L_{A\cdot B}^+ + L_B^+ L_A^-$$

in the form

$$L_Q^- L_P^+ = L_P^+ L_Q^- + L_I^+, \qquad L_P^- L_Q^+ = L_Q^+ L_P^- - L_I^+.$$

Then the adjoint superoperator (23) will be presented as

$$\bar{\mathcal{L}} = G\big[L_Q^+, L_P^+\big]L_P^- - F\big[L_Q^+, L_P^+\big]L_Q^- - \Omega\big[L_Q^+, L_P^+\big],$$

where $\Omega[L_Q^+, L_P^+]$ is a Jordan superoperator function. If instead of q and p we use L_Q^+ and L_P^+, then the function

$$\Omega(q, p) = \frac{\partial G(q, p)}{\partial q} + \frac{\partial F(q, p)}{\partial p}$$

gives $\Omega[L_Q^+, L_P^+]$. As a result, we have

$$\alpha_q(\mathcal{L}) = \bar{\mathcal{L}} = -\mathcal{L} - \Omega\big[L_Q^+, L_P^+\big].$$

If $\mathcal{L}$ is a Hamiltonian superoperator, then $\Omega[L_Q^+, L_P^+] = 0$ and $\bar{\mathcal{L}} = -\mathcal{L}$.

18.6. Weyl multiplication and Weyl scalar product

Weyl multiplication

Let π be a Weyl quantization, and let $A(q, p)$, $B(q, p)$ be real-valued functions on $\mathbb{R}^{2n}$. In general,

$$\pi(AB) \neq \pi(A)\pi(B).$$

Then $\pi(A)\pi(B)$ may not belong to a set of Weyl ordered operator, if $\pi(A)$ and $\pi(B)$ are Weyl ordered. Moreover, $\pi(A)\pi(B)$ is not a self-adjoint operator, and it is not an observable.

Let $\mathcal{M}$ be a set of all observables, and let A, B be elements of $\mathcal{M}$. In general, the operator AB is not an element of $\mathcal{M}$. Then the scalar product $(A|B) = Tr[AB]$, and the trace operation $Tr[AB]$ is not defined on $\mathcal{M}$. Using $Tr[AB] = Tr[BA]$, we can define

$$(A|B) = Tr[A \circ B], \tag{24}$$

where $A \circ B = (1/2)(AB + BA)$. If $A, B \in \mathcal{M}$, then $A \circ B \in \mathcal{M}$.

We shall denote the linear space of all Weyl ordered self-adjoint operators by $\mathcal{M}_W$. In general, a linear space $\mathcal{M}_W$, together with the binary operation $A \circ B$

cannot be considered as an algebra. If A and B are Weyl ordered operators, then, in general, $A \circ B$ is not Weyl ordered. As a result, the scalar product (24) cannot be defined on $\mathcal{M}_W$ by this equation.

If Q, P are self-adjoint operators such that

$$Q \cdot P = I, \qquad Q \cdot Q = P \cdot P = 0, \tag{25}$$

then we can define an element A of $\mathcal{M}_W$ as an operator function $A(Q, P)$ by the equation

$$A(Q, P) = A\big(L_Q^+, L_P^+\big)I.$$

As a result,

$$\mathcal{M}_W = \big\{A(Q, P)\colon\ A(Q, P) = A\big(L_Q^+, L_P^+\big)I\big\}.$$

For $A(Q, P)$, $B(Q, P) \in \mathcal{M}_W$, we define the product $A(Q, P) * B(Q, P)$ as the Weyl ordered self-adjoint operator such that

$$\begin{aligned} A(Q, P) * B(Q, P) &= A\big(L_Q^+, L_P^+\big)B(Q, P) \\ &= A\big(L_Q^+, L_P^+\big)B\big(L_Q^+, L_P^+\big)I. \end{aligned}$$

This operation of multiplication is called the *Weyl multiplication*. If A, $B \in \mathcal{M}_W$, then $A * B \in \mathcal{M}_W$ is an observable.

In general, AB is not observable even if A and B are observable. *Concepts that correspond to impossible observation like "the product of observables that is not observable" should be eliminated from theory*. We should use the Weyl multiplication.

The Weyl multiplication is a rule that assigns to each pair of Weyl ordered operators $A(Q, P)$, $B(Q, P)$ exactly one Weyl ordered operator $C(Q, P)$ such that

$$C\big(L_Q^+, L_P^+\big) = A\big(L_Q^+, L_P^+\big)B\big(L_Q^+, L_P^+\big),$$

i.e., $C(Q, P) = A(L_Q^+, L_P^+)B(L_Q^+, L_P^+)I$.

In the general case,

$$A(Q, P)B(Q, P) \neq A(Q, P) * B(Q, P).$$

Note that from $A \in \mathcal{M}_W$ it does not follow that $A^n \in \mathcal{M}_W$. In general,

$$A(Q, P)^2 \neq A(Q, P) * A(Q, P).$$

Using $L_Q^+ L_P^+ = L_P^+ L_Q^+$, it is not hard to prove that

$$A(Q, P) * B(Q, P) = B(Q, P) * A(Q, P)$$

for all $A(Q, P)$ and $B(Q, P)$ in $\mathcal{M}_W$. With this definition of multiplication, $\mathcal{M}_W$ becomes an algebra.

STATEMENT. *A linear space $\mathcal{M}_W$, together with the binary operation*

$$A(Q, P) * B(Q, P) = A\big(L_Q^+, L_P^+\big)B\big(L_Q^+, L_P^+\big)I$$

is a commutative associative operator algebra of Weyl ordered operators.

Note that this important statement comes from the properties of Jordan superoperator functions.

Weyl representation of quantum mechanics

Setting quantization of kinematics means establishing a general rule assigning a quantum observable $A(Q, P)$ to each classical observable $A(q, p)$. However, quantization π is not uniquely defined by $\pi(q) = Q$ and $\pi(p) = P$. To remove the ambiguity, we apply certain ordering (quantization) rule, i.e., we fix a method by which to each function $A(q, p)$ of the numbers q, p there is a uniquely assigned function $A(Q, P)$ of the operators Q, P. If only functions of this type are used in quantum mechanics, no ambiguity will arise.

There exists a natural requirement that must be satisfied in the quantum theory. All quantum observables must be ordered by an ordering rule. This rule defines the representation of the theory. If only ordered operators of this type are used in quantum theory, then no ambiguity will arise. The Weyl ordering realizes the Weyl representation of quantum mechanics in the algebraic approach. In order to all operators be Weyl ordered, the Weyl multiplication must be used instead of usual multiplication.

A unary operation on a set of quantum observables must assign to each element of $\mathcal{M}_W$ exactly one element of $\mathcal{M}_W$. A binary operation on a set of quantum observables must be a map from $\mathcal{M}_W \times \mathcal{M}_W$ into $\mathcal{M}_W$. The time evolution of quantum systems must be described by superoperators that are maps from $\mathcal{M}_W$ into itself.

Weyl scalar product

The scalar product on $\mathcal{M}_W$ can be defined by

$$(A|B)_W = Tr[A * B] = Tr\big[A\big(L_Q^+, L_P^+\big)B\big(L_Q^+, L_P^+\big)I\big].$$

This product will be called the *Weyl scalar product*.

STATEMENT. *If $A, B \in \mathcal{M}_W$, then*

$$(A|B)_W = (A|B).$$

PROOF. Suppose $\mathcal{L}$ is a Jordan superoperator function, and B is in $\mathcal{M}_W$. Then $(\mathcal{L}B)^* = \mathcal{L}B$, $\bar{\mathcal{L}} = \mathcal{L}$ and

$$Tr\big[(\mathcal{L}B)C\big] = Tr\big[B(\mathcal{L}C)\big].$$

Let $A(L_Q^+, L_P^+)$ be a Jordan superoperator function. Then

$$\begin{aligned}(A|B)_W &= Tr\big[A(Q,P) * B(Q,P)\big] = Tr\big[A\big(L_Q^+, L_P^+\big)B(Q,P)\big] \\ &= Tr\big[I\,A\big(L_Q^+, L_P^+\big)B(Q,P)\big] = Tr\big[\big(A\big(L_Q^+, L_P^+\big)I\big)B(Q,P)\big] \\ &= Tr\big[A(Q,P)B(Q,P)\big] = (A|B).\end{aligned}$$ □

As a result, the Weyl scalar product is equivalent to the usual scalar product in a Hilbert operator space. Then $\mathcal{M}_W$ can be considered as a Liouville space. Note that the Weyl multiplication is not equivalent to the usual multiplication (and to the Jordan product) of operators.

It is not hard to prove the following properties of the Weyl product:

$$Tr[A * B] = Tr[B * A],$$
$$Tr[A * B * C] = Tr[B * C * A] = Tr[C * A * B].$$

Using $A * B = B * A$, we have

$$Tr[A * B * C] = Tr[B * A * C].$$

For the usual multiplication of operators, we can obtain $Tr[ABC] \neq Tr[BAC]$. As a result, we have the following statement.

STATEMENT. *If $A, B, C \in \mathcal{M}_W$, then*

$$Tr[A * B] = Tr[AB].$$

In the general case, there exists the inequality

$$Tr[A * B * C] \neq Tr[ABC].$$

This statement shows that if the Weyl ordered operators are used, then we should generalize the expectation values, the variance, and the correlators.

18.7. Weyl expectation value and Weyl correlators

Weyl expectation value

The observables of a quantum system can be considered as the elements of an operator algebra $\mathcal{M}_W$. The state of the system can be identified with a Weyl ordered

density operator, i.e., with a positive element $\rho \in \mathcal{M}_W$ with unit trace. The expectation value of an observable $A \in \mathcal{M}_W$ on a state $\rho \in \mathcal{M}_W$ is then computed with the formula

$$<A>_W = (\rho|A)_W = (\rho|A) = Tr[\rho A] = <A>.$$

Note that from $A \in \mathcal{M}_W$ it does not follow that $A^2 \in \mathcal{M}_W$. In general, $A^2 \notin \mathcal{M}_W$, and

$$A * A \neq A^2.$$

As a result, $<A^2>$ should be replaced by $<A * A>$. The mean square of an observable A is the expectation $<A * A>_W$. In general,

$$<A * A>_W \neq <A^2>.$$

The variance $D_W A$ of $A \in \mathcal{M}_W$ should be defined as the mean square $<(A - aI) * (A - aI)>_W$ of the difference $A - aI$, where $a = <A>_W$ is the expectation of A. The following formula then holds

$$D_W A = <A * A>_W - <A>_W^2.$$

In the general case, $D_W A \neq DA = <A^2> - <A>^2$.

Note that $Q * Q = Q^2$ and $P * P = P^2$. Then operators Q^2 and P^2 are elements of $\mathcal{M}_W$, and

$$\Delta_W Q = \sqrt{<Q^2>_W - <Q>_W^2} = \sqrt{<Q^2> - <Q>^2} = \Delta Q,$$

$$\Delta_W P = \sqrt{<P^2>_W - <P>_W^2} = \sqrt{<P^2> - <P>^2} = \Delta P.$$

As a result, the Heisenberg uncertainty principle $\Delta Q \Delta P \geqslant \hbar/2$ on $\mathcal{M}_W$ has the form

$$\Delta_W Q \Delta_W P \geqslant \frac{\hbar}{2}.$$

In the general case, we have $\Delta_W A \neq \Delta A$, and $\Delta_W A \Delta_W B \neq \Delta A \Delta B$.

Weyl correlators

If the observables $A \in \mathcal{M}_W$ and $B \in \mathcal{M}_W$ are *mutually independent in* $\mathcal{M}_W$, then

$$<A * B>_W = <A>_W <B>_W. \tag{26}$$

Note that from (26) it does not follow that

$$<AB> = <A><B>, \qquad <BA> = <B><A>.$$

For $A, B \in \mathcal{M}_W$, the *Weyl correlation coefficient* is

$$C_W(A, B) = (D_W A D_W B)^{-1/2} <(A - aI) * (B - bI)>_W,$$

where $a = <A>_W$, and $b = <B>_W$. The correlation coefficient is an elementary measure of dependence between the observables $A, B \in \mathcal{M}_W$. If the observables A and B are independent, then by using (26), we obtain

$$C_W(A, B) = 0.$$

Note that from $C_W(A, B) = 0$ it does not follow that $C(A, B) = 0$.

In general,

$$<A * B>_W = <B * A>_W, \qquad <A * B>_W \neq <AB>.$$

Moreover, AB is not an observable, and $A * B$ is an observable. As a result, the correlator $(A; B) = <AB>$, where $A, B \in \mathcal{M}_W$, cannot be used in the general case. If $A \in \mathcal{M}_W$, then we must define the Weyl correlator

$$(A; B)_W = <A * B>_W,$$

where we can use $<A * B>_W = <A * B>$. The Weyl λ-correlator should be defined by

$$<A; B>_{\lambda,\rho} = Tr\big[A * \rho^{\lambda} * B * \rho^{1-\lambda}\big].$$

Using the fact that $\mathcal{M}_W$ is commutative, we have

$$Tr\big[A * \rho^{\lambda} * B * \rho^{1-\lambda}\big] = Tr\big[A * B * \rho^{\lambda} * \rho^{1-\lambda}\big],$$

where $\rho^{\lambda} * \rho^{1-\lambda} \neq \rho$, in general. The canonical correlator on $\mathcal{M}_W$ will be defined by

$$<A; B>_{\lambda} = \int_0^1 d\lambda \, Tr\big[A * \rho^{\lambda} * B * \rho^{1-\lambda}\big].$$

Weyl expectation and Wigner distribution function

Using the Wigner distribution function $\rho_W(q, p)$, the expectation value $<A> = Tr[\rho A]$ can be written in the form

$$<A> = \int dq \, dp \, A(q, p) \rho_W(q, p), \tag{27}$$

where $A(q, p)$ is a symbol of the Weyl ordered operator A.

We may be interested in the expectation values of certain powers of the observable A. For example, the mean square of an observable A is the expectation $<A^2>$. In general, the operator A^2 is not in the Weyl ordered form, so

that equation (27) cannot be directly applied to it. If, however, we bring it into this form by means of the commutation relations to find its Weyl symbol, then $symb(A^2) \neq (symb\ A)^2$. Therefore,

$$<A^2> \neq \int dq\, dp \left(A(q, p)\right)^2 \rho_W(q, p).$$

If we use the Weyl expectation value, then

$$<A^2>_W = <A * A>_W = \int dp\, dq \left(A(q, p)\right)^2 \rho_W(q, p).$$

The Weyl representation involves only concepts that are common to both quantum and classical mechanics.

Derivation superoperator of order $\leqslant k$ on $\mathcal{M}_W$

Let $\mathcal{A}(\mathcal{M}_W)$ be a set of all superoperators on $\mathcal{M}_W$. We define the Lie multiplication on $\mathcal{A}(\mathcal{M}_W)$ by

$$[L_{A*}, \mathcal{L}] = L_{A*}\mathcal{L} - \mathcal{L}L_{A*},$$

where L_{A*} is a left Weyl multiplication by A, i.e.,

$$L_{A*}B = A * B.$$

It allows us to define a derivation superoperator of order $\leqslant k$.

DEFINITION. A *derivation superoperator of order $\leqslant k$* on a commutative associative algebra $\mathcal{M}_W$ is a superoperator $\mathcal{L}$ such that

$$\left[L_{A_0*}, [L_{A_1*}, \ldots [L_{A_k*}, \mathcal{L} \ldots]\right] = 0$$

for all $A_0, A_1, \ldots, A_k \in \mathcal{M}_W$.

The derivation of order $\leqslant k$ on $\mathcal{M}_W$ is also called the *locally Hamiltonian superoperator of order $\leqslant k$*.

A derivation superoperator of order $\leqslant 1$ is defined by the condition

$$\left[L_{A*}, [L_{B*}, \mathcal{L}]\right]X = 0.$$

For $X = I$, this equation gives the Leibnitz rule

$$\mathcal{L}(A * B) - (\mathcal{L}A) * B - A * (\mathcal{L}B) + A * B * \mathcal{L}(I) = 0.$$

Note that if $\mathcal{L}(I) = 0$, then $\mathcal{L}$ is a globally Hamiltonian superoperator on $\mathcal{M}_W$. A derivation superoperator of order $\leqslant 2$ satisfies the equation

$$\left[L_{A*}, \left[L_{B*}, [L_{C*}, \mathcal{L}]\right]\right]X = 0.$$

For $X = I$, we have

$$\begin{aligned}&\mathcal{L}(A * B * C) - \mathcal{L}(A * B) * C - A * \mathcal{L}(B * C) - B * \mathcal{L}(A * C)\\&\quad + \mathcal{L}(A) * B * C + A * \mathcal{L}(B) * C + A * B * \mathcal{L}(C)\\&\quad - A * B * C * \mathcal{L}(I) = 0.\end{aligned}$$

We shall denote the linear space of all derivation of order $\leqslant k$ on $\mathcal{M}_W$ by $\mathcal{A}_k(\mathcal{M}_W)$. It is a common practice to call the elements of $Der_k(\mathcal{M}_W) = \mathcal{A}_k(\mathcal{M}_W)/\mathcal{A}_{k-1}(\mathcal{M}_W)$ derivations of order k. An element of $Der_k(\mathcal{M}_W)$ is also called the *locally Hamiltonian superoperator of order k*.

18.8. Evolution of state in the Schrödinger picture

Quantization for the Liouvillian picture

Let us consider the Weyl quantization of classical equations in the Liouvillian picture. Then we obtain operator equations in the Schrödinger picture.

In the Liouvillian picture, the time evolution of a classical observable $A(t, q, p)$ is described by the equation

$$\frac{d}{dt}A(t, q, p) = \frac{\partial}{\partial t}A(t, q, p).$$

The Weyl quantization of this equation gives

$$\frac{d}{dt}A_s(t) = \frac{\partial}{\partial t}A_s(t), \tag{28}$$

where $A_s(t) = \pi(A(t, q, p)) = A(t, Q, P)$.

Suppose that a classical system, whose pure state is determined by a point (q, p) in $2n$-dimensional phase-space $\mathbb{R}^{2n}$, is described by the equation

$$\frac{\partial}{\partial t}\varrho(t, q, p) = -\mathcal{L}\varrho(t, q, p) - \Omega(q, p)\varrho(t, q, p), \tag{29}$$

where

$$\Omega(q, p) = -\sum_{k=1}^{n} J_{\mathcal{L}}\big[q^k, p^k\big],$$

$$J_{\mathcal{L}}\big[q^k, p^k\big] = \mathcal{L}\big(\big\{q^k, p^k\big\}\big) - \big\{\mathcal{L}\big(q^k\big), p^k\big\} - \big\{q^k, \mathcal{L}\big(p^k\big)\big\}.$$

This is the classical Liouville equation in the Liouvillian picture.

The Weyl quantization of this Liouville equation gives

$$\frac{\partial}{\partial t}\varrho_s(t) = \Lambda_t\varrho_s(t), \tag{30}$$

where $\varrho_s(t) = \pi(\varrho(t, q, p))$, and

$$\Lambda_t = -\pi\big(\mathcal{L} + \Omega\big[L_q^+, L_p^+\big]\big).$$

The superoperator Λ_t is called the Liouville superoperator. Note, that this quantum Liouville equation is directly derived by the Weyl quantization of the classical Liouville equation. The formal solution of (30) can be written by (chronological) T-exponent:

$$\varrho_s(t) = S_t\varrho_s(0), \qquad S_t = T\left\{\exp\int_0^t d\,\tau\,\Lambda_\tau\right\}. \tag{31}$$

If $\Lambda_t = \Lambda$ is a constant superoperator, then $S_t = \exp(t\Lambda)$. This is the evolution superoperator for $\varrho_s(t)$. In general, $Tr[\varrho_s(t)] \neq 1$.

Trace-preserving equation in the Schrödinger picture

We define the density operator with unit trace by

$$\rho_s(t) = \frac{1}{Tr[\varrho_s(t)]}\varrho_s(t).$$

Differentiation of $\rho_s(t)$ with respect to t gives

$$\frac{d}{dt}\rho_s(t) = \Lambda_t\rho_s(t) - \rho_s(t)\,Tr\big[\Lambda_t\rho_s(t)\big]. \tag{32}$$

This is the *trace-preserving quantum Liouville equation* in the Schrödinger picture. This equation is nonlinear with respect to the density operator.

We define the following nonlinear Liouville superoperator

$$\breve{\Lambda}_t = \Lambda_t - Tr\big[\Lambda_t\rho_s(t)\big]L_I = \Lambda_t - <\bar{\Lambda}_t(I)>_t L_I,$$

where $\bar{\Lambda}_t$ is adjoint of Λ_t. Here $<A>_t$ is an expectation value with respect to $\rho_s(t)$, such that

$$<A>_t = \big(\rho_s(t)|A\big) = Tr\big[\rho_s(t)A\big].$$

Then equation (32) can be written in the form

$$\frac{d}{dt}\rho_s(t) = \breve{\Lambda}_t\rho_s(t).$$

This equation is nonlinear. Note that the formal solution *cannot* be presented in the form

$$\rho_s(t) = \breve{S}_t\rho_s, \qquad \breve{S}_t = T\left\{\exp\int_0^t d\,\tau\,\breve{\Lambda}_\tau\right\}.$$

If S_t is an evolution superoperator for $\varrho_s(t)$ (see equation (31)), then

$$\rho_s(t) = \breve{S}_t \rho_s = \big(Tr[S_t \rho_s]\big)^{-1} S_t \rho_s.$$

Here $\breve{S}_t$ is an evolution superoperator for $\rho_s(t)$.

Schrödinger equation

If Λ is a globally Hamiltonian superoperator, then the quantum Liouville equation has the form

$$\frac{d}{dt}\varrho_s(t) = L_H^- \varrho_s(t). \tag{33}$$

Using $Tr[L_H^- \varrho_s] = 0$, we have $\breve{\Lambda}_t = \Lambda_t = L_H^-$. Then $\rho_s(t) = \varrho_s(t)$. A formal solution of (33) can be written in the form

$$\varrho_s(t) = S_t \varrho_s(0), \qquad S_t = \exp\big(t L_H^-\big).$$

Using

$$L_H^- = \frac{1}{i\hbar}(L_H - R_H), \qquad L_H R_H = R_H L_H,$$

we obtain

$$S_t = L_{U_t} R_{U_t^*}, \qquad U_t = \exp\left\{\frac{1}{i\hbar} t H\right\}.$$

If $\varrho_s(0)$ is a pure state at $t = 0$, i.e., $\varrho_s(0) = |\Psi><\Psi|$, then $\varrho_s(t)$ at $t>0$ is a pure state, and

$$\varrho_s(t) = |\Psi(t)><\Psi(t)|,$$

where $|\Psi(t)> = U_t|\Psi>$.

If Λ_t is a globally Hamiltonian superoperator, then the following properties are satisfied:

(1) U_t is a unitary operator $U_t^* U_t = U_t U_t^* = I$.
(2) S_t is a trace preserving superoperator $Tr[\varrho_s(t)] = Tr[\varrho_s]$.
(3) $\breve{S}_t$ is a linear superoperator, and $\breve{S}_t = S_t$.
(4) $\breve{S}_t = S_t$ is a map from a set of pure state into itself. For quantum Hamiltonian systems, pure states evolve into pure states.

Differentiation of the ket-vector $|\Psi(t)>$ with respect to t gives

$$\frac{d}{dt}|\Psi(t)> = -\frac{i}{\hbar} H|\Psi(t)>. \tag{34}$$

This is the *Schrödinger equation*.

In the coordinate representation, equation (34) gives

$$\frac{d}{dt}<q|\Psi(t)> = -\frac{i}{\hbar}<q|H|\Psi(t)>. \tag{35}$$

Using

$$\int dq' \, |q'><q'| = I,$$

we obtain

$$\frac{\partial}{\partial t}\Psi(q,t) = -\frac{i}{\hbar}\int dq' \, H(q,q')\Psi(q',t),$$

where $\Psi(q,t) = <q|\Psi(t)>$ is the wave function, and $H(q,q') = <q|H|q'>$ is a kernel of the Hamilton operator H. If $H(q,q') = \hat{H}(q)\delta(q-q')$, then the Schrodinger equation has the form

$$\frac{\partial}{\partial t}\Psi(q,t) = -\frac{i}{\hbar}\hat{H}(q)\Psi(q,t).$$

This is the Schrödinger equation in the coordinate representation.

The Schrödinger equations provide a quantitative description of the rate of change of the pure states of quantum Hamiltonian systems.

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Chapter 19

Dynamical Deformation of Algebras of Observables

19.1. Evolution as a map

The dynamical structure of Hamiltonian systems is given by one-parameter groups of automorphisms of the underlying kinematical structure, which represent the motion of the systems with time. In classical Hamiltonian mechanics one has a group of diffeomorphisms on a smooth manifold. In quantum dynamics of Hamiltonian systems, we use a group of unitary operators on a Hilbert space. The time development can be given by a strongly continuous one-parameter group of automorphisms of a C^*-algebra. It is conventional to describe symmetries of systems by group of automorphism of the basic kinematical structures. In non-Hamiltonian quantum mechanics, we cannot use automorphisms and endomorphisms to describe dynamics.

Endomorphism of groupoid

In the quantum mechanics, the observables are given by operators. Let $\mathcal{M}$ be a set of the all initial observables of the quantum systems at the time $t = 0$. Let us denote by $\mathcal{M}_t$ the set of the observables of the systems at any later time $t > 0$. The set $\mathcal{M}$, together with a single binary operation on $\mathcal{M}$, is called a groupoid. This is still rather to wide concept. The dynamical structure of the quantum system can be given by a map Φ_t from $\mathcal{M}$ into $\mathcal{M}_t$, which represents the motion of the system with time.

Let us give more mathematically precise the idea that two groupoids $\mathcal{M}$ and $\mathcal{M}_t$, are structurally the same or isomorphic. Clearly that $\mathcal{M}$ and $\mathcal{M}_t$ are isomorphic if the groupoids are identical except for the names of the elements and operations.

(1) To each element $A \in \mathcal{M}$ is assigned its counterpart $A_t \in \mathcal{M}_t$.
(2) Two different elements A and B in $\mathcal{M}$ should have two different counterparts $A_t = \Phi_t A$ and $B_t = \Phi_t B$, that is, the map Φ_t must be one-to-one.
(3) Every element of $\mathcal{M}_t$ must be counterpart of some element of $\mathcal{M}$, that is, Φ_t must be onto $\mathcal{M}_t$.

(4) If the groupoids are to be structurally the same and if we denote the groupoid operation of $\mathcal{M}$ by g and that of $\mathcal{M}_t$ by g_t, then the counterpart of $g(A, B)$ should be $g_t(A_t, B_t)$, i.e., $\Phi_t(g(A, B))$ must be $g_t(\Phi_t A, \Phi_t B)$.

Usually we drop the notations g and g_t for the operations and use multiplicative notations.

Requirement (2) express the mathematical statement that Φ_t is a monomorphism. A homomorphism Φ_t of $\mathcal{M}$ into $\mathcal{M}_t$ that is a one-to-one map is a monomorphism. Requirement (3) is a statement that Φ_t is an epimorphism. A homomorphism Φ_t of $\mathcal{M}$ into $\mathcal{M}_t$ is an epimorphism if it is onto $\mathcal{M}_t$.

Suppose $\mathcal{M}_t \subset \mathcal{M}$ and $g_t = g$. Then an isomorphism of a groupoid $\mathcal{M}$ with a groupoid $\mathcal{M}_t$ is a one-to-one map Φ_t from $\mathcal{M}$ onto $\mathcal{M}_t$ such that for all A and B in $\mathcal{M}$,

$$\Phi_t(AB) = \Phi_t(A)\Phi_t(B).$$

The groupoids $\mathcal{M}$ and $\mathcal{M}_t$ are then isomorphic. An isomorphism of a groupoid onto itself is an automorphism of the groupoid.

An isomorphism of a groupoid $\mathcal{M}$ with a groupoid $\mathcal{M}_t$ was defined as a one-to-one map Φ_t of $\mathcal{M}$ onto $\mathcal{M}_t$ such that for all A and B in $\mathcal{M}$, $\Phi_t(AB) = \Phi_t(A)\Phi_t(B)$, where $\mathcal{M}_t \subset \mathcal{M}$ and $g_t = g$. If we drop the condition that Φ_t be one-to-one and onto, just retaining $\Phi_t(AB) = \Phi_t(A)\Phi_t(B)$, the map Φ_t is then a homomorphism. This requirement is the only one that distinguishes a homomorphism from just any map of $\mathcal{M}$ into $\mathcal{M}_t$. It asserts that Φ_t is a structure-relating map. The algebraic structure of $\mathcal{M}$ is completely determined by the binary operation on $\mathcal{M}$, and that of $\mathcal{M}_t$ is completely determined by the operation on $\mathcal{M}_t$. The homomorphism condition thus relates the structure of $\mathcal{M}$ to that of $\mathcal{M}_t$.

If $\mathcal{M}_t \subset \mathcal{M}$ and $g_t = g$, then an isomorphism Φ_t of a ring $\mathcal{M}$ with a ring $\mathcal{M}_t$ is a one-to-one mapping $\mathcal{M}$ onto $\mathcal{M}_t$ such that for all A and B in $\mathcal{M}$,

$$\Phi_t(AB) = \Phi_t(A)\Phi_t(B), \qquad \Phi_t(A + B) = \Phi_t(A) + \Phi_t(B).$$

The rings $\mathcal{M}$ and $\mathcal{M}_t$ are then isomorphic.

Time evolution is not endomorphism of an operator ring

Let $\mathcal{M}$ be an operator ring. If the equation

$$\frac{d}{dt}A_t = \mathcal{L}A_t \tag{1}$$

describes a non-Hamiltonian quantum system, then there exist A and B in $\mathcal{M}$ such that

$$Z_{\mathcal{L}}(A, B) = \mathcal{L}(AB) - \mathcal{L}(A)B - A\mathcal{L}(B) \neq 0.$$

Formally, the solution of the operator differential equation is $A_t = \Phi_t A$, where $\Phi_t = \exp\{t\mathcal{L}\}$. Differentiation of the homomorphism condition

$$\Phi_t(AB) = \Phi_t(A)\Phi_t(B)$$

with respect to t gives

$$\frac{d\Phi_t(AB)}{dt} = \frac{d\Phi_t(A)}{dt}\Phi_t(B) + \Phi_t(A)\frac{d\Phi_t(B)}{dt}$$

for all $A, B \in D(\Phi_t)$. For $t = 0$, we obtain

$$\mathcal{L}(AB) = \mathcal{L}(A)B + A\mathcal{L}(B)$$

for all $A, B \in D(\mathcal{L})$ such that $AB \in D(\mathcal{L})$. This equation means that the quantum system is locally Hamiltonian and $Z_{\mathcal{L}}(A, B) = 0$. Therefore, in non-Hamiltonian quantum dynamics, we cannot use endomorphisms of $\mathcal{M}$, together with a multiplicative operation $g_t = g$.

Environment-induced noncommutativity

An endomorphism of an involutive unital operator algebra $\mathcal{M}$ is a bounded superoperator Φ_t such that the following conditions are satisfied:

(1) $\Phi_t(aA + bB) = a\Phi_t(A) + b\Phi_t(B)$ for all $A, B \in \mathcal{M}$, and $a, b \in \mathbb{C}$.
(2) $\Phi_t(0) = 0$.
(3) $\Phi_t(I) = 1$.
(4) $\Phi_t(A)^* = \Phi_t(A^*)$ for all $A \in \mathcal{M}$ such that $A^* \in \mathcal{M}$.
(5) $\Phi_t(AB) = \Phi_t(A)\Phi_t(B)$ for all $A, B \in \mathcal{M}$.

These relations are satisfied for quantum Hamiltonian dynamics. The time evolution of quantum non-Hamiltonian systems is not an endomorphism of algebras of observables if $g_t = g$. If the time evolution of the non-Hamiltonian system is an endomorphism of a linear operator space, then

(1) $\Phi_t(A + B) = \Phi_t(A) + \Phi_t(B)$ for all $A, B \in \mathcal{M}$,
(2) $\Phi_t(cA) = c\Phi_t(A)$ for all $A \in \mathcal{M}$ and $c \in \mathbb{C}$,
(3) $\Phi_t(0) = 0$.

In general, Φ_t is not an endomorphism of the linear space. It is well-known that strange attractors of classical non-Hamiltonian systems are not linear spaces. In quantum theory, there are analogous situations for quantum analogs of (regular or strange) attractors.

STATEMENT. *A time evolution Φ_t of observables of a quantum non-Hamiltonian system is not an endomorphism with respect to Lie, Jordan and associative multiplications. There exist observables $A, B \in \mathcal{M}$ such that*

$$\Phi_t(AB) \neq \Phi_t(A)\Phi_t(B),$$

$$\Phi_t(A \cdot B) \neq \Phi_t(A) \cdot \Phi_t(B),$$

$$\Phi_t(A \circ B) \neq \Phi_t(A) \circ \Phi_t(B).$$

The map Φ_t is an endomorphism of $\mathcal{M}$ with respect to multiplicative binary operations $g_t = g$ (in Lie, Jordan and associative algebras) if and only if the system is locally Hamiltonian.

In general, the time evolution described by Φ_t is not an endomorphism with respect to multiplication in $\mathcal{M}$. There exist observables A and B such that

$$\Delta\Phi_t(A, B) = \Phi_t(AB) - \Phi_t(A)\Phi_t(B) \neq 0.$$

If $\mathcal{L}$ is a constant superoperator, then

$$\Delta\Phi_t(A, B) = tZ_{\mathcal{L}}(A, B) + \cdots.$$

It is easy to see, that if $\Delta\Phi_t(A, B) = 0$ for all $t > 0$, then $Z_{\mathcal{L}}(A, B) = 0$.

In quantum non-Hamiltonian dynamics, there exists an effect of *appearing noncommutativity*.

(1) Let A, B be commutative observables ($[A, B] = 0$). In general, the evolution gives $[A_t, B_t] = [\Phi_t(A), \Phi_t(B)] \neq 0$.
(2) If $[\rho_1(0), \rho_2(0)] = 0$, we can have $[\rho_1(t), \rho_2(t)] \neq 0$ for $t > 0$. This is the "environment-induced noncommutativity" [119].

In general, the time evolution cannot be considered as an endomorphism of an operator algebra. The time evolution of non-Hamiltonian systems is not an endomorphism of a linear space structure, since these exist strange attractors that cannot be considered as linear spaces. It is possible to generalize a kinematical structure such that it will be "invariant" with respect to time evolution. This generalization should be connected with a notion of one-parameter operations and t-deformation of the underlying algebraic structure.

19.2. Rule of term-by-term differentiation

Suppose that a quantum system is described by equation (1). If we consider a Cauchy problem for this equation in which the initial condition is given by A at the time $t = 0$, then its solution can be written in the form $A_t = \Phi_t(A)$. The rule of term-by-term differentiation (the Leibnitz rule) with respect to time has the form

$$\frac{d}{dt}g(A_t, B_t) = g\left(\frac{dA_t}{dt}, B_t\right) + g\left(A_t, \frac{dB_t}{dt}\right),$$

where g is a binary operation on $\mathcal{M}$. If $\mathcal{M}$ is a Lie algebra, then the operation $g(A, B) = A \cdot B = (1/i\hbar)[A, B]$. This Leibnitz rule is a generalization of the rule for the derivative of the multiplication of two functions.

STATEMENT. *If the rule of term-by-term differentiation* (*Leibnitz rule*) *with respect to time and the canonical commutation relations*

$$\begin{aligned}&\big[Q_k(t),\, P_l(t)\big] = i\hbar\delta_{kl} I,\\ &\big[Q_k(t),\, Q_l(t)\big] = \big[P_k(t),\, P_l(t)\big] = 0, \quad k, l = 1, \dots, n,\end{aligned} \tag{2}$$

are valid for all $t > 0$*, then the quantum Helmholtz conditions*

$$J_{\mathcal{L}}\big(Q_k(t),\, P_l(t)\big) = J_{\mathcal{L}}\big(Q_k(t),\, Q_l(t)\big) = J_{\mathcal{L}}\big(P_k(t),\, P_l(t)\big) = 0$$

are satisfied for all $t > 0$*, and the superoperator* $\mathcal{L}$ *is locally Hamiltonian.*

PROOF. Differentiation of the first relation in (2) with respect to time t gives

$$\frac{d}{dt}\big[Q_k(t),\, P_l(t)\big] = 0.$$

The rule of term-by-term differentiation for the commutator $[Q_k(t),\, P_l(t)]$ has the form

$$\frac{d}{dt}\big[Q_k(t),\, P_l(t)\big] = \left[\frac{d}{dt}Q_k(t),\, P_l(t)\right] + \left[Q_k(t),\, \frac{d}{dt}P_l(t)\right].$$

Consequently, we have

$$\left[\frac{d}{dt}Q_k(t),\, P_l(t)\right] + \left[Q_k(t),\, \frac{d}{dt}P_l(t)\right] = 0.$$

Using the equations of motion

$$\frac{dQ_k(t)}{dt} = \mathcal{L}\big(Q_k(t)\big), \qquad \frac{dP_k(t)}{dt} = \mathcal{L}\big(P_k(t)\big),$$

we obtain

$$\big[\mathcal{L}\big(Q_k(t)\big),\, P_l(t)\big] + \big[Q_k(t),\, \mathcal{L}\big(P_l(t)\big)\big] = 0.$$

If $\mathcal{L}(I) = 0$, then

$$\mathcal{L}\big(\big[Q_k(t),\, P_l(t)\big]\big) - \big[\mathcal{L}\big(Q_k(t)\big),\, P_l(t)\big] - \big[Q_k(t),\, \mathcal{L}\big(P_l(t)\big)\big] = 0.$$

As a result, $J_{\mathcal{L}}(Q_k(t),\, P_l(t)) = 0$. Similarly, considering other canonical commutation relations (2), we obtain all of the identities

$$J_{\mathcal{L}}\big(X^k(t),\, X^l(t)\big) = 0,$$

where $X^k = Q_k,\, P_k$. Then, the quantum system is locally Hamiltonian. □

As a result, if the rule of term-by-term differentiations and the canonical commutation relations are valid for all $t \geqslant 0$, then $\mathcal{L}$ is locally Hamiltonian. For

quantum non-Hamiltonian systems, either the canonical commutation relations or the Leibnitz rule for multiplication is not valid.

