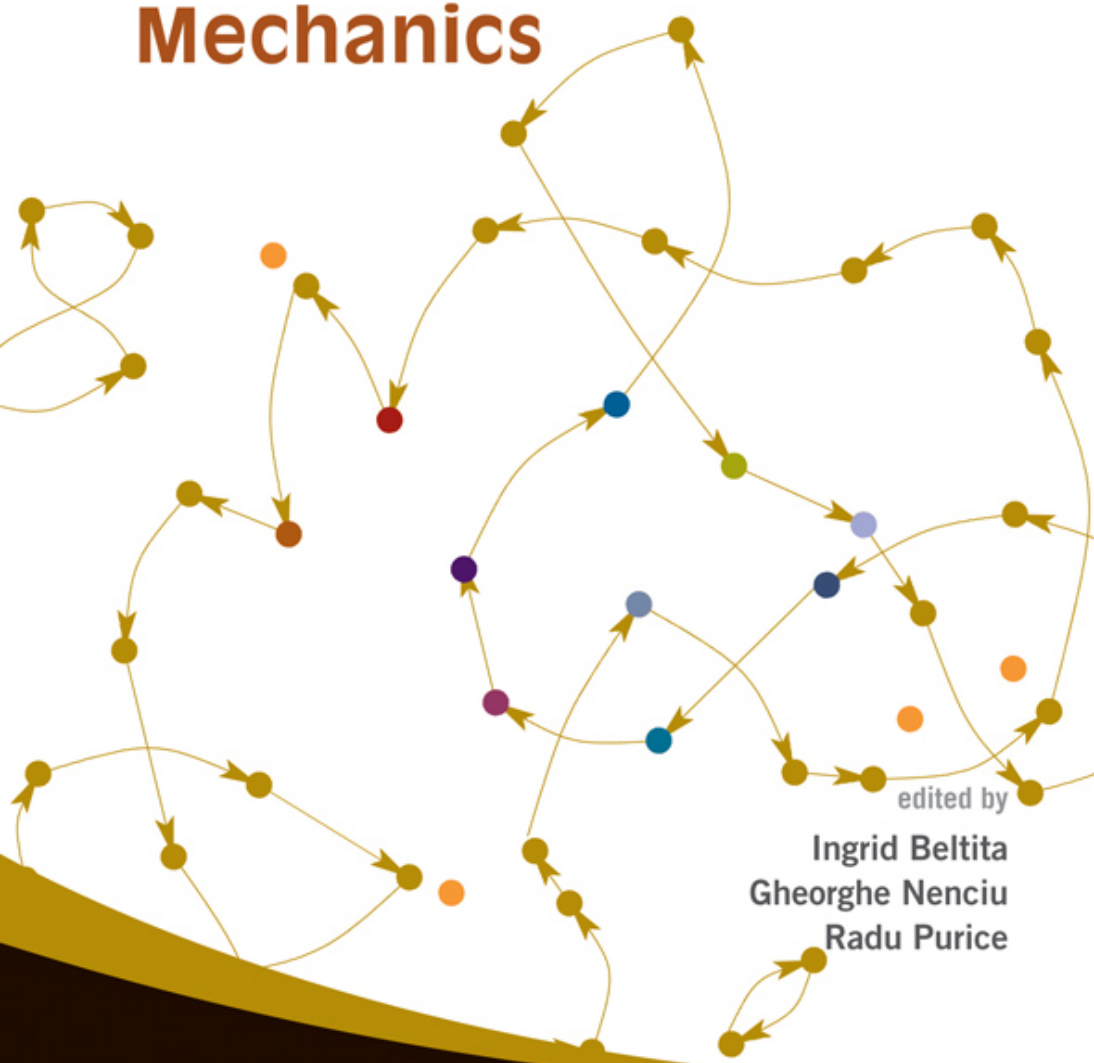
Proceedings of the QMath10 Conference

Mathematical Results In Quantum Mechanics



edited by
Ingrid Beltita
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Mathematical Results In Quantum Mechanics

Moieciu, Romania 10 – 15 September 2007

edited by

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PREFACE

This book continues the series of Proceedings dedicated to the *Quantum Mathematics International Conferences Series* and presents a number of selected refereed papers dealing with some of the topics discussed at its 10-th edition, Moieciu (Romania), September 10 - 15, 2007.

The *Quantum Mathematics* series of conferences started in the seventies, having the aim to present the state of the art in the mathematical physics of Quantum Systems, both from the point of view of the models considered and of the mathematical techniques developed for their study. While at its beginning the series was an attempt to enhance collaboration between mathematical physicists from eastern and western European countries, in the nineties it took a worldwide dimension, being hosted successively in Germany, Switzerland, Czech Republic, Mexico, France and this last one in Romania.

The aim of QMath10 has been to cover a number of topics that present an interest both for theoretical physicists working in several branches of pure and applied physics such as solid state physics, relativistic physics, physics of mesoscopic systems, etc, as well as mathematicians working in operator theory, pseudodifferential operators, partial differential equations, etc. This conference was intended to favour exchanges and give rise to collaborations between scientists interested in the mathematics of Quantum Mechanics. A special attention was paid to young mathematical physicists.

The 10-th edition of the *Quantum Mathematics International Conference* series has been organized as part of the SPECT Programme of the *European Science Foundation* and has taken place in Romania, in the mountain resort Moieciu, in the neighborhood of Brasov. It has been attended by 79 people coming from 17 countries. There have been 13 invited plenary talks and 55 talks in 6 parallel sections:

- *Schrödinger Operators and Inverse Problems* (organized by Arne Jensen),
- *Random Schrödinger Operators and Random Matrices* (organized by Frederic Klopp),

- *Open Systems and Condensed Matter* (organized by Valentin Zagrebnov),
- *Pseudodifferential Operators and Semiclassical Analysis* (organized by Francis Nier),
- *Quantum Field Theory and Relativistic Quantum Mechanics* (organized by Volker Bach),
- *Quantum Information* (organized by Dagmar Bruss).

This book is intended to give a comprehensive glimpse on recent advances in some of the most active directions of current research in quantum mathematical physics. The authors, the editors and the referees have done their best to provide a collection of works of the highest scientific standards, in order to achieve this goal.

We are grateful to the Scientific Committee of the Conference: Yosi Avron, Pavel Exner, Bernard Helffer, Ari Laptev, Gheorghe Nenciu and Heinz Siedentop and to the organizers of the 6 parallel sections for their work to prepare and mediate the scientific sessions of "QMath10".

We would like to thank all the institutions who contributed to support the organization of "QMath10": the European Science Foundation, the International Association of Mathematical Physics, the "Simion Stoilow" Institute of Mathematics of the Romanian Academy, the Romanian National Authority for Scientific Research (through the Contracts CEx-M3-102/2006, CEx06-11-18/2006 and the Comission for Exhibitions and Scientific Meetings), the National University Research Council (through the grant 2RNP/2007), the Romanian Ministry of Foreign Affairs (through the Department for Romanians Living Abroad) and the SOFTWIN Group. We also want to thank the Tourist Complex "Cheile Grădiştei" - Moieciu, for their hospitality.

The Editors
Bucharest, June 2008

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CONTENTS

CHARGE TRANSPORT AND DETERMINANTS

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We review some known facts in the transport theory of mesoscopic systems, including counting statistics, and discuss its relation with the mathematical treatment of open systems.

1. Introduction

The aim of these notes is to introduce to some theoretical developments concerning transport in mesoscopic systems. More specifically, we intend to show how concepts and tools from mathematical physics provide ways and means to put some recent, fundamental results on counting statistics on rigorous ground and in a natural setting. We will draw on concepts like C*-algebras, which have been often used in the mathematical treatment of systems out of equilibrium, see *e.g.* Ref. 7, but also on tools like Fredholm determinants, which have been used for renormalization purposes in quantum field theory. Before going into mathematical details we will review some of the more familiar aspects of transport, and notably noise. That will provide some examples on which to later illustrate the theory.

These notes are not intended for the expert. On the contrary, the style might be overly pedagogical.

2. Noises

Consider two leads joined by a resistor. The value of its conductance, G, is to be meant, for the sake of precision, as corresponding to a two-terminal arrangement, meaning that the voltage V is identified with the difference of

chemical potentials between right movers on the left of the resistor and left movers on its right. We are interested in the average charge $\langle Q \rangle$ transported across the resistance in a time T, and in the variance $\langle\langle Q^2 \rangle\rangle = \langle Q^2 \rangle - \langle Q \rangle^2$, equivalently in the current $\langle Q \rangle / T$ and in the noise $\langle\langle Q^2 \rangle\rangle / T$.

There are two types of noises:

(1) Equilibrium, or thermal, noise occurs in the absence of voltage, $V = 0$, and at positive temperature $\beta^{-1} > 0$. Then

$$\langle Q \rangle = 0\,, \qquad \frac{\langle Q^2 \rangle}{T} = \frac{2}{\beta}\, G\,. \tag{2.1}$$

(Johnson,[8] Nyquist[17]). This is an early instance of the fluctuation-dissipation theorem, those words being here represented as noise and conductance.

(2) Non-equilibrium, or shot, noise occurs in the reverse situation: $V \neq 0$, $\beta^{-1} = 0$. Ohm's law states $\langle Q \rangle / T = GV$, while for the noise different expressions (corresponding to different situations) are available: (a) classical shot noise

$$\langle\langle Q^2 \rangle\rangle = e \langle Q \rangle \tag{2.2}$$

(Schottky[21]), where e is the charge of the carriers, say electrons. The result is interpreted on the basis of the Poisson distribution

$$p_n = \mathrm{e}^{-\lambda} \frac{\lambda^n}{n!}\,, \quad (n = 0, 1, 2, \ldots)$$

of parameter λ, for which

$$\langle n \rangle = \lambda\,, \qquad \langle\langle n^2 \rangle\rangle = \lambda\,.$$

Assuming that electrons arrive independently of one another, the number n of electrons collected in time T is so distributed, whence (2.2) for $Q = en$.