It is interesting to find a generalization $[\ ,\ ]_t$ of the commutator $[\ ,\ ]$, such that the commutation relations

$$\big[Q_k(t), Q_l(t)\big]_t = 0, \qquad \big[P_k(t), P_l(t)\big]_t = 0, \qquad \big[Q_k(t), P_l(t)\big]_t = i\hbar\delta_{kl}$$

are satisfied for all $t \geqslant 0$. This operation $[\ ,\ ]_t$ can be called the *t-invariant commutator* for quantum non-Hamiltonian system. The canonical commutation relations are satisfied for quantum Hamiltonian systems. Then, we have $[A_t, B_t]_t = [A_t, B_t]$, for all $A, B \in \mathcal{M}$ and $t > 0$ if and only if $J_{\mathcal{L}}(A_t, B_t) = 0$.

If $\mathcal{L}$ is a bounded generating superoperator of the one-parameter semi-group

$$\Phi_t = \exp\{t\mathcal{L}\} = \sum_{n=0}^{\infty} \frac{t^n}{n!}\mathcal{L}^n = L_I + t\mathcal{L} + \cdots \quad (t > 0),$$

then $[\ ,\ ]_t$ can be presented by

$$[A, B]_t = [A, B] + J_{\mathcal{L}}[A, B]t + \cdots, \tag{3}$$

where $J_{\mathcal{L}}[A, B] = \mathcal{L}([A, B]) - [\mathcal{L}(A), B] - [A, \mathcal{L}(B)] = i\hbar J_{\mathcal{L}}(A, B)$. Differentiation of equation (3) with respect to time t gives

$$\frac{d}{dt}[A, B]_t = J_{\mathcal{L}}[A, B] + \cdots.$$

For $t = 0$, we obtain

$$\left(\frac{d}{dt}[A, B]_t\right)_{t=0} = J_{\mathcal{L}}[A, B].$$

As a result, the Jacobian $J_{\mathcal{L}}[A, B] = i\hbar J_{\mathcal{L}}(A, B)$ is an infinitesimal commutator.

19.3. Time evolution of binary operations

Suppose M is a set of the all initial observables of the quantum systems at the time $t = 0$. Let us denote by M_t the set of the observables of the systems at any later time $t > 0$. We assume that $M_t \subset \mathcal{M}$. The map Φ_t from M into M_t describes the motion of $A \in M$. Here Φ_t is a one-parameter superoperator from M into M_t.

A set M, together with a single binary operation g on M, is a groupoid $\mathcal{M} = <M, g>$. If the groupoid operation of M_t is $g_t = g$, then we obtain the statement that Φ_t is not an endomorphism of $\mathcal{M} = <M, g>$ The time evolution of non-Hamiltonian system is not endomorphism with respect to operation g:

$$\Phi_t\big(g(A, B)\big) \neq g\big(\Phi_t(A), \Phi_t(B)\big).$$

Let us denote the groupoid operation on M_t by g_t. In general, $g_t \neq g_s$ if $t \neq s$. A set M_t, together with a single binary operation g_t on M_t, is a groupoid $\mathcal{M}_t = <M_t, g_t>$. Then g_t is a *one-parameter binary operation*. If the groupoids $<M, g>$ and $<M_t, g_t>$ are to be structurally the same, then the counterpart of $g(A, B)$ should be $g_t(A_t, B_t)$, i.e., $\Phi_t(g(A, B))$ must be $g_t(\Phi_t A, \Phi_t B)$.

DEFINITION. Suppose Φ_t is a map from a set M into a set M_t for each fixed $t \in \mathbb{R}$, and $A_t = \Phi_t A$, $B_t = \Phi_t B$ are in M_t. A *one-parameter binary operation* on a set M_t is a mapping $g_t : M_t \times M_t \to M_t$ that assigns to each ordered pair of elements $A_t, B_t \in M_t$ some element $g_t(A_t, B_t)$ of the set M_t.

The following are examples of some one-parameter binary operations.

(1) Suppose $\mathcal{M} = <M, g_0>$ is an associative operator algebra, and M is a underlying linear space. If $\mathcal{L}$ is a bounded linear superoperator on $\mathcal{M}$, then we can define a one-parameter binary operation on $M_t = M$ of the form

$$g_t(A, B) = g_0(A, B) + t Z_{\mathcal{L}}(A, B),$$

where

$$Z_{\mathcal{L}}(A, B) = \mathcal{L}\big(g_0(A, B)\big) - g_0\big(\mathcal{L}(A), B\big) - g_0\big(A, \mathcal{L}(B)\big).$$

This is the Leibnitz defect. Note that

$$\frac{dg_t(A, B)}{dt} = Z_{\mathcal{L}}(A, B).$$

As a result, $\mathcal{M}_t = <M, g_t>$ is an operator algebra for each fixed t.

(2) Let Φ_t be a bounded superoperator on a linear operator space $\mathcal{M}$. For each fixed $t \geqslant 0$, we can consider subspace $\mathcal{M}_t = \{\Phi_t A\colon\ A \in \mathcal{M}\}$ of $\mathcal{M}$, together with a one-parameter binary operation g_t such that

$$g_t(A_t, B_t) = \sum_{k=1}^{\infty} t^{k-1} G_k(A_t, B_t),$$

where $A_t = \Phi_t A$, $B_t = \Phi_t B$, and $\{G_k, k \in \mathbb{N}\}$ is an infinite set of binary operations G_k on $\mathcal{M}_t$.

(3) Suppose $\mathcal{M}$ is an associative operator algebra, and M is a underlying linear space. We can consider a one-parameter binary operation on M of the form

$$g_\lambda = \lambda(AB + BA) + (1 - \lambda)(AB - BA),$$

where $\lambda \in [0, 1]$. For $\lambda = 0$, we have $g_0(A, B) = AB - BA$. For $\lambda = 1$, we have $g_1(A, B) = AB + BA$. If $\lambda = 1/2$, then $g_{1/2}(A, B) = AB$. Note that

$$\frac{dg_\lambda(A, B)}{d\lambda} = 2BA.$$

As a result, we have the algebra $\mathcal{M}_\lambda = <M, g_\lambda>$ such that $\mathcal{M}_0 = \mathcal{M}^{(-)}$ and $\mathcal{M}_1 = \mathcal{M}^{(+)}$ and $\mathcal{M}_{1/2} = \mathcal{M}$. Then $\mathcal{M}_\lambda$ is a generalization of the associative algebra $\mathcal{M}$ and the Lie–Jordan algebra $\mathcal{M}^{(\pm)}$.

DEFINITION. A map Φ_t of a groupoid $<\mathcal{M}, g>$ into a groupoid $<\mathcal{M}_t, g_t>$ is a *one-parameter homomorphism* if

$$\Phi_t\big(g(A, B)\big) = g_t(\Phi_t A, \Phi_t B) \tag{4}$$

for all elements A and B in $\mathcal{M}$.

We shall denote the set of all one-parameter homomorphisms from $\mathcal{M}_s$ into $\mathcal{M}_t$ by $\mathrm{Hom}(\mathcal{M}_s, \mathcal{M}_t)$. The binary operation g_t can be considered as a superoperator from $\mathcal{M}_t \times \mathcal{M}_t$ into $\mathcal{M}_t$ that assigns to each pair A_t, B_t of $\mathcal{M}_t$ exactly one operator $C_t = g_t(A_t, B_t)$ of $\mathcal{M}_t$. If there exist $A, B, C \in \mathcal{M}_0$ such that $\Phi_t A = A_t$, $\Phi_t B = B_t$ and $\Phi_t C = C_t$, then in general $g(A, B) \neq C$. If $g(A, B) = C$, then Φ_t is a one-parameter endomorphism.

If $\Phi_t \Phi_s = \Phi_{t+s}$ and $\Phi_0 = L_I$, then

$$g_t\, g_s = g_{t+s}, \quad g_0 = g.$$

As a result, the binary operations g_t, $t > 0$, form a one-parameter semi-group.

Let $t \to \Phi_t$ and $t \to g_t$ be continuous maps (superoperators). Differentiation of equation (4) with respect to t gives

$$\frac{d\Phi_t(g(A, B))}{dt} = g_t\left(\frac{d\Phi_t(A)}{dt}, \Phi_t(B)\right) + g_t\left(\Phi_t(A), \frac{d\Phi_t(B)}{dt}\right) + \frac{dg_t}{dt}\big(\Phi_t(A), \Phi_t(B)\big) \tag{5}$$

for all $A, B \in D(\Phi_t)$.

If $g_t = g$, then $dg_t/dt = 0$ and equation (5) has the form

$$\frac{d\Phi_t(g(A, B))}{dt} = g\left(\frac{d\Phi_t(A)}{dt}, \Phi_t(B)\right) + g\left(\Phi_t(A), \frac{d\Phi_t(B)}{dt}\right). \tag{6}$$

Using

$$\frac{d\Phi_t}{dt} = \mathcal{L}\Phi_t,$$

equation (6) at $t = 0$ has the form $\mathcal{L}(AB) = \mathcal{L}(A)B + A\mathcal{L}(B)$. In general, equation (5) at $t = 0$ gives

$$\mathcal{L}(AB) = \mathcal{L}(A)B + A\mathcal{L}(B) + Z(A, B) \tag{7}$$

where

$$Z(A, B) = \lim_{t \to 0+} \frac{dg_t}{dt}\big(\Phi_t(A), \Phi_t(B)\big).$$

Then $Z(A, B)$ is a Leibnitz defect, i.e., $Z(A, B) = Z_{\mathcal{L}}(A, B)$. As a result, we obtain

$$g_t(A, B) = g(A, B) + tZ_{\mathcal{L}}(A, B) + \cdots.$$

19.4. Bilinear superoperators

Let $\mathcal{M}$ be a linear operator space. A linear superoperator is a map $\mathcal{L}$ from $\mathcal{M}$ into itself, such that the following requirements are satisfied:

(1) $\mathcal{L}(A + B) = \mathcal{L}(A) + \mathcal{L}(B)$ for all $A, B \in \mathcal{D}(\mathcal{L}) \subset \mathcal{M}$.
(2) $\mathcal{L}(aA) = a\mathcal{L}(A)$ for all $A \in \mathcal{D}(\mathcal{L}) \subset \mathcal{M}$ and $a \in \mathbb{C}$.

The *direct product* of sets $\mathcal{M}_1$ and $\mathcal{M}_2$ is the set of all ordered pairs A, B, where $A \in \mathcal{M}_1$ and $B \in \mathcal{M}_2$. The direct product is denoted by $\mathcal{M}_1 \times \mathcal{M}_2$.

DEFINITION. A *bilinear superoperator* is a map $Z(\cdot,\cdot)$ from $\mathcal{M} \times \mathcal{M}$ into $\mathcal{M}$ such that the following requirements are satisfied:

(1) $Z(A, \cdot)$ is a linear superoperator for all $A \in D_1(Z) \subset \mathcal{M}$ with domain $D_2(Z)$.
(2) $Z(\cdot, B)$ is a linear superoperator for all $B \in D_2(Z) \subset \mathcal{M}$ with domain $D_1(Z)$.
(3) $Z(A, \cdot)B = Z(\cdot, B)A = Z(A, B)$ for all $A \in D_1(Z)$ and $B \in D_2(Z)$.

The direct product $D_1(Z) \times D_2(Z) \subset \mathcal{M} \times \mathcal{M}$ is called the domain of Z. We denote this domain by $D(Z)$.

We illustrate this notion with the following examples.

(a) Let $\mathcal{M}$ be an operator algebra with binary operation g. If Φ is a linear superoperator from $\mathcal{M}$ into itself, then we can define the superoperator

$$\Psi(A, B) = \Phi\big(g(A, B)\big) - g\big(\Phi(A), \Phi(B)\big).$$

If Φ is a homomorphism, then $\Psi(A, B) = 0$. In general, $\Psi(A, B) \neq 0$. In this case, Ψ is a bilinear superoperator. Note that Ψ can be considered as a binary operation on $\mathcal{M}$.

(b) Let $\mathcal{L}$ be a linear superoperator on $\mathcal{M}$. Then the Leibnitz defect

$$Z_{\mathcal{L}}(A, B) = \mathcal{L}\big(g(A, B)\big) - g\big(\mathcal{L}(A), B\big) - g\big(A, \mathcal{L}(B)\big) \tag{8}$$

is a bilinear superoperator. The Leibnitz defect of a superoperator $\mathcal{L}$ shows how much the deviation of $\mathcal{L}$ from a derivation superoperator. If $\mathcal{M}$ is an associative operator algebra with multiplication $g(A, B) = AB$, then the Leibnitz defect is

defined by

$$Z_{\mathcal{L}}(A, B) = \mathcal{L}(AB) - \mathcal{L}(A)B - A\mathcal{L}(B).$$

(c) If $\mathcal{M}^{(-)}$ is a Lie algebra, together with the binary operation

$$g(A, B) = A \cdot B = \frac{1}{i\hbar}[A, B] = \frac{1}{i\hbar}(AB - BA),$$

then the Leibnitz defect is called the *Jacobian*. The classic notation to denote the Jacobian is

$$\begin{aligned} J_{\mathcal{L}}(A, B) &= Z_{\mathcal{L}}^{(-)}(A, B) = \mathcal{L}(A \cdot B) - (\mathcal{L}A) \cdot B - A \cdot (\mathcal{L}B) \\ &= \frac{1}{i\hbar}\big(\mathcal{L}\big([A, B]\big) - \big[\mathcal{L}(A), B\big] - \big[A, \mathcal{L}(B)\big]\big). \end{aligned}$$

It is not hard to prove the relation

$$J_{\mathcal{L}}(A, B) = \frac{1}{i\hbar}\big(Z_{\mathcal{L}}(A, B) - Z_{\mathcal{L}}(B, A)\big).$$

The Jacobian is a bilinear superoperator.

(d) If $\mathcal{M}^{(+)}$ is a special Jordan algebra with the binary operation

$$g(A, B) = A \circ B = [A, B]_+ = \frac{1}{2}(AB + BA),$$

then the Leibnitz defect is called the *Jordanian*. The classic notation to denote the Jordanian is

$$K_{\mathcal{L}}(A, B) = Z_{\mathcal{L}}^{(+)}(A, B) = \mathcal{L}\big([A, B]_+\big) - \big[\mathcal{L}(A), B\big]_+ - \big[A, \mathcal{L}(B)\big]_+.$$

Note that

$$K_{\mathcal{L}}(A, B) = \frac{1}{2}\big(Z_{\mathcal{L}}(A, B) + Z_{\mathcal{L}}(B, A)\big).$$

The Jordanian is a bilinear superoperator.

(e) A bilinear superoperator is a binary operation on $\mathcal{M}$. Let $\mathcal{M}$ be an operator algebra with binary operation g. If

$$\begin{aligned} g(aA + bB, C) &= ag(A, C) + bg(B, C), \\ g(C, aA + bB) &= ag(C, A) + bg(C, B), \end{aligned}$$

then g is a bilinear superoperator.

A bilinear superoperator on $\mathcal{M}$ can be considered as a binary operation on $\mathcal{M}$. For quantum Hamiltonian systems the bilinear superoperators $Z_{\mathcal{L}}$, $J_{\mathcal{L}}$, and $K_{\mathcal{L}}$ are degenerated, i.e., all Leibnitz defects vanish

$$Z_{\mathcal{L}}(A, B) = J_{\mathcal{L}}(A, B) = K_{\mathcal{L}}(A, B) = 0$$

for all $A, B \in \mathcal{M}$.

We will consider the superoperator $\mathcal{L}$ such that the bilinear superoperators $Z_{\mathcal{L}}$, $J_{\mathcal{L}}$, and $K_{\mathcal{L}}$ are nondegenerate. Then *the bilinear superoperators $Z_{\mathcal{L}}$, $J_{\mathcal{L}}$, and $K_{\mathcal{L}}$ can be considered as binary algebraic operations on $\mathcal{M}$*. There is an important relationship between these binary operations and the non-Hamiltonian superoperator $\mathcal{L}$.

A binary operation $J_{\mathcal{L}}$ on $\mathcal{M}$ is a skew-symmetric operation,

$$J_{\mathcal{L}}(A, B) = -J_{\mathcal{L}}(B, A)$$

for $A, B \in \mathcal{M}$. A binary operation $K_{\mathcal{L}}$ on $\mathcal{M}$ is commutative

$$K_{\mathcal{L}}(A, B) = K_{\mathcal{L}}(B, A)$$

for $A, B \in \mathcal{M}$.

Let $\mathcal{L}$ be a linear superoperator on an operator algebra $\mathcal{M}$. We can consider a one-parameter binary operation on $\mathcal{M}$ of the form

$$g_t(A, B) = g(A, B) + t Z_{\mathcal{L}}(A, B),$$

where $Z_{\mathcal{L}}(A, B)$ is defined by (8).

19.5. Cohomology groups of bilinear superoperators

Definition of cohomology group

Let us define a cohomology group. For $n \geqslant 0$, we let $C^n(\mathcal{M}^n, \mathcal{M})$ be the commutative group of all maps from $\mathcal{M}^n$ to $\mathcal{M}$:

$$C^n(\mathcal{M}, \mathcal{M}) = \{\Phi\colon \mathcal{M}^n \to \mathcal{M}\}.$$

Its elements are called the *n-cochains*. We further define the group homomorphisms

$$\delta^n\colon C^n(\mathcal{M}, \mathcal{M}) \to C^{n+1}(\mathcal{M}, \mathcal{M})$$

by the equation

$$\delta^n\Phi(A_0, \ldots, A_n) = A_0\Phi(A_1, \ldots, A_n) + (-1)^{n+1}\Phi(A_0, \ldots, A_{n-1})A_n + \sum_{k=0}^{n-1}(-1)^{k+1}\Phi(A_0, \ldots, A_{k-1}, A_kA_{k+1}, A_{k+2}, \ldots, A_n).$$

They are known as the coboundary homomorphisms.

For $n \geqslant 0$, we define the group of n-cocycles as

$$Z^n(\mathcal{M}, \mathcal{M}) = \operatorname{Ker}(\delta^n),$$

and the group of n-coboundaries as

$$B^n(\mathcal{M}, \mathcal{M}) = \mathrm{Im}\big(\delta^{n-1}\big) \quad (n \geqslant 1), \qquad B^0(\mathcal{M}, \mathcal{M}) = 0.$$

Then the cohomology group is defined by

$$H^n(\mathcal{M}, \mathcal{M}) = Z^n(\mathcal{M}, \mathcal{M})/B^n(\mathcal{M}, \mathcal{M}).$$

First cohomology group and derivations

Let $\mathcal{M}$ be an operator algebra. A derivation of $\mathcal{M}$ is a superoperator $\mathcal{L}$ on $\mathcal{M}$ such that the Leibnitz rule

$$\mathcal{L}(AB) = \mathcal{L}(A)B + A\mathcal{L}(B)$$

is valid for all $A, B \in \mathcal{M}$. A superoperator $\mathcal{L}$ is an inner derivation, if there exists $H \in \mathcal{M}$ such that $\mathcal{L}(A) = [H, A]$ for all $A \in \mathcal{M}$.

A derivation is an element of $Z^1(\mathcal{M}, \mathcal{M})$. All elements of $Z^1(\mathcal{M}, \mathcal{M})$ are derivations on $\mathcal{M}$. An inner derivative can be considered as an element of $B^1(\mathcal{M}, \mathcal{M})$. All elements of $B^1(\mathcal{M}, \mathcal{M})$ are inner derivations on $\mathcal{M}$. Then $B^1(\mathcal{M}, \mathcal{M})$ is a subgroup of $Z^1(\mathcal{M}, \mathcal{M})$. The factor group $Z^1(\mathcal{M}, \mathcal{M})/B^1(\mathcal{M}, \mathcal{M})$ is a first cohomology group $H^1(\mathcal{M}, \mathcal{M})$. Then $H^1(\mathcal{M}, \mathcal{M})$ is interpreted as a set of all outer derivations. If $H^1(\mathcal{M}, \mathcal{M}) = 0$, then all derivation of $\mathcal{M}$ are inner.

Derivations	$Der(\mathcal{M})$	$Z^1(\mathcal{M}, \mathcal{M})$
Inner derivations	$Inn(\mathcal{M})$	$B^1(\mathcal{M}, \mathcal{M})$
Outer derivations	$Out(\mathcal{M})$	$H^1(\mathcal{M}, \mathcal{M})$

The first cohomology group $H^1(\mathcal{M}, \mathcal{M})$ can be interpreted as a group of infinitesimal automorphisms. If Φ_t is an automorphism of $\mathcal{M}$, then

$$\mathcal{L} = \left(\frac{d}{dt}\Phi_t\right)_{t=0}$$

is an infinitesimal superoperator on $\mathcal{M}$, i.e., "infinitesimal automorphism" of $\mathcal{M}$.

Let $\mathcal{M}$ be a Lie algebra. An element of $C^1(\mathcal{M}, \mathcal{M})$, the group of 1-cochains of $\mathcal{M}$ with coefficients in itself, is a linear superoperator on $\mathcal{M}$. Then

$$C^1(\mathcal{M}, \mathcal{M}) = \mathcal{A}(\mathcal{M}).$$

The condition $\delta^1(\mathcal{L}) = 0$, where $\mathcal{L} \in C^1(\mathcal{M}, \mathcal{M})$, means that $\mathcal{L}$ is a derivation on $\mathcal{M}$:

$$\big(\delta^1\mathcal{L}\big)(A, B) = \mathcal{L}(A \cdot B) - \mathcal{L}(A) \cdot B - A \cdot \mathcal{L}(B).$$

Then

$$\big(\delta^1\mathcal{L}\big)(A, B) = J_{\mathcal{L}}(A, B)$$

is the Jacobian of $\mathcal{L}$.

If $C^0(\mathcal{M}, \mathcal{M})$ is a group of 0-cochains of the Lie algebra $\mathcal{M}$ with coefficients in itself, then $C^0(\mathcal{M}, \mathcal{M})$ is the algebra $\mathcal{M}$:

$$C^0(\mathcal{M}, \mathcal{M}) = \mathcal{M}.$$

For $A \in \mathcal{M}$, the elements

$$\big(\delta^0 A\big)(B) = -A \cdot B = [A, B]$$

are inner derivations.

Second cohomology group

The second cohomology group $H^2(\mathcal{M}, \mathcal{M})$ of an algebra $\mathcal{M}$ may be interpreted as the group of infinitesimal deformations of $\mathcal{M}$.

Let $\mathcal{M}$ be a Lie operator algebra, together with a binary operation g.

DEFINITION. A *deformation of a Lie algebra* $<\mathcal{M}, g>$ is a one-parameter bilinear superoperator g_t that is a map from $\mathcal{M} \times \mathcal{M} \times \mathbb{R}$ into $\mathcal{M}$ such that

(1) $<\mathcal{M}, g_t>$ is a Lie algebra for each $t \in \mathbb{R}$.
(2) $g_t(A, B) = g(A, B)$ for $t = 0$.

There exists the bilinear (infinitesimal) superoperator

$$G_1(A, B) = \left(\frac{d}{dt} g_t(A, B)\right)_{t=0}.$$

Then the skew-symmetry condition $g_t(A, B) = -g_t(B, A)$ gives

$$G_1(A, B) = -G_1(B, A). \tag{9}$$

Differentiation of the Jacobi identity

$$g_t\big(g_t(A, B), C\big) + g_t\big(g_t(B, C), A\big) + g_t\big(g_t(C, A), B\big) = 0 \tag{10}$$

at $t = 0$ gives

$$\begin{aligned} &G_1\big([A, B], C\big) + G_1\big([B, C], A\big) + G_1\big([C, A], B\big) \\ &\quad + \big[G_1(A, B), C\big] + \big[G_1(B, C), A\big] + \big[G_1(C, A), B\big] = 0. \end{aligned} \tag{11}$$

DEFINITION. Let $\mathcal{M}$ be a Lie algebra. An *infinitesimal deformation* is a bilinear superoperator G_1 such that equations (9) and (11) are valid for all $A, B, C \in \mathcal{M}$.

One-parameter families g_t and f_t of deformations of an algebra $\mathcal{M}$ are called the equivalent deformations if there exists a linear one-parameter automorphism Φ_t of $\mathcal{M}$ such that $\Phi_t(A) = A$ for all $A \in \mathcal{M}$, and

$$\Phi_t\big(f_t(A, B)\big) = g_t\big(\Phi_t(A), \Phi_t(B)\big).$$

If G_1 and F_1 are infinitesimal deformations such that

$$G_1(A, B) = \left(\frac{d}{dt} g_t(A, B)\right)_{t=0}, \qquad F_1(A, B) = \left(\frac{d}{dt} f_t(A, B)\right)_{t=0},$$

then

$$F_1(A, B) = G_1(A, B) + \big[\mathcal{L}(A), B\big] + \big[A, \mathcal{L}(B)\big],$$

where $\mathcal{L} = (d\Phi_t/dt)_{t=0}$. The second cohomology group $H^2(\mathcal{M}, \mathcal{M})$ of $\mathcal{M}$ is interpreted as the group of infinitesimal deformations of $\mathcal{M}$.

If the deformation g_t has the form

$$g_t(A, B) = [A, B] + tG_1(A, B) + t^2 G_2(A, B) + \cdots,$$

then the Jacoby identity (10) gives

$$[A, B, C]_t = P[A, B, C]_0 + tP[A, B, C]_1 + t^2 P[A, B, C]_2 + \cdots,$$

where P is a permutation operation such that

$$P[A, B, C]_k = [A, B, C]_k + [B, C, A]_k + [C, A, B]_k,$$

and

$$\begin{aligned}
&[A, B, C]_t = g_t\big(g_t(A, B), C\big), \qquad [A, B, C]_0 = g\big(g(A, B), C\big),\\
&[A, B, C]_1 = g\big(G_1(A, B), C\big) + G_1\big(g(A, B), C\big),\\
&[A, B, C]_2 = g\big(G_2(A, B), C\big) + G_1\big(G_1(A, B), C\big) + G_2\big(g(A, B), C\big).
\end{aligned}$$

The equation $P[A, B, C]_0 = 0$ is the Jacobi identity for g, and $P[A, B, C]_t = 0$ is the Jacobi identity for g_t. The condition $P[A, B, C]_1 = 0$ gives equation (11). The equation $P[A, B, C]_2 = 0$ gives that $PG_1(G_1(A, B), C)$ is equal to $-P[g(G_2(A, B), C) + G_2(g(A, B), C)]$.

19.6. Deformation of operator algebras

This section contains the definitions and certain theorems of a deformation theory for operator algebras. The deformation of algebras was investigated by M. Gerstenhaber [65]. We consider mainly associative and Lie algebras, but the definitions holds for wider classes of algebras. The second cohomology group $H^2(\mathcal{M}, \mathcal{M})$ of an algebra $\mathcal{M}$ will be interpreted as the group of infinitesimal

deformations of $\mathcal{M}$ in the same way that the first cohomology group $H^1(\mathcal{M}, \mathcal{M})$ (derivations of $\mathcal{M}$ into itself modulo inner derivations) is interpreted as the group of infinitesimal automorphisms.

Infinitesimal deformation of an algebra

Let $\mathcal{M} = <M, g>$ be an associative operator algebra, and M be the underlying linear space of the algebra $\mathcal{M}$. Suppose that there is given a bilinear superoperator from $M \times M$ into M (in particular, the multiplication g on M) expressible in the form

$$g_t(A, B) = AB + tG_1(A, B) + t^2G_2(A, B) + \cdots, \tag{12}$$

where G_k, $k = 1, 2, \ldots$, are bilinear superoperators on $\mathcal{M}$. We set $G_0(A, B) = g(A, B) = AB$, the product in $\mathcal{M}$.

We can consider the algebra $\mathcal{M}_t = <M, g_t>$, whose underlying linear space is M and multiplication is g_t, as the generic element of a *one-parameter family of deformations of* $\mathcal{M} = <M, g>$. The multiplication g_t given by (12) has the trivial special case defined by setting $t = 0$, i.e., the original multiplication g. The *infinitesimal deformation* (or differential) of this family is the bilinear superoperator G_1, considered as a map from $M \times M$ into M.

The following are example of some deformations of operator algebras.

(1) Suppose that $\mathcal{M}_t = <M, g_t>$ is *associative*, i.e.,

$$g_t\big(g_t(A, B), C\big) = g_t\big(A, g_t(B, C)\big) \tag{13}$$

for all A, B, C in M. The condition (13) that g_t be associative is equivalent to the equations

$$\sum_{\substack{k,l\geqslant 0\\ k+l=m}} \big(G_k\big(G_l(A, B), C\big) - G_k\big(A, G_l(B, C)\big)\big) = 0 \tag{14}$$

for all A, B, C in M and all $m = 0, 1, 2, \ldots$. For $m = 0$ this is just the associativity of the original multiplication

$$G_0\big(G_0(A, B), C\big) - G_0\big(A, G_0(B, C)\big) = (AB)C - A(BC) = 0.$$

For $m = 1$, equation (14) can be expressed in the form

$$AG_1(B, C) - G_1(AB, C) + G_1(A, BC) - G_1(A, B)C = 0.$$

In terms of the cohomology group theory, G_1 is an element of the group $Z^2(\mathcal{M}, \mathcal{M})$ of two-cocycles of $\mathcal{M}$ with coefficients in $\mathcal{M}$.

(2) Suppose that $\mathcal{M} = <M, g>$ is an operator Lie algebra, and that g_t defines a one-parameter family of deformations of $\mathcal{M}$ such that we have again a Lie algebra

$\mathcal{M}_t = <M, g_t>$. Then we have

$$g_t(A, B) = -g_t(B, A),$$
$$g_t\big(g_t(A, B), C\big) + g_t\big(g_t(B, C), A\big) + g_t\big(g_t(C, A), B\big) = 0.$$

These conditions are equivalent to the following conditions

$$G_k(A, B) = -G_k(B, A),$$

and

$$\sum_{\substack{k,l\geqslant 0\\ k+l=m}} \big(G_k\big(G_l(A, B), C\big) + G_k\big(G_l(B, C), A\big) + G_k\big(G_l(C, A), B\big)\big) = 0 \tag{15}$$

for all A, B, C in $\mathcal{M}$ and all $k = 0, 1, 2\ldots$. For $k = 0$, these equations express the conditions that $\mathcal{M} = <M, g>$ is a Lie algebra:

$$G_0(A, B) = -G_0(B, A),$$
$$G_0\big(G_0(A, B), C\big) + G_0\big(G_0(B, C), A\big) + G_0\big(G_0(C, A), B\big) = 0.$$

For $k = 1$, we obtain

$$G_1(A, B) = -G_1(B, A),$$

and equation (11). Let $C^2(\mathcal{M}, \mathcal{M})$ be a group of 2-cochains of the Lie algebra $\mathcal{M}$ with coefficients in itself. Considering G_1 as an element of $C^2(\mathcal{M}, \mathcal{M})$, the quantity on the left in equation (11) is just $\delta G_1(A, B, C)$. Therefore equation (11) means that G_1 is again a 2-cocycle.

The analogous computations can be performed for Jordan algebra.

Obstructions

Suppose $\mathcal{M} = <M, g>$ is a Lie or associative ring $\mathcal{M}$. In general, an element G_1 in $Z^2(\mathcal{M}, \mathcal{M})$ need not be the differential of a one-parameter family of deformations of $\mathcal{M}$. If G_1 is the differential, then we say that G_1 is *integrable*. The integrability of G_1 implies an infinite sequence of relations which may be interpreted as the vanishing of the "obstructions" to the integration of G_1.

In the associative case, these obstructions can be derived from (14) by rewriting these equations in the form

$$\sum_{\substack{k,l>0\\ k+l=m}} \big(G_k\big(G_l(A, B), C\big) - G_k\big(A, G_l(B, C)\big)\big) = \delta G_m(A, B, C). \tag{16}$$

For $m = 2$, we obtain

$$G_1\big(G_1(A, B), C\big) - G_1\big(A, G_1(B, C)\big) = \delta G_2(A, B, C). \tag{17}$$

The function of three variables on the left is the associator of the binary operation G_1, and is an element of $Z^3(\mathcal{M}, \mathcal{M})$ whenever G_1 is in $Z^2(\mathcal{M}, \mathcal{M})$. The cohomology class of this element is the first obstruction to the integration of G_1. If G_1 is integrable, this must be the zero class.

If $G_1, \ldots, G_{n-1}$ satisfy (16) for $m = 1, \ldots, n-1$, then the left side of (16) for $m = n$ defines an element of $Z^3(\mathcal{M}, \mathcal{M})$, the $(n-1)$th "obstruction cocycle" which, however, is a function not of G_1 only, but of sequence $G_1, \ldots, G_{n-1}$. If $H^3(\mathcal{M}, \mathcal{M}) = 0$, then all obstructions vanish and every G_1 in $Z^2(\mathcal{M}, \mathcal{M})$ is integrable.

Analogous statements hold for the Lie and Jordan algebras. In these cases, the left hand side of (17) is presented by Jacobian and Jordanian.

Trivial deformations

A one-parameter family of deformations of an associative algebra defined by a multiplication f_t is trivial if there is a non-singular linear mapping Φ_t of M onto itself (an automorphism of M) of the form

$$\Phi_t A = A + t\varphi_1(A) + t^2\varphi_2(A) + \cdots, \tag{18}$$

where $\varphi_k : M \to M$ are linear maps, such that

$$f_t(A, B) = \Phi_t^{-1}\big(\Phi_t(A)\Phi_t(B)\big).$$

Then the algebra $\mathcal{M}_t = <M, f_t>$ is obviously isomorphic to $\mathcal{M}$. The isomorphism is a linear map Φ_t considered as a mapping from $\mathcal{M}_t$ into $\mathcal{M}$. Writing for this multiplication,

$$f_t(A, B) = AB + tF_1(A, B) + \cdots, \tag{19}$$

we obtain

$$F_1(A, B) = \delta\varphi_1(A, B) = \varphi_1(A)B + A\varphi_1(B) - \varphi_1(AB).$$

More generally, if a one-parameter family of deformations of $\mathcal{M}$ is given by equation (12), then we set

$$f_t(A, B) = \Phi_t^{-1} g_t\big(\Phi_t(A), \Phi_t(B)\big), \tag{20}$$

and write $f_t(A, B)$ by (19), then

$$F_1(A, B) = G_1(A, B) + \delta\varphi_1(A, B).$$

It follows that the integrability of an element G_1 of $Z^2(\mathcal{M}, \mathcal{M})$ depends only on its cohomology class. If any element in a class is integrable, then the element of that class may be integrated to give one-parameter families of algebras whose generic elements are isomorphic. We may therefore interpret the classes, i.e., the

elements of $H^2(\mathcal{M}, \mathcal{M})$, as the infinitesimal deformations. In general, the infinitesimal deformation G_1 of a one-parameter family can be zero while the generic element $\mathcal{M}_t$ of the family is not isomorphic to $\mathcal{M}$.

One-parameter families g_t and f_t of deformations of an algebra $\mathcal{M}$ will be called the equivalent deformations if there exists a non-singular linear automorphism Φ_t of M of the form (18) such that (20) holds. The family g_t is trivial if it is equivalent to the identity deformation f_t defined by $f_t(AB) = AB$.

Obstructions to derivations

Let $\mathcal{M}$ be an operator algebra. It is natural to consider the elements $Z^1(\mathcal{M}, \mathcal{M})$ (the derivations of $\mathcal{M}$ into itself) as infinitesimal automorphisms.

Suppose Φ_t is an automorphism of $\mathcal{M}$ such that

$$\Phi_t(A) = \sum_{k=0} t^k \varphi_k(A) = A + t\varphi_t(A) + t^2\varphi_2(A) + \cdots, \tag{21}$$

where φ_k are linear maps from $\mathcal{M}$ into itself, and φ_0 is interpreted as the identity mapping, I. We can consider Φ_t of (21) as a generic element of a one-parameter family of superoperators on $\mathcal{M}$. The condition that Φ_t be an automorphism is

$$\sum_{\substack{k,l\geqslant 0\\ k+l=m}} \varphi_k(A)\varphi_l(B) = \varphi_m(AB). \tag{22}$$

The obstructions are all deducible from (22) by rewriting this equation in the form

$$\sum_{\substack{k,l>0\\ k+l=m}} \varphi_k(A)\varphi_l(B) = -\delta\varphi_m(A, B). \tag{23}$$

The condition is vacuous for $m = 0$. For $m = 1$, the definition of $\delta = \delta^1$ and equation (23) give

$$\delta\varphi_1(A, B) = A\varphi_1(B) - \varphi_1(AB) + \varphi_1(A)B = 0,$$

i.e., φ_1 is a derivation of $\mathcal{M}$, or φ_1 is an element of $Z^1(\mathcal{M}, \mathcal{M})$. For $m = 2$ in equation (22), we have

$$\varphi_2(AB) = A\varphi_2(B) + \varphi_1(A)\varphi_1(B) + \varphi_2(A)B \tag{24}$$

and the definition of $\delta = \delta^1$ gives

$$-\delta\varphi_2(A, B) = -A\varphi_2(B) + \varphi_2(AB) - \varphi_2(A)B. \tag{25}$$

Equations (23) and (25) give

$$-\delta\varphi_2(A, B) = \varphi_1(A)\varphi_1(B). \tag{26}$$

Note that substitution of (24) into (25) gives (26). The function of two variables on the left is just the cup product, $\varphi_1 \smile \varphi_1$ of φ_1 with itself, and is an element of $Z^2(\mathcal{M}, \mathcal{M})$. The cup product is a method of adjoining two cocycles of degrees k and l to form a composite cocycle of degree $k + l$. The product $\varphi_1 \smile \varphi_1$ is the first obstruction to the integration of φ_1. Using (26), $\varphi_1 \smile \varphi_1$ must represent the zero cohomology class, if φ_1 is the differential of a one-parameter family of automorphisms.

Since all the obstructions to the integration of an element of $Z^1(\mathcal{M}, \mathcal{M})$ will be elements of $Z^2(\mathcal{M}, \mathcal{M})$, the vanishing of $H^2(\mathcal{M}, \mathcal{M})$ implies the integrability of any φ_1 in $Z^1(\mathcal{M}, \mathcal{M})$ to a one-parameter family of automorphisms of $\mathcal{M}$.

19.7. Phase-space metric for classical non-Hamiltonian system

The dynamics of Hamiltonian systems is characterized by conservation of phase-space volume under time evolution. This conservation of the phase volume is a cornerstone of conventional statistical mechanics of Hamiltonian systems. At a mathematical level, conservation of phase-space volume is considered as a consequence of the existence of an invariant symplectic form (skew-symmetric phase-space metric) in the phase-space of Hamiltonian systems. This metric defines an "invariant" binary operations on the phase space of Hamiltonian system. Non-Hamiltonian systems are characterized by nonzero phase space compressibility, and the usual phase-space volume is no longer necessarily conserved [125, 186,185].

We can consider an invariant skew-symmetric (antisymmetric) phase-space metric for non-Hamiltonian systems [172]. We say that the metric is an invariant, if the metric tensor field is an integral of motion. We define the phase-space metric such that the Jacobi identity is satisfied. The suggested skew-symmetric phase-space metric allows us to introduce the generalization of the Poisson bracket for non-Hamiltonian systems such that the Jacobi identity is satisfied by the generalized Poisson bracket. As a result the algebra of phase-space functions is time translation invariant. The generalized Poisson bracket defines a Lie algebra in phase-space. The invariant metric structure defines an "invariant" binary operation on the phase space of non-Hamiltonian systems.

Note that the invariant phase space metric can be used in molecular dynamics [172,184,55].

Classical non-Hamiltonian system

The dynamics is described by a smooth vector field $\mathbf{F} = \mathbf{F}(\mathbf{x})$, and the equation $d\mathbf{x}/dt = \mathbf{F}$ with components F^k in basis $\partial_k = \partial/\partial x^k$. For simplicity, we consider the case where the vector field $\mathbf{F}$ is time independent. In local coordinates $\{x^k\}$,

equation of motion has the form

$$\frac{dx^k}{dt} = F^k(x). \tag{27}$$

Consider now the definition of the locally Hamiltonian systems.

DEFINITION. A classical system (27) on the symplectic manifold (M, ω) is called a *locally Hamiltonian system* if the differential 1-form $\omega(F)$ is a closed form $d\omega(F) = 0$, where $\omega(F) = i_F\omega$ is the contraction (interior product) of the 2-form ω with vector $\mathbf{F}$, and d is the exterior derivative.

A classical system (27) on the symplectic manifold (M, ω) is called a *classical non-Hamiltonian system* if the differential 1-form $\omega(F)$ is nonclosed $d\omega(F) \neq 0$.

The classical system (27) is a locally Hamiltonian system if the conditions

$$J_{kl}(\omega, \mathbf{x}, t) = \partial_k\big(\omega_{lm}F^m\big) - \partial_l\big(\omega_{km}F^m\big) = 0 \tag{28}$$

are satisfied [172].

Let us consider the canonical coordinates $\mathbf{x} = (x^1, \ldots, x^n, x^{n+1}, \ldots, x^{2n}) = (q^1, \ldots, q^n, p^1, \ldots, p^n)$, and phase space metric such that

$$\omega = dq^i \wedge dp^i. \tag{29}$$

Equation (27) can be written as

$$\frac{dq^i}{dt} = G^i(q, p), \qquad \frac{dp^i}{dt} = K^i(q, p). \tag{30}$$

THEOREM. *If the right-hand sides of equations* (30) *for the phase-space with* (29) *satisfy the following Helmholtz conditions*

$$\frac{\partial G^i}{\partial p^j} - \frac{\partial G^j}{\partial p^i} = 0, \quad \frac{\partial G^j}{\partial q^i} + \frac{\partial K^i}{\partial p^j} = 0, \quad \frac{\partial K^i}{\partial q^j} - \frac{\partial K^j}{\partial q^i} = 0, \tag{31}$$

then the classical system (30) *is a locally Hamiltonian system.*

PROOF. This theorem is proved in [172]. □

It is interesting to consider an invariant antisymmetric phase-space metric that satisfies the Jacoby identity, and defines the Lie algebra in phase-space. We call the metric is invariant if the metric tensor field is an integral of motion ($d\omega/dt = 0$). This invariant phase-space metric $\omega_{kl}(\mathbf{x}, t)$ defines the invariant phase-space volume form v by the equation $v = (1/n!)\omega^n = \sqrt{g(\mathbf{x}, t)}\, dx^1 \wedge \cdots \wedge dx^{2n}$, where $g(\mathbf{x}, t)$ is the metric determinant $g(\mathbf{x}, t) = \det(\omega_{kl}(\mathbf{x}, t))$ and $dv/dt = 0$. Note that the invariant phase-space metric of some non-Hamiltonian systems can leads

us to the lack of smoothness of the metric. In this case, the phase-space probability distribution can be collapsed onto a fractal set of dimensionality lower than in the Hamiltonian case [73]. Note that classical systems that are Hamiltonian systems in the usual phase-space are non-Hamiltonian systems in the fractional phase-space.

Time evolution of phase-space metric

Let us find a time-dependent symplectic 2-form ω that satisfies the equation $d\omega/dt = 0$. The following theorem is well known.

THEOREM. *If the system* (27) *on the symplectic manifold* (M, ω) *with time-independent symplectic form* $(\partial\omega_{kl}/\partial t = 0)$ *is a locally Hamiltonian system, then differential* 2*-form* ω *is conserved, i.e.,* $d\omega/dt = 0$.

Let us consider a generalization of this statement.

THEOREM. *If the time-dependent metric* $\omega_{kl} = \omega_{kl}(\mathbf{x}, t)$ *is a skew-symmetric metric* $(\omega_{kl} = -\omega_{lk})$ *that is satisfied by the Jacobi identity*

$$\partial_k\omega_{lm} + \partial_l\omega_{mk} + \partial_m\omega_{kl} = 0, \qquad \partial_k = \partial/\partial x^k \tag{32}$$

and the system is defined by equation (27)*, then the total time derivative of the differential* 2*-form*

$$\omega = \omega_{kl}(\mathbf{x}, t)\, dx^k \wedge dx^l,$$

is given by

$$\frac{d\omega}{dt} = \left(\frac{\partial\omega_{kl}}{\partial t} - \partial_k\big(\omega_{lm}F^m\big) + \partial_l\big(\omega_{km}F^m\big)\right) dx^k \wedge dx^l. \tag{33}$$

PROOF. This theorem is proved in [172]. □

If the total derivative (33) is zero, then we have the integral of motion or invariant. It is easy to see that the differentiable 2-form ω is invariant if the phase-space metric $\omega_{kl}(\mathbf{x}, t)$ is satisfied by the equation

$$\frac{\partial\omega_{kl}}{\partial t} = \partial_k\big(\omega_{lm}F^m\big) - \partial_l\big(\omega_{km}F^m\big). \tag{34}$$

This equation can be rewritten in the equivalent form

$$\frac{\partial\omega_{kl}}{\partial t} = \hat{J}^{ms}_{kl}\omega_{ms},$$

where the operator $\hat{J}$ is defined by the equation

$$\hat{J}^{ms}_{kl} = \frac{1}{2}\big(\big(\delta^m_l\partial_k - \delta^m_k\partial_l\big)F^s - \big(\delta^s_l\partial_k - \delta^s_k\partial_l\big)F^m\big). \tag{35}$$

THEOREM. *The differentiable* 2*-form* ω *is invariant* (*is an integral of motion for non-Hamiltonian system* (27)) *if the phase-space metric* $\omega_{kl}(\mathbf{x}, t)$ *is defined by the equation*

$$\omega_{kl}(\mathbf{x}, t) = \big(\exp\big(t\hat{J}\big)\big)^{ms}_{kl}\omega_{ms}(\mathbf{x}, 0). \tag{36}$$

Here $\hat{J}$ *is an operator that is defined by equation* (35).

PROOF. Let us consider the formal solution of equation (34) in the form

$$\omega_{kl}(\mathbf{x}, t) = \sum_{n=1}^{\infty} \frac{t^n}{n!}\omega^{(n)}_{kl}(\mathbf{x}), \tag{37}$$

where $\omega^{(n)}_{kl} = -\omega^{(n)}_{lk}$. In this case, the time-independent tensor fields $\omega^{(n)}_{kl}(\mathbf{x})$ are defined by the recursion relation

$$\omega^{(n+1)}_{kl} = \partial_k\big(\omega^{(n)}_{lm}F^m\big) - \partial_l\big(\omega^{(n)}_{km}F^m\big).$$

This equation can be rewritten in the following equivalent form

$$\omega^{(n+1)}_{kl} = \big(\delta^m_l\partial_k - \delta^m_k\partial_l\big)\big(F^s\omega^{(n)}_{ms}\big).$$

Using the skew symmetry of the $\omega^{(n)}_{ns}$, we have

$$\omega^{(n+1)}_{kl} = \frac{1}{2}\big(\big(\delta^m_l\partial_k - \delta^m_k\partial_l\big)F^s - \big(\delta^s_l\partial_k - \delta^s_k\partial_l\big)F^m\big)\omega^{(n)}_{ms}.$$

This relation can be represented in the form

$$\omega^{(n+1)}_{kl} = \hat{J}^{ms}_{kl}\omega^{(n)}_{ms},$$

where the operator $\hat{J}$ is defined by equation (35). Therefore the invariant phase-space metric is defined by the following equation:

$$\omega_{kl}(\mathbf{x}, t) = \sum_{n=0}^{\infty} \frac{t^n}{n!}\big(\hat{J}^n\big)^{ms}_{kl}\omega_{ms}(\mathbf{x}, 0) = \big(\exp(t\hat{J}\,)\big)^{ms}_{kl}\omega_{ms}(\mathbf{x}, 0).$$

As a result, we have equation (36). □

Example: System with linear friction

Let us consider the non-Hamiltonian system

$$\frac{dq^i}{dt} = \frac{\partial H}{\partial p^i}, \quad \frac{dp^i}{dt} = -\frac{\partial H}{\partial q^i} - K_i(t)p^i, \tag{38}$$

where $H = T(p) + U(q)$ and $i, j = 1, \ldots, n$. Here $T(p)$ is a kinetic energy, $U(q)$ is a potential energy. The term $-K^i_j(t)p^j$ is a friction term. Let us consider

the symplectic form

$$\omega = 2g_{ij}(t)\,dq^i \wedge dp^j.$$

The total time derivative of this form gives

$$\frac{d\omega}{dt} = 2\left(\frac{dg_{ij}}{dt} - g_{ij}K_j\right) dq^i \wedge dp^j.$$

In order to have the invariant phase-space metric ($d\omega/dt = 0$), we use the following equation:

$$\frac{dg_{ij}}{dt} = g_{ij}K_j.$$

The solution of these equations has the form

$$g_{ij}(t) = \delta_{ij} \exp \int_{t_0}^{t} K_j(\tau)\,d\tau.$$

This is the invariant phase-space metric for system (38). For example, the system

$$\frac{dq_1}{dt} = \frac{p_1}{m}, \quad \frac{dp_1}{dt} = -\frac{\partial U(q)}{\partial q_1} - K_1 p_1,$$
$$\frac{dq_2}{dt} = \frac{p_2}{m}, \quad \frac{dp_2}{dt} = -\frac{\partial U(q)}{\partial q_2} - K_2 p_2,$$

has the invariant phase-space metric $\omega_{kl}(t)$ of the form

$$\left\|\omega_{kl}(t)\right\| = \begin{pmatrix} 0 & 0 & e^{K_1 t} & 0 \\ 0 & 0 & 0 & e^{K_2 t} \\ -e^{K_1 t} & 0 & 0 & 0 \\ 0 & -e^{K_2 t} & 0 & 0 \end{pmatrix}.$$

Poisson brackets for non-Hamiltonian systems

Let us consider the skew-symmetric tensor field Ψ^{kl} that is defined by the equations

$$\Psi^{kl}(\mathbf{x}, t)\omega_{lm}(\mathbf{x}, t) = \Psi^{lk}(\mathbf{x}, t)\omega_{ml}(\mathbf{x}, t) = \delta_l^k.$$

This tensor field satisfies the Jacoby identity

$$\Psi^{kl}\partial_l \Psi^{ms} + \Psi^{ml}\partial_l \Psi^{sk} + \Psi^{sl}\partial_l \Psi^{km} = 0.$$

It follows from the Jacoby identity (32) for ω_{kl}.

Equations (33) and (36) give the time-dependent phase-space metric $\omega_{kl}(\mathbf{x}, t)$, which satisfies the Jacoby identity. As a result, we have Lie algebra that is defined

by the brackets:

$$\{A, B\}_t = \Psi^{kl}(\mathbf{x}, t)\partial_k A \partial_l B. \tag{39}$$

It is easy to prove that these brackets are Poisson brackets. These brackets define an "invariant" structure of a Lie algebra for classical observables of non-Hamiltonian systems.

In the general case, the rule of term-by-term differentiation with respect to time that has the form

$$\frac{d}{dt}\{A, B\} = \{\dot{A}, B\} + \{A, \dot{B}\}, \tag{40}$$

where $\dot{A} = dA/dt$, is not valid for non-Hamiltonian systems. In general, we have

$$\frac{d}{dt}\{A, B\}_t = \{\dot{A}, B\}_t + \{A, \dot{B}\}_t + J(A, B)$$

where

$$J(A, B) = \Psi^{kl}_{(1)}(\mathbf{x}, t)\partial_k A \partial_l B, \qquad \Psi^{kl}_{(1)}(\mathbf{x}, t) = \Psi^{km}\Psi^{ls}(\partial_s F_m - \partial_m F_s).$$

Note that time evolution of the Poisson brackets (39) for non-Hamiltonian systems can be considered as t-deformation of the Lie algebra of classical observables on phase-space with the metric (37).

If we use the invariant phase-space metric, then the rule (40) is valid for (39). As a result, the suggested Poisson brackets (39) define an invariant Lie operation, such that the bracket of two constants of motion is a constant of motion and rule (40) is satisfied.

Chapter 20

Fractional Quantum Dynamics

20.1. Fractional power of superoperator

Let L_A be a closed linear superoperator with an everywhere dense domain $D(L_A)$, having a resolvent $R(z, L_A)$ on the negative half-axis, and satisfying the condition

$$\left\| R(-z, L_A) \right\| \leqslant M/z \quad (z > 0). \tag{1}$$

Note that

$$R(-z, L_A) = L^{-1}_{zI+A} = (zL_I + L_A)^{-1}.$$

The superoperator

$$L^{\alpha}_A = \frac{\sin \pi\alpha}{\pi} \int\limits_0^{\infty} dz\, z^{\alpha-1} R(-z, L_A)\, L_A \tag{2}$$

is defined on $D(L_A)$ for $0 < \alpha < 1$. It is called a *fractional power of the left superoperator* and can be denoted by $(L_A)^{\alpha}$. Note that the superoperator L^{α}_A allows a closure.

If a closed superoperator L_A satisfy condition (1), then $L^{\alpha}_A L^{\beta}_A = L^{\alpha+\beta}_A$ for $\alpha, \beta > 0$, and $\alpha + \beta < 1$.

If R_A is a closed right superoperator with an everywhere dense domain $D(R_A)$ such that

$$\left\| (zR_I + R_A)^{-1} \right\| \leqslant M/z \quad (z > 0),$$

then we can define the superoperator

$$R^{\alpha}_A = \frac{\sin \pi\alpha}{\pi} \int\limits_0^{\infty} dz\, z^{\alpha-1} (zR_I + R_A)^{-1},$$

which is called a fractional power of the right superoperator R_A.

Let L_A be a closed generating superoperator of the semi-group $\{\Phi_t | t \geqslant 0\}$. Then the fractional power L_A^α of L_A is given by

$$L_A^\alpha = \frac{1}{\Gamma(-\alpha)} \int_0^\infty dz\, z^{-\alpha-1}(\Phi_z - L_I),$$

which is called the *Balakrishnan formula*.

The resolvent for the superoperator $L_A^\alpha = (L_A)^\alpha$ can be found by the equation

$$R\big(-z, L_A^\alpha\big) = \big(zL_I + (L_A)^\alpha\big)^{-1} = \frac{\sin \pi\alpha}{\pi} \int_0^\infty dx\, \frac{x^\alpha}{z^2 + 2zx^\alpha \cos \pi\alpha + x^{2\alpha}} R(-x, L_A).$$

It is the *Kato's formula*. It follows from this formula that the inequality

$$\big\| R\big(-z, (L_A)^\alpha\big) \big\| \leqslant M/z \quad (z > 0)$$

with the same constant M as for analogous inequality (1) for the superoperator L_A, is valid for $(L_A)^\alpha$.

It follows from the inequality

$$\big\| zR(-z, L_A) \big\| = \big\| z(zL_I + L_A)^{-1} \big\| = \big\| zL_{zI+A}^{-1} \big\| \leqslant M$$

for all $z > 0$ that the superoperator zL_{zI+A}^{-1} is uniformly bounded in every sector of the complex plane $|\arg z| \leqslant \phi$ for ϕ not greater than some number $\pi - \psi$ $(0 < \psi < \pi)$. Then the superoperator $zR(-z, (L_A)^\alpha)$ is uniformly bounded in every sector of the complex plane $|\arg z| \leqslant \phi$ for $\phi < \pi - \alpha\psi$.

Let L_A be a closed generating superoperator of the semi-group $\{\Phi_t | t \geqslant 0\}$. Then the superoperators

$$\Phi_t^{(\alpha)} = \int_0^\infty ds\, f_\alpha(t, s)\Phi_s \quad (t > 0) \tag{3}$$

form a semi-group such that L_A^α is an infinitesimal generator of $\Phi_t^{(\alpha)}$. Equation (3) will be called the *Bochner–Phillips formula*.

In equation (3), we use the function

$$f_\alpha(t, s) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} dz \exp\big(sz - tz^\alpha\big), \tag{4}$$

where $a, t > 0$, $s \geqslant 0$, and $0 < \alpha < 1$. The branch of z^α is so taken that $\mathrm{Re}(z^\alpha) > 0$ for $\mathrm{Re}(z) > 0$. This branch is a one-valued function in the z-plane

cut along the negative real axis. The convergence of this integral is obviously in virtue of the convergence factor $\exp(-tz^{\alpha})$.

The function $f_{\alpha}(t,s)$ has the following properties.

(1) For $t > 0$ and $x > 0$,

$$\int_0^{\infty} ds\, e^{-sx}\, f_{\alpha}(t,s) = e^{-tx^{\alpha}}.$$

(2) For all $s > 0$, the function $f_{\alpha}(t,s)$ is nonnegative: $f_{\alpha}(t,s) \geqslant 0$.

(3) We have

$$\int_0^{\infty} ds\, f_{\alpha}(t,s) = 1.$$

(4) By denoting the path of integration in (4) to the union of two paths $r\exp(-i\theta)$, and $r\exp(+i\theta)$, where $r \in (0,\infty)$, and $\pi/2 \leqslant \theta \leqslant \pi$, we obtain

$$f_{\alpha}(t,s) = \frac{1}{\pi}\int_0^{\infty} dr \exp\bigl(sr\cos\theta - tr^{\alpha}(\alpha\theta)\bigr) \cdot \sin\bigl(sr\sin\theta - tr^{\alpha}\sin(\alpha\theta) + \theta\bigr). \tag{5}$$

(5) If $\alpha = 1/2$, then we have, by taking $\theta = \pi$,

$$f_{1/2}(t,s) = \frac{1}{\pi}\int_0^{\infty} dr\, e^{-sr}\sin(t\sqrt{r}\,) = \frac{t}{2\sqrt{\pi}s^{3/2}}e^{-t^2/4s}.$$

20.2. Fractional Lindblad equation and fractional semi-group

Let us consider the equation

$$\frac{d}{dt}A_t = -\frac{1}{i\hbar}[H, A_t] + \frac{1}{2\hbar}\sum_{k=1}^{\infty}\bigl(V_k^*[A_t, V_k] + \bigl[V_k^*, A_t\bigr]V_k\bigr). \tag{6}$$

This is the *Lindblad equation* for quantum observable A_t. We rewrite this equation in the form

$$\frac{d}{dt}A_t = -\mathcal{L}_V A_t, \quad \mathcal{L}_V = L_H^- + \frac{i}{2}\sum_{k=1}^{\infty}\bigl(L_{V_k^*}L_{V_k}^- - L_{V_k^*}^- R_{V_k}\bigr), \tag{7}$$

where $\mathcal{L}_V$ is the Lindblad superoperator. If all operators V_k are equal to zero, then $\mathcal{L}_0 = L_H^-$, and equation (7) gives the Heisenberg equation for Hamiltonian system.

It is interesting to obtain a fractional generalization of equation (7). We will consider here concept of fractional power for $\mathcal{L}_V$. If $\mathcal{L}_V$ is a closed linear superoperator with an everywhere dense domain $D(\mathcal{L}_V)$, having a resolvent $R(z, \mathcal{L}_V) = (zL_I - \mathcal{L}_V)^{-1}$ on the negative half-axis, and satisfying the condition

$$\left\| R(-z, \mathcal{L}_V) \right\| \leqslant M/z \quad (z > 0),$$

then there exists the superoperator

$$-(\mathcal{L}_V)^\alpha = \frac{\sin \pi\alpha}{\pi} \int_0^\infty dz\, z^{\alpha-1} R(-z, \mathcal{L}_V)\, \mathcal{L}_V \tag{8}$$

defined on $D(\mathcal{L}_V)$ for $0 < \alpha < 1$. The superoperator $(\mathcal{L}_V)^\alpha$ is a *fractional power of the Lindblad superoperator*. Note that $(\mathcal{L}_V)^\alpha (\mathcal{L}_V)^\beta = (\mathcal{L}_V)^{\alpha+\beta}$ for $\alpha, \beta > 0$, and $\alpha + \beta < 1$.

As a result, we obtain the equation

$$\frac{d}{dt} A_t = -(\mathcal{L}_V)^\alpha A_t, \tag{9}$$

where t, $H/\hbar$ and $V_k/\sqrt{\hbar}$ are dimensionless variables. This is the *fractional Lindblad equation*.

If $V_k = 0$, then equation (9) gives the fractional Heisenberg equation

$$\frac{d}{dt} A_t = -\left(L_H^-\right)^\alpha A_t. \tag{10}$$

The superoperator $(L_H^-)^\alpha$ is a *fractional power of the Lie left superoperator*. Note that this equation cannot be presented in the form

$$\frac{d}{dt} A_t = -L_{H_{new}}^- A_t = \frac{i}{\hbar}[H_{new}, A_t]$$

with some operator H_{new}. Therefore, quantum systems described by (10) are not Hamiltonian systems. These systems will be called the *fractional Hamiltonian systems* (FHS). Usual Hamiltonian systems can be considered as a special case of FHS.

If we consider the Cauchy problem for equation (7) in which the initial condition is given at the time $t = 0$ by A_0, then its solution can be written in the form $A_t = \Phi_t A_0$. The one-parameter superoperators Φ_t, $t \geqslant 0$, have the properties

$$\Phi_t \Phi_s = \Phi_{t+s} \quad (t, s > 0), \quad \Phi_0 = L_I.$$

As a result, the superoperators Φ_t form a semi-group, and the superoperator $\mathcal{L}_V$ is a generating superoperator of the semi-group $\{\Phi_t | t \geqslant 0\}$.

Let us consider the Cauchy problem for fractional Lindblad equation (9) in which the initial condition is given by A_0. Then its solution can be presented in the form

$$A_t(\alpha) = \Phi_t^{(\alpha)} A_0,$$

where the superoperators $\Phi_t^{(\alpha)}$, $t > 0$, form a semi-group, which can be called the *fractional semi-group*. The superoperator $(\mathcal{L}_V)^\alpha$ is a generating superoperator of the semi-group $\{\Phi_t^{(\alpha)} | t \geqslant 0\}$.

Properties of the fractional semi-group

Let us consider some properties of fractional semi-groups $\{\Phi_t^{(\alpha)} | t > 0\}$.

(1) The superoperators $\Phi_t^{(\alpha)}$ can be constructed in terms of Φ_t by the Bochner–Phillips formula

$$\Phi_t^{(\alpha)} = \int_0^\infty ds\ f_\alpha(t, s) \Phi_s \quad (t > 0), \tag{11}$$

where $f_\alpha(t, s)$ is defined in (4). If A_t is a solution of the Lindblad equation (7), then formula (11) gives the solution

$$A_t(\alpha) = \int_0^\infty ds\ f_\alpha(t, s) A_s \quad (t > 0)$$

of fractional equation (9).

(2) Let Φ_t, $t > 0$, be a positive one-parameter superoperator, i.e., $\Phi_t A \geqslant 0$ for $A \geqslant 0$. Using the Bochner–Phillips formula and the property $f_\alpha(t, s) \geqslant 0$ ($s > 0$), it is easy to prove that the superoperator $\Phi_t^{(\alpha)}$ is also positive, i.e., $\Phi_t^{(\alpha)} A \geqslant 0$ for $A \geqslant 0$.

(3) A linear superoperator Φ_t is completely positive if

$$\sum_{i,j} B_i \Phi_t \left(A_i^* A_j\right) B_j \geqslant 0$$

for any A_i, $B_i \in \mathcal{M}$.

THEOREM. *If $\{\Phi_t | t > 0\}$ is a completely positive semi-group of superoperator Φ_t on $\mathcal{M}$, then fractional superoperators $\Phi_t^{(\alpha)}$, $t > 0$, form a completely positive semi-group.*

PROOF. The Bochner–Phillips formula gives

$$\sum_{i,j} B_i \Phi_t^{(\alpha)}\big(A_i^* A_j\big) B_j = \int_0^\infty ds\ f_\alpha(t,s) \sum_{i,j} B_i \Phi_s\big(A_i^* A_j\big) B_j$$

for $t > 0$. Using

$$\sum_{i,j} B_i \Phi_s\big(A_i^* A_j\big) B_j \geqslant 0, \quad f_\alpha(t,s) \geqslant 0\ (s > 0),$$

we obtain

$$\sum_{i,j} B_i \Phi_t^{(\alpha)}\big(A_i^* A_j\big) B_j \geqslant 0. \qquad \square$$

(4) Let $\mathcal{M}$ be a Hilbert operator space, together with a scalar product $(\,|\,)$. If Φ_t is a superoperator on $\mathcal{M}$, then an *adjoint superoperator* of Φ_t is a superoperator $\bar{\Phi}_t$ on $\mathcal{M}^*$, such that

$$\big(\bar{\Phi}_t(A)|B\big) = \big(A|\Phi_t(B)\big) \tag{12}$$

for all $B \in D(\Phi_t) \subset \mathcal{M}$ and some $A \in \mathcal{M}^*$. Using the Bochner–Phillips formula, we obtain the following theorem.

THEOREM. *If $\bar{\Phi}_t$ is an adjoint superoperator of Φ_t, then the superoperator*

$$\bar{\Phi}_t^{(\alpha)} = \int_0^\infty ds\ f_\alpha(t,s) \bar{\Phi}_s \quad (t > 0)$$

is an adjoint superoperator of $\Phi_t^{(\alpha)}$.

PROOF. Suppose $\bar{\Phi}_t$ is an adjoint of Φ_t, i.e. equation (12) is satisfied. Then

$$\begin{aligned}\big(\bar{\Phi}_t^{(\alpha)} A\big|B\big) &= \int_0^\infty ds\ f_\alpha(t,s)(\bar{\Phi}_s A|B) \\ &= \int_0^\infty ds\ f_\alpha(t,s)(A|\Phi_s B) = \big(A\big|\Phi_t^{(\alpha)} B\big).\end{aligned} \qquad \square$$

(5) Let $\{\bar{\Phi}_t | t > 0\}$ be a completely positive semi-group, such that the density operator $\rho_t = \bar{\Phi}_t \rho_0$ is described by

$$\frac{d}{dt}\rho_t = -\bar{\mathcal{L}}_V \rho_t, \tag{13}$$

where $\bar{\mathcal{L}}_V$ is adjoint of the Lindblad superoperator $\mathcal{L}_V$. The superoperator $\bar{\mathcal{L}}_V$ can be presented by

$$\bar{\mathcal{L}}_V \rho_t = -\frac{1}{i\hbar}[H, \rho_t] + \frac{1}{\hbar}\sum_{k=1}^{\infty}\big(V_k \rho_t V_k^* - \big(\rho_t V_k^* V_k + V_k^* V_k \rho_t\big)\big).$$

Note that equation (13) with $V_k = 0$ gives the von Neumann equation

$$\frac{d}{dt}\rho_t = \frac{1}{i\hbar}[H, \rho_t].$$

The semi-group $\{\bar{\Phi}_t^{(\alpha)} | t > 0\}$ describes the evolution of the density operator

$$\rho_t(\alpha) = \bar{\Phi}_t^{(\alpha)} \rho_0$$

by the fractional equation

$$\frac{d}{dt}\rho_t(\alpha) = -(\bar{\mathcal{L}}_V)^{\alpha} \rho_t(\alpha).$$

This is the *fractional Lindblad equation for density operator*. For $V_k = 0$, this equation gives

$$\frac{d}{dt}\rho_t = -\big(-L_H^-\big)^{\alpha} \rho_t.$$

This is the *fractional von Neumann equation*.

(6) In quantum theory, the most important is the class of real superoperators. Let $A^* \in \mathcal{M}^*$ be adjoint of $A \in \mathcal{M}$. A *real superoperator* is a superoperator Φ_t on $\mathcal{M}$, such that $(\Phi_t A)^* = \Phi_t(A^*)$ for all $A \in D(\Phi_t) \subset \mathcal{M}$. A quantum observable is a self-adjoint operator. If Φ_t is a real superoperator and A is a self-adjoint operator $A^* = A$, then the operator $A_t = \Phi_t A$ is self-adjoint, i.e., $(\Phi_t A)^* = \Phi_t A$. Let $\mathcal{M}$ be a set of observables. Then superoperators on $\mathcal{M}$ into $\mathcal{M}$ should be real. All possible dynamics, i.e., temporal evolutions of quantum observables, must be described by a set of all real superoperators.

THEOREM. *If Φ_t is a real superoperator, then $\Phi_t^{(\alpha)}$ is real.*

PROOF. The Bochner–Phillips formula gives

$$\big(\Phi_t^{(\alpha)} A\big)^* = \int_0^{\infty} ds\, f_{\alpha}^*(t, s)(\Phi_s A)^* \quad (t > 0).$$

Using (5), it is easy to see that $f_{\alpha}^*(t, s) = f_{\alpha}(t, s)$ is a real-valued function. Then $(\Phi_t A)^* = \Phi_t A^*$ leads to $(\Phi_t^{(\alpha)} A)^* = \Phi_t^{(\alpha)}(A^*)$ for all $A \in D(\Phi_t^{(\alpha)}) \subset \mathcal{M}$. □

(7) It is known that $\bar{\Phi}_t$ is a real superoperator if Φ_t is real. Analogously, if $\Phi_t^{(\alpha)}$ is a real superoperator, then $\bar{\Phi}_t^{(\alpha)}$ is real.

Fractional Heisenberg equation for harmonic oscillator

Let us consider the Hamiltonian

$$H = \frac{1}{2m} P^2 + \frac{m\omega^2}{2} Q^2, \tag{14}$$

where t and P are dimensionless variables. Then equation (10) describes a harmonic oscillator. For $A = Q$, and $A = P$, equation (10) for $\alpha = 1$ gives

$$\frac{d}{dt} Q_t = \frac{1}{m} P_t, \qquad \frac{d}{dt} P_t = -m\omega^2 Q_t.$$

The well-known solutions of these equations are

$$\begin{aligned} Q_t &= Q_0 \cos(\omega t) + \frac{1}{m\omega} P_0 \sin(\omega t), \\ P_t &= P_0 \cos(\omega t) - m\omega Q_0 \sin(\omega t). \end{aligned} \tag{15}$$

Using these solutions and the Bochner–Phillips formula, we can obtain solutions of the following fractional Heisenberg equations

$$\frac{d}{dt} Q_t = -\left(L_H^-\right)^\alpha Q_t, \qquad \frac{d}{dt} P_t = -\left(L_H^-\right)^\alpha P_t, \tag{16}$$

where H is defined by (14). The solutions of fractional equations (16) have the forms

$$\begin{aligned} Q_t(\alpha) &= \Phi_t^{(\alpha)} Q_0 = \int_0^\infty ds\, f_\alpha(t,s) Q_s, \\ P_t(\alpha) &= \Phi_t^{(\alpha)} P_0 = \int_0^\infty ds\, f_\alpha(t,s) P_s. \end{aligned} \tag{17}$$

Substitution of (15) into (17) gives

$$Q_t = Q_0 C_\alpha(t) + \frac{1}{m\omega} P_0 S_\alpha(t), \qquad P_t = P_0 C_\alpha(t) - m\omega Q_0 S_\alpha(t), \tag{18}$$

where

$$C_\alpha(t) = \int_0^\infty ds\, f_\alpha(t,s) \cos(\omega s), \qquad S_\alpha(t) = \int_0^\infty ds\, f_\alpha(t,s) \sin(\omega s).$$

Equations (18) describe solutions of the fractional Heisenberg equations (16) for quantum harmonic oscillator.

If $\alpha = 1/2$, then

$$C_{1/2}(t) = \frac{t}{2\sqrt{\pi}} \int\limits_0^\infty ds\, \frac{\cos(\omega s)}{s^{3/2}}\, e^{-t^2/4s},$$

$$S_{1/2}(t) = \frac{t}{2\sqrt{\pi}} \int\limits_0^\infty ds\, \frac{\sin(\omega s)}{s^{3/2}}\, e^{-t^2/4s}.$$

These functions can be presented through the Macdonald function (see [123], Sec. 2.5.37.1), which is also called the modified Bessel function of the third kind.

It is not hard to obtain the expectation values

$$<Q_t> = x_0 C_\alpha(t) + \frac{1}{m\omega}\, p_0 S_\alpha(t),$$
$$<P_t> = p_0 C_\alpha(t) - m\omega x_0 S_\alpha(t),$$

and the dispersions

$$D_t(Q) = \frac{b^2}{2} C_\alpha^2(t) + \frac{\hbar^2}{2b^2 m^2 \omega^2} S_\alpha^2(t),$$
$$D_t(P) = \frac{\hbar^2}{2b^2} C_\alpha^2(t) + \frac{b^2 m^2 \omega^2}{2} S_\alpha^2(t).$$

Here we use the coordinate representation and the pure state

$$\Psi(x) = <x|\Psi> = (b\sqrt{\pi}\,)^{-1/2} \exp\left(-\frac{(x - x_0)^2}{2b} + \frac{i}{\hbar} p_0 x \right). \tag{19}$$

The expectation value and dispersion are defined by the equations

$$<A_t> = Tr\big[|\Psi><\Psi|A_t\big] = <\Psi|A_t|\Psi>,$$
$$D_t(A) = <A_t^2> - <A_t>^2 = <\Psi|A_t^2|\Psi> - <\Psi|A_t|\Psi>^2.$$

Example of fractional Lindblad equation

The basic assumption is that the general form of a bounded completely dissipative superoperator given by Lindblad equation is also valid for an unbounded completely dissipative superoperator $\mathcal{L}_V$. Another simple condition imposed to the operators H, V_k is that they are functions of the basic operators Q and P of such that $V_k = V_k(Q, P)$ are at most the first degree polynomials in Q and P, and $H = H(Q, P)$ is at most a second degree polynomial in Q and P. Then V_k and H are chosen in the forms:

$$V_k = a_k P + b_k Q, \qquad H = \frac{1}{2m} P^2 + \frac{m\omega^2}{2} Q^2 + \frac{\mu}{2}(PQ + QP), \tag{20}$$

where a_k, b_k are complex numbers, $k = 1, 2$. It is easy to obtain

$$\mathcal{L}_V Q = \frac{1}{m} P + \mu Q - \lambda Q, \qquad \mathcal{L}_V P = -m\omega^2 Q - \mu P - \lambda P,$$

where

$$\lambda = \mathrm{Im}\left(\sum_{k=1}^{n=2} a_k b_k^* \right) = -\mathrm{Im}\left(\sum_{k=1}^{n=2} a_k^* b_k \right).$$

Let us define the following matrices

$$A = \begin{pmatrix} Q \\ P \end{pmatrix}, \qquad M = \begin{pmatrix} \mu - \lambda & \frac{1}{m} \\ -m\omega^2 & -\mu - \lambda \end{pmatrix}.$$

In this case, the Lindblad equation for A_t becomes

$$\frac{d}{dt} A_t = M A_t, \tag{21}$$

where $\mathcal{L}_V A_t = M A_t$. The solution of (21) is

$$A_t = \Phi_t A_0 = \sum_{n=0}^{\infty} \frac{t^n}{n!} \mathcal{L}_V^n A_0 = \sum_{n=0}^{\infty} \frac{t^n}{n!} M^n A_0.$$

The matrix M can be presented in the form $M = N^{-1} F N$, where F is a diagonal matrix. Let ν be a complex parameter such that $\nu^2 = \mu^2 - \omega^2$. Then, we have

$$N = \begin{pmatrix} m\omega^2 & \mu + \nu \\ m\omega^2 & \mu - \nu \end{pmatrix}, \qquad F = \begin{pmatrix} -(\lambda + \nu) & 0 \\ 0 & -(\lambda - \nu) \end{pmatrix}.$$

Using

$$\Phi_t = \sum_{n=0}^{\infty} \frac{t^n}{n!} M^n = N^{-1} \left(\sum_{n=0}^{\infty} \frac{t^n}{n!} F^n \right) N,$$

we obtain the superoperator Φ_t in the form

$$\begin{aligned} \Phi_t &= e^{tM} = N^{-1} e^{tF} N \\ &= e^{-\lambda t} \begin{pmatrix} \cosh(\nu t) + \frac{\mu}{\nu} \sinh(\nu t) & \frac{1}{m\nu} \sinh(\nu t) \\ -\frac{m\omega^2}{\nu} \sinh(\nu t) & \cosh(\nu t) - \frac{\mu}{\nu} \sinh(\nu t) \end{pmatrix}, \end{aligned}$$

where sinh and cosh are hyperbolic sine and cosine.