(b) quantum shot noise. Consider the leads and the resistor as modelled by a 1-dimensional scattering problem with matrix

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}\,, \tag{2.3}$$

where r, t (resp. r', t') are the reflection and transmission amplitudes from the left and from the right. Then

$$\langle\langle Q^2 \rangle\rangle = e \langle Q \rangle (1 - |t|^2) \tag{2.4}$$

(Khlus,[10] Lesovik[12]). In this case the result may be attributed to a binomial distribution with the success probability p and with N attempts:

$$p_n = \binom{N}{n} p^n (1-p)^{N-n}\,,$$
$$\langle n\rangle = Np\,, \quad \langle\langle n^2\rangle\rangle = Np(1-p)\,.$$

This yields (2.4) for $p = |t|^2$ being the probability of transmission. For small p it reduces to (2.2). It should be noticed that in the case of thermal noise, the origin of fluctuations is in the source of electrons, or in the incoming flow, depending on the point of view. By contrast, in the interpretation of the quantum shot noise the flow is assumed ordered, as signified by the fixed number of attempts, and fluctuations arise only because of the uncertainty of transmission.

We refer to Ref. 6 for a more complete exposition of these matters. We conclude the section by recalling that noises are quantitative evidence to atomism. Thermal noise determines $\beta^{-1} = k\cdot$temperature, and hence Boltzmann's constant k as well as Avogadro's number $N_0 = R/k$ (somewhat in analogy to its determination from Brownian motion[5,23]). Shot noise determines the charge of carriers. In some instances of the fractional quantum Hall effect this yielded $e/3$[19] or $e/5$.[18]

3. A setup for counting statistics

Before engaging in quantum mechanical computations of the transported charge we should describe how it is measured, at least in the sense of a thought experiment. Consider a device (dot, resistor, or the like) connected to several leads, or reservoirs, one of which is distinguished ('the lead'). The measurement protocol consists of three steps:

- measure the charge present *initially* in the lead, given a prepared state of the whole system.
- act on the system during some time by driving its controls (like gate voltages in a dot), but not by performing measurements. This includes the possibility of just waiting.
- measure the charge present in the lead *finally*.

The transported charge is then identified as the difference, n, of the outcome of the measurements. For simplicity we assume that n takes only integer values, interpreted as the number of transferred electrons. Let p_n

be the corresponding probabilities. They are conveniently encoded in the generating function

$$\chi(\lambda) = \sum_{n\in\mathbb{Z}} p_n \mathrm{e}^{\mathrm{i}\lambda n} \tag{3.1}$$

of the moments of the distribution,

$$\langle n^k\rangle = \left(-\mathrm{i}\frac{d}{d\lambda}\right)^k \chi(\lambda)\bigg|_{\lambda=0} .$$

Similarly, $\log\chi(\lambda)$ generates the cumulants $\langle\!\langle n^k\rangle\!\rangle$, inductively defined by

$$\langle n^k\rangle = \sum_{\mathcal{P}} \prod_{\alpha\in\mathcal{P}} \langle\!\langle n^{|\alpha|}\rangle\!\rangle ,$$

where $\mathcal{P} = \{\alpha_1, \ldots, \alpha_m\}$ runs over all partitions of $\{1, \ldots, k\}$. Alternative protocols with measurements extending over time will be discussed later.

4. Quantum description

The three steps of the procedure just described can easily be implemented quantum mechanically by means of two projective measurements and by a Hamiltonian evolution in between.

Let $\mathcal{H}$ be the Hilbert space of pure states of a system, ρ a density matrix representing a mixed state, and $A = \sum_i \alpha_i P_i$ an observable with its spectral decomposition. A single measurement of A is associated, at least practically, with the 'collapse of the wave function' resulting in the replacement

$$\rho \rightsquigarrow \sum_i P_i \rho P_i , \tag{4.1}$$

where $\mathrm{tr}(P_i\rho P_i) = \mathrm{tr}(\rho P_i)$ is the probability for the outcome α_i. Two measurements of A, separated by an evolution given as a unitary U, result in the replacement.[22]

$$\rho \rightsquigarrow \sum_{i,j} P_j U P_i \rho P_i U^* P_j , \tag{4.2}$$

where $\mathrm{tr}(P_j U P_i \rho P_i U^* P_j) = \mathrm{tr}(U^* P_j U P_i \rho P_i)$ is the probability of the history (α_i, α_j) of outcomes. We can so compute the moment generating function (3.1):

$$\begin{aligned}\chi(\lambda) &= \sum_{i,j} \mathrm{tr}(U^* P_j U P_i \rho P_i) \mathrm{e}^{\mathrm{i}\lambda(\alpha_j - \alpha_i)} \\ &= \sum_i \mathrm{tr}(U^* \mathrm{e}^{\mathrm{i}\lambda A} U P_i \rho P_i) \mathrm{e}^{-\mathrm{i}\lambda\alpha_i} .\end{aligned} \tag{4.3}$$

The expression simplifies if

$$[A, \rho] = 0\,; \tag{4.4}$$

then $P_i \rho P_i = P_i \rho$, whence the r.h.s. of (4.1) still equals ρ (no collapse at first measurement) and

$$\chi(\lambda) = \mathrm{tr}(U^* \mathrm{e}^{\mathrm{i}\lambda A} U \mathrm{e}^{-\mathrm{i}\lambda A} \rho)\,. \tag{4.5}$$

If ρ is a pure state, $\rho = \Omega(\Omega, \cdot)$, then

$$\chi(\lambda) = (\Omega, U^* \mathrm{e}^{\mathrm{i}\lambda A} U \mathrm{e}^{-\mathrm{i}\lambda A} \Omega)\,. \tag{4.6}$$

5. Independent, uncorrelated fermions

We intend to apply (4.5) to many-body systems consisting of fermionic particles which are uncorrelated in the initial state. The particles shall contribute additively to the observable to be considered and evolve independently of one another. The ingredients can therefore be specified at the level of a single particle. At the risk of confusion we denote them like the related objects in the previous section: A Hilbert space $\mathcal{H}$ with operators A, U, ρ. However, the meaning of ρ is now that of a 1-particle density matrix $0 \leq \rho \leq 1$ specifying an uncorrelated many-particle state, to the extent permitted by the Pauli principle: any eigenstate of $|\nu\rangle$ of ρ, $\rho|\nu\rangle = \nu|\nu\rangle$, is occupied in the many-particle state with probability given by its eigenvalue ν. Common examples are the vacuum $\rho = 0$ and, in terms of a single-particle Hamiltonian H, the Fermi-Dirac distribution $\rho = (1 + \mathrm{e}^{\beta H})^{-1}$ or its zero temperature limit, $\beta^{-1} \to 0$, the Fermi sea $\rho = \Theta(-H)$.

The corresponding many-particle objects are obtained through second quantization, which amounts to the following replacements:

$$\mathcal{H} \rightsquigarrow \mathcal{F}(\mathcal{H}) = \bigoplus_{n=0}^{\infty} \bigwedge^n \mathcal{H} \qquad \text{(Fock space)} \tag{5.1}$$

$$A \rightsquigarrow \mathrm{dd}\Gamma(A) \tag{5.2}$$

$$U \rightsquigarrow \Gamma(U) \tag{5.3}$$

where $\mathrm{dd}\Gamma(A)$ and $\Gamma(U)$ act on the subspaces $\bigwedge^n \mathcal{H} \subset \mathcal{F}(\mathcal{H})$ as

$$\mathrm{dd}\Gamma(A) = \sum_{i=1}^{n} 1 \otimes \cdots \otimes A \otimes \cdots \otimes 1\,,$$

$$\Gamma(U) = U \otimes \cdots \otimes U\,.$$

Moreover, the state is replaced as

$$\rho \rightsquigarrow \frac{\Gamma(\rho/\rho')}{\mathrm{Tr}_{\mathcal{F}(\mathcal{H})}\Gamma(\rho/\rho')}\,, \qquad (\rho' = 1-\rho)\,. \tag{5.4}$$

Indeed, if ρ splits with respect to $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$, then the many-body state (5.4) factorizes w.r.t. $\mathcal{F}(\mathcal{H}) = \mathcal{F}(\mathcal{H}_1) \otimes \mathcal{F}(\mathcal{H}_2)$. In particular if $\rho|\nu\rangle = \nu|\nu\rangle$, this entails the following state on $\mathcal{F}[|\nu\rangle] = \oplus_{n=0}^{1} \wedge^n [|\nu\rangle]$

$$\frac{1_0 + \frac{\nu}{\nu'}1_1}{1+\frac{\nu}{\nu'}} = \nu' 1_0 + \nu 1_1\,,$$

confirming that ν is the occupation number of $|\nu\rangle$. We note that

$$\mathrm{Tr}_{\mathcal{F}(\mathcal{H})}\Gamma(M) = \det{}_{\mathcal{H}}(1+M)\,,$$

provided that M is a trace-class operator on $\mathcal{H}$, in which case the r.h.s. is a Fredholm determinant. We will comment on that condition later. Under the replacements (5.1-5.4) the assumption $[A,\rho] = 0$ is inherited by the corresponding second quantized observables, $[\mathrm{dd}\Gamma(A), \Gamma(\rho/\rho')] = 0$. As a result (4.5) applies and becomes the Levitov-Lesovik formula

$$\chi(\lambda) = \det(\rho' + \mathrm{e}^{\mathrm{i}\lambda U^* A U}\mathrm{e}^{-\mathrm{i}\lambda A}\rho)\,. \tag{5.5}$$

Indeed,

$$\begin{aligned}\chi(\lambda) &= \frac{\mathrm{Tr}_{\mathcal{F}(\mathcal{H})}(\Gamma(U)^*\mathrm{e}^{\mathrm{i}\lambda \mathrm{dd}\Gamma(A)}\Gamma(U)\mathrm{e}^{-\mathrm{i}\lambda \mathrm{dd}\Gamma(A)}\Gamma(\rho/\rho'))}{\mathrm{Tr}_{\mathcal{F}(\mathcal{H})}\Gamma(\rho/\rho')} \\ &= \frac{\mathrm{Tr}_{\mathcal{F}(\mathcal{H})}\Gamma(U^*\mathrm{e}^{\mathrm{i}\lambda A}U\mathrm{e}^{-\mathrm{i}\lambda A}\rho/\rho')}{\mathrm{Tr}_{\mathcal{F}(\mathcal{H})}\Gamma(\rho/\rho')} = \frac{\det(1+U^*\mathrm{e}^{\mathrm{i}\lambda A}U\mathrm{e}^{-\mathrm{i}\lambda A}(\rho/\rho'))}{\det(1+(\rho/\rho'))} \\ &= \det(\rho' + U^*\mathrm{e}^{\mathrm{i}\lambda A}U\mathrm{e}^{-\mathrm{i}\lambda A}\rho)\,.\end{aligned}$$