As a result, we obtain

$$Q_t = e^{-\lambda t} \left[\cosh(\nu t) + \frac{\mu}{\nu} \sinh(\nu t) \right] Q_0 + \frac{1}{m\nu} e^{-\lambda t} \sinh(\nu t) P_0, \tag{22}$$

$$P_t = -\frac{m\omega^2}{\nu} e^{-\lambda t} \sinh(\nu t) Q_0 + e^{-\lambda t} \left[\cosh(\nu t) - \frac{\mu}{\nu} \sinh(\nu t) \right] P_0. \tag{23}$$

The fractional Lindblad equations for Q_t and P_t are

$$\frac{d}{dt}Q_t = -(\mathcal{L}_V)^\alpha Q_t, \qquad \frac{d}{dt}Q_t = -(\mathcal{L}_V)^\alpha Q_t, \tag{24}$$

where t and $V_k/\sqrt{\hbar}$ are dimensionless variables. The solutions of these fractional equations are given by the Bochner–Phillips formula

$$Q_t(\alpha) = \Phi_t^{(\alpha)} Q_0 = \int_0^\infty ds\ f_\alpha(t,s) Q_s \quad (t > 0), \tag{25}$$

$$P_t(\alpha) = \Phi_t^{(\alpha)} P_0 = \int_0^\infty ds\ f_\alpha(t,s) P_s \quad (t > 0), \tag{26}$$

where Q_s and P_s are presented in equations (22) and (23). The function $f_\alpha(t,s)$ is defined in (4). Substitution of (22) and (23) into (25) and (26) gives

$$Q_t(\alpha) = \left[Ch_\alpha(t) + \frac{\mu}{\nu} Sh(t)\right] Q_0 + \frac{1}{m\nu} Ch_\alpha(t) P_0, \tag{27}$$

$$P_t(\alpha) = -\frac{m\omega^2}{\nu} Sh_\alpha(t) Q_0 + \left[Ch_\alpha(t) - \frac{\mu}{\nu} Sh_\alpha(t)\right] P_0, \tag{28}$$

where

$$Ch_\alpha(t) = \int_0^\infty ds\ f_\alpha(t,s) e^{-\lambda s} \cosh(\nu s),$$

$$Sh_\alpha(t) = \int_0^\infty ds\ f_\alpha(t,s) e^{-\lambda s} \sinh(\nu s).$$

If $\alpha = 1/2$, then we have

$$Ch_{1/2}(t) = \frac{t}{2\sqrt{\pi}} \int_0^\infty ds\ \frac{\cosh(\nu s)}{s^{3/2}} e^{-t^2/4s - \lambda s},$$

$$Sh_{1/2}(t) = \frac{t}{2\sqrt{\pi}} \int_0^\infty ds\ \frac{\sinh(\nu s)}{s^{3/2}} e^{-t^2/4s - \lambda s}.$$

These functions can be presented through the Macdonald function (see [123], Sec. 2.4.17.2) such that

$$Ch_{1/2}(t) = \frac{t}{2\sqrt{\pi}} \big[V(t, \lambda, -\nu) + V(t, \lambda, \nu)\big],$$

$$Sh_{1/2}(t) = \frac{t}{2\sqrt{\pi}}\big[V(t,\lambda,-\nu) - V(t,\lambda,\nu)\big].$$

Here

$$V(t,\lambda,\nu) = \left(\frac{t^2+4\nu}{4\lambda}\right)^{1/4} K_{-1/2}\left(2\sqrt{\frac{\lambda(t^2+4\nu)}{4}}\right),$$

where $\mathrm{Re}(t^2) > \mathrm{Re}(\nu)$, $\mathrm{Re}(\lambda) > 0$, and $K_\alpha(z)$ is the Macdonald function [115, 134], which is also called the modified Bessel function of the third kind.

20.3. Quantization of fractional derivatives

From fractional derivative operator to superoperator

The theory of derivatives and integrals of noninteger order goes back to Leibniz, Liouville, Grunwald, Letnikov and Riemann [81,115,134]. Derivatives of fractional order, and fractional differential equations have found many applications in recent studies in physics [199–201].

The fractional derivative ${}_0D_x^\alpha$ on $[0,\infty)$ in the Riemann–Liouville form is defined by the equation

$${}_0D_x^\alpha A(x) = \frac{1}{\Gamma(m-\alpha)}\frac{d^m}{dx^m}\int_0^x \frac{A(y)\,dy}{(x-y)^{\alpha-m+1}},$$

where m is the first whole number greater than or equal to α. The derivative of powers n of x is

$${}_0D_x^\alpha x^n = \frac{\Gamma(n+1)}{\Gamma(n+1-\alpha)}x^{n-\alpha}, \tag{29}$$

where $n \geqslant 1$, and $\alpha \geqslant 0$. Here $\Gamma(z)$ is a Gamma function.

Let $A(x)$ be an analytic function for $x \in (0,b)$. The fractional Riemann–Liouville derivative can be presented [134] in the form

$${}_0D_x^\alpha A(x) = \sum_{n=0}^{\infty} a(n,\alpha)x^{n-\alpha}\frac{d^n A(x)}{dx^n},$$

where

$$a(n,\alpha) = \frac{\Gamma(\alpha+1)}{\Gamma(n+1)\Gamma(\alpha-n+1)\Gamma(n-\alpha+1)}.$$

If $A(q, p)$ is an analytic function on $\mathbb{R}^{2n}$, then we can define the fractional derivatives

$$ {}_0D^{\alpha}_{q_k} A(q, p) = \sum_{n=0}^{\infty} a(n, \alpha) q_k^{n-\alpha} \frac{\partial^n}{\partial q_k^n} A(q, p), \tag{30} $$

$$ {}_0D^{\alpha}_{p_k} A(q, p) = \sum_{n=0}^{\infty} a(n, \alpha) p_k^{n-\alpha} \frac{\partial^n}{\partial p_k^n} A(q, p), \tag{31} $$

where $k = 1, \ldots, n$. Using the operators

$$ L^+_{q_k} A(q, p) = q_k A(q, p), \qquad L^+_{p_k} A(q, p) = p_k A(q, p), $$

$$ L^-_{q_k} A(q, p) = \frac{\partial A(q, p)}{\partial p_k}, \qquad L^-_{p_k} A(q, p) = -\frac{\partial A(q, p)}{\partial q_k}, $$

equations (30) and (31) can be rewritten in the form

$$ {}_0D^{\alpha}_{q_k} A(q, p) = \sum_{n=0}^{\infty} a(n, \alpha) \big(L^+_{q_k}\big)^{n-\alpha} \big(-L^-_{p_k}\big)^n A(q, p), $$

$$ {}_0D^{\alpha}_{p_k} A(q, p) = \sum_{n=0}^{\infty} a(n, \alpha) \big(L^+_{p_k}\big)^{n-\alpha} \big(L^-_{q_k}\big)^n A(q, p). $$

As a result, the fractional derivatives are defined by

$$ {}_0D^{\alpha}_{q_k} = \sum_{n=0}^{\infty} a(n, \alpha) \big(L^+_{q_k}\big)^{n-\alpha} \big(-L^-_{p_k}\big)^n, \tag{32} $$

$$ {}_0D^{\alpha}_{p_k} = \sum_{n=0}^{\infty} a(n, \alpha) \big(L^+_{p_k}\big)^{n-\alpha} \big(L^-_{q_k}\big)^n. \tag{33} $$

The Weyl quantization π of q_k and p_k gives the operators

$$ Q_k = \pi(q_k), \qquad P_k = \pi(p_k). $$

The Weyl quantization of the operators $L^{\pm}_{q^k}$ and $L^{\pm}_{p^k}$ is defined by the equation

$$ \pi_W\big(L^+_{q_k}\big) = L^+_{Q_k}, \qquad \pi_W\big(L^-_{q_k}\big) = L^-_{Q_k}, $$

$$ \pi_W\big(L^+_{p_k}\big) = L^+_{P_k}, \qquad \pi_W\big(L^-_{p_k}\big) = L^-_{P_k}, $$

where

$$ L^+_Q A = \frac{1}{2}(QA + AQ), \qquad L^+_P A = \frac{1}{2}(PA + AP), \tag{34} $$

$$ L^-_Q A = \frac{1}{i\hbar}(QA - AQ), \qquad L^-_P A = \frac{1}{i\hbar}(PA - AP). \tag{35} $$

As a result, the quantization of the fractional derivatives (32) and (33) gives the superoperators

$$ {}_0\mathcal{D}^{\alpha}_{Q_k} = \pi\left({}_0D^{\alpha}_{q_k}\right) = \sum_{n=0}^{\infty} a(n,\alpha)\left(L^{+}_{Q_k}\right)^{n-\alpha}\left(-L^{-}_{P_k}\right)^{n}, \tag{36} $$

$$ {}_0\mathcal{D}^{\alpha}_{P_k} = \pi\left({}_0D^{\alpha}_{p_k}\right) = \sum_{n=0}^{\infty} a(n,\alpha)\left(L^{+}_{P_k}\right)^{n-\alpha}\left(L^{-}_{Q_k}\right)^{n}. \tag{37} $$

Equations (36) and (37) can be considered as definitions of the *fractional derivation superoperators* on an operator space.

It is not hard to prove that

$$ {}_0\mathcal{D}^{\alpha}_{Q}\,Q^n = \frac{\Gamma(n+1)}{\Gamma(n+1-\alpha)}\,Q^{n-\alpha}, \qquad {}_0\mathcal{D}^{\alpha}_{P}\,P^n = \frac{\Gamma(n+1)}{\Gamma(n+1-\alpha)}\,P^{n-\alpha}, $$

where $n \geqslant 1$, and $\alpha \geqslant 0$.

Quantization of Riemann–Liouville derivative

We remind of the formula for the Fourier transform $\tilde{A}(a)$ of some function $A(x)$:

$$ \tilde{A}(a) = \mathcal{F}\left\{A(x)\right\} = \frac{1}{(2\pi)^{1/2}}\int\limits_{\mathbb{R}} dx\; A(x)\exp\{-iax\}, $$

which is valid for all $A(x)$ with

$$ \int\limits_{\mathbb{R}} dx\,\left|A(x)\right| < \infty. $$

If we require

$$ \left\|A(x)\right\|_2 = \int\limits_{\mathbb{R}} dx\,\left|A(x)\right|^2 < \infty, $$

then the Parseval formula $\|\tilde{A}\|_2 = \|A\|_2$ holds.

Let $\mathcal{F}$ be an extension of this Fourier transformation to a unitary isomorphism on $L_2(\mathbb{R})$. We define the operators

$$ \mathcal{L} = \mathcal{F}^{-1}L(a)\mathcal{F}. $$

It is well defined, if the function $L(a)$ is measurable. These operators form a commutative algebra. Let $\mathcal{L}_1$ and $\mathcal{L}_2$ be operators associated with the functions $L_1(a)$ and $L_2(a)$. If $\mathcal{L}_{12}$ is an operator associated with $L_{12}(a) = L_1(a)L_2(a)$, then

$$ \mathcal{L}_{12} = \mathcal{L}_1\mathcal{L}_2 = \mathcal{L}_2\mathcal{L}_1. $$

As a result, we may present explicit formulas for a fractional derivative. If the Fourier transforms exists, then the operator D_x^α is

$$D_x^\alpha A(x) = \mathcal{F}^{-1}(ia)^\alpha \tilde{A}(a) = \mathcal{F}^{-1}(ia)^\alpha \mathcal{F} A(x),$$

where

$$(ia)^\alpha = |a|^\alpha \exp\left(\frac{\pi\alpha}{2}\operatorname{sgn}(a)\right).$$

For $A(x) \in L_2(\mathbb{R})$, we have the integral representation

$$D_x^\alpha A(x) = \frac{1}{2\pi}\int\limits_{\mathbb{R}^2} da\, dx'\, (ia)^\alpha A(x') \exp\{ia(x-x')\}. \tag{38}$$

Some elementary manipulations lead to the well-known Riemann–Liouville integral representation

$$D_x^\alpha A(x) = {}_{-\infty}D_x^\alpha A(x) = \frac{1}{\Gamma(m-\alpha)}\frac{d^m}{dx^m}\int\limits_{-\infty}^{x} dx'\, \frac{A(x')}{(x-x')^{\alpha+1-m}}.$$

This form cannot be used to quantization. For Weyl quantization, we consider the representation (38).

Let $A(q,\, p)$ be a function of $L_2(\mathbb{R}^2)$ on the phase space $\mathbb{R}^2$. Then equation (38) can be presented in the form

$$\begin{aligned} &D_q^\alpha D_p^\beta A(q,\, p) \\ &\quad = \int\limits_{\mathbb{R}^4} \frac{da\, db\, dq'\, dp'}{(2\pi\hbar)^2}(ia)^\alpha (ib)^\beta A(q',\, p') e^{\frac{i}{\hbar}(a(q-q')+b(p-p'))}. \end{aligned} \tag{39}$$

Using the Weyl quantization of $A(q,\, p)$ in the form

$$A(Q,\, P) = \pi\big(A(q,\, p)\big) = \int\limits_{\mathbb{R}^4} \frac{da\, db\, dq\, dp}{(2\pi\hbar)^2} A(q,\, p) e^{\frac{i}{\hbar}(a(Q-qI)+b(P-pI))},$$

we obtain the following result of the Weyl quantization of (39):

$$\begin{aligned} D_Q^\alpha D_P^\beta A(Q,\, P) &= \pi\big(D_q^\alpha D_p^\beta A(q,\, p)\big) \\ &= \frac{1}{(2\pi\hbar)^2}\int\limits_{\mathbb{R}^4} da\, db\, dq\, dp (ia)^\alpha (ib)^\beta A(q,\, p) \\ &\quad \times \exp\frac{i}{\hbar}\big(a(Q-qI)+b(P-pI)\big). \end{aligned} \tag{40}$$

This equation can be considered as a definition of D_Q^α and D_P^β on a set of quantum observables.

Note that the general quantization of $A(q, p)$ is defined by

$$A_F(Q, P) = \int_{\mathbb{R}^4} \frac{da\,db\,dq\,dp}{(2\pi\hbar)^2} F(a, b) A(q, p) \times \exp \frac{i}{\hbar}\big(a(Q - qI) + b(P - pI)\big).$$

For the Weyl quantization, $F(a, b) = 1$. If $F(a, b) = \cos(ab/2\hbar)$, then we have the Rivier quantization. Equation (40) can be considered as a general quantization of $A(q, p)$ with the function

$$F(a, b) = (ia)^\alpha (ib)^\beta.$$

This function has zeros on the real a, b axis. It is clear that there is no dual operator basis.

20.4. Quantization of Weierstrass nondifferentiable function

We consider a function $W(x)$ on $\mathbb{R}$. Under certain circumstances the graph

$$\text{graph}\, W(x) = \big\{\big(x, W(x)\big)\colon x \in \mathbb{R}\big\}$$

regarded as a subset of the (x, y)-coordinate plane may be fractal. If $W(x)$ has a continuous derivative, then it is not difficult to prove that the graph has dimension 1. However, it is possible for a continuous function to be sufficiently irregular to have a graph of dimension strictly greater than 1. The well-known example is

$$W(x) = \sum_{k=0}^{\infty} a^{(s-2)k} \sin\big(a^k x\big),$$

where $1 < s < 2$, and $a > 1$. This function has the box-counting dimension $D = s$.

Fractality of pure quantum states

Some general approach to quantum fractal construction was proposed by D. Wojcik, I. Bialynicki-Birula, and K. Zyczkowski [189].

The Weierstrass function

$$W(x) = \sum_{k=0}^{\infty} a^n \sin\big(b^n x\big),$$

where $0 < a < 1 < b$, $ab > 1$, is an example of a continuous, nowhere differentiable function. The box-counting dimension of its graph is the noninteger number

$$D = 2 - \left|\frac{\ln a}{\ln b}\right|.$$

We can consider the wave function

$$\Psi_M(t, x) = N_M \sum_{k=0}^{M} a^{k(s-2)} \sin\bigl(a^k x\bigr) e^{-ia^{2k}t},$$

where $a = 2, 3, \ldots$ and $s \in (0, 2)$. In the physically interesting case of any finite M the wave function $\Psi_M(t, x)$ is a solution of the Schrödinger equation. The limit case

$$\Psi(t, x) = \lim_{M\to\infty} \Psi_M(t, x) = N \sum_{k=0}^{\infty} a^{k(s-2)} \sin\bigl(a^k x\bigr) e^{-ia^{2k}t}$$

with the normalization constant

$$N = \sqrt{\frac{2}{\pi}\bigl(1 - a^{2(s-2)}\bigr)}$$

is continuous but nowhere differentiable. In analogy with the theory of distribution, it can be considered as a solution of the Schrödinger equation in the weak sense. It was shown that the probability density $P(t, x) = |\Psi(t, x)|^2$ has a fractal nature and the surface $P(t, x)$ has the box-counting dimension

$$D = 2 + \frac{s}{2}.$$

Weierstrass superoperator functions

The complex Weierstrass function has the form

$$W_0(x) = \bigl(1 - a^2\bigr)^{-1/2} \sum_{k=0}^{\infty} a^k \exp\bigl\{2\pi i b^k x\bigr\},$$

where $b > 1$ is a real number, and $a = b^{D-2}$ $(1 < D < 2)$. It can be proved that this function is continuous, but it is not differentiable. Note that $W_0(x)$ is continuous and differentiable if $D < 1$.

Let us consider this function on the phase space $\mathbb{R}^2$, and $x = q$ or $x = p$. Using the operators

$$L_q^+ A(q, p) = qA(q, p), \qquad L_p^+ A(q, p) = pA(q, p),$$

the complex Weierstrass function can be presented in the operator form

$$W_0\big(L_x^+\big) = \big(1-a^2\big)^{-1/2} \sum_{k=0}^{\infty} a^k \exp\big\{2\pi i b^k L_x^+\big\}. \tag{41}$$

The basic assumption is that the general properties of the Weyl quantization given by the equations

$$\pi\big(L_q^+\big) = L_Q^+, \qquad \pi\big(L_q^+\big) = L_Q^+,$$
$$\pi\left(\sum_k A_k(q,p)\right) = \sum_k \pi\big(A_k(q,p)\big)$$

are also valid for infinite sums. Then the Weyl quantization of (41) gives

$$W_0\big(L_X^+\big) = \pi\big(W_0\big(L_x^+\big)\big) = \big(1-a^2\big)^{-1/2} \sum_{k=0}^{\infty} a^k \exp\big\{2\pi i b^k L_X^+\big\}, \tag{42}$$

where $X = Q = \pi(q)$ or $X = P = \pi(p)$, and L_X^+ is defined by (34). As a result, equation (42) defines the Weierstrass superoperator functions $W_0(L_Q^+)$ and $W_0(L_P^+)$ on an operator algebra. In the Wigner representation of quantum mechanics these superoperators are represented by the Weierstrass functions $W_0(q)$ and $W_0(p)$ on the phase space $\mathbb{R}^2$.

We can formally consider the operators

$$W_0\big(L_x^-\big) = \big(1-a^2\big)^{-1/2} \sum_{k=0}^{\infty} a^k \exp\big\{2\pi i b^k L_x^-\big\}, \tag{43}$$

where $x = q$ or p, and

$$L_q^- A(q,p) = \frac{\partial A(q,p)}{\partial p}, \qquad L_p^- A(q,p) = -\frac{\partial A(q,p)}{\partial q}.$$

Using the functions

$$\Psi(x) = \exp(\lambda x) \quad (x \in \mathbb{R}),$$

we obtain

$$L_q^- \Psi(q) = \lambda \Psi(q), \qquad L_p^- \Psi(p) = -\lambda \Psi(p).$$

Then $\Psi(x)$ are eigenfunctions of the operators L_x^- with the eigenvalues $\pm\lambda$. The box-counting dimension of its spectrum graphs $(\lambda, \pm\lambda)$ is 1. The operators (43) give

$$W_0\big(L_q^-\big)\Psi(q) = W_0(\lambda)\Psi(q), \qquad W_0\big(L_p^-\big)\Psi(p) = W_0(-\lambda)\Psi(p).$$

As a result, the Weierstrass functions $W_0(\pm\lambda)$ are eigenvalues of the operators (43) with the eigenfunction $\Psi(x)$. Then the spectrum graphs $(\lambda, W_0(\pm\lambda))$ of these operators are fractal sets. The box-counting dimensions of these graph are noninteger numbers.

Using the formulas

$$\pi_W\bigl(L_p^+\bigr) = L_P^+, \qquad \pi_W\bigl(L_p^-\bigr) = L_P^-,$$

we can realize the Weyl quantization of the operators (43). As a result, we obtain the superoperators of the form

$$W_0\bigl(L_X^-\bigr) = \pi\bigl(W_0\bigl(L_x^-\bigr)\bigr) = \bigl(1-a^2\bigr)^{-1/2}\sum_{k=0}^{\infty} a^k \exp\bigl\{2\pi i b^k L_X^-\bigr\}, \tag{44}$$

where $X = Q = \pi(q)$ or $X = P = \pi(p)$, and L_X^- is defined by (35). Equation (44) defines the Weierstrass superoperator functions $W_0(L_Q^-)$ and $W_0(L_P^-)$ on a set of quantum observables. In the Wigner representation of quantum mechanics these superoperators are represented by the operators $W_0(L_q^-)$ and $W_0(L_p^-)$ with the fractal spectrum graphs $(\lambda, W_0(\pm\lambda))$.

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Chapter 21

Stationary States of Non-Hamiltonian Systems

21.1. Pure stationary states

Classical non-Hamiltonian and dissipative systems can have regular or strange attractors. Regular attractors of a non-Hamiltonian system can be considered as a set of (stationary) states for Hamiltonian system that corresponds to the non-Hamiltonian system. Quantization of time evolution equations in phase space allows one to derive quantum analogs of non-Hamiltonian classical systems with regular attractors. Quantum analogs of dissipative systems with strange attractors such as Lorenz-like system and Rössler systems can be obtained by quantization. Then it is interesting to consider quantum analogs for regular and strange attractors. The regular "quantum" attractors can be considered as stationary states of non-Hamiltonian quantum systems. The existence of stationary states for non-Hamiltonian quantum systems is an interesting fact.

The condition given by Davies [39] defines the stationary state of non-Hamiltonian quantum system. An example, where the stationary state is unique and approached by all states for long times is considered by Lindblad [96] for Brownian motion of quantum harmonic oscillator. In Refs. [146,147] Spohn derives sufficient condition for the existence of a unique stationary state for the non-Hamiltonian quantum system described by Lindblad equation [95]. The stationary solution of the Wigner function evolution equation for non-Hamiltonian quantum system was discussed in [6,76]. Quantum effects in the steady states of the dissipative map are considered in [47]. Stationary pure states of quantum non-Hamiltonian systems are considered in [164,166]. For classical non-Hamiltonian systems, stationary states are presented in [170,167,171].

In this chapter, we consider stationary pure states of some non-Hamiltonian quantum systems. In the pure stationary states, these non-Hamiltonian systems look like Hamiltonian quantum systems. We consider the quantum analog of dynamical bifurcations that are used for classical dynamical systems. Non-Hamiltonian quantum systems with pure stationary states of linear harmonic oscillator are suggested. We derive stationary states for the Lindblad equation. The suggested approach allows one to use theory of bifurcations for a wide class

of quantum non-Hamiltonian systems. We consider the example of bifurcation of pure stationary states for non-Hamiltonian quantum systems.

In the general case, the time evolution of the quantum state $|\rho_t)$ can be described by the Liouville–von Neumann equation

$$\frac{d}{dt}|\rho_t) = \Lambda|\rho_t), \tag{1}$$

where Λ is a Liouville superoperator, $|\rho)$ is a density operator. For Hamiltonian systems, the Liouville superoperator has the form

$$\Lambda = -\frac{i}{\hbar}(L_H - R_H) \quad \text{or} \quad \Lambda = L_H^-, \tag{2}$$

where $H = H(Q, P)$ is a Hamilton operator. If Λ can be represented in the form (2), then the quantum system is called globally Hamiltonian.

The stationary state is defined by the condition:

$$\Lambda|\rho_t) = 0. \tag{3}$$

For Hamiltonian quantum systems (2), this condition has the simple form:

$$L_H|\rho_t) = R_H|\rho_t) \quad \text{or} \quad L_H^-|\rho_t) = 0. \tag{4}$$

In the general case, we can consider the Liouville superoperator as a superoperator function:

$$\Lambda = \Lambda\big(L_X^-, L_X^+\big) \quad \text{or} \quad \Lambda = \Lambda(L_X, R_X),$$

where X is a set of linear operators. For example, $X = \{Q, P, H\}$ or $X = \{H_1, \ldots, H_s\}$. We will use the special form of the superoperator Λ such that

$$\Lambda = -\frac{i}{\hbar}(L_H - R_H) + \sum_{k=1}^{s} F_k N_k(L_H, R_H),$$

where $N_k(L_H, R_H)$ are some superoperator functions and F^k are arbitrary nonzero superoperators.

It is known that a pure state $|\rho_\Psi)$ is a stationary state of a Hamiltonian quantum system (1), (2), if the state $|\rho_\Psi)$ is an eigenvector of the superoperators L_H and R_H such that

$$L_H|\rho_\Psi) = |\rho_\Psi)E, \qquad R_H|\rho_\Psi) = |\rho_\Psi)E. \tag{5}$$

Equivalently, the state $|\rho_\Psi)$ is an eigenvector of superoperators L_H^+ and L_H^- such that

$$L_H^+|\rho_\Psi) = |\rho_\Psi)E, \qquad L_H^-|\rho_\Psi) = |\rho_\Psi) \cdot 0 = 0.$$

The energy variable E can be defined by

$$E = (I|L_H|\rho_\Psi) = (I|R_H|\rho_\Psi) = (I|L_H^+|\rho_\Psi).$$

The superoperators L_H and R_H for linear harmonic oscillator are

$$L_H = \frac{1}{2m}L_P^2 + \frac{m\omega^2}{2}L_Q^2, \qquad R_H = \frac{1}{2m}R_P^2 + \frac{m\omega^2}{2}R_Q^2. \tag{6}$$

It is known that pure stationary states $\rho_{\Psi_n} = \rho_{\Psi_n}^2$ of linear harmonic oscillator (6) exists if the variable E is equal to

$$E_n = \frac{1}{2}\hbar\omega(2n+1). \tag{7}$$

21.2. Stationary states of non-Hamiltonian systems

Let us consider the Liouville–von Neumann equation (1) for the non-Hamiltonian quantum system in the form

$$\frac{d}{dt}|\rho_t) = -\frac{i}{\hbar}(L_H - R_H)|\rho_t) + \sum_{k=1}^{s} F_k N_k(L_H, R_H)|\rho_t). \tag{8}$$

Here F^k are some superoperators and $N_k(L_H, R_H)$, where $k = 1, \ldots, s$, are superoperator functions.

Let $|\rho_\Psi)$ be a pure stationary state of the Hamiltonian quantum system defined by Hamilton operator H. If equations (5) are satisfied, then the state $|\rho_\Psi)$ is a stationary state of the Hamiltonian system associated with the non-Hamiltonian system (8) and defined by

$$\frac{d}{dt}|\rho_t) = -\frac{i}{\hbar}(L_H - R_H)|\rho_t). \tag{9}$$

If the vector $|\rho_\Psi)$ is an eigenvector of operators L_H and R_H, then the Liouville–von Neumann equation (8) for the pure state $|\rho_\Psi)$ has the form

$$\frac{d}{dt}|\rho_\Psi) = \sum_{k=1}^{s} F_k|\rho_\Psi)\, N_k(E, E),$$

where the functions $N_k(E, E)$ are defined by

$$N_k(E, E) = (I|N_k(L_H, R_H)|\rho_\Psi).$$

If all functions $N_k(E, E)$ are equal to zero

$$N_k(E, E) = 0, \tag{10}$$

then the stationary state $|\rho_\Psi)$ of the Hamiltonian quantum system (9) is the stationary state of the non-Hamiltonian quantum system (8).

Note that functions $N_k(E, E)$ are eigenvalues and $|\rho_\Psi)$ is the eigenvector of superoperators $N_k(L_H, R_H)$, since

$$N_k(L_H, R_H)|\rho_\Psi) = |\rho_\Psi)N_k(E, E).$$

Therefore stationary states of the non-Hamiltonian quantum system (8) are defined by zero eigenvalues of superoperators $N_k(L_H, R_H)$.

21.3. Non-Hamiltonian systems with oscillator stationary states

In this section simple examples of non-Hamiltonian quantum systems (8) are considered.

(1) Let us consider the nonlinear oscillator with friction defined by the equation

$$\frac{d}{dt}\rho_t = -\frac{i}{\hbar}\big[\tilde{H}, \rho_t\big] - \frac{i}{2\hbar}\beta\big[Q^2, P^2\rho_t + \rho_t P^2\big], \tag{11}$$

where the operator $\tilde{H}$ is the Hamilton operator of the nonlinear oscillator:

$$\tilde{H} = \frac{P^2}{2m} + \frac{m\Omega^2 Q^2}{2} + \frac{\gamma Q^4}{2}.$$

Equation (11) can be rewritten in the form

$$\frac{d}{dt}|\rho_t) = L_H^-|\rho_t) + 2m\beta L_{Q^2}^-\left(\frac{1}{2m}\big(L_P^+\big)^2 + \frac{\gamma}{2m\beta}\big(L_Q^+\big)^2 - \frac{\Delta}{4\beta}L_I\right)|\rho_t), \tag{12}$$

where $\Delta = \Omega^2 - \omega^2$ and the superoperator L_H^- is defined for the Hamilton operator H of the linear harmonic oscillator by equations (2) and (6). Equation (12) has the form (8), with

$$N(L_H, R_H) = \frac{1}{2}(L_H + R_H) - \frac{\Delta}{2\beta}L_I, \qquad F = 2m\beta L_{Q^2}^-.$$

In this case the function $N(E, E)$ has the form

$$N(E, E) = E - \frac{\Delta}{2\beta}.$$

Let $\gamma = \beta m^2\omega^2$. The non-Hamiltonian quantum system (11) has one stationary state of the linear harmonic oscillator with energy $E_n = (\hbar\omega/2)(2n + 1)$, if $\Delta = 2\beta\hbar\omega(2n + 1)$, where n is an integer nonnegative number. This stationary state is one of the stationary states of the linear harmonic oscillator with the mass m

and frequency ω. In this case we can have the quantum analog of dynamical Hopf bifurcation.

(2) Let us consider the non-Hamiltonian quantum system described by the equation

$$\frac{d}{dt}|\rho_t) = L_H^-|\rho_t) + L_Q^- \cos\left(\frac{\pi}{\varepsilon_0}L_H^+\right)|\rho_t), \tag{13}$$

where the superoperator L_H^- is defined by formulas (2) and (6). Equation (13) has the form (8) if the superoperators F and $N(L_H, R_H)$ are defined by

$$F = -\frac{i}{\hbar}(L_Q - R_Q),$$

and

$$\begin{aligned} N(L_H, R_H) &= \cos\left(\frac{\pi}{2\varepsilon_0}(L_H + R_H)\right) \\ &= \sum_{m=0}^{\infty} \frac{1}{(2m)!}\left(\frac{i\pi}{2\varepsilon_0}\right)^{2m}(L_H + R_H)^{2m}. \end{aligned} \tag{14}$$

The function $N(E, E)$ has the form

$$N(E, E) = \cos\left(\frac{\pi E}{\varepsilon_0}\right) = \sum_{m=0}^{\infty} \frac{1}{(2m)!}\left(\frac{i\pi E}{\varepsilon_0}\right)^{2m}.$$

The stationary state condition (10) has the solution

$$E = \frac{\varepsilon_0}{2}(2n + 1),$$

where n is an integer number. If parameter ε_0 is equal to $\hbar\omega$, then quantum system (13) and (14) has pure stationary states of the linear harmonic oscillator with the energy (7). As a result, stationary states of the non-Hamiltonian quantum system (13) coincide with pure stationary states of linear harmonic oscillator. If the parameter ε_0 is equal to $\hbar\omega(2m + 1)$, then quantum system (13) and (14) has stationary states of the linear harmonic oscillator with $n(k, m) = 2km + k + m$ and

$$E_{n(k,m)} = \frac{\hbar\omega}{2}(2k + 1)(2m + 1).$$

(3) Let us consider the superoperator function $N_k(L_H, R_H)$ in the form

$$N_k(L_H, R_H) = \frac{1}{2\hbar}\sum_{n,m} v_{kn}v_{km}^*\left(2L_H^n R_H^m - L_H^{n+m} - R_H^{n+m}\right),$$

and let all superoperators F_k are equal to L_I. In this case, the Liouville–von Neumann equation (8) can be represented by the Lindblad equation:

$$\frac{d}{dt}|\rho_t) = -\frac{i}{\hbar}(L_H - R_H)|\rho_t) + \frac{1}{2\hbar}\sum_j (2L_{V_k}R_{V_k^*} - L_{V_k}L_{V_k^*} - R_{V_k^*}R_{V_k})|\rho_t) \tag{15}$$

with linear operators V_k defined by

$$V_k = \sum_n v_{kn}H^n, \qquad V_k^* = \sum_m v_{km}^* H^m. \tag{16}$$

If $|\rho_\Psi)$ is a pure stationary state (5), then all functions $N_k(E, E)$ are equal to zero and this state $|\rho_\Psi)$ is a stationary state of the non-Hamiltonian quantum system (15).

If the Hamilton operator H is defined by

$$H = \frac{1}{2m}P^2 + \frac{m\omega^2}{2}Q^2 + \frac{\lambda}{2}(QP + PQ), \tag{17}$$

then we have some generalization of the quantum model for the Brownian motion of a harmonic oscillator considered in [96]. Note that in the model [96] operators V_k are linear $V_k = a_k P + b_k Q$, but in our generalization (15) and (16) these operators are nonlinear. For example, we can use

$$V_k = a_k P + b_k Q + c_k P^2 + d_k Q^2 + e_k(QP + PQ).$$

The case $c_k = d_k = e_k = 0$ is considered in Ref. [96]. Let real parameters α and β exist and

$$b_k = \alpha a_k, \quad c_k = \beta a_k, \quad d_k = m^2\omega^2\beta a_k, \quad e_k = m\lambda\beta a_k.$$

In this case, the pure stationary states of the linear oscillator (17) exist if $\omega > \lambda$ and the variable E is equal to

$$E_n = \frac{1}{2}\hbar\omega(2n+1)\sqrt{1 - \lambda^2/\omega^2}.$$

Stationary states of non-Hamiltonian quantum systems can coincide with pure stationary states of Hamiltonian systems. As an example, we suggest non-Hamiltonian quantum systems with pure stationary states of linear oscillator. Note that using equation (8), it is easy to get non-Hamiltonian (dissipative) quantum systems with stationary states of hydrogen atom. For a special case of non-Hamiltonian systems, we can use the theory of bifurcation and catastrophe. Quantum analogs of classical dynamical bifurcations can be derived.

21.4. Dynamical bifurcations and catastrophes

Let us consider a special case of non-Hamiltonian quantum systems (8) such that the vector function

$$N_k(E, E) = (I|N_k(L_H, R_H)|\rho),$$

is a globally potential function and the Hamilton operator H can be represented in the form

$$H = \sum_{k=1}^{s} H_k.$$

In this case, we have a function $V(E)$ called potential, such that the following conditions are satisfied:

$$\frac{\partial V(E)}{\partial E_k} = N_k(E, E),$$

where $E_k = (I|L_{H_k}|\rho) = (I|R_{H_k}|\rho)$. If potential $V(E)$ exists, then the stationary state condition (10) for the non-Hamiltonian quantum system (8) is defined by critical points of the potential $V(E)$. If the system has one variable E, then the function $N(E, E)$ is always a potential function. In general, the vector function $N_k(E, E)$ is globally potential, if

$$\frac{\partial N_k(E, E)}{\partial E_l} = \frac{\partial N_l(E, E)}{\partial E_k},$$

and the set of variables $E = \{E_k|k = 1, \ldots, s\}$ is a simply connected region of $\mathbb{R}^s$. A region is simply connected if it is path-connected and every path between two points can be continuously transformed into every other. A region where any two points can be joined by a path is called path-connected.

Stationary states of the non-Hamiltonian quantum system (8) with potential vector function $N_k(E, E)$ are determined by critical points of the potential $V(E)$. It allows one to use the theory of bifurcations and catastrophes for the parametric set of functions $V(E)$. Note that a bifurcation in a linear space of variables $E = \{E_k|k = 1, \ldots, s\}$ is a bifurcation in the linear space of eigenvalues of the Hamilton operators H_k.

For the polynomial superoperator function $N_k(L_H, R_H)$, we have

$$N_k(L_H, R_H) = \sum_{n=0}^{N} \sum_{m=0}^{n} a_{n,m}^{(k)} L_H^m R_H^{n-m}.$$

In general case, m and n are multi-indices. The function $N_k(E, E)$ is the polynomial

$$N_k(E, E) = \sum_{n=0}^{N} \alpha_n^{(k)} E^n,$$

where the coefficients $\alpha_n^{(k)}$ are defined by

$$\alpha_n^{(k)} = \sum_{m=0}^{n} a_{n,m}^{(k)}.$$

We can define the variables $x_l = E_l - a_l$ $(l = 1, \ldots, s)$, such that functions $N_k(E, E) = N_k(x + a, x + a)$ have no the terms x_l^{n-1}.

$$\begin{aligned} N_k(x + a, x + a) &= \sum_{n=0}^{N} \alpha_n^{(k)} \left(x + a^{(k)}\right)^n \\ &= \sum_{n=0}^{N} \sum_{m=0}^{n} \alpha_n^{(k)} \frac{n!}{m!(n-m)!} x^m \left(a^{(k)}\right)^{n-m}. \end{aligned}$$

If the coefficient of the term $x_l^{n_l-1}$ is equal to zero

$$\alpha_{n_l}^{(k)} \frac{n_l!}{(n_l - 1)!} a_l^{(k)} + \alpha_{n_l-1}^{(k)} = \alpha_{n_l}^{(k)} n_l a_l^{(k)} + \alpha_{n_l-1}^{(k)} = 0,$$

then we have the following coefficients

$$a_l^{(k)} = -\frac{\alpha_{n_l-1}^{(k)}}{n_l \alpha_{n_l}^{(k)}}.$$

If we change parameters $\alpha_n^{(k)}$, then non-Hamiltonian quantum system can have pure stationary states. For example, the bifurcation with the birth of linear oscillator pure stationary state is a quantum analog of dynamical Hopf bifurcation for classical dynamical system.