Before discussing the mathematical fine points of (5.5), let us compute the first two cumulants of charge transport. In line with the discussion in the previous section, let $A = Q$ be the projection onto single-particle states located in the distinguished lead. Then (5.5) yields

$$\begin{aligned}\langle Q\rangle &= -\mathrm{i}\chi'(0) = \mathrm{tr}\rho(\Delta Q)\,, \\ \langle\!\langle Q^2\rangle\!\rangle &= -(\log\chi)''(0) = \mathrm{tr}\rho(\Delta Q)(1-\rho)\Delta Q \\ &= \mathrm{tr}(\rho(1-\rho)(\Delta Q)^2) + \frac{1}{2}\mathrm{tr}(\mathrm{i}[\Delta Q,\rho])^2\,,\end{aligned} \tag{5.6}$$

where $\Delta Q = U^*QU - Q$ is the operator of transmitted charge. The split (5.6) of the noise $\langle\!\langle Q^2\rangle\!\rangle$ into two separately non negative contributions is of some interest ([3] by a different approach,[1]): The commutator $[\Delta Q, \rho]$ expresses the uncertainty of transmission ΔQ in the given state

ρ; the second term in (5.6) may thus be viewed as *shot noise*. The factor $\rho(1-\rho)$ expresses the fluctuation $\nu(1-\nu)$ in the occupation of single particle states $|\nu\rangle$. It refers to the initial state, or source, and its term may be viewed as *thermal noise*; indeed it vanishes for pure states, $\rho = \rho^2$, while for $\rho = (1+\mathrm{e}^{\beta H})^{-1}$ the energy width of $\rho(1-\rho)$ is proportional to β^{-1}, *cf.* 2.1).

6. Alternative approaches

We present alternatives and variants of the two-step measurement procedures discussed in Sect. 3. We discuss them in the first quantized setting of Sect. 4. The corresponding second quantized versions can then easily obtained from the replacements (5.1-5.4).

i)[14] One could envisage a single measurement of the difference $U^*AU - A$. On the basis of (4.2) its generating function is

$$\chi(\lambda) = \mathrm{tr}(\mathrm{e}^{\mathrm{i}\lambda(U^*AU-A)}\rho)\,.$$

It remains unclear how to realize a von Neumann measurement for this observable, since its two pieces are associated with two different times. Moreover, its second quantized version

$$\chi(\lambda) = \det(\rho' + \mathrm{e}^{\mathrm{i}\lambda(U^*AU-A)}\rho)$$

generates cumulants which, as a rule beginning with $n = 3$, differ from those of (5.5).

ii)[20] We keep the two-measurement setup, but refrain from making assumption (4.4), *i.e.*, the first measurement is allowed to induce a "collapse of the wave function". We do however assume that the eigenvalues α_i of A are integers, in line with the application made at the end of the previous section, where $A \rightsquigarrow \mathrm{dd}\Gamma(Q)$ with Q a projection. Then (4.3) yields

$$\begin{aligned}\chi(\lambda) &= \sum_{n,m} \mathrm{tr}(U^*\mathrm{e}^{\mathrm{i}\lambda A}UP_n\rho P_m)\delta_{mn}\mathrm{e}^{-\mathrm{i}\lambda n} \\ &= \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\mathrm{d}\tau\, \mathrm{tr}(U^*\mathrm{e}^{\mathrm{i}\lambda A}U\mathrm{e}^{-\mathrm{i}(\lambda+\tau)A}\rho\mathrm{e}^{\mathrm{i}\tau A})\end{aligned}$$

by using $\delta_{mn} = (2\pi)^{-1}\int_0^{2\pi}\mathrm{d}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\tau(m-n)}$.

iii)[13] Here neither (3.1) nor (4.4) is assumed. The system is coupled to a spin-$\frac{1}{2}$ resulting in a total state space $\mathcal{H}\otimes\mathbb{C}^2$. Specifically, the total Hamiltonian is obtained by conjugating the system Hamiltonian by $\mathrm{e}^{-\mathrm{i}\frac{\lambda}{2}A\otimes\sigma_3}$, where λ is a coupling constant and σ_3 a Pauli matrix; equivalently, the same holds true for the evolution U, which becomes

$$\widehat{U} = \mathrm{e}^{-\mathrm{i}\frac{\lambda}{2}A\otimes\sigma_3}(U\otimes 1)\mathrm{e}^{\mathrm{i}\frac{\lambda}{2}A\otimes\sigma_3}\,.$$

We note that

$$\widehat{U}(\psi\otimes|\sigma\rangle) = (U_{\sigma\cdot\lambda}\psi)\otimes|\sigma\rangle\,,\qquad(\sigma=\pm1)\,,$$

where $\sigma_3|\sigma\rangle = \sigma|\sigma\rangle$ and $U_\lambda = \mathrm{e}^{-\mathrm{i}\frac{\lambda}{2}A}U\mathrm{e}^{\mathrm{i}\frac{\lambda}{2}A}$. The joint initial state is assumed of the form $\rho\otimes\rho_\mathrm{i}$ with ρ being that of the system and

$$\rho_\mathrm{i} = \big(\langle\sigma|\rho_\mathrm{i}|\sigma'\rangle\big)_{\sigma,\sigma'=\pm1} = \begin{pmatrix}\rho_{++} & \rho_{+-}\\ \rho_{-+} & \rho_{--}\end{pmatrix}$$

that of the spin. The final state is $\widehat{U}(\rho\otimes\rho_\mathrm{i})\widehat{U}^*$ and, after tracing out the system,

$$\rho_\mathrm{f} = \mathrm{tr}_{\mathcal{H}}\widehat{U}(\rho\otimes\rho_\mathrm{i})\widehat{U}^*$$

with matrix elements

$$\langle\sigma|\rho_\mathrm{f}|\sigma'\rangle = \mathrm{tr}(U_{\sigma\lambda}\rho U^*_{\sigma'\lambda})\langle\sigma|\rho_\mathrm{i}|\sigma'\rangle\,.$$

In other words,

$$\rho_\mathrm{f} = \begin{pmatrix}\rho_{++} & \rho_{+-}\chi(\lambda)\\ \rho_{-+}\chi(-\lambda) & \rho_{--}\end{pmatrix}$$

with

$$\chi(\lambda) = \mathrm{tr}(\mathrm{e}^{\mathrm{i}\frac{\lambda}{2}A}U^*\mathrm{e}^{-\mathrm{i}\lambda A}U\mathrm{e}^{\mathrm{i}\frac{\lambda}{2}A}\rho)\,.$$

We remark that $\chi(\lambda)$ agrees with (4.5) under the assumption (4.4) of the latter. It can be determined from the average spin precession, since $\langle\sigma|\rho_\mathrm{f}|\sigma'\rangle$ reflects that measurement. On the other hand no probability interpretation, *cf.* (3.1), is available for $\chi(\lambda)$, since its Fourier transform is non-positive in general.[9]

7. The thermodynamic limit

The derivation of (5.5) was heuristic. It therefore seems appropriate to investigate whether the resulting determinant, cast as $\det(1+M)$, is well-defined, which is the case if M is a trace-class operator. This happens to be the case if the leads are of finite extent and the energy range finite, essentially because the single-particle Hilbert space becomes finite dimensional. While these conditions may be regarded as effectively met in practice, it is nevertheless useful to idealize these quantities as being infinite. There are two physical reasons for that. First, any bound on these quantities ought to be irrelevant, because the transport occurs across the dot (compact in space) and near the Fermi energy (compact in energy); second, the infinite settings allows to conveniently formulate non-equilibrium stationary states. However this idealization needs some care. In fact, in the attempt of extending eq. (5.5) to infinite systems, the determinant becomes ambiguous and ill-defined. The cure is a regularization which rests on the heuristic identity

$$\mathrm{tr}(U^*\rho QU - \rho Q) = 0\,, \tag{7.1}$$

obtained by splitting the trace and using its cyclicity. It consists in multiplying the determinant by

$$\det(\mathrm{e}^{-\mathrm{i}\lambda U^*\rho QU})\cdot\det(\mathrm{e}^{\mathrm{i}\lambda\rho Q}) = \mathrm{e}^{-\mathrm{i}\lambda\mathrm{tr}(U^*\rho QU-\rho Q)} = 1\,, \tag{7.2}$$

thereby placing one factor on each of its sides. The straightforward result is (see Ref. 2, and in the zero-temperature case Ref. 16)

$$\chi(\lambda) = \det(\mathrm{e}^{-\mathrm{i}\lambda\rho_U Q_U}\rho'\mathrm{e}^{\mathrm{i}\lambda\rho Q} + \mathrm{e}^{\mathrm{i}\lambda\rho'_U Q_U}\rho\mathrm{e}^{-\mathrm{i}\lambda\rho' Q})\,, \tag{7.3}$$

where $\rho' = 1-\rho$, $\rho_U = U^*\rho U$, and similarly for ρ'_U and Q_U.

Remark 7.1. 1. We observe a manifest particle-hole symmetry:

$$\chi_\rho(\lambda) = \chi_{\rho'}(-\lambda)\,.$$

2. We will see that the determinant (7.3) is Fredholm under reasonable hypotheses.
3. The regularization bears some resemblance to $\det_2(1+M) = \det(1+M)\mathrm{e}^{-\mathrm{tr}M}$, though the latter typically changes the value of the determinant.

To the extent that the regularization is regarded as a modification at all, it affects only the first cumulant, because the term $-\mathrm{i}\lambda\mathrm{tr}(\rho_U Q_U - \rho Q)$, which by (7.2) has been added to the generating function $\log\chi(\lambda)$, is linear in λ.

The mean is thus changed from $\langle n\rangle = \mathrm{tr}\rho(Q_U - Q)$ to $\langle n\rangle = \mathrm{tr}(\rho - \rho_U)Q_U$. In line with Sections 3 and 5 we interpret Q as the projection onto single-particle states in the distinguished lead and U as the evolution preserving the initial state ρ, except for changes in the dot. We then expect that $Q_U - Q$ is non-trivial on states of any energy, while $\rho - \rho_U$ is so only on states which are located near the dot and near the Fermi energy. As a result, the second expression for $\langle n\rangle$, but not the first one, appears to be well-defined.

8. A more basic approach

The regularization (7.1) remains an ad hoc procedure, though it may be motivated as a cancellation between right and left movers, see Ref. 2. The point we wish to make here is that eq. (7.3) is obtained without any recourse to regularization if the second quantization is based upon a state of positive density (rather than the vacuum, *cf.* Sect. 5), as it is appropriate for an open system.

To this end let us briefly recall the defining elements of quantum mechanics of infinitely many degrees of freedom: (local) observables are represented by elements of a C*-algebra $\mathcal{A}$ and states by normalized, positive, continuous linear functionals on $\mathcal{A}$. A state ω, together with its local perturbations, may be given a Hilbert space realization through the GNS construction: it consists of a Hilbert space $\mathcal{H}_\omega$, a representation π_ω of $\mathcal{A}$ on $\mathcal{H}_\omega$, and a cyclic vector $\Omega_\omega \in \mathcal{H}_\omega$ such that

$$\omega(A) = (\Omega_\omega, \pi_\omega(A)\Omega_\omega)\,, \qquad (A \in \mathcal{A})\,.$$

Notice that the state ω is realized as a vector, Ω_ω, regardless of whether it is pure. Rather, it is pure iff the commutant $\pi_\omega(\mathcal{A})' \subset \mathcal{L}(\mathcal{H}_\omega)$ is trivial. The closure of $\pi_\omega(\mathcal{A})$ yields the von Neumann algebra $\overline{\pi_\omega(\mathcal{A})}$. Besides of local observables $\pi_\omega(A)$ it also contains some global ones, whose existence and meaning presupposes ω. An example occurring in the following is the charge present in the (infinite) lead in excess of the (infinite) charge attributed to ω.

The C*-algebra of the problem at hand is $\mathcal{A}(\mathcal{H})$, the algebra of canonical anti-commutation relations over the single-particle Hilbert space $\mathcal{H}$. It is the algebra with unity generated by the elements $a(f)$, $a(f)^*$ (anti-linear, resp. linear in $f \in \mathcal{H}$) satisfying

$$\{a(f), a^*(g)\} = (f, g)1\,, \qquad \{a(f), a(g)\} = 0 = \{a^*(f), a^*(g)\}\,.$$

A unitary U induces a *-automorphism of the algebra by $a(f) \mapsto a(Uf)$ (Bogoliubov automorphism). A single-particle density matrix $0 \leq \rho \leq 1$

defines a state ω on $\mathcal{A}(\mathcal{H})$ through

$$\omega(a^*(f)a(g)) = (g, \rho f)\,, \qquad \omega(a(f)a(g)) = 0 = \omega(a^*(f)a^*(g))$$

and the use of Wick's lemma for the ccomputation of higher order correlators. States of this form are known as gauge-invariant quasi-free states; they describe uncorrelated fermions. It is possible to give an explicit construction of their GNS representation, known as Araki-Wyss representation, but we will not need it.

For clarity we formulate the main result first for pure state and then for mixed states. In both cases we assume $[\rho, Q] = 0$, *cf.* (4.4).

Theorem 8.1 (Pure states). *Let $\rho = \rho^2$. We assume that*

$$\rho - U\rho U^* \tag{8.1}$$

is trace class. Then

(1) The algebra automorphisms $a(f) \mapsto a(Uf)$ and $a(f) \mapsto a(\mathrm{e}^{\mathrm{i}\lambda Q} f)$ are unitarily implementable: There exists (non-unique) unitaries $\widehat{U}$ and $\mathrm{e}^{\mathrm{i}\lambda\widehat{Q}}$ on $\mathcal{H}_\omega$ such that

$$\widehat{U}\pi_\omega(a(f)) = \pi_\omega(a(Uf))\widehat{U}\,, \qquad \mathrm{e}^{\mathrm{i}\lambda\widehat{Q}}\pi_\omega(a(f)) = \pi_\omega(a(\mathrm{e}^{\mathrm{i}\lambda Q} f))\mathrm{e}^{\mathrm{i}\lambda\widehat{Q}}\,.$$

(2) $\widehat{Q}$ is an observable, in the sense that any bounded function thereof is in $\overline{\pi_\omega(\mathcal{A}(\mathcal{H}))}$.

(3) The above properties define $\widehat{U}$ uniquely up to a phase and $\widehat{Q}$ up to an additive constant.

(4) The generating function of cumulants, cf. (4.6), equals the regularized determinant (7.3):

$$(\Omega_\omega, \widehat{U}^*\mathrm{e}^{\mathrm{i}\lambda\widehat{Q}}\widehat{U}\mathrm{e}^{-\mathrm{i}\lambda\widehat{Q}}\Omega_\omega) = \det(\mathrm{e}^{-\mathrm{i}\lambda\rho_U Q_U}\rho'\mathrm{e}^{\mathrm{i}\lambda\rho Q} + \mathrm{e}^{\mathrm{i}\lambda\rho'_U Q_U}\rho\mathrm{e}^{-\mathrm{i}\lambda\rho' Q})\,,$$

where the determinant is Fredholm.

Eq. (8.1) demands that the evolution U preserves ρ, except for creating excitations of finite energy within an essentially finite region of space. This assumption is appropriate for the evolution induced by a compact device operating smoothly during a finite time interval.

The generalization to mixed states is as follows.

Theorem 8.2 (Mixed states). *Let $0 < \rho < 1$. Assume, instead of (8.1), that $\rho^{1/2} - U\rho^{1/2}U^*$ and $(\rho')^{1/2} - U(\rho')^{1/2}U^*$ are trace class; moreover that*

$$(\rho\rho')^{1/2}Q \tag{8.2}$$

is, too. Then the above results (i-iv) hold true, upon replacing (iii) by

- *Properties (i-ii) define $\widehat{U}$ uniquely up to left multiplication with an element from the commutant $\pi_\omega\big(\mathcal{A}(\mathcal{H})\big)'$, and $\widehat{Q}$ up to an additive constant. In particular, $\widehat{U}^* \mathrm{e}^{\mathrm{i}\lambda\widehat{Q}}\widehat{U}\mathrm{e}^{-\mathrm{i}\lambda\widehat{Q}}$ is unaffected by the ambiguities.*

Notice that the most general case, $0 \leq \rho \leq 1$, is not covered. The physical origin of the extra assumption (8.2) needed in the mixed state case is as follows. In both cases, pure or mixed, the expected charge contained in a portion of the lead is of order of its length L, or zero if renormalized by subtraction of a background charge. In the pure case however, the Fermi sea is an eigenvector of the charge operator, while for the mixed state, the variance of the charge must itself be of order L, because the occupation of the one-particle states is fluctuating, due to $\rho\rho' \neq 0$. Hence, in this latter situation, the measurement of the renormalized charge yields finite values only as long as L is finite, of which eq. (8.2) is a mathematical abstraction. In the limit $L \to \infty$ all but a finite part of the fluctuation of the source is affecting the transmitted noise. That suggests perhaps that there is a better formulation of the result. Indeed, the expression for the transmitted noise, *cf.* the first term (5.6), is finite if $(U^*QU - Q)(\rho\rho')^{1/2}$ is trace class. This condition turns out to be sufficient for property (i), for making the determinant Fredholm and $\widehat{U^*QU - Q}$ an observable, but not for (ii, iii).

For proofs we refer to Ref. 2.

9. An application

We discuss a very simple application to illustrate the working of the regularization. The system consists of two leads in guise of circles of length T, joined at one point. Particles run in the positive sense along the circles C at velocity 1, whence it takes them time T to make a turn, and may scatter from one to the other circle at the junction. Initially states in the two circles are populated up to Fermi energies $\mu_L < \mu_R$. This is formalized as follows. The single particle Hilbert space is

$$\mathcal{H} = L^2(C) \oplus L^2(C) \ni \psi = \begin{pmatrix} \psi_L(x) \\ \psi_R(x) \end{pmatrix},$$

the evolution over time T is

$$(U\psi)(x) = S\psi(x)$$

with S as in (2.3). The momentum operator is $p = -\mathrm{i}d/dx$ and the initial state is $\rho = \rho_L \oplus \rho_R$ with $\rho_i = \theta(\mu_i - p)$, $(i = L, R)$. The projection onto the right lead is $Q = 0 \oplus 1$.

Quite generally, for $\rho = \rho^2$ a pure state, eq. (7.3) reads

$$\chi(\lambda) = \det_{\mathcal{H}}(1 + (\mathrm{e}^{-\mathrm{i}\lambda} - 1)Q_U\rho_U\rho' + (\mathrm{e}^{\mathrm{i}\lambda} - 1)Q_U\rho'_U\rho)\,,$$

and in the present situation that determinant reduces to

$$\chi(\lambda) = \det_{L^2(C)}(1 + (\mathrm{e}^{\mathrm{i}\lambda} - 1)\rho'_R\rho_L|t|^2)\,.$$

It is to be noted that $\rho'_R\rho_L$ selects a finite energy interval, $(\mu_L, \mu_R]$, unlike the determinant without regularization. Using eigenstates of momentum $p \in (2\pi/T)\mathbb{Z}$ we find

$$\begin{aligned}\chi(\lambda) &= \prod_{\mu_L < p \le \mu_R} (1 + (\mathrm{e}^{\mathrm{i}\lambda} - 1)|t|^2) \\ &= (1 - |t|^2 + \mathrm{e}^{\mathrm{i}\lambda}|t|^2)^N = (q + \mathrm{e}^{\mathrm{i}\lambda}p)^N\end{aligned}$$

with $N = \#\{p \mid \mu_L < p \le \mu_R\} \cong (\mu_L - \mu_R)T/2\pi$. This is a binomial distribution with probability $p = |t|^2$ and N attempts, reproducing (2.4). In particular, it yields Ohm's law $\langle Q\rangle/T = GV$ with $G = (2\pi)^{-1}|t|^2$.[4,11]

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THE INTEGRATED DENSITY OF STATES IN STRONG MAGNETIC FIELDS

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In this work we consider three-dimensional Schrödinger operators with constant magnetic fields and random ergodic electric potentials. We study the strong-magnetic-field asymptotic behaviour of the integrated density of states in two energy regimes: *far from the Landau levels* and *near a given Landau level*. These energy regimes are defined by the threshold distribution in the absolutely continuous spectrum of the unperturbed operator.