Let a linear space of energy variables E be a one-dimensional space. If the function $N(E, E)$ is equal to

$$N(E, E) = \pm \alpha_n E^n + \sum_{j=1}^{n-1} \alpha_j E^j, \quad n \geqslant 2,$$

then the potential $V(x)$ is defined by the equation

$$V(x) = \pm x^{n+1} + \sum_{j=1}^{n-1} a_j x^j, \quad n \geqslant 2,$$

and we have catastrophe of type $A_{\pm n}$.

If we have s variables E_l, where $l = 1, 2, \ldots, s$, then quantum analogs of elementary catastrophes $A_{\pm n}$, $D_{\pm n}$, $E_{\pm 6}$, E_7 and E_8 can be realized for non-Hamiltonian quantum systems. Let us write the full list of potentials $V(x)$, which leads to elementary catastrophes (zero modal) defined by $V(x) = V_0(x) + Q(x)$,

where

$$A_{\pm n}\colon\ V_0(x) = \pm x_1^{n+1} + \sum_{j=1}^{n-1} a_j x_1^j, \quad n \geqslant 2,$$

$$D_{\pm n}\colon\ V_0(x) = x_1^2 x_2 \pm x_2^{n-1} + \sum_{j=1}^{n-3} a_j x_2^j + \sum_{j=n-2}^{n-1} x_1^{j-(n-3)},$$

$$E_{\pm 6}\colon\ V_0(x) = \left(x_1^3 \pm x_2^4\right) + \sum_{j=1}^{2} a_j x_2^j + \sum_{j=3}^{5} a_j x_1 x_2^{j-3},$$

$$E_7\colon\ V_0(x) = x_1^3 + x_1 x_2^3 + \sum_{j=1}^{4} a_j x_2^j + \sum_{j=5}^{6} a_j x_1 x_2^{j-5},$$

$$E_8\colon\ V_0(x) = x_1^3 + x_2^5 + \sum_{j=1}^{3} a_j x_2^j + \sum_{j=4}^{7} a_j x_1 x_2^{j-4}.$$

Here $Q(x)$ is the nondegenerate quadratic form with variables $x_2, x_3, \ldots, x_s$ for $A_{\pm n}$ and parameters $x_3, \ldots, x_s$ for other cases.

21.5. Fold catastrophe

In this section, we suggest an example of the non-Hamiltonian quantum system with catastrophe A_2 called fold.

Let us consider the Liouville–von Neumann equation (8) for a nonlinear quantum oscillator with friction, where multiplication superoperators L_H and R_H are defined by equation (6) and superoperators F and $N(L_H, R_H)$ are given by the equations:

$$F = -2L_Q^- L_P^+, \tag{18}$$

$$N(L_H, R_H) = \alpha_0 L_I^+ + \alpha_1 L_H^+ + \alpha_2 (L_H^+)^2. \tag{19}$$

In this case, the function $N(E, E)$ is equal to

$$N(E, E) = \alpha_0 + \alpha_1 E + \alpha_2 E^2.$$

A pure stationary state $|\rho_\Psi)$ of the linear harmonic oscillator is a stationary state of the non-Hamiltonian quantum system (19), if $N(E, E) = 0$. Let us define the new real variable x and parameter λ by the equations

$$x = E + \frac{\alpha_1}{2\alpha_2}, \qquad \lambda = \frac{4\alpha_0\alpha_2 - \alpha_1^2}{4\alpha_2^2}.$$

Then we have the stationary condition $N(E, E) = 0$ in the form $x^2 - \lambda = 0$. If $\lambda \leqslant 0$, then the non-Hamiltonian quantum system has no stationary states. If $\lambda > 0$, then we have pure stationary states for a discrete set of parameter values λ. If the parameters α_1, α_2 and λ satisfy the following conditions

$$-\frac{\alpha_1}{2\alpha_2} = \hbar\omega\left(n + \frac{1}{2} + \frac{m}{2}\right), \qquad \lambda = \hbar^2\omega^2\frac{m^2}{4},$$

where $n, m \in \mathbb{N}$, then the non-Hamiltonian quantum system (18) and (19) has two pure stationary states of the linear harmonic oscillator. The energies of these states are equal to

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \qquad E_{n+m} = \hbar\omega\left(n + m + \frac{1}{2}\right).$$

Chapter 22

Quantum Dynamical Methods

22.1. Resolvent method for non-Hamiltonian systems

If we consider a Cauchy problem for the quantum Liouville equation

$$\partial_t \varrho_s(t) = \Lambda \varrho_s(t) \tag{1}$$

in which the initial condition is given by ϱ_s at $t = 0$, then its solution can be written in the form $\varrho_s(t) = S_t \varrho_s$. The superoperator $S(t) = S_t$ can be defined by the superoperator equation

$$\partial_t S(t) = \Lambda S(t) \tag{2}$$

with the initial condition $S(0) = L_I$, where L_I is a unit superoperator.

The method of the resolvent superoperator can be applied to solve the quantum Liouville equation. It begins with the construction of the Laplace transform $\tilde{\varrho}_s(z)$ of the operator $\varrho_s(t)$:

$$\tilde{\varrho}_s(z) = \int_0^\infty dt\, \varrho_s(t) e^{-zt} = Lap\big[\varrho_s(t)\big],$$

where $z \in \mathbb{C}$. If $\tilde{\varrho}_s(z)$ is known, then $\varrho_s(t)$ is obtained through the inversion formula

$$\varrho_s(t) = \frac{1}{2\pi i} \int_C dz\, e^{zt} \tilde{\varrho}_s(z). \tag{3}$$

The path C of integration is parallel to the $\mathrm{Im}(z)$ axis with all singularities of $\tilde{\varrho}_s(z)$ to its left. Closing the contour in a semicircle to the left we have convergence for $t > 0$.

The Laplace transformation of the quantum Liouville equation (1) gives

$$z\tilde{\varrho}_s(z) - \varrho_s(0) = \Lambda \tilde{\varrho}_s(z).$$

Then

$$\tilde{\varrho}_s(z) = (zL_I - \Lambda)^{-1}\varrho_s(0).$$

The inverse Laplace transform (3) gives

$$\varrho_s(t) = \frac{1}{2\pi i}\int\limits_C dz\, e^{zt}(zL_I - \Lambda)^{-1}\varrho_s(0). \tag{4}$$

Using the resolvent superoperator

$$R(z, \Lambda) = (zL_I - \Lambda)^{-1},$$

the solution (4) can be presented as

$$\varrho_s(t) = \frac{1}{2\pi i}\int\limits_C dz\, e^{zt} R(z, \Lambda)\varrho_s(0).$$

Using the equation $\varrho_s(t) = S(t, 0)\varrho_s(0)$, it is not hard to see

$$S(t) = \frac{1}{2\pi i}\int\limits_C dz\, e^{zt} R(z, \Lambda). \tag{5}$$

The solution of the Cauchy problem with initial condition $\varrho_s(0)$ for the non-homogeneous equation

$$\partial_t \varrho_s(t) = \Lambda\varrho_s(t) + F(t),$$

where $F(t)$ is a bounded operator, can be written, using the evolution superoperator $S_0(t)$ for the corresponding homogeneous equation, in the form

$$\varrho_s(t) = S_0(t)\varrho_s(0) + \int\limits_0^t d\tau\, S_0(\tau)F(t - \tau).$$

The Liouville superoperator Λ can be presented in the form $\Lambda = \Lambda_0 + \Lambda_{nh}$, where Λ_0 is a Hamiltonian superoperator and Λ_{nh} is non-Hamiltonian. Then equation (2) has the form

$$\partial_t S(t) = \Lambda_0 S(t) + \Lambda_{nh} S(t).$$

The non-Hamiltonian part can be considered as the source term $F(t) = \Lambda_{nh} S(t)$, and the quantum Liouville equation will be considered as an inhomogeneous equation.

Let $S_0(t)$ be a solution of the equation

$$\partial_t S_0(t) = \Lambda_0 S_0(t).$$

Then instead of the quantum Liouville equation we take the equivalent integral equation

$$S(t) = S_0(t) + \int_0^t d\tau\, S_0(\tau)\Lambda_{nh}S(t-\tau). \tag{6}$$

The convolution is a binary operation $\bullet$ such that

$$A \bullet B = \int_0^t d\tau\, A(t-\tau)B(\tau) = \int_0^t d\tau\, A(\tau)B(t-\tau).$$

This operation is associative and distributive. Using the convolution, equation (6) will be presented in the form

$$S(t) = S_0(t) + S_0(t) \bullet \big(\Lambda_{nh}S(t)\big).$$

Successive iterations lead to the following approximations:

$$S(t) = S_0(t) + S_0(t) \bullet \big(\Lambda_{nh}S_0(t)\big),$$
$$S(t) = S_0(t) + S_0(t) \bullet \big(\Lambda_{nh}S_0(t)\big) + S_0(t) \bullet \big(\Lambda_{nh}S_0(t)\big) \bullet \big(\Lambda_{nh}S_0(t)\big),$$

and so on. As a result, we obtain

$$S(t) = \sum_{k=0}^{\infty} S_0(t)\big[\bullet\big(\Lambda_{nh}S_0(t)\big)\big]^k. \tag{7}$$

This is the formal solution of the quantum Liouville equation in the form of infinite series, such that each term contains only the superoperators $S_0(t)$, Λ_{nh}, and it can be calculated explicitly.

Let consider relation (5). In the resolvent $R(z, \Lambda) = (zL_I - \Lambda)^{-1}$, for the Liouville superoperator $\Lambda = \Lambda_0 + \Lambda_{nh}$, we can use the relation between the complete and unperturbed resolvents.

Using the equation

$$\frac{1}{A-B} = \frac{1}{A} + \frac{1}{A}B\frac{1}{A-B},$$

the resolvent $R(z, \Lambda) = (zL_I - \Lambda)^{-1}$, for the Liouville superoperator $\Lambda = \Lambda_0 + \Lambda_{nh}$, gives

$$R(z, \Lambda) = R(z, \Lambda_0) + R(z, \Lambda_0)\Lambda_{nh}R(z, \Lambda),$$

where $R(z, \Lambda_0) = (zL_I - \Lambda_0)^{-1}$. This superoperator equation represents the integral quantum Liouville equation (6). This form of the resolvent equation demonstrates the well-known property of Laplace transformation: a convolution

maps into a usual multiplication. Successive iteration of the resolvent superoperator equation leads to the following series

$$R(z, \Lambda) = \sum_{k=0}^{\infty} \big[R(z, \Lambda_0)\Lambda_{nh}\big]^k R(z, \Lambda_0).$$

This expression is more simple than (7), since it has the usual multiplication instead of the convolution.

22.2. Wigner function method for non-Hamiltonian systems

Quantum Markovian equations

In the Schrödinger dynamical representation, the quantum Liouville equation for the density operator $\rho_s(t)$ has the form

$$\frac{d\rho_s(t)}{dt} = \Lambda\rho_s(t), \quad \rho_s(t) = S_t\rho_s(0).$$

Here S_t denotes the dynamical semi-group describing the evolution of the non-Hamiltonian quantum system in Schrödinger representation. The Liouville superoperator Λ is the infinitesimal generator of the dynamical semi-group S_t. Using the Lindblad theorem, which gives the most general form of a bounded completely dissipative generator Λ, we write the explicit form of the most general quantum Liouville equation of Markovian type:

$$\frac{d\rho_s(t)}{dt} = -\frac{i}{\hbar}\big[H, \rho_s(t)\big] + \frac{1}{2\hbar}\sum_{k=1}^{m}\big(\big[V_k\rho_s(t), V_k^*\big] + \big[V_k, \rho_s(t)V_k^*\big]\big). \tag{8}$$

Here H is the Hamiltonian operator of the system and V_k, V_k^* are bounded operators on a Hilbert space $\mathcal{H}$. We make the assumption that the general form (8) of the quantum Liouville equation with a bounded generator is also valid for an unbounded generator. To study the one-dimensional case, we consider the operators H, V_k, V_k^* as functions of the observables P and Q of the one-dimensional quantum system (with $[Q, P] = i\hbar I$, where I is the identity operator). For simplicity, we assume that the operators V_k, V_k^* are first degree polynomials in P and Q. In the complex linear space of the first degree polynomials in P and Q there exist only two linear independent operators

$$V_k = a_k P + b_k Q \quad (k = 1, 2), \tag{9}$$

where a_k, b_k are complex numbers. The constant term cI is omitted because its contribution to the generator Λ is equivalent to terms in H linear in P and Q

which for simplicity are chosen to be zero. Then H has the form

$$H = \frac{1}{2m}P^2 + U(Q) + \frac{\mu}{2}(PQ + QP), \tag{10}$$

where $U(Q)$ is the potential energy and m is the mass of the particle. We introduce the notations

$$d_{qq} = \frac{\hbar}{2}\sum_{k=1,2}|a_k|^2, \qquad d_{pp} = \frac{\hbar}{2}\sum_{k=1,2}|b_k|^2, \tag{11}$$

$$d_{pq} = d_{qp} = -\frac{\hbar}{2}\,\mathrm{Re}\sum_{k=1,2}a_k^* b_k, \qquad \lambda = -\,\mathrm{Im}\sum_{k=1,2}a_k^* b_k, \tag{12}$$

where a_k^* and b_k^* denote the complex conjugate of a_k, and b_k respectively. Using these H, V_k, V_k^*, equation (8) takes the form:

$$\begin{aligned}\frac{d\rho_s}{dt} = &-\frac{i}{\hbar}[H_0, \rho_s] \\ &+ \frac{i(\lambda-\mu)}{2\hbar}[P, \rho_s Q + Q\rho_s] - \frac{i(\lambda+\mu)}{2\hbar}[Q, \rho_s P + P\rho_s] \\ &- \frac{d_{pp}}{\hbar^2}\big[Q, [Q, \rho_s]\big] - \frac{d_{qq}}{\hbar^2}\big[P, [P, \rho_s]\big] + \frac{2d_{pq}}{\hbar^2}\big[P, [Q, \rho_s]\big].\end{aligned} \tag{13}$$

Here the quantum diffusion coefficients d_{pp}, d_{qq}, d_{pq} and the friction constant λ satisfy the fundamental inequalities:

$$d_{pp} > 0, \quad d_{qq} > 0, \quad d_{pp}d_{qq} - {d_{pq}}^2 \geqslant \lambda^2\hbar^2/4. \tag{14}$$

These are the *Sandulescu–Scutaru inequalities* [133]. The necessary and sufficient condition for Λ to be translationally invariant is $\mu = \lambda$.

Equation for Wigner distribution of Hamiltonian systems

A quantum Hamiltonian systems can be described by quantum Lindblad equation (8) with $V_k = 0$. Instead of operator differential equation (8) with $V_k = 0$, we can use the following phase-space equation which determines the time evolution of the Wigner distribution function:

$$\begin{aligned}i\hbar\frac{\partial\rho_W(t, q, p)}{\partial t} = &H(q, p)\left(\exp\frac{\hbar\mathcal{P}}{2i}\right)\rho_W(t, q, p) \\ &- \rho_W(t, q, p)\left(\exp\frac{\hbar\mathcal{P}}{2i}\right)H(q, p),\end{aligned} \tag{15}$$

where $H(q, p)$ is the Weyl symbol of the Hamiltonian operator H of the system. Equation (15) can be rewritten in the form

$$\frac{\partial\rho_W(t, q, p)}{\partial t} = -\frac{2}{\hbar}H(q, p)\left(\sin\frac{\hbar\mathcal{P}}{2}\right)\rho_W(t, q, p). \tag{16}$$

Note that if we take the $\hbar \to 0$ limit of this equation, we obtain the classical Liouville equation

$$\frac{\partial \rho_W(t,q,p)}{\partial t} = -\frac{\partial H(q,p)}{\partial p}\frac{\partial \rho_W(t,q,p)}{\partial q} + \frac{\partial H(q,p)}{\partial q}\frac{\partial \rho_W(t,q,p)}{\partial p}$$

for the function $\rho_W(t,q,p)$.

Equation for Wigner distribution of non-Hamiltonian systems

The Wigner distribution functions are useful not only as calculation tools, but can also provide the connection between classical and quantum mechanics. The Wigner distribution was introduced to study quantum corrections to classical statistical mechanics [187]. The Wigner distribution function has found many applications primarily in statistical mechanics or in purely quantum mechanical problems [11,177,93,196], but also in areas such as quantum chemistry [121] and quantum optics [135], quantum chaos [196], and density functional theory [117]. The applicability of Wigner distribution function to the Lindblad equations is considered in [76,77].

The time evolution of the Wigner distribution function corresponding to the Lindblad master equation (8), can be obtained from equation (15) by adding in the right-hand side the Weyl symbol of the non-Hamiltonian part of equation (8), i.e., the sum of commutators. We use the equation

$$\begin{aligned} C(q,p) &= A(q,p)\left(\exp\frac{\hbar\mathcal{P}}{2i}\right)B(q,p) \\ &= B(q,p)\left(\exp\left(-\frac{\hbar\mathcal{P}}{2i}\right)\right)A(q,p), \end{aligned} \tag{17}$$

where $C = AB$ and $\mathcal{P}$ is given by

$$\mathcal{P} = \overleftarrow{\partial_p}\overrightarrow{\partial_q} - \overleftarrow{\partial_q}\overrightarrow{\partial_p}, \tag{18}$$

and the arrows indicate in which direction the derivatives act. As a result, we obtain the evolution equation for the Wigner distribution:

$$\begin{aligned} \frac{\partial \rho_W}{\partial t} = &-\frac{2}{\hbar}H\left(\sin\frac{\hbar\mathcal{P}}{2}\right)\rho_W + \frac{1}{2\hbar}\sum_k\Bigg[2V_k\left(\exp\frac{\hbar\mathcal{P}}{2i}\right)\rho_W\left(\exp\frac{\hbar\mathcal{P}}{2i}\right)V_k^* \\ &- V_k^*\left(\exp\frac{\hbar\mathcal{P}}{2i}\right)V_k\left(\exp\frac{\hbar\mathcal{P}}{2i}\right)\rho_W \\ &- \rho_W\left(\exp\frac{\hbar\mathcal{P}}{2i}\right)V_k^*\left(\exp\frac{\hbar\mathcal{P}}{2i}\right)V_k\Bigg], \end{aligned} \tag{19}$$

where V_k and V_k^* are the Weyl symbol of the operators V_k and V_k^*, respectively, and V_k^* is the complex conjugate of V_k. If the operators V_k are taken of the form

(9), then equation (19) becomes the evolution equation for the Wigner distribution corresponding to equation (13):

$$\frac{\partial \rho_W}{\partial t} = -\frac{2}{\hbar} H\left(\sin\frac{\hbar\mathcal{P}}{2}\right)\rho_W + \lambda\frac{\partial}{\partial q}(q\rho_W) + \lambda\frac{\partial}{\partial p}(p\rho_W) + d_{qq}\frac{\partial^2\rho_W}{\partial q^2} + d_{pp}\frac{\partial^2\rho_W}{\partial p^2} + 2d_{pq}\frac{\partial^2\rho_W}{\partial p\partial q}. \tag{20}$$

The first term on the right-hand side generates the evolution in phase-space of a Hamiltonian system and gives the Poisson bracket and the higher derivatives containing the quantum contribution. The following terms represent the contribution from the non-Hamiltonian terms.

Suppose $U(q)$ is an analytic. Then for a Hamiltonian operator of the form (10) equation (20) takes the form:

$$\frac{\partial \rho_W}{\partial t} = -\frac{p}{m}\frac{\partial \rho_W}{\partial q} + \frac{\partial U}{\partial q}\frac{\partial \rho_W}{\partial p} + \sum_{n=1}^{\infty}\frac{(-1)^n(\hbar)^{2n}}{2^{2n}(2n+1)!}\frac{\partial^{2n+1}U(q)}{\partial q^{2n+1}}\frac{\partial^{2n+1}\rho_W}{\partial p^{2n+1}} + D(\rho_W), \tag{21}$$

where we use the notation

$$D(\rho_W) = (\lambda-\mu)\frac{\partial}{\partial q}(q\rho_W) + (\lambda+\mu)\frac{\partial}{\partial p}(p\rho_W) + d_{qq}\frac{\partial^2\rho_W}{\partial q^2} + d_{pp}\frac{\partial^2\rho_W}{\partial p^2} + 2d_{pq}\frac{\partial^2\rho_W}{\partial p\partial q}. \tag{22}$$

The following are remarks to equation (21).

(1) If equation (21) has only the first two terms on the right-hand side, then $\rho_W(t, q, p)$ evolves along the classical flow in phase-space.

(2) The terms containing λ and μ are the dissipative terms. They cause a contraction of each volume element in phase-space.

(3) The terms containing d_{pp}, d_{qq} and d_{pq} are the diffusion terms and produce an expansion of the volume elements. The diffusion terms are responsible for the destruction of interference, by erasing the structure of the Wigner function on small scales.

(4) The infinite sum (the power series), together with the first two terms make up the unitary part of the evolution. Hence, up to corrections of order $\hbar^2$, unitary evolution corresponds to approximately classical evolution of the Wigner function.

(5) The higher corrections can often be assumed as negligible and give structures on small scales. There are, however, important examples where they cannot be neglected, e.g., in chaotic systems. From equation (21) it is clear that, as a consequence of the quantum correction terms with higher derivatives, the Wigner

function of a nonlinear system does not follow the classical Liouville equation. The higher derivative terms are generated by the nonlinearities in the potential $U(q)$.

(6) There are two well-known limits in which equation (21) can go over into a classical equation: (a) U is at most quadratic in q; (b) $\hbar \to 0$.

(7) Because of the extra diffusion terms, we get yet a third classical limit. In the limit of large d_{pp}, the diffusion smoothing becomes so effective that it damps out all the momentum-derivatives in the infinite sum and equation (21) approaches the Liouville equation with diffusion, an equation of Fokker–Planck type. This is an example of how systems start to behave classically (decoherence), since the diffusion coefficients are roughly proportional to the size of these objects. Thus a system will evolve according to classical dynamics if it has a strong interaction with its environment.

Special cases of Lindblad equations

The following are some special cases of equation (21) that are considered in [76, 77].

(1) In the case of a free particle, i.e., $U(q) = 0$, equation (21) takes the form:

$$\frac{\partial \rho_W}{\partial t} = -\frac{p}{m}\frac{\partial \rho_W}{\partial q} + D(\rho_W). \tag{23}$$

(2) The linear potential $U = \gamma q$ (for example, $\gamma = mg$ for the free fall or $\gamma = eE$ for the motion in a uniform electric field) gives

$$\frac{\partial \rho_W}{\partial t} = -\frac{p}{m}\frac{\partial \rho_W}{\partial q} + \gamma\frac{\partial \rho_W}{\partial p} + D(\rho). \tag{24}$$

(3) In the case of the harmonic oscillator with $U = m\omega^2 q^2/2$, equation (21) takes the form:

$$\frac{\partial \rho_W}{\partial t} = -\frac{p}{m}\frac{\partial \rho_W}{\partial q} + m\omega^2 q\frac{\partial \rho_W}{\partial p} + D(\rho_W). \tag{25}$$

Since the coefficients are linear in the variables q and p and the diffusion coefficients are constant with respect to q and p, equations (23)–(25) describe an Ornstein–Uhlenbeck process. Equations (23)–(25) are exactly equations of the Fokker–Planck type. Equation (25) represents an exactly solvable model that is studied in [76,77].

Note that not every function $\rho(0, q, p)$ on the phase-space is the Weyl symbol of a density operator. Hence, the quantum mechanics appears now in the restrictions imposed on the initial condition $\rho_W(0, q, p)$ for equation (21). The most frequently used choice for $\rho_W(0, q, p)$ is a Gaussian function and equations (23)–(25) preserve this Gaussian type, i.e., $\rho_W(t, q, p)$ is always a Gaussian function in

time, so that the differences between quantum and classical mechanics are completely lost in this representation of the master equation.

(4) For the exponential potential $U(q) = \alpha \exp(-\beta q)$, the Wigner equation is the infinite order partial differential equation

$$\frac{\partial \rho_W}{\partial t} = -\frac{p}{m}\frac{\partial \rho_W}{\partial q} - \alpha\beta e^{-\beta q}\frac{\partial \rho_W}{\partial p} + \sum_{n=1}^{\infty} \frac{(-1)^{3n+1}(\hbar)^{2n}\alpha\beta^{2n+1}}{2^{2n}(2n+1)!} e^{-\beta q}\frac{\partial^{2n+1}\rho_W}{\partial p^{2n+1}} + D(\rho_W). \tag{26}$$

In the case of a potential of the finite polynomial form $U(q) = \sum_{n=1}^{N} a_n q^n$, the sum keeps only finite number of the terms. As an example, we can consider an anharmonic oscillator with the potential $U_{anh}(q) = m\omega^2 q^2/2 + cq^4$. In this case, equation (21) becomes

$$\frac{\partial \rho}{\partial t} = -\frac{p}{m}\frac{\partial \rho_W}{\partial q} + \left(m\omega^2 q + 4cq^3\right)\frac{\partial \rho_W}{\partial p} - c\hbar^2 q\frac{\partial^3 \rho_W}{\partial p^3} + D(\rho_W). \tag{27}$$

This equation has one term with third derivative, associated with the nonlinear potential $U_{anh}(q)$. In fact, the first three terms on the right-hand side of equation (27) give the usual Wigner equation of an isolated anharmonic oscillator. The third derivative term is of order $\hbar^2$ and is the quantum correction. In the classical limit, when this term is neglected, the Wigner equation becomes the Fokker–Planck type equation.

(5) For a periodic potential $U(q) = U_0 \cos(kq)$,

$$\frac{\partial^{2n+1} U}{\partial q^{2n+1}} = (-1)^n k^{2n}\frac{\partial U}{\partial q}, \tag{28}$$

and we obtain

$$\frac{\partial \rho_W}{\partial t} = -\frac{p}{m}\frac{\partial \rho_W}{\partial q} + \frac{\partial U}{\partial q}\Delta\rho_W + D(\rho_W), \tag{29}$$

where

$$\Delta\rho_W = \frac{\rho_W(t, q, p + \hbar k/2) - \rho_W(t, q, p - \hbar k/2)}{\hbar k}. \tag{30}$$

Equation (29) takes a simpler form when $\hbar k$ is large compared to the momentum spread Δp of the particle, i.e., when the spatial extension of the wave packet representing the particle is large compared to the spatial period of the potential. Imposing the condition $\hbar k \gg \Delta p$ on equation (30), we have that $\Delta\rho_W$ is small ($\Delta\rho_W \approx 0$) for any p that yields an appreciable value of the Wigner distribution function. Equation (29) is then reduced to the equation (23) for a free particle moving in an environment.

From the examples (1)–(3), we see that for Hamiltonians at most quadratic in q and p, the equation of motion of the Wigner distribution *contains only the classical part* and the contributions from the non-Hamiltonian properties of the system and obeys classical Fokker–Planck equations of motion (23)–(25). In general, the potential U has terms of order higher than q^2 and one has to deal with a partial differential equation of order higher than two or generally of infinite order. When the potential deviates only slightly from the harmonic potential, one can take the classical limit $\hbar \to 0$ in equation (21) as the lowest-order approximation to the quantum dynamics and construct higher-order approximations that contain quantum corrections to the classical behavior using the perturbation technique.

Phase-space representation of quantum dynamics provides a natural framework to study the consequences of the chaotic dynamics and its interplay with decoherence. Equation (21) can be applied in order to investigate the process of decoherence for quantum chaos. Since decoherence induces a transition from quantum to classical mechanics, it can be used to find the connection between the classical and quantum chaotic systems.

(6) Equation (21) was considered in [119], for the special case of the high temperature limit of the environment: $\mu = \lambda = \gamma$, where γ is the relaxation rate, $d_{qq} = 0$, $d_{pq} = 0$ and the diffusion coefficient $d_{pp} = D = 2m\gamma k_B T$, where T is the temperature of the environment. In this model the symmetry between q and p is broken, and coupling with the environment through position gives momentum diffusion only. It is possible to use a similar equation in which the diffusion term is symmetric, namely $D(\partial_{pp}^2 + \partial_{qq}^2)\rho_W$.

(7) The power series involving third and higher derivative terms can be neglected. The diffusion terms may smooth out the Wigner function, suppressing contributions from the higher-order terms. When these terms can be neglected, the Wigner function evolution equation (21) then becomes

$$\frac{\partial \rho_W}{\partial t} = -\frac{p}{m}\frac{\partial \rho_W}{\partial q} + \frac{\partial U}{\partial q}\frac{\partial \rho_W}{\partial p} + D(\rho_W). \tag{31}$$

In the case of a thermal bath and

$$\lambda = \mu = \gamma, \quad d_{qq} = d_{pq} = 0, \quad d_{pp} = D = 2m\gamma k_B T,$$

equation (31) becomes the Kramer equation

$$\frac{\partial \rho_W}{\partial t} = -\frac{p}{m}\frac{\partial \rho_W}{\partial q} + \frac{\partial U}{\partial q}\frac{\partial \rho_W}{\partial p} + 2\gamma\frac{\partial}{\partial p}(p\rho_W) + 2m\gamma k_B T\frac{\partial^2 \rho_W}{\partial p^2}. \tag{32}$$

It has the stationary solution

$$\rho_W(q, p) = Z^{-1}\exp -\frac{H_0(q, p)}{k_B T}, \tag{33}$$

where $H_0(q, p) = p^2/2m + U(q)$ and Z^{-1} is a normalization factor. It is a Wigner function only if the potential is such that $\exp[-U(q)/k_BT]$ is normalizable. This requires $U(q) \to \infty$ as $q \to \pm\infty$ faster than $\ln|q|$. In this case, the stationary distribution is the Weyl symbol of the thermal state

$$\rho_W(Q, P) = Z^{-1} \exp -\frac{H_0(Q, P)}{k_BT}, \qquad Z = Tr \exp\bigl(-H_0(Q, P)/k_BT\bigr),$$

for large temperatures T. All solutions of equation (32) approach the stationary solutions (33) as $t \to \infty$. Hence all initial states tend towards the thermal state in the long-time limit.

The phase-space formulation of the Lindblad equation represents an alternative to the standard formulation. The main difficulty with the phase-space formulation is that the time development of the phase-space Wigner distribution is given in terms of an infinite order partial differential equation (see equation (21)). This difficulty is a result of the fact that superoperator Λ is not a Weyl ordered superoperator.

Equation (21) is the infinite order differential equation. If Λ is a Weyl ordered superoperator, then we obtain a finite order differential equation for Wigner distribution $\rho_W(q, p)$. The Weyl ordered superoperator $\Lambda = \Lambda[L_Q^{\pm}, L_P^{\pm}]$ gives an operator equation with Weyl ordered operators. As a result, the correspondent equation for the Wigner distribution is finite order.

22.3. Integrals of motion of non-Hamiltonian systems

Let $\mathcal{M}$ be an operator algebra of observables, and let $\mathcal{L}$ be a superoperator on $\mathcal{M}$. In the general case, the restriction of derivation superoperators is not necessary. We then can define a quantum system by the equation

$$\frac{d}{dt}A = \frac{\partial}{\partial t}A + \mathcal{L}(A) \tag{34}$$

for a quantum observable $A \in \mathcal{M}$. The operators $A_k \in \mathcal{M}$ satisfying

$$\frac{\partial}{\partial t}A_k + \mathcal{L}(A_k) = 0 \tag{35}$$

can be called the integrals of motion (invariants).

Let us consider a set of operators $I_k \in \mathcal{M}$, which are closed under the action of the superoperator $\mathcal{L}$, i.e.,

$$\mathcal{L}(I_k) = L_{kl}(t)I_l,$$

where $L_{kl}(t)$ are time dependent functions. If the I_l appearing in the $\mathcal{L}(I_k)$ is not closed, the set of I_k must be extended. We shall denote the linear space generated by I_k as $\mathcal{M}_I$.

We now look for an invariant $A(t)$, which is an element of the space $\mathcal{M}_I$ such that

$$A(t) = \sum_{k=1}^{m} \lambda_k(t) I_k(t).$$

The time development of $I_k(t)$ is given by (34), and the dynamical invariant $I_k(t)$ is characterized by (35). Then equation of motion gives

$$\sum_{k=1}^{m} \left(\frac{d}{dt}\lambda_k(t) + \sum_{l=1}^{m} \lambda_l(t) L_{lk}(t) \right) I_k = 0.$$

As a result, we obtain

$$\frac{d}{dt}\lambda_k(t) + \sum_{l=1}^{m} \lambda_l(t) L_{lk}(t) = 0.$$

This is the system of linear first order differential equations for functions $\lambda_k(t)$. Solution of the system gives the integral $A(t)$ of motion for non-Hamiltonian system.

Chapter 23

Path Integral for Non-Hamiltonian Systems

23.1. Non-Hamiltonian evolution of mixed states

Unitary evolution is not the most general type of state change possible for quantum systems. The most general state change of a quantum system is a quantum operation. One can describe a quantum operation starting from a unitary evolution of some closed (Hamiltonian) system if the quantum non-Hamiltonian system is a subsystem of the closed system. However, situations can arise where it is difficult or impossible to find a closed system comprising the given quantum system. This would render theory of quantum operations a fundamental generalization of the unitary evolution of the quantum system.

All processes occur in time. It is naturally to consider time dependence for quantum operations. We will consider the path integral approach to general time-dependent quantum operations. The quantum operation is considered as a real completely positive trace-preserving superoperator on the operator space. We derive a path integral for a completely positive quantum operation satisfied Lindblad equation. For example, we consider a path integral for a quantum operation with a simple infinitesimal generator. Note that the path integral approach to non-Hamiltonian, open and dissipative quantum systems is considered in [3,32,33, 53,107,109,153,158–160,168].

The quantum Liouville equation can be represented as the linear equation

$$\frac{d}{dt}|\varrho_t) = \hat{\Lambda}_t|\varrho_t). \tag{1}$$

The superoperator language allows one to use the analogy with Dirac's notations. This leads quite simple to the derivation of the appropriate equations.

Here $\hat{\Lambda}_t$ is a linear Liouville superoperator. For the globally Hamiltonian quantum systems this superoperator is defined by the Hamiltonian H: $\hat{\Lambda}_t = -(i/\hbar)(L_H - R_H)$. For non-Hamiltonian systems, the Liouville superoperator has the form

$$\hat{\Lambda}_t = -\frac{i}{\hbar}(L_H - R_H) + \hat{D}. \tag{2}$$

In general, the operator $|\varrho_t)$ is an unnormalized density operator, i.e., $Tr\,\varrho_t = (I|\varrho_t) \neq 1$.

Equation (1) has the formal solution

$$|\varrho_t) = \hat{\mathcal{E}}(t, t_0)|\varrho_{t_0}), \tag{3}$$

where $\hat{\mathcal{E}}(t, t_0)$ is a linear quantum operation defined by

$$\hat{\mathcal{E}}(t, t_0) = T \exp \int_{t_0}^{t} d\tau\ \hat{\Lambda}_\tau. \tag{4}$$

The symbol T is a time-ordering operator. The quantum operation (4) satisfies the quantum Liouville equation (1). We can define a normalized density operator $|\rho_t)$ by

$$|\rho_t) = |\varrho_t)(I|\varrho_t)^{-1} \quad \text{or} \quad |\rho_t) = \frac{\hat{\mathcal{E}}(t, t_0)|\varrho)}{(I|\hat{\mathcal{E}}(t, t_0)|\varrho)},$$

i.e., $\rho_t = \varrho_t / Tr[\varrho_t]$. The evolution equation for the normalized density operator ρ_t can be written in the form

$$\frac{d}{dt}|\rho_t) = \hat{\Lambda}_t|\rho_t) - |\rho_t)(I|\hat{\Lambda}_t|\rho_t).$$

In general, this equation is a nonlinear equation. A formal solution of this equation is connected with the nonlinear quantum operation

$$|\rho_t) = \hat{\mathcal{N}}_t|\rho_{t_0}) = \frac{\hat{\mathcal{E}}(t, t_0)|\rho_{t_0})}{(I|\hat{\mathcal{E}}(t, t_0)|\rho_{t_0})}.$$

The equation of motion has the form

$$\frac{d}{dt}\hat{\mathcal{N}}_t|\rho_{t_0}) = \hat{\Lambda}_t\hat{\mathcal{N}}_t|\rho) - \hat{\mathcal{N}}_t|\rho)(I|\hat{\Lambda}_t\hat{\mathcal{N}}_t|\rho).$$

Unitary evolution is not the most general type of state change possible for quantum systems. The most general state change of a quantum system is a positive trace-preserving map which is called a quantum operation. A quantum operation is a superoperator $\hat{\mathcal{E}}$ which maps the density operator $|\rho)$ to the density operator $|\rho')$. If $|\rho)$ is a density operator, then $|\rho') = \hat{\mathcal{E}}|\rho)$ should also be a density operator. Any density operator ρ is a self-adjoint ($\rho_t^* = \rho_t$), positive ($\rho_t > 0$) operator with unit trace ($Tr\,\rho_t = 1$). Therefore, the requirements for a superoperator $\hat{\mathcal{E}}$ to be the quantum operation are as follows:

(1) $\hat{\mathcal{E}}$ is a *real* superoperator, i.e., $(\hat{\mathcal{E}}(A))^* = \hat{\mathcal{E}}(A^*)$ for all A. The real superoperator $\hat{\mathcal{E}}$ maps the self-adjoint operator ρ to the self-adjoint operator $\hat{\mathcal{E}}(\rho)$: $(\hat{\mathcal{E}}(\rho))^* = \hat{\mathcal{E}}(\rho)$.