Keywords: Schrödinger operators, integrated density of states, magnetic field.

1. Introduction

During the last decades the spectral analysis of quantum Hamiltonians in strong magnetic fields was approached by different authors. Many domains of investigation of the mathematical physics are concerned, let us mention here the problem of the stability of the matter,[2,3,5,15,22] the study of eigenvalue distributions[7,16,19,23–26] and the the investigation of the scattering phase,[6] the magnetic response of quantum gases and the quantum Hall effect,[10,14] and finally, the asymptotic analysis of the integrated density of states in strong magnetic fields,[21,26,27] which is the main theme of the present note.

We consider here a three-dimensional Schrödinger operator with con-

stant magnetic field $\mathbf{B} := (0, 0, b)$, $b > 0$ being the intensity of the field. The precise definition of this operator is given in Section 2 below. We analyze the behavior of the integrated density of states as $b \to \infty$. Our results described in Section 3 have been proved in Ref. 4. Here we give some additional comments on the motivation, the physical interpretation, and the possible extensions of our results.

2. Self-adjointness

In this section we introduce the class of random self-adjoint operators considered in the note. We first recall some basic facts. The potential vector is chosen as $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{x}$ then the free magnetic Schrödinger operator is defined on $L^2(\mathbb{R}^3)$ by

$$H_0(b) = H_{\perp,0}(b) \otimes \mathbb{I}_1 + \mathbb{I}_2 \otimes -\partial_{x_3}^2, \quad b > 0,$$

where $\mathbb{I}_n$ is the identity operator on $L^2(\mathbb{R}^n)$, $n = 1, 2$, and

$$H_{\perp,0}(b) = \left(i\frac{\partial}{\partial x_1} - \frac{bx_2}{2}\right)^2 + \left(i\frac{\partial}{\partial x_2} + \frac{bx_1}{2}\right)^2 - b,$$

is the Landau Hamiltonian on $L^2(\mathbb{R}^2)$ up to the additive constant $-b$. It is well known that $H_{\perp,0}(b)$ is a self-adjoint operator having only pure point spectrum which coincides with the set $\{2bq, q \in \mathbb{Z}_+\}$. The eigenvalues of the Landau operator, called usually *Landau levels*, have infinite multiplicity.[1]

It is well-known[1] that $H_0(b), b \geq 0$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$ and its spectrum $\sigma(H_0(b)) = [0, \infty)$ is purely absolutely continuous.

We consider now on $L^2(\mathbb{R}^3)$ a perturbation of the free operator

$$H(b) = H_0(b) + V, \quad b > 0,$$

where V is a real random electric potential defined in the following way.

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a complete probability space. Introduce the random field $\Omega \times \mathbb{R}^3 \ni (\omega, x) \mapsto V_\omega(x) \in \mathbb{R}$ which is supposed to be measurable with respect to the product σ-algebra $\mathcal{F} \times \mathcal{B}(\mathbb{R}^3)$ where $\mathcal{B}(\mathbb{R}^3)$ is the σ-algebra of the Borel sets in $\mathbb{R}^3$. Let $\mathbb{G} = \mathbb{R}$ or $\mathbb{G} = \mathbb{Z}$. We assume that V is a $\mathbb{G}^3$- ergodic real random field[12,20] satisfying

$$\mathbb{E}\left(\int_{\mathcal{C}} |V_\omega(\mathbf{x})|^4 d\mathbf{x}\right) < \infty, \tag{2.1}$$

where $\mathbb{E}$ is the mathematical expectation with respect to the probability measure $\mathbb{P}$, and $\mathcal{C} := \left(-\frac{1}{2}, \frac{1}{2}\right)^3$. Note that if $\mathbb{G} = \mathbb{R}$, i.e. if V_ω is $\mathbb{R}^3$- ergodic, then (2.1) can be formulated as $\mathbb{E}(|V_\omega(\mathbf{0})|^4) < \infty$. The ergodicity of

V_ω combined with (2.1) implies[17] that with probability one the operator $H_\omega(b) = H_0(b) + V_\omega$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. Moreover, there exists a real subset Σ such that the spectrum $\sigma(H_\omega(b))$ of the operator $H_\omega(b)$ coincides almost surely with Σ.

Finally, in the formulation of our main results, we suppose that V_ω is $\mathbb{G}$- ergodic in the direction of the magnetic field $\mathbf{B}$.[4,21]

Most of random ergodic fields used in condensed matter physics for modelling amorphous materials satisfy our assumptions. For example, the *Gaussian random fields* whose correlation function is continuous at the origin and decays at infinity are $\mathbb{R}^3$-ergodic, and $\mathbb{R}$-ergodic in any direction. The same is true for appropriate *Poisson* potentials. On the other hand the *Anderson-type* potentials (called also *alloy-type* potentials) are $\mathbb{Z}^3$-ergodic, and $\mathbb{Z}$-ergodic in any direction.[11,12]

Finally, we recall that the operators with periodic or almost periodic electric potentials also fit in the general scheme of the present note. We refer the reader to Ref. 12 for the relationship between periodic and almost periodic functions on one side, and ergodic random fields on the other.

3. Main Results

The main object of study in the present note is the integrated density of states (IDS). We define the IDS $\varrho_{V,b}$ associated with $H_\omega(b)$ by the Shubin-Pastur formula

$$\varrho_{V,b}(E) := \mathbb{E}\left(\mathrm{Tr}\left(\chi_{\mathcal{C}}\chi_{(-\infty,E)}(H_\omega(b))\chi_{\mathcal{C}}\right)\right), \quad E \in \mathbb{R},$$

where $\chi_{\mathcal{C}}$ is the multiplier by the characteristic function of the cube $\mathcal{C}$, and $\chi_{(-\infty,E)}(H_\omega(b))$ is the spectral projection of the operator $H_\omega(b)$ corresponding to the interval $(-\infty, E)$. The correctness of this definition of the IDS, and its equivalence to the traditional definition involving a thermodynamic limit are discussed in Refs. 9,17. The aim of the note is to study the asymptotic behaviour as $b \to \infty$ of the quantities

$$\varrho_{V,b}(\mathcal{E}b + \lambda_2) - \varrho_{V,b}(\mathcal{E}b + \lambda_1),$$

the parameters $\mathcal{E} \in [0, \infty)$, λ_1, λ_2, $\lambda_1 \leq \lambda_2$, being fixed. It is reasonable to distinguish two asymptotic regimes: asymptotics near a given Landau level which corresponds to $\mathcal{E} \in 2\mathbb{Z}_+$, and asymptotics far from the Landau levels which corresponds to $\mathcal{E} \in (0, \infty) \setminus 2\mathbb{Z}_+$. This distinction is justified already by the elementary calculation yielding the leading asymptotic term as $b \to \infty$ of the free IDS $\varrho_{0,b}$ corresponding to $V_\omega = 0$. The explicit form

of $\varrho_{0,b}$ is well-known:

$$\varrho_{0,b}(E) = \frac{b}{2\pi^2} \sum_{q=0}^{\infty} (E - 2bq)_+^{1/2}, \quad E \in \mathbb{R},$$

and we find easily that the leading asymptotic term as $b \to \infty$ of the variation of $\varrho_{0,b}$ is of order b near any fixed Landau level, and of order $b^{1/2}$ far from the Landau levels.

In order to formulate our results concerning the asymptotics of the IDS $\varrho_{V,b}$ near a given Landau level, we need some additional notations. For $\mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$ we denote by $x_\perp = (x_1, x_2) \in \mathbb{R}^2$ the variables on the plane perpendicular to the magnetic field. Fix $x_\perp \in \mathbb{R}^2$. Since by assumption V is ergodic in direction of the magnetic field, the random field $\mathbb{R} \ni x_3 \mapsto V_\omega(x_\perp, x_3) \in \mathbb{R}$ is ergodic, and the operator

$$h_V(x_\perp) := -\frac{d^2}{dx_3^2} + V(x_\perp, x_3) \tag{3.1}$$

is almost surely essentially self-adjoint on $C_0^\infty(\mathbb{R})$ (see Ref. 12). Denote by $\rho_V(\lambda; x_\perp)$, $\lambda \in \mathbb{R}$, the IDS for the operator $h_V(x_\perp)$. By Ref. 21, if V is $\mathbb{R}$-ergodic (respectively, $\mathbb{Z}$-ergodic) in the direction of the magnetic field, then the IDS $\rho_V(\lambda; x_\perp)$ is independent of $x_\perp \in \mathbb{R}^2$ (respectively, $\rho_V(\lambda; x_\perp)$ is $\mathbb{Z}$-periodic with respect to $x_\perp$). Set

$$k_V(\lambda) := \int_{(-\frac{1}{2}, \frac{1}{2})^2} \rho_V(\lambda; x_\perp) dx_\perp.$$

Thus, in the case of $\mathbb{R}$-ergodicity we have $k_V(\lambda) = \rho(\lambda; 0)$. Moreover, since the operator $h_V(x_\perp)$ is an ordinary differential operator, the function $\mathbb{R} \ni \lambda \mapsto k_V(\lambda) \in \mathbb{R}$ is continuous.[12]

Theorem 3.1. [4] *Assume that the random potential $V : \Omega \times \mathbb{R}^3 \to \mathbb{R}$ is measurable with respect to the product σ-algebra $\mathcal{F} \times \mathcal{B}(\mathbb{R}^3)$, and that (2.1) holds. Moreover, suppose that V is $\mathbb{R}^3$-ergodic or $\mathbb{Z}^3$-ergodic, and is $\mathbb{R}$-ergodic or $\mathbb{Z}$-ergodic in the direction of the magnetic field.*
i) Let $\mathcal{E} \in (0, \infty) \setminus 2\mathbb{Z}_+$, and $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$. Then we have

$$\lim_{b \to \infty} b^{-1/2} \left(\varrho_{V,b}(\mathcal{E}b + \lambda_2) - \varrho_{V,b}(\mathcal{E}b + \lambda_1) \right) = \frac{\lambda_2 - \lambda_1}{4\pi^2} \sum_{q=0}^{[\mathcal{E}/2]} (\mathcal{E} - 2q)^{-1/2}. \tag{3.2}$$

ii) Let $\mathcal{E} \in 2\mathbb{Z}_+$, and $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$. Then we have

$$\lim_{b \to \infty} b^{-1} \left(\varrho_{V,b}(\mathcal{E}b + \lambda_2) - \varrho_{V,b}(\mathcal{E}b + \lambda_1) \right) = \frac{1}{2\pi} \left(k_V(\lambda_2) - k_V(\lambda_1) \right). \tag{3.3}$$

Let us discuss briefly our results, the methods applied in their proofs, as well as several possible extensions and generalizations.