(2) $\hat{\mathcal{E}}$ is a *positive* superoperator, i.e., $\hat{\mathcal{E}}$ maps positive operators to positive operators: $\hat{\mathcal{E}}(A^2) > 0$ for all $A \neq 0$ or $\hat{\mathcal{E}}(\rho) \geqslant 0$.
(3) $\hat{\mathcal{E}}$ is a *trace-preserving* superoperator, i.e., $(I|\hat{\mathcal{E}}|\rho) = (\hat{\mathcal{E}}^*(I)|\rho) = 1$ or $\hat{\mathcal{E}}^*(I) = I$.

We have to assume the superoperator $\hat{\mathcal{E}}$ to be not merely positive but completely positive.

Let $\hat{\mathcal{E}}$ be a *convex linear* superoperator on the set of density operators, i.e.,

$$\hat{\mathcal{E}}\left(\sum_s \lambda_s \rho_s\right) = \sum_s \lambda_s \hat{\mathcal{E}}(\rho_s),$$

where all λ_s are $0 < \lambda_s < 1$ and $\sum_s \lambda_s = 1$. Any convex linear map of density operators can be uniquely extended to a *linear* superoperator on self-adjoint operators. Note that any linear completely positive superoperator can be represented by

$$\hat{\mathcal{E}} = \sum_{k=1}^{m} L_{A_k} R_{A_k^*}: \quad \hat{\mathcal{E}}(\rho) = \sum_{k=1}^{m} A_k \rho A_k^*.$$

The restriction to linear quantum operations is unnecessary. Let us consider a linear real completely positive superoperator $\hat{\mathcal{E}}$ which is not trace-preserving. Suppose $(I|\hat{\mathcal{E}}|\rho) = Tr(\hat{\mathcal{E}}(\rho))$ is the probability that the process represented by the superoperator $\hat{\mathcal{E}}$ occurs. Since the probability is nonnegative and never exceed 1, it follows that the superoperator $\hat{\mathcal{E}}$ is a trace-decreasing superoperator: $0 \leqslant (I|\hat{\mathcal{E}}|\rho) \leqslant 1$ or $\hat{\mathcal{E}}^*(I) \leqslant I$. In general, any real linear completely positive trace-decreasing superoperator is not a quantum operation, since it can be not trace-preserving. The quantum operation can be defined as a *nonlinear trace-preserving* operation $\hat{\mathcal{N}}$ by

$$\hat{\mathcal{N}}|\rho) = \hat{\mathcal{E}}|\rho)(I|\hat{\mathcal{E}}|\rho)^{-1} \quad \text{or} \quad \hat{\mathcal{N}}(\rho) = \frac{\hat{\mathcal{E}}(\rho)}{Tr(\hat{\mathcal{E}}(\rho))},$$

where $\hat{\mathcal{E}}$ is a real linear completely positive trace-decreasing superoperator.

All processes occur in time. It is naturally to consider time dependence for quantum operations $\hat{\mathcal{E}}(t, t_0)$. Let the linear superoperators $\hat{\mathcal{E}}(t, t_0)$ form a completely positive semi-group such that

$$\frac{d}{dt}\hat{\mathcal{E}}(t, t_0) = \hat{\Lambda}_t \hat{\mathcal{E}}(t, t_0).$$

23.2. Path integral for quantum operations

In the coordinate representation the kernel

$$\varrho(q, q', t) = (q, q'|\varrho_t)$$

of the density operator $|\varrho_t)$ evolves according to the equation

$$\varrho(q, q', t) = \int dq_0\, dq_0'\, \mathcal{E}(q, q', q_0, q_0', t, t_0)\varrho(q_0, q_0', t_0),$$

where we use equation (3). The function

$$\mathcal{E}(q, q', q_0, q_0', t, t_0) = \big(q, q'\big|\hat{\mathcal{E}}(t, t_0)\big|q_0, q_0'\big) \tag{5}$$

is a kernel of the linear quantum operation $\hat{\mathcal{E}}(t, t_0)$. Let the Liouville superoperator $\hat{\Lambda}_t$ be time independent, i.e., the quantum operation $\hat{\mathcal{E}}(t, t_0)$ is given by

$$\hat{\mathcal{E}}(t, t_0) = \exp\big\{(t - t_0)\hat{\Lambda}\big\}. \tag{6}$$

Let us give the basic theorem regarding path integrals of non-Hamiltonian systems [159,160,168].

THEOREM. *Let* $\{\hat{\mathcal{E}}(t, t_0)|t \geqslant t_0\}$ *be a superoperator semi-group such that*

$$\hat{\mathcal{E}}(t_0, t_0) = \hat{I}, \qquad \hat{\mathcal{E}}(t, t_0) = \hat{\mathcal{E}}(t, t_1)\hat{\mathcal{E}}(t_1, t_0),$$

where $t \geqslant t_1 \geqslant t_0$. *If the infinitesimal generator* $\hat{\Lambda}$ *of this semi-group is defined by* (6)*, then the path integral for kernel* (5) *of the quantum operation* $\hat{\mathcal{E}}(t, t_0)$ *has the form*:

$$\mathcal{E}(q, q', q_0, q_0', t, t_0) = \int \mathcal{D}q\mathcal{D}q'\mathcal{D}p\mathcal{D}p' \exp \int_{t_0}^{t} dt \left(\frac{\imath}{\hbar}[\dot{q}\, p - \dot{q}'\, p'] + \Lambda_S(q, q', p, p') \right). \tag{7}$$

This integral is over all trajectories in the double phase space with the constraints $q(t_0) = q_0$, $q(t) = q$, $q'(t_0) = q_0'$, $q'(t) = q'$, *and the measure*

$$\mathcal{D}q = \prod_t dq(t), \qquad \mathcal{D}p = \prod_t \frac{dp(t)}{2\pi\hbar}.$$

The symbol $\Lambda_S(q, q', p, p')$ *of the Liouville superoperator* $\hat{\Lambda}$ *is connected with the kernel* $\Lambda(q, q', y, y')$ *by*

$$\Lambda_S(q, q', p, p') = \int dy\, dy'\, \Lambda(q, q', y, y') \cdot \exp -\frac{\imath}{\hbar}\big[(q - y)p - (q' - y')p'\big],$$

where $\Lambda(q, q', y, y') = (q, q'|\hat{\Lambda}|y, y')$ *and*

$$\Lambda(q, q', y, y') = \frac{1}{(2\pi\hbar)^{2n}} \int dp\, dp'\, \Lambda_S(q, q', p, p')$$

$$\cdot \exp \frac{\imath}{\hbar}\big[(q-y)p-(q'-y')p'\big].$$

This theorem is proved in the paper [168].

COROLLARY. *If the superoperator Λ is defined by equation (2), then the path integral for the quantum operation kernel (5) has the form*

$$\mathcal{E}(q,q',q_0,q_0',t,t_0) = \int \mathcal{D}q\mathcal{D}p\mathcal{D}q'\mathcal{D}p' \exp\left(\frac{\imath}{\hbar}\big(\mathcal{A}(q,p)-\mathcal{A}(p',q')\big)+D(q,q',p,p')\right).$$

Here $\mathcal{A}(q,p)$ and $\mathcal{A}(p',q')$ are the action functionals

$$\mathcal{A}(q,p) = \int_{t_0}^{t} dt\,\big(\dot{q}p - H(q,p)\big),$$

$$\mathcal{A}(p',q') = \int_{t_0}^{t} dt\,\big(\dot{q}'p' - H(p',q')\big). \tag{8}$$

The functional $D(q,q',p,p')$ is a time integral of the symbol D_S of the superoperator $\hat{D}$.

The functional $D(q,q',p,p')$ describes the dissipative part of evolution.

COROLLARY. *If the quantum system is a globally Hamiltonian system, then $D(q,q',p,p') = 0$ and the path integral for the quantum operation (5) takes the form*

$$\mathcal{E}(q,q',q_0,q_0',t,t_0) = U^*(q,q_0,t,t_0)U(q',q_0',t,t_0),$$

where

$$U(q',q_0',t,t_0) = \int \mathcal{D}q'\mathcal{D}p' \exp -\frac{\imath}{\hbar}\mathcal{A}(q',p'),$$

$$U^*(q,q_0,t,t_0) = \int \mathcal{D}q\mathcal{D}p \exp \frac{\imath}{\hbar}\mathcal{A}(q,p).$$

The path integral for the dissipative quantum systems and the corresponding quantum operations cannot be separated and this path integral can only be defined in the double phase space.

Liouville superoperator for globally Hamiltonian systems can be presented as $\Lambda = -(i/\hbar)(L_H - R_H)$. Using that the kernel of the superoperator Λ is the kernel

of the operator $\Lambda(\hat{P}(y, y'))$, we obtain

$$\Lambda(q, q', y, y') = <\hat{P}(q, q')|\Lambda\big(\hat{P}(y, y')\big)> = <q|\Lambda\big(\hat{P}(y, y')\big)|q'>.$$

As a result, the kernel of Λ for quantum Hamiltonian systems is

$$\Lambda(q, q', p, p') = -\frac{i}{\hbar}\big[H(q, p) - H(p', q')\big]. \tag{9}$$

The kernel (5) for quantum Hamiltonian systems has the form

$$\mathcal{E}(q, q', q_0, q_0', t, t_0) = \int \mathcal{D}q\mathcal{D}p \exp\frac{i}{\hbar}\int_{t_0}^{t} dt\,\big(\dot{q}\,p - H(q, p)\big)$$

$$\cdot \int \mathcal{D}q'\mathcal{D}p' \exp -\frac{i}{\hbar}\int_{t_0}^{t} dt\,\big(\dot{q}'p' - H(p', q')\big).$$

We can rewrite this amplitude in the form [136,168]

$$\mathcal{E}(q, q', q_0, q_0', t, t_0) = \int \mathcal{D}q\mathcal{D}p\mathcal{D}q'\mathcal{D}p' \exp\frac{i}{\hbar}\big(\mathcal{A}(q, p) - \mathcal{A}(p', q')\big),$$

where $\mathcal{A}(q, p)$ and $\mathcal{A}(p', q')$ are defined by (8).

It is easy to see that the kernel (5) for Hamiltonian systems splits (decomposes) into two independent Feynman's path integrals:

$$\mathcal{E}(q, q', q_0, q_0', t, t_0) = U(q, q_0, t, t_0)U^*(q', q_0', t, t_0),$$

where

$$U(q, q_0, t, t_0) = \int \mathcal{D}q\mathcal{D}p \exp\frac{i}{\hbar}\mathcal{A}(q, p).$$

23.3. Path integral for completely positive quantum operations

There exists a one-to-one correspondence between the completely positive norm continuous semi-group of superoperators $\hat{\mathcal{E}}(t, t_0)$ and superoperator $\hat{\Lambda}$ such that the adjoint superoperator $\mathcal{L} = \bar{\Lambda}^*$ is completely dissipative. The Lindblad theorem [95,67,68] gives the most general form of the bounded completely dissipative Liouville superoperator $\hat{\Lambda}$. The quantum Liouville equation for a completely positive evolution is the Lindblad equation

$$\frac{d\rho_t}{dt} = -\frac{i}{\hbar}[H, \rho_t] + \frac{1}{2\hbar}\sum_{k=1}^{m}\big([V_k\rho_t, V_k^*] + [V_k, \rho_t V_k^*]\big). \tag{10}$$

This equation in an operator Hilbert space can be written as

$$\frac{d}{dt}|\rho_t) = \hat{\Lambda}|\rho_t),$$

where the Liouville superoperator $\hat{\Lambda}$ is given by

$$\hat{\Lambda} = -\frac{i}{\hbar}(L_H - R_H) + \frac{1}{2\hbar}\sum_{k=1}^{m}\bigl(2L_{V_k}R_{V_k^*} - L_{V_k}L_{V_k^*} - \hat{R}_{V_k^*}\hat{R}_{V_k}\bigr). \tag{11}$$

The basic assumption is that the general form of a bounded superoperator $\hat{\Lambda}$, given by the Lindblad theorem, is also valid for an unbounded superoperator. Another condition imposed on the operators H, V_k, V_k^* is that they are functions of the observables P and Q (with $[Q, P] = i\hbar I$) of the one-dimensional quantum system. Let us consider $V_k = a_k P + b_k Q$, were $k = 1, 2$, and a_k, b_k are complex numbers, and the Hamiltonian operator

$$H = \frac{1}{2m}P^2 + \frac{m\omega^2}{2}Q^2 + \frac{\mu}{2}(PQ + QP).$$

Then with the notation:

$$d_{qq} = \frac{\hbar}{2}\sum_{k=1,2}|a_k|^2, \qquad d_{pp} = \frac{\hbar}{2}\sum_{k=1,2}|b_k|^2,$$

$$d_{pq} = -\frac{\hbar}{2}\,\mathrm{Re}\Bigl(\sum_{k=1,2}a_k^* b_k\Bigr), \qquad \lambda = -\mathrm{Im}\Bigl(\sum_{k=1,2}a_k^* b_k\Bigr)$$

equation (10) can be written as

$$\begin{aligned}\frac{d}{dt}|\rho_t) = {}& \frac{1}{2m}L_P^+ L_P^- \\ & + \frac{m\omega^2}{2}L_Q^+ L_Q^- - (\lambda - \mu)L_P^- L_Q^+|\rho_t) + (\lambda + \mu)L_Q^- L_P^+|\rho_t) \\ & + d_{pp}L_Q^- L_Q^-|\rho_t) + d_{qq}L_P^- L_P^-|\rho_t) - 2d_{pq}L_P^- L_Q^-|\rho_t),\end{aligned} \tag{12}$$

where $L_A^{\pm}$ are the left superoperators

$$L_A^- = \frac{1}{i\hbar}(L_A - R_A), \qquad L_A^+ = \frac{1}{2}(L_A + R_A).$$

Equation (12) is a superoperator form of the well-known phenomenological dissipative model [43,133].

Let us give the basic theorem [159,160,168] regarding path integrals for completely positive quantum operations with the Liouville superoperator (11).

THEOREM. *Let* $\{\hat{\mathcal{E}}(t, t_0),\ t \geqslant t_0\}$ *be a completely positive semi-group of linear real trace-preserving superoperators such that the infinitesimal generator* $\hat{\Lambda}$ *of this semi-group is defined by* (11). *Then the path integral for the kernel of the completely positive quantum operation* $\hat{\mathcal{E}}(t, t_0)$ *has the form*

$$\mathcal{E}(q, q', q_0, q_0', t, t_0) = \int \mathcal{D}q\mathcal{D}p\mathcal{D}q'\mathcal{D}p'\mathcal{F}(q, q', p, p') \times \exp\frac{\imath}{\hbar}\big(\mathcal{A}(q, p) - \mathcal{A}(p', q')\big), \tag{13}$$

where $\mathcal{A}(q, p)$ *and* $\mathcal{A}(p', q')$ *are action functionals* (8) *and the functional* $\mathcal{F}(q, q', p, p')$ *is defined as*

$$\mathcal{F}(q, q', p, p') = \exp -\frac{1}{2\hbar}\int_{t_0}^{t} dt \sum_{k=1}^{m}\big((V_k^* V_k)(q, p) + (V_k^* V_k)(p', q') - 2V_k(q, p)V_k^*(p', q')\big). \tag{14}$$

PROOF. The kernel of superoperator (11) is

$$\begin{aligned}\Lambda(q, q', y, y') &= (q, q_k'|\hat{\Lambda}|y, y') \\ &= -\frac{\imath}{\hbar}\big(<y'|q'><q|H|y> - <q|y><y'|H|q'>\big) \\ &\quad + \frac{1}{\hbar}\sum_{k=1}^{m} <q|V_k|y><y'|V_k^*|q'> \\ &\quad - \frac{1}{2\hbar}\sum_{k=1}^{m}\big(<y'|q'><q|V_k^* V_k|y> \\ &\quad - <q|y><y'|V_k^* V_k|q'>\big).\end{aligned}$$

The symbol $\Lambda_S(q, q', p, p')$ of the Liouville superoperator $\hat{\Lambda}$ can be derived by

$$\begin{aligned}\Lambda(q, q', y, y') = \int dp\, dp' \Bigg(&-\frac{\imath}{\hbar}\big(<y'|p'><p'|q'><q|H_1|p><p|y> \\ &- <q|p><p|y><y'|p'><p'|H_2|q'>\big) \\ &+ \frac{1}{\hbar}\sum_{k=1}^{m} <q|V_k|p><p|y><y'|p'><p'|V_k^*|q'>\Bigg),\end{aligned}$$

where the operators H_1 and H_2 are defined by the relations

$$H_1 \equiv H - \frac{\imath}{2}\sum_{k=1}^{m} V_k^* V_k, \qquad H_2 \equiv H + \frac{\imath}{2}\sum_{k=1}^{m} V_k^* V_k.$$

Then the symbol $\Lambda_S(q, q', p, p')$ of the Liouville superoperator (11) can be written in the form

$$\Lambda_S(q, q', p, p') = -\frac{\imath}{\hbar}\left(H_1(q, p) - H_2(p', q') + i\sum_{k=1}^{m} V_k(q, p)V_k^*(p', q')\right),$$

or

$$\Lambda_S(q, q', p, p') = -\frac{\imath}{\hbar}\big[H(q, p) - H(p', q')\big] - \frac{1}{2\hbar}\sum_{k=1}^{m}\big((V_k^*V_k)(q, p) + (V_k^*V_k)(p', q') - 2V_k(q, p)V_k^*(p', q')\big),$$

where $H(q, p)$ is a qp-symbol of the Hamilton operator H and $H(p, q)$ is a pq-symbol of the operator H.

The path integral for a completely positive quantum operation kernel has the form

$$\mathcal{E}(q, q', q_0, q_0', t, t_0) = \int \mathcal{D}q\mathcal{D}p\mathcal{D}q'\mathcal{D}p'\,\mathcal{F}(q, q', p, p') \times \exp\frac{\imath}{\hbar}\big(\mathcal{A}(q, p) - \mathcal{A}(p', q')\big).$$

Here $\mathcal{A}(q, p)$ and $\mathcal{A}(p', q')$ are action functionals (8), and the functional $\mathcal{F}(q, q', p, p')$ is defined by (14). □

The functional $\mathcal{F}(q, q', p, p')$ describes the dissipative part of the evolution and can be called a *double phase space influence functional*. The completely positive quantum operation is described by the functional (14).

COROLLARY. *For the phenomenological dissipative model* (12) *the double phase space path integral has the form* (13) *with the functional*

$$\mathcal{F}(q, q', p, p') = \exp\frac{1}{\hbar^2}\int_{t_0}^{t} dt\,\big(2d_{qp}(q - q')(p - p') - d_{qq}(p - p')^2 - d_{pp}(q - q')^2 + i\hbar\lambda(pq' - qp') + i\hbar\mu(q'p' - qp)\big). \tag{15}$$

Using the well-known connection between the phase space (Hamiltonian) path integral and the configuration space (Lagrangian) path integral, we can derive the following theorem.

THEOREM. *If the symbol $\Lambda_s(q, q', p, p')$ of the Liouville superoperator can be represented in the form*

$$\Lambda_S(q, q', p, p') = -\frac{\imath}{\hbar}\big[H(q, p) - H(p', q')\big] + D_S(q, q', p, p'), \tag{16}$$

where

$$H(q, p) = \frac{1}{2}a_{kl}^{-1}(q)p_k p_l - b_k(q)p_k + c(q), \tag{17}$$

$$D_S(q, q', p, p') = -d_k(q, q')p_k + d'_k(q, q')p'_k + e(q, q'), \tag{18}$$

then the double phase space path integral (7) can be represented as the double configuration space path integral

$$\mathcal{E}(q, q', q_0, q'_0, t, t_0) = \int \mathcal{D}q\mathcal{D}q'\,\mathcal{F}(q, q')\exp\frac{\imath}{\hbar}\big(\mathcal{A}(q) - \mathcal{A}(q')\big), \tag{19}$$

where

$$\begin{aligned}
\mathcal{A}(q) &= \int_{t_0}^{t} dt\,\mathcal{L}(q, \dot{q}),\\
\mathcal{L}(q, \dot{q}) &= \frac{1}{2}a_{kl}(q)\dot{q}_k\dot{q}_l + a_{kl}(q)b_k(q)\dot{q}_l\\
&\quad + \frac{1}{2}a_{kl}(q)b_k(q)b_l(q) - c(q).
\end{aligned} \tag{20}$$

This Lagrangian $\mathcal{L}(q, \dot{q})$ is related to the Hamiltonian (17) by the usual relations

$$\mathcal{L}(q, \dot{q}) = \dot{q}_k p_k - H(q, p), \quad p_k = \frac{\partial\mathcal{L}}{\partial\dot{q}}.$$

PROOF. Substituting (16) in (7), we obtain the kernel of the corresponding quantum operation. Integrating (7) in p and p', we obtain relation (19) with the functional

$$\begin{aligned}
\mathcal{F}(q, q') = \exp -\frac{1}{\hbar^2}\int_{t_0}^{t} dt\,\Bigg(&d_k(q, q')a_{kl}(q)\bigg[b_l(q) - \frac{i}{2\hbar}d_l(q, q')\bigg]\\
&+ d'_k(q, q')a_{kl}(q')\bigg[b_l(q') - \frac{i}{2\hbar}d'_l(q, q')\bigg]\\
&+ e(q, q') + \delta(0)\Delta(q, q')\Bigg),
\end{aligned}$$

where

$$\Delta(q,q') = -\frac{\hbar^2}{2}\left(\ln\left[\det\left(a_{kl}(q)\right)\right] + \ln\left[\det\left(a_{kl}(q')\right)\right]\right). \qquad \square$$

In equation (19) the functional $\mathcal{F}(q,q')$ is the Feynman–Vernon influence functional [58]. The Feynman path integral is defined for configuration space. The most general form of quantum mechanical path integral is defined for the phase space. The Feynman path integral can be derived from the phase space path integral for the special form of the Hamiltonian. It is known that the path integral for the configuration space is correct only for the Hamiltonian (17). The Feynman–Vernon path integral is defined in the double configuration space. Therefore, *Feynman–Vernon path integral is a special form of path integral for non-Hamiltonian systems* (7) *that is the double phase space path integral*. The Feynman–Vernon path integral is correct only for the Liouville superoperator (16), (17), (18). Note that the symbol $\Lambda_s(q,q',p,p')$ for most of the dissipative and non-Hamiltonian systems (with completely positive quantum operations) cannot be represented in the form (16).

COROLLARY. *In the general case, the completely positive quantum operation cannot be represented as the double configuration space path integral* (19).

For example, the double phase space path integral (15) for the phenomenological dissipative model (12) has the term pp'. Therefore the Liouville symbol $\Lambda_s(q,q',p,p')$ for this model cannot be represented in the form (16), (17), (18).

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Chapter 24

Non-Hamiltonian Systems as Quantum Computers

24.1. Quantum state and qubit

The usual models of a quantum computer deal only with unitary gates on pure states. In these models it is difficult or impossible to deal formally with measurements, dissipation and decoherence. It turns out that the restriction to pure states and unitary gates is unnecessary. Understanding the dynamics of non-Hamiltonian systems is important for studying quantum noise processes [63,137,138], quantum error correction [145,122,20], decoherence effects in quantum computations [116,13,110,94,198] and performing simulations of open and non-Hamiltonian quantum systems [180,181,9,99,197,165], see also [79,80,131,179].

We generalize the usual model of a quantum computer to a model in which a state is a density operator and gates are general superoperators (quantum operations), not necessarily unitary. The pure state of n two-level closed quantum systems is an element of 2^n-dimensional Hilbert space and it allows us to consider a quantum computer model with two-valued logic. The gates of this computer model are unitary operators act on a such state. In the general case, the mixed state (density operator) of n two-level quantum systems is an element of 4^n-dimensional operator Hilbert space (Liouville space). It allows us to use a quantum computer model with four-valued logic [165]. The gates of this model are general superoperators (quantum operations) which act on general n-ququat state. A ququat is a quantum state in a four-dimensional (operator) Hilbert space. Unitary two-valued logic gates and quantum operations for an n-qubit non-Hamiltonian system are considered as four-valued logic gates acting on n-ququat. We discuss universality for general quantum four-valued logic gates acting on ququats.

Pure states

A quantum system in a pure state is described by a unit vector in a Hilbert space $\mathcal{H}$. In the Dirac notation a pure state is denoted by $|\Psi>$. The Hilbert space $\mathcal{H}$ is a linear space with an inner product. The inner product for $|\Psi_1>$,

$|\Psi_2> \in \mathcal{H}$ is denoted by $<\Psi_1|\Psi_2>$. A quantum bit or qubit, the fundamental concept of quantum computations, is a two-state quantum system. The two basis states labeled $|0>$ and $|1>$ are orthogonal unit vectors, i.e., $<k|l> = \delta_{kl}$, where $k, l \in \{0, 1\}$. The Hilbert space of the qubit is $\mathcal{H}_2 = \mathbb{C}^2$. The quantum system which corresponds to a quantum computer (quantum circuit) consists of n quantum two-state particles. The Hilbert space $\mathcal{H}^{(n)}$ of such a system is a tensor product of n Hilbert spaces $\mathcal{H}_2$ of one two-state particle: $\mathcal{H}^{(n)} = \mathcal{H}_2 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_2$. The space $\mathcal{H}^{(n)}$ is a 2^n-dimensional complex linear space. Let us choose a basis for $\mathcal{H}^{(n)}$ which consists of the 2^n orthonormal states $|k>$, where k is in binary representation. The pure state $|k>$ is a tensor product of states $|k_i>$ in $\mathcal{H}^{(n)}$:

$$|k> = |k_1> \otimes |k_2> \otimes \cdots \otimes |k_n> = |k_1 k_2 \cdots k_n>,$$

where $k_i \in \{0, 1\}$ and $i = 1, 2, \ldots, n$. This basis is usually called the computational basis which has 2^n elements. A pure state $|\Psi(t)> \in \mathcal{H}^{(n)}$ is generally a superposition of the basis states.

Mixed states

In general, a quantum system is not in a pure state. Quantum systems are not really isolated from the rest of the universe, so it does not have a well-defined pure state. A density operator is a self-adjoint ($\rho^* = \rho$), nonnegative ($\rho \geqslant 0$) operator on $\mathcal{H}^{(n)}$ with unit trace ($Tr\,\rho = 1$). Pure states can be characterized by idempotent condition $\rho^2 = \rho$. A pure state can be represented by the operator $\rho(t) = |\Psi(t)><\Psi(t)|$.

One can represent an arbitrary density operator $\rho(t)$ for n-qubit in terms of tensor products of Pauli matrices σ_μ:

$$\rho(t) = \frac{1}{2^n} \sum_{\mu_1 \ldots \mu_n} P_{\mu_1 \ldots \mu_n}(t) \sigma_{\mu_1} \otimes \cdots \otimes \sigma_{\mu_n}, \tag{1}$$

where $\mu_i \in \{0, 1, 2, 3\}$ and $i = 1, \ldots, n$. Here σ_μ are Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{2}$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \sigma_0 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{3}$$

The real expansion coefficients $P_{\mu_1 \ldots \mu_n}(t)$ are given by

$$P_{\mu_1 \ldots \mu_n}(t) = Tr\big(\sigma_{\mu_1} \otimes \cdots \otimes \sigma_{\mu_n} \rho(t)\big).$$

Normalization ($Tr\,\rho = 1$) requires that $P_{0 \ldots 0}(t) = 1$. Since the eigenvalues of the Pauli matrices are ± 1, the expansion coefficients satisfy $|P_{\mu_1 \ldots \mu_n}(t)| \leqslant 1$.

24.2. Finite-dimensional Liouville space and superoperators

Finite-dimensional Liouville space

The space of linear operators acting on a 2^n-dimensional Hilbert space $\mathcal{H}^{(n)}$ is a $(2^n)^2 = 4^n$-dimensional complex linear space $\overline{\mathcal{H}}^{(n)}$. We denote an element A of $\overline{\mathcal{H}}^{(n)}$ by a ket-vector $|A)$. The inner product of two elements $|A)$ and $|B)$ of $\overline{\mathcal{H}}^{(n)}$ is defined as

$$(A|B) = Tr(A^* B). \tag{4}$$

The norm $\|A\| = \sqrt{(A|A)}$ is the Hilbert–Schmidt norm of operator A. A new Hilbert space $\overline{\mathcal{H}}^{(n)}$ with scalar product (4) is called the Liouville space attached to $\mathcal{H}^{(n)}$ or the associated Hilbert space.

Let $\{|k>\}$ be an orthonormal basis of $\mathcal{H}^{(n)}$:

$$<k|k'> = \delta_{kk'}, \qquad \sum_{k=0}^{2^n-1} |k><k| = I.$$

Then $|k, l) = ||k><l|)$ is an orthonormal basis of the Liouville space $\overline{\mathcal{H}}^{(n)}$:

$$(k, l|k', l') = \delta_{kk'}\delta_{ll'}, \qquad \sum_{k=0}^{2^n-1}\sum_{l=0}^{2^n-1} |k, l)(k, l| = \hat{I}. \tag{5}$$

This operator basis has 4^n elements. Note that

$$|k, l) = |k_1, l_1) \otimes |k_2, l_2) \otimes \cdots \otimes |k_n, l_n), \tag{6}$$

where $k_i, l_i \in \{0, 1\}$, $i = 1, \ldots, n$, and

$$|k_i, l_i) \otimes |k_j, l_j) = \big||k_i> \otimes |k_j>, <l_i| \otimes <l_j|\big).$$

For an arbitrary element $|A)$ of $\overline{\mathcal{H}}^{(n)}$, we have

$$|A) = \sum_{k=0}^{2^n-1}\sum_{l=0}^{2^n-1} |k, l)(k, l|A) \tag{7}$$

with $(k, l|A) = Tr(|l><k|A) = <k|A|l> = A_{kl}$.

Operators which act on $\overline{\mathcal{H}}^{(n)}$ are called superoperators and we denote them in general by the hat. For an arbitrary superoperator $\hat{\mathcal{E}}$ on $\overline{\mathcal{H}}^{(n)}$, we have

$$(k, l|\hat{\mathcal{E}}|A) = \sum_{k'=0}^{2^n-1}\sum_{l'=0}^{2^n-1} (k, l|\hat{\mathcal{E}}|k', l')(k', l'|A) = \sum_{k'=0}^{2^n-1}\sum_{l'=0}^{2^n-1} \mathcal{E}_{klk'l'} A_{k'l'}.$$

A superoperator $\hat{\mathcal{E}}$ is called unital if $\hat{\mathcal{E}}|I) = |I)$.

Quantum operations

Unitary evolution is not the most general type of state change possible for quantum systems. A most general state change is a positive map $\hat{\mathcal{E}}$ which is called a quantum operation or superoperator. In the formalism of quantum operations a final (output) state ρ' is assigned to the initial (input) state ρ by the map

$$\rho \to \rho' = \frac{\hat{\mathcal{E}}(\rho)}{Tr(\hat{\mathcal{E}}(\rho))}. \tag{8}$$

The trace in the denominator is induced in order to preserve the trace condition, $Tr(\rho') = 1$. In the general case, the map (8) is nonlinear, where $\hat{\mathcal{E}}$ is a linear positive map. The quantum operation $\hat{\mathcal{E}}$ can be considered as a completely positive map of the form.

$$\hat{\mathcal{E}} = \sum_{j=1}^{m} L_{A_j} R_{A_j^*}.$$

If ρ is an initial state that $Tr(\hat{\mathcal{E}}(\rho))$ is a probability that the process represented by $\hat{\mathcal{E}}$ occurs. The probability never exceed 1. As a result, $\hat{\mathcal{E}}$ must be trace-decreasing, i.e., $Tr(\hat{\mathcal{E}}(\rho)) \leqslant 1$ for all density operators ρ. This condition can be expressed as the operator inequality

$$\sum_{j=1}^{m} A_j^* A_j \leqslant I.$$

The normalized state is defined by (8). The map (8) is a nonlinear trace-preserving map. If $\hat{\mathcal{E}}$ is trace-preserving, then $Tr(\hat{\mathcal{E}}(\rho)) = 1$, and

$$\sum_{j=1}^{m} A_j^* A_j = I.$$

Note that a trace-preserving quantum operation $\hat{\mathcal{E}}(\rho) = A\rho A^*$ is unitary ($A^*A = AA^* = I$).

As an example of nonunitary dynamics, we consider a measurement. A quantum system being measured is no longer a closed system, since it is interacting with a measuring device. The usual way to describe a measurement is a set of projections P_k such that

$$P_k P_l = \delta_{kl} P_k, \qquad P_k^* = P_k, \qquad \sum_k P_k = \hat{I}.$$

The measurement gives

$$\hat{\mathcal{E}}_k(\rho) = P_k \rho P_k.$$

The probability of this measurement result is given by

$$p(k) = Tr\big(\hat{\mathcal{E}}_k(\rho)\big).$$

The normalization condition, $\sum_k p(k) = 1$ for density operators, is equivalent to the completeness condition $\sum_k P_k = I$. If ρ is an initial state, then the normalized state after the measurement is

$$\rho' = p^{-1}(k)\hat{\mathcal{E}}_k(\rho).$$

24.3. Generalized computational basis and ququats

Let us introduce a generalized computational basis and generalized computational states for 4^n-dimensional operator Hilbert space (Liouville space).

Pauli representation

Pauli matrices (2) and (3) can be considered as a basis for operator space $\overline{\mathcal{H}}^{(1)}$. Let us write the Pauli matrices (2) and (3) in the form

$$\sigma_1 = |0><1| + |1><0| = |0,1) + |1,0),$$
$$\sigma_2 = -i|0><1| + i|1><0| = -i(|0,1) - |1,0)),$$
$$\sigma_3 = |0><0| - |1><1| = |0,0) - |1,1),$$
$$\sigma_0 = I = |0><0| + |1><1| = |0,0) + |1,1).$$

We can use the equations

$$|0,0) = \frac{1}{2}\big(|\sigma_0) + |\sigma_3)\big), \qquad |1,1) = \frac{1}{2}\big(|\sigma_0) - |\sigma_3)\big),$$
$$|0,1) = \frac{1}{2}\big(|\sigma_1) + i|\sigma_2)\big), \qquad |1,0) = \frac{1}{2}\big(|\sigma_1) - i|\sigma_2)\big).$$

It allows us to rewrite the operator basis

$$|k,l) = |k_1,l_1) \otimes |k_2,l_2) \otimes \cdots \otimes |k_n,l_n)$$

by the complete basis operators

$$|\sigma_\mu) = |\sigma_{\mu_1} \otimes \sigma_{\mu_2} \otimes \cdots \otimes \sigma_{\mu_n}),$$

where $\mu_i = 2k_i + l_i$, i.e., $\mu_i \in \{0,1,2,3\}$ and $i = 1,\ldots,n$. The basis $|\sigma_\mu)$ is orthogonal

$$(\sigma_\mu|\sigma_{\mu'}) = 2^n\delta_{\mu\mu'}$$

and it is a complete operator basis, i.e.,

$$\frac{1}{2^n}\sum_{\mu}^{N-1}|\sigma_\mu)(\sigma_\mu| = \hat{I},$$

where $N = 4^n$. For an arbitrary element $|A)$ of $\overline{\mathcal{H}}^{(n)}$, we have the Pauli representation

$$|A) = \frac{1}{2^n}\sum_{\mu=0}^{N-1}|\sigma_\mu)(\sigma_\mu|A)$$

with the complex coefficients $(\sigma_\mu|A) = Tr(\sigma_\mu A)$. We can rewrite formula (1) using the complete operator basis $|\sigma_\mu)$ in $\overline{\mathcal{H}}^{(n)}$:

$$|\rho(t)) = \frac{1}{2^n}\sum_{\mu=0}^{N-1}|\sigma_\mu)P_\mu(t),$$

where $\sigma_\mu = \sigma_{\mu_1}\otimes\cdots\otimes\sigma_{\mu_n}$, $\mu = (\mu_1\ldots\mu_n)$, $N = 4^n$ and $P_\mu(t) = (\sigma_\mu|\rho(t))$.

The density operator $\rho(t)$ is a self-adjoint nonnegative operator of unit trace. It follows that

$$P_\mu^*(t) = P_\mu(t), \quad P_0(t) = \big(\sigma_0|\rho(t)\big) = 1.$$

In the general case,

$$\frac{1}{2^n}\sum_{\mu=0}^{N-1}P_\mu^2(t) = \big(\rho(t)|\rho(t)\big) = Tr\big(\rho^2(t)\big) \leqslant 1. \tag{9}$$

Note that the Schwarz inequality $|(A|B)|^2 \leqslant (A|A)(B|B)$ gives

$$\big|\big(I|\rho(t)\big)\big|^2 \leqslant (I|I)\big(\rho(t)|\rho(t)\big).$$

We rewrite this inequality in the form

$$1 = \big|Tr\,\rho(t)\big|^2 \leqslant 2^n\,Tr\big(\rho^2(t)\big) = \sum_{\mu=0}^{N-1}P_\mu^2(t), \tag{10}$$

where $N = 4^n$. Using (9) and (10), we have

$$\frac{1}{\sqrt{2^n}} \leqslant Tr\big(\rho^2(t)\big) \leqslant 1 \quad \text{or} \quad 1 \leqslant \sum_{\mu=0}^{N-1}P_\mu^2(t) \leqslant 2^n.$$

Generalized computational basis

Let us define the orthonormal basis of Liouville space. In the general case, the state $\rho(t)$ of the n-qubit system is an element of Hilbert space $\overline{\mathcal{H}}^{(n)}$. The basis for $\overline{\mathcal{H}}^{(n)}$ consists of the $2^{2n} = 4^n$ orthonormal basis elements denoted by $|\mu)$.

DEFINITION. The basis for a Liouville space $\overline{\mathcal{H}}^{(n)}$ is defined by

$$|\mu) = |\mu_1 \dots \mu_n) = \frac{1}{\sqrt{2^n}}|\sigma_\mu) = \frac{1}{\sqrt{2^n}}|\sigma_{\mu_1} \otimes \cdots \otimes \sigma_{\mu_n}), \tag{11}$$

where $N = 4^n$, $\mu_i \in \{0, 1, 2, 3\}$ and

$$(\mu|\mu') = \delta_{\mu\mu'}, \qquad \sum_{\mu=0}^{N-1} |\mu)(\mu| = \hat{I} \tag{12}$$

is called the *generalized computational basis*.