- Relation (3.2) implies that far from the Landau levels the main asymptotic term of the IDS is independent of the potential V_ω. Note that the r.h.s. of (3.2) is proportional to the length of the interval $(\mathcal{E}b + \lambda_1, \mathcal{E}b + \lambda_2)$. It is likely that if we impose more restrictive assumptions on the regularity of the realizations of V_ω, we would be able to obtain a more precise asymptotic expansion of the IDS, and the lower-order terms will depend on the random potential
- Relation (3.3) shows us that at energies close to the Landau levels, the three-dimensional quantum particle behaves like an one-dimensional particle whose motion in the direction of the magnetic field is "averaged" with respect to the variables in the plane perpendicular to the magnetic field. A similar picture has been encountered in the investigation of the asymptotic behaviour of many other spectral characteristics of quantum Hamiltonians in strong magnetic fields, such as the ground state energy, the discrete-eigenvalue counting function, the scattering phase, etc. This picture is in accordance with the physical intuition born by the elementary analysis of the trajectory of a classical three-dimensional particle in constant magnetic field. Generically, this trajectory is a helix whose axis is parallel to the magnetic field, and whose radius is inversely proportional to the intensity of the field.[7]
- In the proof of (3.3) we apply the Helffer-Sjöstrand formula[8] for the representation of a smooth compactly supported function φ of a self-adjoint operator L via a quasi-analytic extension of φ, and the resolvent of L. Moreover, we make use of appropriate estimates of the resolvents of H_0 and $H_\omega(b)$.
  For the proof of (3.2), we apply the so called suspension method,[12,20] consisting of a standard extension of a $\mathbb{Z}^3$-ergodic random field defined on $\Omega \times \mathbb{R}^3$, to a $\mathbb{R}^3$-ergodic random field. Once this extension is constructed, (3.2) follows quite easily from (3.3).
- We have formulated our assumptions on the random potential V_ω seeking for a reasonable compromise between generality and comprehensibility. If more special classes of random potentials are considered, then probably condition (2.1) could be relaxed in some cases.
- We have considered the asymptotic behaviour of the IDS only for positive energies, near or far from the Landau levels. An interesting problem would be to consider this behaviour at *negative* energies in the cases

when it is known that the spectrum of the operator $H_\omega(b)$ almost surely covers the real axis (e.g. in the case of Gaussian or attractive Poisson potentials).

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GEOMETRICAL OBJECTS ON MATRIX ALGEBRA

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In this paper we present some geometric objects (derivations, differential forms, distributions, linear connections, their curvature and their torsion) on matrix algebra using the framework of noncommutative geometry.

Keywords: noncommutative geometry, matrix algebras

1. Introduction

We study some differential calculi on the matrix algebra $M_n(\mathbb{C})$ (most of them used the techniques from noncommutative geometry), which have been used in some different areas from mathematics and physics, here we mention some of them: quantum groups,[12] graded matrix algebra,[20,21] the noncommutative differential geometry of matrix algebras.[1,2,16–18,24,25,30–32]

The basic idea of noncommutative geometry is to replace an algebra of smooth functions defined on a smooth manifold by an abstract associative algebra A which is not necessarily commutative. In the context of noncommutative geometry the basic role is the generalization of the notion of differential forms (on a manifold). To any associative algebra A over the real field or complex field k one associates a differential algebra, which is a $\mathbb{Z}$-graded algebra $\Omega(A) = \oplus_{n\geq 0}\Omega^n(A)$ (where $\Omega^n(A)$ are A-bimodules and $\Omega^0(A) = A$) together with a linear operator $d : \Omega^n(A) \to \Omega^{n+1}(A)$ satisfying $d^2 = 0$ and $d(\omega\omega') = (d\omega)\omega' + (-1)^n\omega d\omega'$, $\omega \in \Omega^n(A)$. The algebra $\Omega(A)$ is also called the (noncommutative) differential calculus on the algebra A.

A generalization of a differential calculus $\Omega(A)$ of an associative algebra A is the ρ-differential calculus associated with a ρ-(commutative) algebra A, where A is a G-graded algebra, G is a commutative group and ρ is a twisted cocycle. The differential calculus over a ρ-algebra A was introduced

in Ref. 3 and continued in some recent papers Refs. 5–11,28,29.

The "classical" noncommutative differential calculus and linear connections on the algebra $M_n(\mathbb{C})$ were studied in Ref. 16,18,26,27. The ρ-differential calculi and the linear connections on matrix algebra are introduced in Ref. 7. However, distributions, tensors and metrics on the algebra $M_n(\mathbb{C})$ were not introduced in that paper, and introducing these objects is the aim of the present paper.

In the second section we review the basic geometrical objects about the ρ-algebras as ρ-derivations, ρ-differential calculi, tensors, linear connections and distributions. In the last section we apply the mentioned notions on the matrix algebra $M_n(\mathbb{C})$.

2. ρ-algebras

In this section we present briefly the class of the noncommutative algebras, namely the ρ-algebras. For more details see Ref. 3.

Let G be an abelian group, additively written. A ρ-algebra A is a G-graded algebra over that field k (which may be either the real or the complex field), endowed with a cyclic cocycle $\rho : G \times G \to k$ which fulfills the properties

$$\rho(a,b) = \rho(b,a)^{-1} \text{ and } \rho(a+b,c) = \rho(a,c)\rho(b,c) \tag{2.1}$$

for any a, b ,$c \in G$.

Notation 2.1. From now on, if M is a graded set, then $Hg\,(M)$ will stand for the set of homogeneous elements in M. The G-degree of a (nonzero) homogeneous element f of M is denoted $|f|$.

A G-graded algebra A with a given cocycle ρ will be called ρ- **commutative** (or **almost commutative algebra**) if $fg = \rho(|f|\,,|g|)gf$ for all $f, g \in Hg\,(A)$.

Example 2.1.

(1) Any usual (commutative) algebra is a ρ-algebra with the trivial group G.
(2) Let be the group $G = \mathbb{Z}$ ($\mathbb{Z}_2$) and the cocycle $\rho(a,b) = (-1)^{ab}$, for any $a, b \in G$. In this case any ρ-(commutative) algebra is a super(commutative) algebra.
(3) The N-dimensional quantum hyperplane[3,5,6,11] S_N^q is the algebra generated by the unit element and N linearly independent elements

$x_1, \ldots, x_N$ satisfying the relations

$$x_i x_j = q x_j x_i, \qquad i < j,$$

for some fixed $q \in k$, $q \neq 0$. Then S_N^q is a $\mathbb{Z}^N$-graded algebra

$$S_N^q = \bigoplus_{n_1,\ldots,n_N}^{\infty} (S_N^q)_{n_1 \ldots n_N},$$

with $(S_N^q)_{n_1 \ldots n_N}$ the one-dimensional subspace spanned by products $x^{n_1} \cdots x^{n_N}$. The $\mathbb{Z}^N$-degree of these elements is denoted by

$$|x^{n_1} \cdots x^{n_N}| = n = (n_1, \ldots, n_N).$$

Define the function $\rho : \mathbb{Z}^N \times \mathbb{Z}^N \to k$ as

$$\rho(n, n') = q^{\sum_{j,k=1}^{N} n_j n'_k \alpha_{jk}},$$

with $\alpha_{jk} = 1$ for $j < k$, 0 for $j = k$ and -1 for $j > k$. It is clear that S_N^q is a ρ-commutative algebra.

(4) The algebra of matrix $M_n(\mathbb{C})^7$ is a $\rho-$commutative algebra, as follows: Let p, $q \in M_n(\mathbb{C})$,

$$p = \begin{pmatrix} 1 & 0 \ldots 0 \\ 0 & \varepsilon \ldots 0 \\ \ldots & \\ 0 & 0 \ldots \varepsilon^{n-1} \end{pmatrix} \quad \text{and} \quad q = \begin{pmatrix} 0 & 0 & \ldots 0 & 1 \\ \varepsilon & 0 & \ldots 0 & 0 \\ 0 & \varepsilon^2 & \ldots 0 & 0 \\ \ldots & & & \\ 0 & 0 & \ldots \varepsilon^{n-1} & 0 \end{pmatrix},$$

where $\varepsilon^n = 1$, $\varepsilon \neq 1$. Then $pq = \varepsilon qp$ and $M_n(\mathbb{C})$ is generated by the set $B = \{p^a q^b | a, b = 0, 1, \ldots, n-1\}$. It is easy to see that $p^a q^b = \varepsilon^{ab} q^b p^a$ and $q^b p^a = \varepsilon^{-ab} p^a q^b$ for any $a, b = 0, 1, \ldots, n-1$. Let $G := \mathbb{Z}_n \oplus \mathbb{Z}_n$, $\alpha = (\alpha_1, \alpha_2) \in G$ and $x_\alpha := p^{\alpha_1} q^{\alpha_2} \in M_n(\mathbb{C})$. Setting $\rho(\alpha, \beta) = \varepsilon^{\alpha_2 \beta_1 - \alpha_1 \beta_2}$, one sees that $x_\alpha x_\beta = \rho(\alpha, \beta) x_\beta x_\alpha$, for any $\alpha, \beta \in G$, x_α, $x_\beta \in B$. It is clear that the map $\rho : G \times G \to \mathbb{C}$, $\rho(\alpha, \beta) = \varepsilon^{\alpha_2 \beta_i - \alpha_1 \beta_2}$ is a cocycle and $M_n(\mathbb{C})$ is a ρ -commutative algebra.

2.1. *ρ-derivations*

Definition 2.1.[7] Let $\alpha, \beta \in G$. A ρ-derivation of the order(α, β) is a linear map $X : A \to A$, which fulfills the properties

(1) $X \colon A_* \to A_{*+\beta}$,
(2) $X(fg) = (Xf)g + \rho(\alpha, |f|) f(Xg)$, for any $f \in A_{|f|}$ and $g \in A$.

The left product between the element $f \in A$ and a derivation X of the order (α, β) is defined in a natural way: $fX : A \to A$, $(fX)(g) = fX(g)$ for any $g \in A$. Remark that fX is a derivation of the order $(|f| + \alpha, |f| + \beta)$ if and only if the algebra A is ρ-commutative.

Next we study the case when A is a ρ-commutative algebra.

Let X be a ρ-derivation of the order (α, β) and X' a ρ-derivation of the order (α', β'). The ρ-bracket of X and X' is $[X, X'] = X \circ X' - \rho(\alpha, \beta')X' \circ X$ and satisfies the following property: $[X, X']$ is a ρ-derivation of the order $(\alpha + \alpha', \beta + \beta')$ if and only if $\rho(\alpha, \beta)\rho(\alpha', \beta') = 1$.

Definition 2.2.[3] We say that $X \colon A \to A$ is a ρ-derivation if it has the order $(|X|, |X|)$, i.e., $X \colon A_* \to A_{*+|X|}$ and $X(fg) = (Xf)g + \rho(|X|, |f|)f(Xg)$ for any $f \in A_{|f|}$ and $g \in A$.

It is known[3] that the ρ-commutator $[X, Y]_\rho = XY - \rho(|X|, |Y|)YX$ of two ρ -derivations is also a ρ-derivation and the linear space of all ρ-derivations is a ρ-Lie algebra, denoted by ρ-Der$A$.

One verifies immediately that for such an algebra A, ρ -Der$A$ is not only a ρ-Lie algebra, but also a left A-module with the action of A on ρ -Der$A$ defined by $(fX)g = f(Xg)$, for f, $g \in A$ and $X \in \rho$-Der$A$.

Let M be a G-graded left module over a ρ-commutative algebra A, with the usual properties, in particular $|f\psi| = |f| + |\psi|$ for $f \in A$, $\psi \in M$. Then M is also a right A-module with the right action on M defined by $\psi f = \rho(|\psi|, |f|)f\psi$, for any $\psi \in Hg(M)$ and $f \in Hg(A)$. In fact M is a bimodule over A, i.e., $f(\psi g) = (f\psi)g$ for any f, $g \in A$, $\psi \in M$.

2.2. *Differential calculi on a ρ-algebra*

We generalize the classical notions of differential graded algebra and the differential graded superalgebras by defining so called *differential graded ρ -algebras.*

Denote by $G' = \mathbb{Z} \times G$ and define the cocycle $\rho' : G' \times G' \to k$ through

$$\rho'((n, \alpha), (m, \beta)) = (-1)^{nm} \rho(\alpha, \beta).$$

It is easy to see that the function ρ' satisfies the properties (2.1).

Definition 2.3. We say that $\Omega = \bigoplus_{(n,\beta) \in G'} \Omega^n_\beta$ is a ρ-differential graded algebra (DG $\rho-$ algebra) if there is an element $\alpha \in G$ and a map $d \colon \Omega^n_\beta \to \Omega^{n+1}_\beta$ of degree $(1, \alpha) \in G'$ and the G'-degree $|d|' = (1, 0)$ such that $d^2 = 0$ and

$$d(\omega\theta) = (d\omega)\theta + (-1)^n \rho(\alpha, |\omega|)\omega d\theta$$

for any $\omega \in \Omega^n_{|\omega|}$ and $\theta \in \Omega$.

If we denote $|\omega|' = (n, |\omega|)$ the G'-degree of $\omega \in \Omega^n_{|\omega|}$, then the last equality becomes

$$d(\omega\theta) = (d\omega)\theta + \rho'(|d|', |\omega|')\omega d\theta.$$

It follows that Ω is a ρ'-algebra.

Example 2.2.

(1) In the case where the group G is trivial, then Ω is the classical differential graded algebra.
(2) When the group G is $\mathbb{Z}_2$ and the map ρ is given by $\rho(a,b) = (-1)^{ab}$, then Ω is a differential graded superalgebra (see Refs. 22,23).

Definition 2.4. Let A be a ρ-algebra. Then

$$\left(\Omega(A) = \bigoplus_{(n,\alpha)\in G'} \Omega^n_\alpha(A), d\right)$$

is a ρ-differential calculus over A if $\Omega(A)$ is a ρ-differential graded algebra, $\Omega(A)$ is an A-bimodule and $\Omega^0(A) = A$.

The first example of a ρ-differential calculus over the ρ -commutative algebra A is the algebra of forms $(\Omega(A), d)$ of A from Ref. 3. The second example of a ρ-differential calculus over a ρ-algebra is the universal differential calculus of A from the next paragraph.

2.2.1. *The algebra of forms of a ρ-algebra*

In this paragraph we construct the algebra of forms $\Omega(A)$ of an almost commutative algebra A (see Ref. 3).

The algebra of forms of an the ρ-algebra A is given in the classical manner: $\Omega^0(A) := A$ and $\Omega^p(A)$ for $p = 1, 2, \ldots$ as the G -graded space of p-linear maps $\alpha_p : \times^p \rho\text{- Der}A \to A$, p-linear in sense of left A-modules

$$\alpha_p(fX_1, \ldots, X_p) = f\alpha_p(X_1, \ldots, X_p),$$
$$\alpha_p(X_1, \ldots, X_j f, X_{j+1,} \ldots, X_p) = \alpha_p(X_1, \ldots, X_j, fX_{j+1,} \ldots X_p)$$

and ρ-alternating, that is,

$$\alpha_p(X_1, \ldots, X_j, X_{j+1,} \ldots, X_p)$$
$$= -\rho(|X_j|, |X_{j+1}|)\alpha_p(X_1, \ldots, , X_{j+1}, X_{j,} \ldots, X_p)$$

for $j = 1, \ldots, p-1$, $X_k \in \rho\text{-Der}(A)$, $k = 1, \ldots p$, $f \in A$, and where Xf is the right A-action on ρ -Der$A$.

Then $\Omega^p(A)$ is in natural way a G-graded right A-module with

$$|\alpha_p| = |\alpha_p(X_1, \ldots, X_p)| - (|X_1| + \cdots + |X_p|)$$

and with the right action of A defined as

$$(\alpha_p f)(X_1, \ldots, X_p) = \alpha_p(X_1, \ldots, X_p)f.$$

From the previous considerations, it follows that $\Omega(A) = \bigoplus_{p=0}^{\infty} \Omega^p(A)$ is a G-graded A-bimodule.

Exterior differentiation is defined to be a linear map $d\colon \Omega^p(A) \to \Omega^{p+1}(A)$, for all $p \geq 0$, given by

$$df(X) = X(f),$$

and for $p = 1, 2, \ldots,$

$$\begin{aligned} &d\alpha_p(X_1, \ldots, X_{p+1}) \\ &:= \sum_{j=1}^{p+1} (-1)^{j-1} \rho(\sum_{i=1}^{j-1} |X_i|, |X_j|) X_j \alpha_p(X_1, \ldots, \widehat{X}_j, \ldots, X_{p+1}) \\ &\quad + \sum_{1 \leq j < k \leq p+1} (-1)^{j+k} \rho(\sum_{i=1}^{j-1} |X_i|, |X_j|) \rho(\sum_{i=1}^{j-1} |X_i|, |X_k|) \\ &\times \rho(\sum_{i=j+1}^{k-1} |X_i|, |X_k|) \alpha_p([X_j, X_k]_\rho, \ldots, X_1, \ldots, \widehat{X}_j, \ldots, \widehat{X}_k, \ldots X_{p+1}). \end{aligned}$$

One can show that d has degree 0, and that $d^2 = 0$.

There is an exterior product $\Omega^p(A) \times \Omega^q(A) \to \Omega^{p+q}(A)$, $(\alpha_p, \beta_q) \mapsto \alpha_p \wedge \beta_q$, defined by the ρ-antisymmetrization formula

$$\begin{aligned} &\alpha_p \wedge \beta_q (X_1, \ldots, X_{p+q}) \\ &= \sum_{\sigma} \text{sign}(\sigma) \, (\rho\text{-factor}) \, \alpha_p \left(X_{\sigma(1)}, \ldots, X_{\sigma(p)}\right) \beta_q \left(X_{\sigma(p+1)}, \ldots, X_{\sigma(p+q)}\right). \end{aligned}$$

The sum is over all permutations σ of the cyclic group S_{p+q} such that $\sigma(1) < \cdots < \sigma(p)$ and $\sigma(p+1) < \cdots < \sigma(p+q)$. The ρ-factor is the product of all $\rho(|X_{\sigma(j)}|, |\alpha_p|)$ for $p+1 \leq j \leq p+q$ and all $\rho(|X_{\sigma(j)}|, |X_{\sigma(k)}|)^{-1}$ for $j < k$ and $\sigma(j) > \sigma(k)$.

The algebra $\Omega(A)$ is a G'-graded algebra with the group $G' = \mathbb{Z} \times G$. Denote the G' degree of α_p by $|\alpha_p|' = (p, |\alpha_p|)$. It is easy to see that the map $\rho' : G' \times G' \to k$ defined by $\rho'((p,a),(q,b)) = (-1)^{pq}\rho(a,b)$ is a cocycle and that $\Omega(A)$ is a ρ'-commutative algebra. Moreover, the map d is a ρ'-derivation of $\Omega(A)$ with G'-degree $|d|' = (+1, 0)$.

2.2.2. *The algebra of universal differential forms of a ρ-algebra*

We present here our construction of algebra of universal differential forms $\Omega_\alpha A$ of the ρ-algebra A (not necessarily ρ -commutative) for a given element $\alpha \in G$.