Here μ is a four-valued representation of the form

$$\mu = \mu_1 4^{n-1} + \cdots + \mu_{n-1} 4 + \mu_n. \tag{13}$$

The pure state of n two-level closed quantum systems is an element of 2^n-dimensional function Hilbert space $\mathcal{H}^{(n)}$. It leads to a quantum computer model with two-valued logic. *In the general case, the mixed state $\rho(t)$ of n two-level (open or closed) quantum system is an element of 4^n-dimensional operator Hilbert space $\overline{\mathcal{H}}^{(n)}$. It leads to a four-valued logic model for the quantum computer.*

The state $|\rho(t))$ at $t > 0$ is a superposition of basis elements,

$$\big|\rho(t)\big) = \sum_{\mu=0}^{N-1} |\mu)\rho_\mu(t), \tag{14}$$

where $\rho_\mu(t) = (\mu|\rho(t))$ are real numbers (functions) satisfying normalized condition

$$\rho_0(t) = \frac{1}{\sqrt{2^n}}\big(\sigma_0|\rho(t)\big) = \frac{1}{\sqrt{2^n}}\,Tr\big(\rho(t)\big) = \frac{1}{\sqrt{2^n}}. \tag{15}$$

Generalized computational states

Generalized computational basis elements $|\mu)$ are not quantum states for $\mu \neq 0$. It follows from normalized condition (15). The general quantum state in the Pauli representation has the form (14). Let us define simple computational quantum states.

DEFINITION. Quantum states in the space $\overline{\mathcal{H}}^{(n)}$ defined by

$$|\mu] = \frac{1}{2^n}\big(|\sigma_0) + |\sigma_\mu)(1 - \delta_{\mu 0})\big) \tag{16}$$

or

$$|\mu] = \frac{1}{\sqrt{2^n}}\big(|0) + |\mu)(1 - \delta_{\mu 0})\big) \tag{17}$$

are called the *generalized computational states*.

Note that all states $|\mu]$, where $\mu \neq 0$, are pure states, since $[\mu|\mu] = 1$. The state $|0]$ is a maximally mixed state. The states $|\mu]$ are elements of $\overline{\mathcal{H}}^{(n)}$.

The quantum state in a four-dimensional Hilbert space is usually called ququat [165], qu-quart [24] or qudit [34,23] with $d = 4$. Usually the ququat is considered as a four-level quantum system. We consider the ququat as a general quantum state in a four-dimensional operator Hilbert space.

DEFINITION. A quantum state in a four-dimensional Liouville space (operator Hilbert space) $\overline{\mathcal{H}}^{(1)}$ associated with a single qubit of space $\mathcal{H}^{(1)} = \mathcal{H}_2$ is called the *single ququat*. A quantum state in 4^n-dimensional Liouville space $\overline{\mathcal{H}}^{(n)}$ associated with an n-qubit system is called the *n-ququat*.

For example, the states $|\mu]$ of the single ququat are

$$|0] = \frac{1}{2}|\sigma_0), \qquad |k] = \frac{1}{2}\big(|\sigma_0) + |\sigma_k)\big),$$

or

$$|0] = \frac{1}{\sqrt{2}}|0), \qquad |k] = \frac{1}{\sqrt{2}}\big(|0) + |k)\big).$$

It is convenient to use matrices for quantum states. In matrix representation the single ququat computational basis $|\mu)$ can be represented by

$$|0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |1) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |2) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |3) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

In this representation single ququat generalized computational states $|\mu]$ are represented by

$$|0] = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |1] = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix},$$

$$|2] = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\\0\end{pmatrix}, \quad |3] = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}.$$

A general single ququat quantum state $|\rho) = \sum_{\mu=0}^{3} |\mu)\rho_\mu$ is represented by

$$|\rho) = \begin{pmatrix}\rho_0\\\rho_1\\\rho_2\\\rho_3\end{pmatrix},$$

where $\rho_0 = 1/\sqrt{2}$ and $\rho_1^2 + \rho_2^2 + \rho_3^2 \leqslant \sqrt{2}$.

We can use the other matrix representation for the states $|\rho]$ which have no coefficient $1/\sqrt{2^n}$. In this representation single ququat generalized computational states $|\mu]$ are represented by

$$|0] = \begin{bmatrix}1\\0\\0\\0\end{bmatrix}, \quad |1] = \begin{bmatrix}1\\1\\0\\0\end{bmatrix}, \quad |2] = \begin{bmatrix}1\\0\\1\\0\end{bmatrix}, \quad |3] = \begin{bmatrix}1\\0\\0\\1\end{bmatrix}.$$

A general single ququat quantum state

$$|\rho] = \begin{bmatrix}1\\P_1\\P_2\\P_3\end{bmatrix},$$

where $P_1^2 + P_2^2 + P_3^2 \leqslant 1$, is a superposition of generalized computational states

$$|\rho] = |0](1 - P_1 - P_2 - P_3) + |1]P_1 + |2]P_2 + |3]P_3.$$

24.4. Quantum four-valued logic gates

Superoperators and quantum gates

Unitary evolution is not the most general type of state change possible for quantum systems. The most general state change is a positive map which is called the quantum operation or superoperator.

Quantum operations can be considered as generalized quantum gates acting on general (mixed) states. Let us define a quantum four-valued logic gate.

DEFINITION. A *quantum four-valued logic gate* is a superoperator $\hat{\mathcal{E}}$ on a Liouville space $\overline{\mathcal{H}}^{(n)}$ which maps a density operator $|\rho)$ of n-ququat to a density operator $|\rho')$ of n-ququat.

If $|\rho)$ is a density operator, then $\hat{\mathcal{E}}|\rho)$ should also be a density operator. Therefore we have some requirements for superoperator $\hat{\mathcal{E}}$. The requirements for a superoperator $\hat{\mathcal{E}}$ on $\mathcal{H}^{(n)}$ to be the quantum four-valued logic gate are as follows:

(1) The superoperator $\hat{\mathcal{E}}$ is a *real* superoperator, i.e., $(\hat{\mathcal{E}}(A))^* = \hat{\mathcal{E}}(A^*)$ for all A or $(\hat{\mathcal{E}}(\rho))^* = \hat{\mathcal{E}}(\rho)$. The real superoperator $\hat{\mathcal{E}}$ is a map that assigns to each self-adjoint operator ρ exactly one self-adjoint operator $\hat{\mathcal{E}}(\rho)$ such that $(\hat{\mathcal{E}}(\rho))^* = \hat{\mathcal{E}}(\rho)$.

(2) The superoperator $\hat{\mathcal{E}}$ is a *positive* superoperator, i.e., $\hat{\mathcal{E}}$ is a map that assigns to each positive operator exactly one positive operator: $\hat{\mathcal{E}}(A^2) > 0$ for all $A \neq 0$ or $\hat{\mathcal{E}}(\rho) \geqslant 0$.

We have to assume the superoperator $\hat{\mathcal{E}}$ to be not merely positive but completely positive. The superoperator $\hat{\mathcal{E}}$ is a *completely positive* map, i.e., the positivity remains if we extend the Liouville space $\overline{\mathcal{H}}^{(n)}$ by adding more qubits. That is, the superoperator $\hat{\mathcal{E}} \otimes \hat{I}^{(m)}$ must be positive, where $\hat{I}^{(m)}$ is the identity superoperator on $\overline{\mathcal{H}}^{(m)}$.

(3) The superoperator $\hat{\mathcal{E}}$ is a *trace-preserving* map, i.e.,

$$(I|\hat{\mathcal{E}}|\rho) = (\hat{\mathcal{E}}^*(I)|\rho) = 1 \quad \text{or} \quad \hat{\mathcal{E}}^*(I) = I. \tag{18}$$

As a result, we have the following definition.

DEFINITION. A *quantum four-valued logic gate* is a real positive (or completely positive) trace-preserving superoperator $\hat{\mathcal{E}}$ on a Liouville space $\overline{\mathcal{H}}^{(n)}$.

In the general case, we can consider linear and nonlinear quantum four-valued logic gates. Let $\hat{\mathcal{E}}$ be a *convex linear* map on the set of density operators, i.e.,

$$\hat{\mathcal{E}}\left(\sum_s \lambda_s \rho_s\right) = \sum_s \lambda_s \hat{\mathcal{E}}(\rho_s),$$

where all λ_s are $0 < \lambda_s < 1$ and $\sum_s \lambda_s = 1$. Any convex linear map of density operators can be uniquely extended to a *linear* map on self-adjoint operators. Note that any linear completely positive superoperator can be represented by

$$\hat{\mathcal{E}} = \sum_{j=1}^{m} \hat{L}_{A_j} \hat{R}_{A_j^*}.$$

If this superoperator is a trace-preserving superoperator, then

$$\sum_{j=1}^{m} A_j^* A_j = I,$$

i.e., the condition (18) is satisfied.

The restriction to linear gates is unnecessary. Let us consider a linear real completely positive superoperator $\hat{\mathcal{E}}$ which is not trace-preserving. This superoperator is not a quantum gate. Let $(I|\hat{\mathcal{E}}|\rho) = Tr(\hat{\mathcal{E}}(\rho))$ be a probability that the process represented by the superoperator $\hat{\mathcal{E}}$ occurs. Since the probability is non-negative and never exceed 1, it follows that $\hat{\mathcal{E}}$ is a trace-decreasing superoperator:

$$0 \leqslant (I|\hat{\mathcal{E}}|\rho) \leqslant 1 \quad \text{or} \quad \hat{\mathcal{E}}^*(I) \leqslant I.$$

In general, any linear real completely positive trace-decreasing superoperator generates a quantum four-valued logic gate.

The quantum four-valued logic gate can be defined as *nonlinear* superoperator $\hat{\mathcal{N}}$ by

$$\hat{\mathcal{N}}|\rho) = (I|\hat{\mathcal{E}}|\rho)^{-1}\hat{\mathcal{E}}|\rho) \quad \text{or} \quad \hat{\mathcal{N}}(\rho) = \frac{\hat{\mathcal{E}}(\rho)}{Tr(\hat{\mathcal{E}}(\rho))},$$

where $\hat{\mathcal{E}}$ is a linear real completely positive trace-decreasing superoperator.

In the generalized computational basis the gate $\hat{\mathcal{E}}$ can be represented by

$$\hat{\mathcal{E}} = \frac{1}{2^n}\sum_{\mu=0}^{N-1}\sum_{\nu=0}^{N-1}\mathcal{E}_{\mu\nu}|\sigma_\mu)(\sigma_\nu|, \tag{19}$$

where $N = 4^n$, μ and ν are four-valued representations of

$$\mu = \mu_1 4^{N-1} + \cdots + \mu_{N-1}4 + \mu_N,$$
$$\nu = \nu_1 4^{N-1} + \cdots + \nu_{N-1}4 + \nu_N,$$
$$\sigma_\mu = \sigma_{\mu_1} \otimes \cdots \otimes \sigma_{\mu_n},$$

$\mu_i, \nu_i \in \{0, 1, 2, 3\}$ and $\mathcal{E}_{\mu\nu}$ are elements of some matrix.

General quantum operation as four-valued logic gates

Unitary gates and quantum operations for a quantum computer with pure states can be considered as quantum four-valued logic gates acting on mixed states.

THEOREM 1. *In the generalized computational basis $|\mu)$ any linear quantum operation $\hat{\mathcal{E}}$ acting on n-qubit mixed (or pure) states can be represented as a quantum four-valued logic gate $\hat{\mathcal{E}}$ on n-ququat by*

$$\hat{\mathcal{E}} = \sum_{\mu=0}^{N-1}\sum_{\nu=0}^{N-1}\mathcal{E}_{\mu\nu}|\mu)(\nu|, \tag{20}$$

where $N = 4^n$,

$$\mathcal{E}_{\mu\nu} = \frac{1}{2^n}\,Tr\big(\sigma_\mu\hat{\mathcal{E}}(\sigma_\nu)\big), \tag{21}$$

and $\sigma_\mu = \sigma_{\mu_1} \otimes \cdots \otimes \sigma_{\mu_n}$.

PROOF. The state ρ' in the generalized computational basis $|\mu)$ has the form

$$|\rho') = \sum_{\mu=0}^{N-1} |\mu)\rho'_\mu,$$

where $N = 4^n$ and

$$\rho'_\mu = (\mu|\rho') = \frac{1}{\sqrt{2^n}}\, Tr(\sigma_\mu \rho').$$

The quantum operation $\hat{\mathcal{E}}$ defines a quantum four-valued logic gate by

$$|\rho') = \hat{\mathcal{E}}|\rho) = \big|\hat{\mathcal{E}}(\rho)\big) = \sum_{\nu=0}^{N-1} \big|\hat{\mathcal{E}}(\sigma_\nu)\big) \frac{1}{\sqrt{2^n}} \rho_\nu.$$

Then

$$(\mu|\rho') = \sum_{\nu=0}^{N-1} \big(\sigma_\mu|\hat{\mathcal{E}}(\sigma_\nu)\big) \frac{1}{2^n} \rho_\nu.$$

Finally, we obtain

$$\rho'_\mu = \sum_{\nu=0}^{N-1} \mathcal{E}_{\mu\nu}\rho_\nu,$$

where

$$\mathcal{E}_{\mu\nu} = \frac{1}{2^n}\big(\sigma_\mu|\hat{\mathcal{E}}(\sigma_\nu)\big) = \frac{1}{2^n}\, Tr\big(\sigma_\mu \hat{\mathcal{E}}(\sigma_\nu)\big).$$

This formula defines a relation between quantum operation $\hat{\mathcal{E}}$ and the real $4^n \times 4^n$ matrix $\mathcal{E}_{\mu\nu}$ of a quantum four-valued logic gate. □

Quantum four-valued logic gates $\hat{\mathcal{E}}$ can be represented by $4^n \times 4^n$ matrices $\mathcal{E}_{\mu\nu}$. The matrix of the gate $\hat{\mathcal{E}}$ is

$$\mathcal{E} = \begin{pmatrix} \mathcal{E}_{00} & \mathcal{E}_{01} & \dots & \mathcal{E}_{0a} \\ \mathcal{E}_{10} & \mathcal{E}_{11} & \dots & \mathcal{E}_{1a} \\ \dots & \dots & \dots & \dots \\ \mathcal{E}_{a0} & \mathcal{E}_{a1} & \dots & \mathcal{E}_{aa} \end{pmatrix},$$

where $a = N - 1 = 4^n - 1$. In the matrix representation, the gate $\hat{\mathcal{E}}$ maps the state $|\rho) = \sum_{\nu=0}^{N-1} |\nu)\rho_\nu$ to the state $|\rho') = \sum_{\mu=0}^{N-1} |\mu)\rho'_\mu$ by

$$\rho'_\mu = \sum_{\nu=0}^{N-1} \mathcal{E}_{\mu\nu}\rho_\nu, \tag{22}$$

where $\rho'_0 = \rho_0 = 1/\sqrt{2^n}$. It can be written in the form

$$\begin{pmatrix} \rho'_0 \\ \rho'_1 \\ \dots \\ \rho'_a \end{pmatrix} = \begin{pmatrix} \mathcal{E}_{00} & \mathcal{E}_{01} & \dots & \mathcal{E}_{0a} \\ \mathcal{E}_{10} & \mathcal{E}_{11} & \dots & \mathcal{E}_{1a} \\ \dots & \dots & \dots & \dots \\ \mathcal{E}_{a0} & \mathcal{E}_{a1} & \dots & \mathcal{E}_{aa} \end{pmatrix} \begin{pmatrix} \rho_0 \\ \rho_1 \\ \dots \\ \rho_a \end{pmatrix}.$$

Since $P_\mu = \sqrt{2^n}\rho_\mu$ and $P'_\mu = \sqrt{2^n}\rho'_\mu$, it follows that representation (22) for linear gate $\hat{\mathcal{E}}$ is equivalent to

$$P'_\mu = \sum_{\nu=0}^{N-1} \mathcal{E}_{\mu\nu} P_\nu. \tag{23}$$

It can be written in the form

$$\begin{bmatrix} P'_0 \\ P'_1 \\ \dots \\ P'_a \end{bmatrix} = \begin{pmatrix} \mathcal{E}_{00} & \mathcal{E}_{01} & \dots & \mathcal{E}_{0a} \\ \mathcal{E}_{10} & \mathcal{E}_{11} & \dots & \mathcal{E}_{1a} \\ \dots & \dots & \dots & \dots \\ \mathcal{E}_{a0} & \mathcal{E}_{a1} & \dots & \mathcal{E}_{aa} \end{pmatrix} \begin{bmatrix} P_0 \\ P_1 \\ \dots \\ P_a \end{bmatrix},$$

where $P_0 = P'_0 = 1$. Note that if we use different matrix representations of state we can use identical matrices for gate $\hat{\mathcal{E}}$.

THEOREM 2. *In the generalized computational basis $|\mu)$ the matrix $\mathcal{E}_{\mu\nu}$ of the linear quantum four-valued logic gate*

$$\hat{\mathcal{E}} = \sum_{j=1}^{m} \hat{L}_{A_j} \hat{R}_{A_j^*} \tag{24}$$

is real, i.e., $\mathcal{E}^*_{\mu\nu} = \mathcal{E}_{\mu\nu}$ for all μ and ν. Any real matrix $\mathcal{E}_{\mu\nu}$ associated with linear trace-preserving gate (24) has

$$\mathcal{E}_{0\nu} = \delta_{0\nu}. \tag{25}$$

PROOF. Using

$$\mathcal{E}_{\mu\nu} = \frac{1}{2^n} \sum_{j=1}^{m} Tr\big(\sigma_\mu A_j \sigma_\nu A_j^*\big) = \frac{1}{2^n} \sum_{j=1}^{m} (A_j^* \sigma_\mu | \sigma_\nu A_j^*),$$

we obtain

$$\begin{aligned} \mathcal{E}^*_{\mu\nu} &= \frac{1}{2^n} \sum_{j=1}^{m} (A_j^* \sigma_\mu | \sigma_\nu A_j^*)^* = \frac{1}{2^n} \sum_{j=1}^{m} (\sigma_\nu A_j^* | A_j^* \sigma_\mu) \\ &= \frac{1}{2^n} \sum_{j=1}^{m} Tr(A_j \sigma_\nu A_j^* \sigma_\mu) = \frac{1}{2^n} \sum_{j=1}^{m} Tr(\sigma_\mu A_j \sigma_\nu A_j^*) = \mathcal{E}_{\mu\nu}. \end{aligned}$$

Let us consider the $\mathcal{E}_{0\nu}$ for (24):

$$\mathcal{E}_{0\nu} = \frac{1}{2^n} Tr\big(\sigma_0 \mathcal{E}(\sigma_\nu)\big) = \frac{1}{2^n} Tr\big(\mathcal{E}(\sigma_\nu)\big)$$
$$= \frac{1}{2^n} Tr\left(\sum_{j=1}^{m} A_j \sigma_\nu A_j^*\right) = \frac{1}{2^n} Tr\left(\left(\sum_{j=1}^{m} A_j^* A_j\right)\sigma_\nu\right)$$
$$= \frac{1}{2^n} Tr\,\sigma_\nu = \delta_{0\nu}. \qquad \square$$

In the general case, a linear quantum four-valued logic gate acts on $|0)$ by

$$\hat{\mathcal{E}}|0) = |0) + \sum_{k=1}^{N-1} T_k |k).$$

For example, a single ququat quantum gate acts by

$$\hat{\mathcal{E}}|0) = |0) + T_1|1) + T_2|2) + T_3|3).$$

If all T_k, where $k = 1, \ldots, N-1$ are equal to zero, then $\hat{\mathcal{E}}|0) = |0)$. The linear quantum gates with $T = 0$ conserve the maximally mixed state $|0]$ invariant.

DEFINITION. A quantum four-valued logic gate $\hat{\mathcal{E}}$ is called a *unital gate* or gate with $T = 0$ if the maximally mixed state $|0]$ is invariant under the action of this gate: $\hat{\mathcal{E}}|0] = |0]$.

The output state of a linear quantum four-valued logic gate $\hat{\mathcal{E}}$ is $|0]$ if and only if the input state is $|0]$. If $\hat{\mathcal{E}}|0] \neq |0]$, then $\hat{\mathcal{E}}$ is not a unital gate.

THEOREM 3. *The matrix $\mathcal{E}_{\mu\nu}$ of linear real trace-preserving superoperator $\hat{\mathcal{E}}$ on n-ququat is an element of group $TGL(4^n - 1, \mathbb{R})$ which is a semidirect product of general linear group $GL(4^n - 1, \mathbb{R})$ and translation group $T(4^n - 1, \mathbb{R})$.*

PROOF. This theorem follows from Theorem 2. Any element (matrix $\mathcal{E}_{\mu\nu}$) of group $TGL(4^n - 1, \mathbb{R})$ can be represented by

$$\mathcal{E}(T, R) = \begin{pmatrix} 1 & 0 \\ T & R \end{pmatrix},$$

where T is a column with $4^n - 1$ elements, 0 is a line with $4^n - 1$ zero elements, and R is a real $(4^n - 1) \times (4^n - 1)$ matrix $R \in GL(4^n - 1, \mathbb{R})$. If R is orthogonal $(4^n - 1) \times (4^n - 1)$ matrix ($R^T R = I$), then we have the motion group. The group multiplication of elements $\mathcal{E}(T, R)$ and $\mathcal{E}(T', R')$ is defined by

$$\mathcal{E}(T, R)\mathcal{E}(T', R') = \mathcal{E}(T + RT', RR').$$

In particular, we have

$$\mathcal{E}(T, R) = \mathcal{E}(T, I)\mathcal{E}(0, R)\,, \qquad \mathcal{E}(T, R) = \mathcal{E}(0, R)\mathcal{E}\big(R^{-1}T, I\big),$$

where I is a unit $(4^n - 1) \times (4^n - 1)$ matrix. □

Any linear real trace-preserving superoperator can be decompose into unital superoperator and translation superoperator. It allows us to consider two types of linear trace-preserving superoperators:

(1) Unital superoperators $\hat{\mathcal{E}}^{(T=0)}$ with the matrices $\mathcal{E}(0, R)$. The n-ququat unital superoperator can be represented by

$$\hat{\mathcal{E}}^{(T=0)} = |0)(0| + \sum_{k=1}^{N-1}\sum_{l=1}^{N-1} R_{kl}|k)(l|,$$

where $N = 4^n$.

(2) Translation superoperators $\hat{\mathcal{E}}^{(T)}$ defined by matrices $\mathcal{E}(T, I)$ and

$$\hat{\mathcal{E}}^{(T)} = \sum_{\mu=0}^{N-1} |\mu)(\mu| + \sum_{k=1}^{N-1} T_k|k)(0|.$$

Decomposition for linear superoperators

Let us consider the n-ququat linear real superoperator

$$\hat{\mathcal{E}} = |0)(0| + \sum_{\mu=1}^{N-1} T_\mu|\mu)(0| + \sum_{\mu=1}^{N-1}\sum_{\nu=1}^{N-1} R_{\mu\nu}|\mu)(\nu|, \tag{26}$$

where $N = 4^n$.

THEOREM 4. *Any real matrix R can be written in the form $R = \mathcal{U}_1 D \mathcal{U}_2^T$, where $\mathcal{U}_1$ and $\mathcal{U}_2$ are real orthogonal $(N-1) \times (N-1)$ matrices and $D = diag(\lambda_1, \ldots, \lambda_{N-1})$ is a diagonal $(N-1) \times (N-1)$ matrix such that $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{N-1} \geqslant 0$.*

PROOF. This theorem is proved in [139,62]. □

In the general case, we have the following theorem.

THEOREM 5. *Any linear real superoperator (26) can be represented by*

$$\hat{\mathcal{E}} = \hat{\mathcal{E}}^{(T)}\hat{\mathcal{U}}_1\,\hat{D}\,\hat{\mathcal{U}}_2, \tag{27}$$

where the following superoperators are used:

$\hat{\mathcal{U}}_1$ *and* $\hat{\mathcal{U}}_2$ *are unital orthogonal superoperators, such that*

$$\hat{\mathcal{U}}_i = |0)(0| + \sum_{\mu=1}^{N-1}\sum_{\nu=1}^{N-1} \mathcal{U}^{(i)}_{\mu\nu}|\mu)(\nu|. \tag{28}$$

$\hat{D}$ *is a unital diagonal superoperator, such that*

$$\hat{D} = |0)(0| + \sum_{\mu=1}^{N-1} \lambda_\mu |\mu)(\mu| \quad (\lambda_\mu \geqslant 0). \tag{29}$$

$\hat{\mathcal{E}}^{(T)}$ *is a translation superoperator, such that*

$$\hat{\mathcal{E}}^{(T)} = |0)(0| + \sum_{\mu=1}^{N-1} |\mu)(\mu| + \sum_{\mu=1}^{N-1} T_\mu |\mu)(0|. \tag{30}$$

PROOF. The proof of this theorem can be easily realized in matrix representation by using Theorems 3 and 4. □

As a result, we have that any linear real trace-preserving superoperator can be realized by three types of superoperators:

(1) unital orthogonal superoperators $\hat{\mathcal{U}}$;
(2) unital diagonal superoperators $\hat{D}$;
(3) nonunital translation superoperators $\hat{\mathcal{E}}^{(T)}$.

THEOREM 6. *If the quantum operation* $\hat{\mathcal{E}}$ *has the form*

$$\hat{\mathcal{E}}(\rho) = \sum_{j=1}^{m} A_j \rho A_j^*,$$

where A *is a self-adjoint operator* ($A_j^* = A_j$), *then quantum four-valued logic gate* $\hat{\mathcal{E}}$ *is described by symmetric matrix* $\mathcal{E}_{\mu\nu} = \mathcal{E}_{\nu\mu}$. *This gate is trace-preserving if* $\mathcal{E}_{\mu 0} = \mathcal{E}_{0\mu} = \delta_{\mu 0}$.

PROOF. If $A_j^* = A_j$, then

$$\mathcal{E}_{\mu\nu} = \frac{1}{\sqrt{2^n}} \sum_{j=1}^{m} Tr(\sigma_\mu A_j \sigma_\nu A_j) = \frac{1}{\sqrt{2^n}} \sum_{j=1}^{m} Tr(\sigma_\nu A_j \sigma_\mu A_j) = \mathcal{E}_{\nu\mu}.$$

Using Theorem 2, we have that this gate is trace-preserving if $\mathcal{E}_{\mu 0} = \mathcal{E}_{0\mu} = \delta_{\mu 0}$. □

Unitary two-valued logic gates as orthogonal four-valued logic gates

Let us consider a unitary two-valued logic gate defined by unitary operator U acting on pure states. The map $\hat{\mathcal{U}} : \rho \to U\rho U^*$ induced by a unitary operator U is a particular case of quantum operation.

THEOREM 7. *In the generalized computational basis any unitary quantum two-valued logic gate U that acts on pure n-qubit states can be considered as a quantum four-valued logic gate $\hat{\mathcal{U}}$ acting on n-ququat*:

$$\hat{\mathcal{U}} = \sum_{\mu=0}^{N-1} \sum_{\nu=0}^{N-1} \mathcal{U}_{\mu\nu} |\mu)(\nu|, \tag{31}$$

where $\mathcal{U}_{\mu\nu}$ is a real matrix such that

$$\mathcal{U}_{\mu\nu} = \frac{1}{2^n} Tr(\sigma_\nu U \sigma_\mu U^*). \tag{32}$$

PROOF. Using Theorem 1 and the equation

$$|\rho') = \hat{\mathcal{U}}|\rho) = |U\rho U^*),$$

we get this theorem. □

Equations (31) and (32) define a relation between the unitary quantum two-valued logic gate U and the real $4^n \times 4^n$ matrix $\mathcal{U}$ of quantum four-valued logic gate $\hat{\mathcal{U}}$.

THEOREM 8. *Any four-valued logic gate associated with unitary two-valued logic gate by* (31) *and* (32) *is a unital gate, i.e., gate matrix $\mathcal{U}$ defined by* (32) *has $\mathcal{U}_{\mu 0} = \mathcal{U}_{0\mu} = \delta_{\mu 0}$.*

PROOF.

$$\mathcal{U}_{\mu 0} = \frac{1}{2^n} Tr(\sigma_\mu U \sigma_0 U^*) = \frac{1}{2^n} Tr(\sigma_\mu U U^*) = \frac{1}{2^n} Tr\, \sigma_\mu.$$

Using $Tr\, \sigma_\mu = \delta_{\mu 0}$, we get $\mathcal{U}_{\mu 0} = \delta_{\mu 0}$. □

Let us denote the gate $\hat{\mathcal{U}}$ associated with unitary two-valued logic gate U by $\hat{\mathcal{E}}^{(U)}$.

THEOREM 9. *If U is a unitary two-valued logic gate, then in the generalized computational basis a quantum four-valued logic gate $\hat{\mathcal{U}} = \hat{\mathcal{E}}^{(U)}$ associated with*

U is represented by the orthogonal matrix $\mathcal{E}^{(U)}$:

$$\mathcal{E}^{(U)}\big(\mathcal{E}^{(U)}\big)^T = \big(\mathcal{E}^{(U)}\big)^T\mathcal{E}^{(U)} = I. \tag{33}$$

PROOF. Let $\hat{\mathcal{E}}^{(U)}$ be defined by

$$\hat{\mathcal{E}}^{(U)}|\rho) = |U\rho U^*), \qquad \hat{\mathcal{E}}^{(U^*)}|\rho) = |U^*\rho U).$$

If $UU^* = U^*U = I$, then

$$\hat{\mathcal{E}}^{(U)}\hat{\mathcal{E}}^{(U^*)} = \hat{\mathcal{E}}^{(U^*)}\hat{\mathcal{E}}^{(U)} = \hat{I}.$$

In the matrix representation, we have

$$\sum_{\alpha=0}^{N-1}\mathcal{E}^{(U)}_{\mu\alpha}\mathcal{E}^{(U^*)}_{\alpha\nu} = \sum_{\alpha=0}^{N-1}\mathcal{E}^{(U^*)}_{\mu\alpha}\mathcal{E}^{(U)}_{\alpha\nu} = \delta_{\mu\nu},$$

i.e., $\mathcal{E}^{(U^*)}\mathcal{E}^{(U)} = \mathcal{E}^{(U)}\mathcal{E}^{(U^*)} = I$. Note that

$$\mathcal{E}^{(U^*)}_{\mu\nu} = \frac{1}{2^n}\,Tr(\sigma_\mu U^*\sigma_\nu U) = \frac{1}{2^n}\,Tr(\sigma_\nu U\sigma_\mu U^*) = \mathcal{E}^{(U)}_{\nu\mu},$$

i.e., $\mathcal{E}^{(U^*)} = (\mathcal{E}^{(U)})^T$. Finally, we obtain (33). □

THEOREM 10. *If $\hat{\mathcal{E}}^*$ is an adjoint superoperator for linear trace-preserving superoperator $\hat{\mathcal{E}}$, then matrices of the superoperators are connected by transposition $\mathcal{E}^* = \mathcal{E}^T$, i.e.,*

$$(\mathcal{E}^*)_{\mu\nu} = \mathcal{E}_{\nu\mu}. \tag{34}$$

PROOF. Using

$$\hat{\mathcal{E}} = \sum_{j=1}^{m}\hat{L}_{A_j}\hat{R}_{A_j^*}, \qquad \hat{\mathcal{E}}^* = \sum_{j=1}^{m}\hat{L}_{A_j^*}\hat{R}_{A_j},$$

we obtain

$$\mathcal{E}_{\mu\nu} = \frac{1}{2^n}\sum_{j=1}^{m}Tr(\sigma_\mu A_j\sigma_\nu A_j^*),$$

$$(\mathcal{E}^*)_{\mu\nu} = \frac{1}{2^n}\sum_{j=1}^{m}Tr(\sigma_\mu A_j^*\sigma_\nu A_j) = \frac{1}{2^n}\sum_{j=1}^{m}Tr(\sigma_\nu A_j\sigma_\mu A_j^*) = \mathcal{E}_{\nu\mu}.$$

Obviously, if we define the superoperator $\hat{\mathcal{E}}$ by (20), then the adjoint superoperator has the form

$$\hat{\mathcal{E}}^* = \sum_{\mu=0}^{N-1}\sum_{\nu=0}^{N-1}\mathcal{E}_{\nu\mu}|\mu)(\nu|.$$

□

THEOREM 11. *If $\hat{\mathcal{E}}^*\hat{\mathcal{E}} = \hat{\mathcal{E}}\hat{\mathcal{E}}^* = \hat{I}$, then $\hat{\mathcal{E}}$ is an orthogonal quantum four-valued logic gate, i.e., $\mathcal{E}^T\mathcal{E} = \mathcal{E}\mathcal{E}^T = I$.*

PROOF. If $\hat{\mathcal{E}}^*\hat{\mathcal{E}} = \hat{I}$, then

$$\sum_{\alpha=0}^{N-1}(\mu|\hat{\mathcal{E}}^*|\alpha)(\alpha|\hat{\mathcal{E}}|\nu) = (\mu|\hat{I}|\nu): \quad \sum_{\alpha=0}^{N-1}(\mathcal{E}^*)_{\mu\alpha}\mathcal{E}_{\alpha\nu} = \delta_{\mu\nu}.$$

Using Theorem 10, we have

$$\sum_{\alpha=0}^{N-1}(\mathcal{E}^T)_{\mu\alpha}\mathcal{E}_{\alpha\nu} = \delta_{\mu\nu},$$

i.e., $\mathcal{E}^T\mathcal{E} = I$. □

Note that n-qubit unitary two-valued logic gate U is an element of Lie group $SU(2^n)$. The dimension of this group is equal to $\dim SU(2^n) = (2^n)^2 - 1 = 4^n - 1$. The matrix of n-ququat orthogonal linear gate $\hat{\mathcal{U}} = \hat{\mathcal{E}}^{(U)}$ can be considered as an element of Lie group $SO(4^n - 1)$. The dimension of this group is equal to $\dim SO(4^n - 1) = (4^n - 1)(2 \cdot 4^{n-1} - 1)$.

For example, if $n = 1$, then $\dim SU(2^1) = 3$, $\dim SO(4^1 - 1) = 3$. If $n = 2$, then $\dim SU(2^2) = 15$, $\dim SO(4^2 - 1) = 105$. Therefore, not all orthogonal quantum four-valued logic gates for mixed and pure states are connected with unitary two-valued logic gates for pure states.

Single ququat orthogonal gates

Let us consider a single ququat quantum four-valued logic gate $\hat{\mathcal{U}}$ associated with unitary single qubit two-valued logic gate U.

THEOREM 12. *Any single qubit unitary quantum two-valued logic gate can be realized as the product of single ququat simple rotation quantum four-valued logic gates $\hat{\mathcal{U}}^{(1)}(\alpha)$, $\hat{\mathcal{U}}^{(2)}(\theta)$ and $\hat{\mathcal{U}}^{(1)}(\beta)$ defined by*

$$\hat{\mathcal{U}}^{(1)}(\alpha) = |0)(0| + |3)(3| + \cos\alpha\big(|1)(1| + |2)(2|\big) + \sin\alpha\big(|2)(1| - |1)(2|\big),$$

$$\hat{\mathcal{U}}^{(2)}(\theta) = |0)(0| + |2)(2| + \cos\theta\big(|1)(1| + |3)(3|\big) + \sin\theta\big(|1)(3| - |3)(1|\big),$$

where α, θ and β are Euler angles.

PROOF. This theorem has been proved in [165]. □

Let us introduce simple reflection gates by

$$\hat{\mathcal{R}}^{(1)} = |0)(0| - |1)(1| + |2)(2| + |3)(3|,$$

$$\hat{\mathcal{R}}^{(2)} = |0)(0| + |1)(1| - |2)(2| + |3)(3|,$$
$$\hat{\mathcal{R}}^{(3)} = |0)(0| + |1)(1| + |2)(2| - |3)(3|.$$

THEOREM 13. *Any single ququat linear quantum four-valued logic gate* $\hat{\mathcal{E}}$ *defined by orthogonal matrix* $\mathcal{E}$: $\mathcal{E}\mathcal{E}^T = I$ *can be realized by*

- *simple rotation gates* $\hat{\mathcal{U}}^{(1)}$ *and* $\hat{\mathcal{U}}^{(2)}$,
- *inversion gate* $\hat{\mathcal{I}}$ *defined by* $\hat{\mathcal{I}} = |0)(0| - |1)(1| - |2)(2| - |3)(3|$.

PROOF. Using Theorem 10 and

$$\hat{\mathcal{R}}^{(3)} = \hat{\mathcal{U}}^{(1)}\hat{\mathcal{I}}, \qquad \hat{\mathcal{R}}^{(2)} = \hat{\mathcal{U}}^{(2)}\hat{\mathcal{I}}, \qquad \hat{\mathcal{R}}^{(1)} = \hat{\mathcal{U}}^{(1)}\hat{\mathcal{U}}^{(1)}\hat{\mathcal{I}},$$

we get this theorem. □

EXAMPLE 1. In the generalized computational basis the Pauli matrices as two-valued logic gates are the quantum four-valued logic gates with diagonal 4×4 matrices. The gate $I = \sigma_0$ is

$$\hat{\mathcal{U}}^{(\sigma 0)} = \sum_{\mu=0}^{3} |\mu)(\mu| = \hat{I},$$

i.e., $\mathcal{U}_{\mu\nu}^{(\sigma 0)} = (1/2)\, Tr(\sigma_\mu \sigma_\nu) = \delta_{\mu\nu}$.

For the unitary quantum two-valued logic gates that are equal to the Pauli matrix σ_k, where $k \in \{1, 2, 3\}$, we have the quantum four-valued logic gates

$$\hat{\mathcal{U}}^{(\sigma k)} = \sum_{\mu,\nu=0}^{3} \mathcal{U}_{\mu\nu}^{(\sigma k)} \, |\mu)(\nu|,$$

with the matrix

$$\mathcal{U}_{\mu\nu}^{(\sigma k)} = 2\delta_{\mu 0}\delta_{\nu 0} + 2\delta_{\mu k}\delta_{\nu k} - \delta_{\mu\nu}. \tag{35}$$

EXAMPLE 2. In the generalized computational basis the unitary NOT gate ("negation") of two-valued logic

$$X = |0><1| + |1><0| = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

is represented by the quantum four-valued logic gate

$$\hat{\mathcal{U}}^{(X)} = |0)(0| + |1)(1| - |2)(2| - |3)(3|.$$

EXAMPLE 3. The Hadamard two-valued logic gate

$$H = \frac{1}{\sqrt{2}}(\sigma_1 + \sigma_3)$$

can be represented as a quantum four-valued logic gate by

$$\hat{\mathcal{E}}^{(H)} = |0)(0| - |2)(2| + |3)(1| + |1)(3|,$$

with the matrix

$$\mathcal{E}^{(H)}_{\mu\nu} = \delta_{\mu 0}\delta_{\nu 0} - \delta_{\mu 2}\delta_{\nu 2} + \delta_{\mu 3}\delta_{\nu 1} + \delta_{\mu 1}\delta_{\nu 3}.$$

Measurements as quantum four-valued logic gates

It is known that the von Neumann measurement superoperator $\hat{\mathcal{E}}$ is defined by

$$\hat{\mathcal{E}}|\rho) = \sum_{k=1}^{r} |P_k \rho P_k), \tag{36}$$

where $\{P_k | k = 1, \ldots, r\}$ is a (not necessarily complete) sequence of orthogonal projection operators on $\mathcal{H}^{(n)}$.

Let P_k be projections onto the pure states $|k>$, which define a basis $\{|k>\}$ for $\mathcal{H}^{(n)}$, i.e.,

$$P_k = |k><k|.$$

THEOREM 14. *A nonlinear quantum four-valued logic gate $\hat{\mathcal{N}}$ for von Neumann measurement* (36) *of the state $\rho = \sum_{\alpha=0}^{N-1} |\alpha)\rho_\alpha$ is defined by*

$$\hat{\mathcal{N}} = \sum_{k=1}^{r} \frac{1}{p(r)} \sum_{\mu=0}^{N-1} \sum_{\nu=0}^{N-1} \mathcal{E}^{(k)}_{\mu\nu} |\mu)(\nu|, \tag{37}$$

where

$$\mathcal{E}^{(k)}_{\mu\nu} = \frac{1}{2^n} Tr(\sigma_\mu P_k \sigma_\nu P_k), \qquad p(r) = \sqrt{2^n} \sum_{k=1}^{r} \sum_{\alpha=0}^{N-1} \mathcal{E}^{(k)}_{0\alpha} \rho_\alpha. \tag{38}$$

PROOF. The trace-decreasing superoperator $\hat{\mathcal{E}}_k$ is defined by

$$|\rho) \to |\rho') = \hat{\mathcal{E}}_k|\rho) = |P_k \rho P_k).$$

This superoperator has the form $\hat{\mathcal{E}}_k = \hat{L}_{P_k} \hat{R}_{P_k}$. Then

$$\rho'_\mu = (\mu|\rho') = (\mu|\hat{\mathcal{E}}_k|\rho) = \sum_{\nu=0}^{N-1} (\mu|\hat{\mathcal{E}}_k|\nu)(\nu|\rho) = \sum_{\nu=0}^{N-1} \mathcal{E}^{(k)}_{\mu\nu} \rho_\nu,$$

where

$$\mathcal{E}^{(k)}_{\mu\nu} = (\mu|\hat{\mathcal{E}}_k|\nu) = \frac{1}{2^n}\, Tr(\sigma_\mu P_k \sigma_\nu P_k).$$

The probability that the process represented by $\hat{\mathcal{E}}_k$ occurs is

$$p(k) = Tr\big(\hat{\mathcal{E}}_k(\rho)\big) = (I|\hat{\mathcal{E}}_k|\rho) = \sqrt{2^n}\rho'_0 = \sqrt{2^n}\sum_{\alpha=0}^{N-1}\mathcal{E}^{(k)}_{0\alpha}\rho_\alpha.$$

If

$$p(r) = \sqrt{2^n}\sum_{k=1}^{r}\sum_{\alpha=0}^{N-1}\mathcal{E}^{(k)}_{0\alpha}\rho_\alpha \neq 0,$$

then the matrix for nonlinear trace-preserving gate $\hat{\mathcal{N}}$ is

$$\mathcal{N}_{\mu\nu} = \sum_{k=1}^{r} p^{-1}(r)\mathcal{E}^{(k)}_{\mu\nu}.$$

□

EXAMPLE 1. Let us consider the single ququat projection operator

$$P_0 = |0><0| = \frac{1}{2}(\sigma_0 + \sigma_3).$$

Using formula (38), we derive

$$\begin{aligned}\mathcal{E}^{(0)}_{\mu\nu} &= \frac{1}{8}\, Tr\big(\sigma_\mu(\sigma_0+\sigma_3)\sigma_\nu(\sigma_0+\sigma_3)\big)\\ &= \frac{1}{2}(\delta_{\mu0}\delta_{\nu0} + \delta_{\mu3}\delta_{\nu3} + \delta_{\mu3}\delta_{\nu0} + \delta_{\mu0}\delta_{\nu3}).\end{aligned}$$

The corresponding matrix is

$$\mathcal{E}^{(0)} = \begin{pmatrix} 1/2 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 \end{pmatrix}.$$

The linear trace-decreasing superoperator for von Neumann measurement projection $|0><0|$ onto the pure state $|0>$ is

$$\hat{\mathcal{E}}^{(0)} = \frac{1}{2}\big(|0)(0| + |3)(3| + |0)(3| + |3)(0|\big).$$

EXAMPLE 2. Let us consider the projection operator

$$P_1 = |1><1| = \frac{1}{2}(\sigma_0 - \sigma_3).$$

Using equation (38), we obtain

$$\mathcal{E}^{(1)}_{\mu\nu} = \frac{1}{2}(\delta_{\mu 0}\delta_{\nu 0} + \delta_{\mu 3}\delta_{\nu 3} - \delta_{\mu 3}\delta_{\nu 0} - \delta_{\mu 0}\delta_{\nu 3}).$$

The linear superoperator $\hat{\mathcal{E}}^{(1)}$ for the von Neumann measurement projection onto the pure state $|1>$ is

$$\hat{\mathcal{E}}^{(1)} = \frac{1}{2}\big(|0)(0| + |3)(3| - |0)(3| - |3)(0|\big).$$

The superoperators $\hat{\mathcal{E}}^{(0)}$ and $\hat{\mathcal{E}}^{(1)}$ are not trace-preserving. The probabilities that processes represented by the superoperators occur are

$$p(0) = \frac{1}{\sqrt{2}}(\rho_0 + \rho_3), \qquad p(1) = \frac{1}{\sqrt{2}}(\rho_0 - \rho_3).$$

24.5. Classical four-valued logic gates

Let us consider some elements of classical four-valued logic. For the concept of many-valued logic, see [126,127,193].

Elementary classical gates

A function $g(x_1, \ldots, x_n)$ describes a classical four-valued logic gate if the following conditions are satisfied:

- all $x_i \in \{0, 1, 2, 3\}$, where $i = 1, \ldots, n$.
- $g(x_1, \ldots, x_n) \in \{0, 1, 2, 3\}$.

It is known that the number of all classical logic gates with n-arguments $x_1, \ldots, x_n$ is equal to 4^{4^n}. The number of classical logic gates $g(x)$ with single argument is equal to $4^{4^1} = 256$.

The number of classical logic gates $g(x_1, x_2)$ with two-arguments is equal to $4^{4^2} = 4^{16} = 42949677296$.

Let us define some elementary classical four-valued logic gates by equations.

- Luckasiewicz negation: $\sim x = 3 - x$.
- Circular shift: $\bar{x} = x + 1 (\mathrm{mod}\ 4)$.
- Functions $I_i(x)$, where $i = 0, \ldots, 3$, such that $I_i(x) = 3$ if $x = i$ and $I_i(x) = 0$ if $x \neq i$.
- $\Box x = 0$ for $x \in \{0, 1, 2\}$, and $\Box x = 3$ for $x = 3$.
- $\Diamond x = 0$ for $x = 0$, and $\Diamond x = 0$ for $x \in \{1, 2, 3\}$.
- Generalized conjunction: $x_1 \wedge x_2 = \min(x_1, x_2)$.
- Generalized disjunction: $x_1 \vee x_2 = \max(x_1, x_2)$.

- Generalized Sheffer–Webb function:

$$V_4(x_1, x_2) = \max(x_1, x_2) + 1 (\mathrm{mod}\, 4).$$

The generalized conjunction and disjunction satisfy the following laws:

- Commutative laws

$$x_1 \wedge x_2 = x_2 \wedge x_1, \qquad x_1 \vee x_2 = x_2 \vee x_1.$$

- Associative laws

$$(x_1 \vee x_2) \vee x_3 = x_1 \vee (x_2 \vee x_3), \qquad (x_1 \wedge x_2) \wedge x_3 = x_1 \wedge (x_2 \wedge x_3).$$

- Distributive laws

$$x_1 \vee (x_2 \wedge x_3) = (x_1 \vee x_2) \wedge (x_1 \vee x_3),$$
$$x_1 \wedge (x_2 \vee x_3) = (x_1 \wedge x_2) \vee (x_1 \wedge x_3).$$

Note that the Luckasiewicz negation satisfies the properties:

$$\sim (\sim x) = x, \qquad \sim (x_1 \wedge x_2) = (\sim x_1) \vee (\sim x_2).$$

The following usual negation rules are not satisfied by the circular shift:

$$\bar{\bar{x}} \neq x, \qquad \overline{x_1 \wedge x_2} \neq \overline{x_1} \vee \overline{x_2}.$$

The analog of the disjunction normal form of the n-argument classical four-valued logic gate is

$$g(x_1, \ldots, x_n) = \bigvee_{(k_1, \ldots, k_n)} I_{k_1}(x_1) \wedge \cdots \wedge I_{k_n}(x_n) \wedge g(k_1, \ldots, k_n).$$

Let us consider (functional) complete sets [193] of classical four-valued logic gates.

THEOREM 15. *The set* $\{0, 1, 2, 3, I_0, I_1, I_2, I_3, x_1 \wedge x_2, x_1 \vee x_2\}$ *is a complete set.*

The set $\{\overline{x}, x_1 \vee x_2\}$ *is a complete set.*

The gate $V_4(x_1, x_2)$ *is complete.*

PROOF. This theorem is proved in [193]. □

Quantum gates for single argument classical gates

Let us consider linear trace-preserving quantum gates for classical gates $\sim$, $\bar{x}$, I_0, I_1, I_2, I_3, 0, 1, 2, 3, $\diamond$, $\square$.

THEOREM 16. *Any single argument classical four-valued logic gate $g(\nu)$ can be realized as a linear trace-preserving quantum four-valued logic gate by*

$$\hat{\mathcal{E}}^{(g)} = |0)(0| + \sum_{k=1}^{3} |g(k))(k| + (1 - \delta_{0g(0)})\left(|g(0))(0| - \sum_{\mu=0}^{3}\sum_{\nu=0}^{3}(1 - \delta_{\mu g(\nu)})|\mu)(\nu| \right). \tag{39}$$

PROOF. The proof is by direct calculation in

$$\hat{\mathcal{E}}^{(g)}|\alpha] = |g(\alpha)]: \quad \hat{\mathcal{E}}^{(g)}|\alpha] = \frac{1}{\sqrt{2}}\big(\hat{\mathcal{E}}^{(g)}|0) + \hat{\mathcal{E}}^{(g)}|\alpha)\big). \qquad \square$$

The following are examples of some classical gates.

(1) The Luckasiewicz negation gate is

$$\hat{\mathcal{E}}^{(\sim)} = |0)(0| + |1)(2| + |2)(1| + |3)(0| - |3)(3|.$$

(2) The four-valued logic gate I_0 can be realized by

$$\hat{\mathcal{E}}^{(I_0)} = |0)(0| + |3)(0| - \sum_{k=1}^{3} |3)(k|.$$

(3) The gates $I_k(x)$, where $k = 1, 2, 3$ are

$$\hat{\mathcal{E}}^{(I_k)} = |0)(0| + |3)(k|.$$

(4) The gate $\bar{x}$ can be realized by

$$\hat{\mathcal{E}}^{(\bar{x})} = |0)(0| + |1)(0| + |2)(1| + |3)(2| - \sum_{k=1}^{3} |1)(k|.$$

(5) The constant gates 0 and $k = 1, 2, 3$ can be realized by

$$\hat{\mathcal{E}}^{(0)} = |0)(0|, \qquad \hat{\mathcal{E}}^{(k)} = |0)(0| + |k)(0|.$$

(6) The gate $\diamond x$ is realized by

$$\hat{\mathcal{E}}^{(\diamond)} = |0)(0| + \sum_{k=1}^{3} |3)(k|.$$

(7) The gate $\Box x = \sim \Diamond x$ is

$$\hat{\mathcal{E}}^{(\Box)} = |0)(0| + |3)(3|.$$

Note that the quantum four-valued logic gates $\hat{\mathcal{E}}^{(\sim)}$, $\hat{\mathcal{E}}^{(I_0)}$, $\hat{\mathcal{E}}^{(k)}$, $\hat{\mathcal{E}}^{(g_1)}$ are not unital gates.

Quantum gates for two-arguments classical gates

Let us consider quantum four-valued logic gates for two-arguments classical four-valued logic gates.

(1) The generalized conjunction $x_1 \wedge x_2 = \min(x_1, x_2)$ and generalized disjunction $x_1 \wedge x_2 = \max(x_1, x_2)$ can be realized by a two-ququat quantum four-valued logic gate with $T = 0$:

$$\hat{\mathcal{E}}|x_1, x_2] = |x_1 \vee x_2, x_1 \wedge x_2].$$

Let us write this quantum gate in the generalized computational basis by

$$\hat{\mathcal{E}} = \sum_{\mu=0}^{N-1}\sum_{\nu=0}^{N-1} |\mu\nu)(\mu\nu| + \sum_{k=1}^{3}\big(|0k) - |k0)\big)(k0|$$
$$+ \sum_{k=2}^{3}\big(|1k) - |k1)\big)(k1| + \big(|23) - |32)\big)(32|.$$

(2) The Sheffer–Webb function gate $|x_1, x_2] \to |V_4(x_1, x_2), \sim V_4(x_1, x_2)]$ can be realized by a two-ququat quantum gate with $T \neq 0$:

$$\hat{\mathcal{E}}^{(SW)} = |00)(00| + |12)(00| - \sum_{\mu=0}^{3}\sum_{\nu=1}^{3} |12)(\mu\nu| + |21)(10|$$
$$+ |21)(11| + |30)(02| + |30)(20| + |30)(12| + |30)(21|$$
$$+ |30)(22| + |03)(03| + |03)(13| + |03)(23| + \sum_{\mu=0}^{3} |03)(3\mu|.$$

Note that this Sheffer–Webb function gate is not a unital quantum gate and

$$\hat{\mathcal{E}}^{(SW)} \neq |V_4(x_1, x_2), \sim V_4(x_1, x_2))(x_1, x_2|.$$

24.6. To universal set of quantum four-valued logic gates

The condition for performing arbitrary unitary operations to realize a quantum computation by dynamics of a Hamiltonian quantum system is well understood

[14,44,98]. Using quantum unitary gates, a quantum computer with pure states may realize the time sequence of operations corresponding to any unitary dynamics. Almost any two-qubit quantum unitary gate is universal for a quantum computer with pure states. It is known [14,44,98] that a set of quantum gates, which consists of all one-qubit unitary gates and the two-qubit exclusive-OR (XOR) gate, is universal for quantum computer with pure states in the sense that all unitary operations on arbitrary many qubits can be expressed as compositions of these unitary gates.

The same is not true for the general quantum operations (superoperators) corresponding to the dynamics of non-Hamiltonian quantum systems. In the paper [9], a single qubit of non-Hamiltonian quantum system with Markovian dynamics was considered and the resources needed for universality of general quantum operations were studied. An analysis of completely positive trace-preserving superoperators on single qubit density operators was realized in papers [61,82,130].

Let us study universality for quantum four-valued logic gates.

DEFINITION. A set of quantum four-valued logic gates is *universal* if and only if all quantum gates on arbitrary many ququats can be expressed as compositions of these gates.

Single ququat gates cannot map two initially un-entangled ququats into an entangled state. Therefore, the single ququat gates or set of single ququat gates are not universal gates for a quantum computer with mixed states. Quantum gates which are realizations of classical gates cannot be universal by definition, since these gates evolve generalized computational states to generalized computational states and never to the superposition of them.

The matrix $\mathcal{E}$ of the linear real superoperator $\hat{\mathcal{E}}$ on $\overline{\mathcal{H}}^{(n)}$ is an element of Lie group $TGL(4^n - 1, \mathbb{R})$. The linear superoperator $\hat{\mathcal{E}}$ on $\overline{\mathcal{H}}^{(n)}$ is a quantum four-valued logic gate (completely positive trace-preserving superoperator) if and only if the matrix $\mathcal{E}$ is a completely positive element of Lie group $TGL(4^n - 1, \mathbb{R})$. The matrix $\mathcal{N}$ of a nonlinear real trace-preserving superoperator $\hat{\mathcal{N}}$ on $\overline{\mathcal{H}}^{(n)}$ is a quantum four-valued logic gate defined by

$$\hat{\mathcal{N}}(\rho) = \frac{\hat{\mathcal{E}}(\rho)}{Tr(\hat{\mathcal{E}}(\rho))} \tag{40}$$

if the matrix $\mathcal{E}$ of the linear trace-decreasing superoperator $\hat{\mathcal{E}}$ is a completely positive element of Lie group $GL(4^n, \mathbb{R})$. The condition of complete positivity leads to difficult inequalities for matrix elements [35,61,82,130]. In order to satisfy the condition of complete positivity we use the following representation:

$$\hat{\mathcal{E}} = \sum_{j=1}^{m} \hat{L}_{A_j} \hat{R}_{A_j^*}, \tag{41}$$

where $\hat{L}_A$ and $\hat{R}_A$ are left and right multiplication superoperators on $\overline{\mathcal{H}}^{(n)}$ defined by $\hat{L}_A|B) = |AB)$, $\hat{R}_A|B) = |BA)$. It is known that any linear completely positive superoperator $\hat{\mathcal{E}}$ can be represented by (41). Any trace-decreasing superoperator (41) generates a quantum four-valued logic gate by (40). *To find the universal set of completely positive (linear or nonlinear) superoperators, i.e., quantum four-valued logic gates, we suggest to consider the universal set of the superoperators* $\hat{L}_{A_j}$ *and* $\hat{R}_{A_j^*}$. Let the superoperators $\hat{L}_{A_j}$ and $\hat{R}_{A_j^*}$ will be called the *pseudo-gates*. A set of pseudo-gates is universal if and only if all pseudo-gates on arbitrary many ququats can be expressed as compositions of these pseudo-gates. The matrices of the superoperators $\hat{L}_A$ and $\hat{R}_{A^*}$ are connected by complex conjugation. The set of these matrices forms a group $GL(4^n, \mathbb{C})$. Obviously, the universal set of pseudo-gates $\hat{L}_A$ is connected with a universal set of completely positive superoperators $\hat{\mathcal{E}}$ of the quantum four-valued logic gates.

The trace-preserving condition for linear superoperator (41) is equivalent to the requirement $\mathcal{E}_{0\mu} = \delta_{0\mu}$ for gate matrix $\mathcal{E}$. The trace-decreasing condition can be satisfied by inequality of the following theorem.

THEOREM 17. *If the matrix elements* $\mathcal{E}_{\mu\nu}$ *of* $\hat{\mathcal{E}}$ *satisfy the inequality*

$$\sum_{\mu=0}^{N-1} (\mathcal{E}_{0\mu})^2 \leqslant 1, \tag{42}$$

then $\hat{\mathcal{E}}$ *is a trace-decreasing superoperator.*

PROOF. Using the Schwarz inequality

$$\left(\sum_{\mu=0}^{N-1} \mathcal{E}_{0\mu}\rho_\mu \right)^2 \leqslant \sum_{\mu=0}^{N-1} (\mathcal{E}_{0\mu})^2 \sum_{\nu=0}^{N-1} (\rho_\nu)^2,$$

and the property

$$Tr\,\rho^2 = (\rho|\rho) = \sum_{\nu=0}^{N-1} (\rho_\nu)^2 \leqslant 1,$$

we have

$$\left|Tr\,\hat{\mathcal{E}}(\rho)\right|^2 = \left|(0|\hat{\mathcal{E}}|\rho)\right|^2 = \left(\sum_{\mu=0}^{N-1} \mathcal{E}_{0\mu}\rho_\mu \right)^2 \leqslant \sum_{\mu=0}^{N-1} (\mathcal{E}_{0\mu})^2.$$

Using (42), we get $|\,Tr\,\hat{\mathcal{E}}(\rho)| \leqslant 1$. Since $\hat{\mathcal{E}}$ is a completely positive (or positive) superoperator ($\hat{\mathcal{E}}(\rho) \geqslant 0$), it follows that

$$0 \leqslant Tr\,\hat{\mathcal{E}}(\rho) \leqslant 1,$$

i.e., $\hat{\mathcal{E}}$ is a trace-decreasing superoperator. □

Let us consider the superoperators $\hat{L}_A$ and $\hat{R}_{A^*}$. These superoperators can be represented by

$$\hat{L}_A = \sum_{\mu=0}^{N-1}\sum_{\nu=0}^{N-1} L_{\mu\nu}^{(A)}|\mu)(\nu|, \qquad \hat{R}_{A^*} = \sum_{\mu=0}^{N-1}\sum_{\nu=0}^{N-1} R_{\mu\nu}^{(A^*)}|\mu)(\nu|, \tag{43}$$

where matrices $L_{\mu\nu}^{(A)}$ and $R_{\mu\nu}^{(A^*)}$ are defined by

$$L_{\mu\nu}^{(A)} = \frac{1}{2^n}\,Tr(\sigma_\mu A\sigma_\nu) = \frac{1}{2^n}\,Tr(\sigma_\alpha\sigma_\mu A),$$
$$R_{\mu\nu}^{(A^*)} = \frac{1}{2^n}\,Tr(\sigma_\mu\sigma_\nu A^*) = \frac{1}{2^n}\,Tr(A^*\sigma_\mu\sigma_\nu).$$

THEOREM 18. *The matrix $\mathcal{E}_{\mu\nu}$ of the completely positive superoperator (41) can be represented by*

$$\mathcal{E}_{\mu\nu} = \sum_{j=1}^{m}\sum_{\alpha=0}^{N-1} L_{\mu\alpha}^{(jA)} R_{\alpha\nu}^{(jA^*)}. \tag{44}$$

PROOF. Let us write the matrix $\mathcal{E}_{\mu\nu}$ by matrices of superoperators $\hat{L}_{A_j}$ and $\hat{R}_{A_j}$:

$$\mathcal{E}_{\mu\nu} = (\mu|\hat{\mathcal{E}}|\nu) = \sum_{j=1}^{m}(\mu|\hat{L}_{A_j}\hat{R}_{A_j^*}|\nu)$$
$$= \sum_{j=1}^{m}\sum_{\alpha=0}^{N-1}(\mu|\hat{L}_{A_j}|\alpha)(\alpha|\hat{R}_{A_j^*}|\nu) = \sum_{j=1}^{m}\sum_{\alpha=0}^{N-1} L_{\mu\alpha}^{(jA)} R_{\alpha\nu}^{(jA^*)}.$$

Finally, we obtain (44), where

$$L_{\mu\alpha}^{(jA)} = (\mu|\hat{L}_A|\alpha) = \frac{1}{2^n}(\sigma_\mu|\hat{L}_{A_j}|\sigma_\alpha)$$
$$= \frac{1}{2^n}\,Tr(\sigma_\mu A_j\sigma_\alpha) = \frac{1}{2^n}\,Tr(\sigma_\alpha\sigma_\mu A_j),$$

and

$$R_{\alpha\nu}^{(jA^*)} = (\alpha|\hat{R}_{A_j^*}|\nu) = \frac{1}{2^n}(\sigma_\alpha|\hat{R}_{A_j^*}|\sigma_\nu)$$
$$= \frac{1}{2^n}\,Tr(\sigma_\alpha\sigma_\nu A_j^*) = \frac{1}{2^n}\,Tr(A_j^*\sigma_\alpha\sigma_\nu).$$

The matrix elements can be rewritten in the form

$$L^{(jA)}_{\mu\alpha} = \frac{1}{2^n}(\sigma_\mu\sigma_\alpha|A_j), \qquad R^{(jA^*)}_{\alpha\nu} = \frac{1}{2^n}(A_j|\sigma_\alpha\sigma_\nu). \tag{45}$$

□

EXAMPLE. Let us consider the single ququat pseudo-gate $\hat{L}_A$. The elements of pseudo-gate matrix $L^{(A)}$ are defined by

$$L^{(A)}_{\mu\nu} = \frac{1}{2}\,Tr(\sigma_\mu A\sigma_\nu).$$

Let us denote

$$a_\mu = \frac{1}{2}\,Tr(\sigma_\mu A).$$

Using

$$L^{(A)}_{kl} = \frac{1}{2}\,Tr(\sigma_l\sigma_k A) = \frac{1}{2}\delta_{kl}\,Tr\,A + \frac{i}{2}\varepsilon_{lkm}\,Tr(\sigma_m A),$$

where $k, l, m = 1, 2, 3$, we obtain

$$\hat{L}_A = \sum_{\mu=0}^{3} a_0|\mu)(\mu| + \sum_{k=0}^{3} a_k\big(|0)(k| + |k)(0|\big) + ia_1\big(|3)(2| - |2)(3|\big) + ia_2\big(|1)(3| - |3)(1|\big) + ia_3\big(|2)(1| - |1)(2|\big).$$

The pseudo-gate matrix is

$$L^{(A)}_{\mu\nu} = \delta_{\mu\nu}\,Tr\,A + \sum_{m=1}^{3}(\delta_{\mu0}\delta_{\nu m} + \delta_{\mu m}\delta_{\nu0})\,Tr(\sigma_m A) + i\sum_{m=1}^{3}\delta_{\mu k}\delta_{\nu l}\varepsilon_{lkm}\,Tr(\sigma_m A). \tag{46}$$

Let us consider the properties of the matrix elements $L^{(jA)}_{\mu\alpha}$ and $R^{(jA^*)}_{\mu\alpha}$.

THEOREM 19. *The matrices $L^{(jA)}_{\mu\alpha}$ and $R^{(jA^*)}_{\mu\alpha}$ are complex $4^n \times 4^n$ matrices and their elements are connected by complex conjugation*:

$$\big(L^{(jA)}_{\mu\alpha}\big)^* = R^{(jA^*)}_{\mu\alpha}. \tag{47}$$

PROOF. Using complex conjugation of the matrix elements (45), we obtain

$$\big(L^{(jA)}_{\mu\alpha}\big)^* = \frac{1}{2^n}(\sigma_\mu\sigma_\alpha|A_j)^* = \frac{1}{2^n}(A_j|\sigma_\mu\sigma_\alpha) = R^{(jA^*)}_{\mu\alpha}.$$

We can write the gate matrix (44) in the form

$$\mathcal{E}_{\mu\nu} = \sum_{j=1}^{m} \sum_{\alpha=0}^{N-1} L_{\mu\alpha}^{(jA)} \bigl(L_{\alpha\nu}^{(jA)}\bigr)^*. \tag{48}$$

□

THEOREM 20. *The matrices $L_{\mu\alpha}^{(jA)}$ and $R_{\mu\alpha}^{(jA^*)}$ of the n-ququat quantum four-valued logic gate* (41) *are the elements of Lie group $GL(4^n, \mathbb{C})$. The set of these matrices is a group.*

A superoperator $\hat{\mathcal{E}}$ on $\overline{\mathcal{H}}^{(2)}$ is called *primitive*, if $\hat{\mathcal{E}}$ maps the tensor product of single ququats to the tensor product of single ququats, i.e., if $|\rho_1)$ and $|\rho_2)$ are ququats, then we can find ququats $|\rho_1')$ and $|\rho_2')$ such that

$$\hat{\mathcal{E}}|\rho_1 \otimes \rho_2) = |\rho_1' \otimes \rho_2').$$

The superoperator $\hat{\mathcal{E}}$ is called imprimitive if $\hat{\mathcal{E}}$ is not primitive.

It can be shown that almost every pseudo-gate that operates on two or more ququats is a universal pseudo-gate.

THEOREM 21. *The set of all single ququat pseudo-gates and any imprimitive two-ququat pseudo-gate form a universal set of pseudo-gates.*

PROOF. Let us consider some points of the proof. Expressed in group theory language, all n-ququat pseudo-gates are elements of the Lie group $GL(4^n, \mathbb{C})$. Two-ququat pseudo-gates $\hat{L}$ are elements of Lie group $GL(16, \mathbb{C})$. The question of universality is the same as that of what set of superoperators $\hat{L}$ is sufficient to generate $GL(16, \mathbb{C})$. The group $GL(16, \mathbb{C})$ has $(16)^2 = 256$ independent one-parameter subgroups $GL_{\mu\nu}(16, \mathbb{C})$ of one-parameter pseudo-gates $\hat{L}^{(\mu\nu)}(t)$ such that $\hat{L}^{(\mu\nu)}(t) = t|\mu)(\nu|$. Infinitesimal generators of Lie group $GL(4^n, \mathbb{C})$ are defined by

$$\hat{H}_{\mu\nu} = \left(\frac{d}{dt}\hat{L}^{(\mu\nu)}(t)\right)_{t=0}, \tag{49}$$

where $\mu, \nu = 0, 1, \ldots, 4^n - 1$. The generators $\hat{H}_{\mu\nu}$ of the one-parameter subgroup $GL_{\mu\nu}(4^n, \mathbb{R})$ are superoperators of the form $\hat{H}_{\mu\nu} = |\mu)(\nu|$ on $\overline{\mathcal{H}}^{(n)}$ which can be represented by $4^n \times 4^n$ matrices $H_{\mu\nu}$ with elements

$$(H_{\mu\nu})_{\alpha\beta} = \delta_{\alpha\mu}\delta_{\beta\nu}.$$

The set of superoperators $\hat{H}_{\mu\nu}$ is a basis (Weyl basis) of Lie algebra $gl(16, \mathbb{R})$ such that

$$\bigl[\hat{H}_{\mu\nu}, \hat{H}_{\alpha\beta}\bigr] = \delta_{\nu\alpha}\hat{H}_{\mu\beta} - \delta_{\mu\beta}\hat{H}_{\nu\alpha},$$

where $\mu, \nu, \alpha, \beta = 0, 1, \ldots, 15$. Any element $\hat{H}$ of the algebra $gl(16, \mathbb{C})$ can be represented by

$$\hat{H} = \sum_{\mu=0}^{15} \sum_{\nu=0}^{15} h_{\mu\nu} \hat{H}_{\mu\nu},$$

where $h_{\mu\nu}$ are complex coefficients.

As a basis of Lie algebra $gl(16, \mathbb{C})$ we can use 256 linearly independent self-adjoint superoperators

$$H_{\alpha\alpha} = |\alpha)(\alpha|, \qquad H^r_{\alpha\beta} = |\alpha)(\beta| + |\beta)(\alpha|,$$
$$H^i_{\alpha\beta} = -i\big(|\alpha)(\beta| - |\beta)(\alpha|\big),$$

where $0 \leqslant \alpha \leqslant \beta \leqslant 15$. The matrices of these generators are Hermitian 16×16 matrices. The matrix elements of 256 Hermitian 16×16 matrices $H_{\alpha\alpha}$, $H^r_{\alpha\beta}$ and $H^i_{\alpha\beta}$ are defined by

$$(H_{\alpha\alpha})_{\mu\nu} = \delta_{\mu\alpha}\delta_{\nu\alpha},$$
$$\big(H^r_{\alpha\beta}\big)_{\mu\nu} = \delta_{\mu\alpha}\delta_{\nu\beta} + \delta_{\mu\beta}\delta_{\nu\alpha},$$
$$\big(H^i_{\alpha\beta}\big)_{\mu\nu} = -i\,(\delta_{\mu\alpha}\delta_{\nu\beta} - \delta_{\mu\beta}\delta_{\nu\alpha}).$$

For any Hermitian generator $\hat{H}$ there exists a one-parameter pseudo-gate $\hat{L}(t)$ which can be represented in the form $\hat{L}(t) = \exp it\hat{H}$ such that $\hat{L}^*(t)\hat{L}(t) = \hat{I}$.

Let us write the main operations which allow us to derive new pseudo-gates $\hat{L}$ from a set of pseudo-gates.

(1) We introduce general SWAP (twist) pseudo-gate $\hat{T}^{(SW)}$. A new pseudo-gate $\hat{L}^{(SW)}$ defined by $\hat{L}^{(SW)} = \hat{T}^{(SW)}\hat{L}\hat{T}^{(SW)}$ is obtained directly from $\hat{L}$ by exchanging two ququats.

(2) Any superoperator $\hat{L}$ on $\overline{\mathcal{H}}^{(2)}$ generated by the commutator $i[\hat{H}_{\mu\nu}, \hat{H}_{\alpha\beta}]$ can be obtained from $\hat{L}_{\mu\nu}(t) = \exp it\hat{H}_{\mu\nu}$ and $\hat{L}_{\alpha\beta}(t) = \exp it\hat{H}_{\alpha\beta}$ because

$$\exp t\big[\hat{H}_{\mu\nu}, \hat{H}_{\alpha\beta}\big] = \lim_{n\to\infty} \big(\hat{L}_{\alpha\beta}(-t_n)\hat{L}_{\mu\nu}(t_n)\hat{L}_{\alpha\beta}(t_n)\hat{L}_{\mu\nu}(-t_n)\big)^n,$$

where $t_n = 1/\sqrt{n}$. Thus we can use the commutator $i[\hat{H}_{\mu\nu}, \hat{H}_{\alpha\beta}]$ to generate pseudo-gates.

(3) Every transformation $\hat{L}(a, b) = \exp i\hat{H}(a, b)$ of $GL(16, \mathbb{C})$ generated by superoperator $\hat{H}(a, b) = a\hat{H}_{\mu\nu} + b\hat{H}_{\alpha\beta}$, where a and b are complex, can obtained from $\hat{L}_{\mu\nu}(t) = \exp it\hat{H}_{\mu\nu}$ and $\hat{L}_{\alpha\beta}(t) = \exp it\hat{H}_{\alpha\beta}$ by

$$\exp i\hat{H}(a, b) = \lim_{n\to\infty} \left[\hat{L}_{\mu\nu}\left(\frac{a}{n}\right)\hat{L}_{\alpha\beta}\left(\frac{b}{n}\right)\right]^n. \qquad \square$$

Control of quantum gates

Quantum non-Hamiltonian systems can be used for quantum computations. The computations are realized by quantum operations, not necessarily unitary. Mixed states subject to the general quantum operations could increase efficiency. This increase is connected with the increasing number of computational basis elements for Hilbert space. A pure state of n two level quantum systems is an element of 2^n-dimensional function Hilbert space. A mixed state of the system is an element of 4^n-dimensional operator Hilbert space. The conventional quantum two-valued logic is replaced by quantum four-valued logic. Therefore the increased efficiency can be formalized in terms of a four-valued logic replacing the conventional two-valued logic. Unitary gates and quantum operations for a quantum computer with pure states and two-valued logic can be considered as four-valued logic gates of a mixed-state quantum computer. Quantum algorithms [120] on a quantum computer with mixed states are expected to run on a smaller network than with pure state implementation.

In the quantum computer model with pure states, control of quantum unitary gates is realized by classical parameters of the Hamilton operator. Quantum systems can be described by the equation:

$$\frac{\partial}{\partial t}\rho(t) = \hat{\Lambda}\rho(t), \tag{50}$$

where $\hat{\Lambda}$ is the Liouville superoperator. For Hamiltonian quantum systems this superoperator is defined by Hamiltonian H:

$$\hat{\Lambda} = -\frac{i}{\hbar}\big(\hat{L}_H - \hat{R}_H\big),$$

where $\hat{L}_H$ and $\hat{R}_H$ are superoperators defined by $\hat{L}_H\rho = H\rho$ and $\hat{R}_H\rho = \rho H$. Quantum unitary gates on pure states are controlled by classical parameters entering the Hamiltonian H. For non-Hamiltonian quantum systems with completely positive evolution, the Liouville superoperator $\hat{\Lambda}$ is given by

$$\hat{\Lambda} = -\frac{i}{\hbar}\big(\hat{L}_H - \hat{R}_H\big) + \frac{1}{2\hbar}\sum_{k=1}^{\infty}\big(2\hat{L}_{V_k}\hat{R}_{V_k^*} - \hat{L}_{V_k}\hat{L}_{V_k^*} - \hat{R}_{V_k^*}\hat{R}_{V_k}\big),$$

where $\{V_k\}$ is a set of operators. Quantum four-valued logic gates on mixed states are controlled by classical parameters of the Hamiltonian H and the operators V_k.

Universality for general quantum four-valued logic gates acting on mixed states should be studied. The matrices of the quantum gates can be considered as elements of some matrix group but these matrices are completely positive (or positive) elements of this matrix group. The condition of complete positivity leads to difficult inequalities for matrix elements [35,61,82,130]. The completely positive

condition for quantum four-valued logic gates can be satisfied by Kraus representation (41). To find the universal set of quantum four-valued logic gates we suggest to consider the universal set of the superoperators (43) called pseudo-gates. Pseudo-gates are not necessarily completely positive and the set of pseudo-gates matrices is a group. Almost any two-ququat pseudo-gate is universal.

In the usual quantum computer model a measurement of the final pure state is described by projection operators $P_k = |k><k|$. In the non-Hamiltonian model a measurement of the final mixed state can be described by projection superoperators described by $\hat{\mathcal{P}}_\mu = |\mu)(\mu|$, where $|\mu)$ are defined by (11) and (12).

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