Let α be an arbitrary element of G. By definition, the algebra of *universal differential forms* (also called the *algebra of noncommutative differential forms*) of the ρ-algebra A is the algebra $\Omega_\alpha A$ generated by the algebra A and the symbols da, $a \in A$, which satisfies the following relations:

(1) da is linear in a.
(2) The $\rho-$Leibniz rule: $d(ab) = d(a)b + \rho(\alpha, |a|)adb$.
(3) $d(1) = 0$.

Let $\Omega^n_\alpha A$ the space of $n-$forms $a_0 da_1 \dots da_n$, $a_i \in A$ for any $0 \leq i \leq n$. The space $\Omega^n_\alpha A$ is an A-bimodule with the left multiplication

$$a(a_0 da_1 \dots da_n) = aa_0 da_1 \dots da_n,$$

and the right multiplication is given by

$$\begin{aligned}(a_0 da_1 \cdots da_n)a_{n+1} \\ = \sum_{i=1}^{n}(-1)^{n-i}\rho(\alpha, \sum_{j=i+1}^{n}|a_j|)(a_0 da_1 \dots d(a_i a_{i+1}) \dots da_{n+1}) \\ +(-1)^n \rho(\alpha, \sum_{i=1}^{n}|a_j|)a_0 a_1 da_2 \dots da_{n+1.}\end{aligned}$$

The algebra $\Omega_\alpha A = \bigoplus_{n\in\mathbb{Z}} \Omega^n_\alpha A$ is a $\mathbb{Z}$-graded algebra with the multiplication $\Omega^n_\alpha A \cdot \Omega^m_\alpha A \subset \Omega^{n+m}_\alpha A$ given by

$$\begin{aligned}(a_0 da_1 \dots da_n)(a_{n+1} da_{n+2} \dots da_{m+n}) \\ = ((a_0 da_1 \dots da_n)a_{n+1})da_{n+2} \dots da_{m+n}).\end{aligned}$$

for any $a_i \in A$, $0 \leq i \leq n+m$, $n, m \in \mathbb{N}$.

We define the $G-$degree of the n-form $a_0 da_1 \dots da_n$ by

$$|a_0 da_1 \dots da_n| = \sum_{i=0}^{n} |a_i|\,.$$

It is clear that $|\omega_n \cdot \omega_m| = |\omega_n| + |\omega_m|$ for any homogeneous forms $\omega_n \in \Omega^n_\alpha A$ and $\omega_m \in \Omega^m_\alpha A$.

The algebra $\Omega_\alpha A$ is a $G' = \mathbb{Z} \times G$-graded algebra with the G' degree of the n-form $a_0 da_1 \dots da_n$ given by $|a_0 da_1 \dots da_n|' = (n, \sum_{i=0}^{n} |a_i|)$.

We may define the cocycle $\rho' : G' \times G' \to k$ on the algebra $\Omega_\alpha A$

$$\rho'(|\omega_n|', |\omega_m|') = (-1)^{nm} \rho(|\omega_n|, |\omega_m|)$$

for any $\omega_n \in \Omega_\alpha^n A$, $\omega_m \in \Omega_\alpha^m A$. Then $\Omega_\alpha A$ is a ρ'-algebra. We note here that G'-degree of the map d is $(1,0)$ i.e. $d : \Omega^n_{|\omega|} \to \Omega^{n+1}_{|\omega|}$, and the G'-degree of an element $x \in A$ is $|x|' = (0, |x|)$.

Theorem 2.1.[7] *1. The mapping $d : \Omega_\alpha^* A \to \Omega_\alpha^{*+1} A$ satisfies*

$$d(\omega\theta) = (d\omega)\theta + (-1)^n \rho(\alpha, |\omega|)\omega d\theta$$

for any $\omega \in \Omega_\alpha^n A$, $\theta \in \Omega_\alpha^m A$.

2. $(\Omega_\alpha A, d)$ is a ρ-differential calculus over A.

Example 2.3. In the case where the group G is trivial, A is the usual associative algebra and $\Omega_\alpha A$ is the algebra of universal differential forms of A.

Example 2.4. If the group G is $\mathbb{Z}_2$ and the cocycle is as in Example 2.2, then A is a superalgebra. In the case where $\alpha = 1$ $\Omega_\alpha A$ is the superalgebra of universal differential forms of A in Ref. 23.

2.3. *Tensors*

In this subsection we present briefly the ρ-tensor algebra $T(A)$ of the almost commutative algebra A. For more details see Ref. 28. Here $\Omega(A)$ is the algebra of forms of A.

For $\alpha_1, \ldots, \alpha_p \in Hg\left(\Omega^1(A)\right)$ and $X_1, \ldots, X_p \in Hg\left(\rho\text{-Der}(A)\right)$ we set $\alpha = \alpha_1 \otimes_\rho \cdots \otimes_\rho \alpha_p$ to be the ρ-p-linear map defined by

$$(\alpha_1 \otimes_\rho \cdots \otimes_\rho \alpha_p)(X_1, \ldots, X_p) := \prod_{i=1}^{p} \alpha_i(X_i) \prod_{k=1}^{p-1} \rho\Big(\sum_{j=k+1}^{p} |X_j|, |\alpha_k|\Big)$$

For example $(\alpha_1 \otimes_\rho \alpha_2)(X_1, X_2) = \alpha_1(X_1)\,\alpha_2(X_2)\,\rho(|X_2|, |\alpha_1|)$.

It is easy to check that

$$\alpha(fX_1, \ldots, X_p) = f\alpha(X_1, \ldots, X_p)$$

and

$$\alpha(X_1, \ldots, X_i f, \ldots, X_p) = \alpha(X_1, \ldots, fX_{j+1}, \ldots, X_p).$$

Then $\alpha = \alpha_1 \otimes_\rho \cdots \otimes_\rho \alpha_p$ is a homogeneous map of G-degree $|\alpha| = \sum_{i=1}^{p} |\alpha_i|$.

The ρ-tensor product be extended to obtain the products of non homogeneous forms such that if $\beta = \sum_{i=1}^{p} \beta_i$ then

$$\alpha_1 \otimes_\rho \cdots \otimes_\rho \beta \otimes_\rho \cdots \otimes_\rho \alpha_p = \sum_{i=1}^{p} \alpha_1 \otimes_\rho \cdots \otimes_\rho \beta_i \otimes_\rho \cdots \otimes_\rho \alpha_p.$$

The set $T^{\otimes_\rho^p}$ is the $A-A$ bimodule generated by the elements $\alpha_1 \otimes_\rho \cdots \otimes_\rho \alpha_p$ defined above with the natural actions

$$(\alpha_1 \otimes_\rho \cdots \otimes_\rho \alpha_p) f = \alpha_1 \otimes_\rho \cdots \otimes_\rho \alpha_p f$$

and

$$f(\alpha_1 \otimes_\rho \cdots \otimes_\rho \alpha_p) = (f\alpha_1) \otimes_\rho \cdots \otimes_\rho \alpha_p$$

for $f \in Hg(A)$. Of course, the natural property

$$\alpha_1 \otimes_\rho \cdots \otimes_\rho \alpha_i f \otimes_\rho \cdots \otimes_\rho \alpha_p = \alpha_1 \otimes_\rho \cdots \otimes_\rho f\alpha_{i+1} \otimes_\rho \cdots \otimes_\rho \alpha_p$$

also holds.

2.3.1. *ρ-tensor algebra*

The ρ-tensor algebra $T^{\otimes_\rho} = \bigoplus_{n\geq 0} T^{\otimes_\rho^n}$, $T^{\otimes_\rho^0} = A$ is the direct sum of linear spaces. There is a natural algebra structure $\otimes_\rho$ defined on homogeneous elements of $T^{\otimes_\rho}$ by

$$(T^p \otimes_\rho T^q)(X_1, \ldots, X_{p+q})$$
$$= T^p(X_1, \ldots, X_p)\, T^q(X_1, \ldots, X_q)\, \rho\Big(\sum_{j=1}^{q} |X_{p+j}|, |T^p|\Big),$$

for all $T^p \in T^{\otimes_\rho^n}$, $T^q \in T^{\otimes_\rho^q}$ and $X_1, \ldots, X_{p+q} \in Hg(\rho\text{-Der}(A))$, and extended linearly on $T^{\otimes_\rho}$, and which coincides on A with initial product in A.

Remark that $|T^p \otimes_\rho T^q| = |T^p| + |T^q|$, the product $\otimes_\rho$ is associative, and $T_1 f \otimes_\rho T_2 = T_1 \otimes_\rho fT_2$ for any $f \in Hg(A)$ and $T_1, T_2 \in Hg(T^{\otimes_\rho})$.

2.4. *Connections on a ρ-bimodule over a ρ-algebra*

Let A be a ρ-algebra and M a ρ-bimodule on A.

Definition 2.5.[6] A linear connection on M is a linear map of ρ -Der$A$ into the linear endomorphisms of M, $\nabla : \rho - \mathrm{A} \to End(M)$ such that

$$\nabla_X : M_p \to M_{p+|X|},$$
$$\nabla_{aX}(m) = a\nabla_X(m)$$

and

$$\nabla_X(ma) = \rho(|X|, |m|)mX(a) + \nabla_X(m)a$$

if we use the right structure of M, or

$$\nabla_X(am) = X(a)m + \rho(|X|, |a|)a\nabla_X(m),$$

if M is considered a left bimodule, for all $p \in G$, $a \in A$, $X \in Hg\,(\rho\text{-Der}A)$ and $m \in Hg\,(M)$.

We say that the distribution $\mathcal{D}$ in the ρ-algebra A over the ρ-differential calculus $(\Omega\,(A) = \oplus_{n\geq 0}\Omega^n\,(A), d)$ is *parallel* with respect to the connection $\nabla : \rho\text{-Der}A \to End(\Omega^1\,(A))$ if

$$\nabla_X(m) = 0 \quad \text{for any } X \in \rho\text{-Der}A \text{ and for any } m \in \mathcal{D}.$$

The *curvature* R of the connection ∇ on M is defined in a natural way by

$$R : (\rho\text{-Der}A) \times (\rho\text{-Der}A) \to End(M);\ (X, Y) \longmapsto R_{X,Y},$$
$$R_{X,Y}(m) = \nabla_X\nabla_Y - \rho(|X|, |Y|)\nabla_Y\nabla_X(m) - \nabla_{[X,Y]_\rho}(m)$$

for any $X, Y \in \rho\text{-Der}A$, and $m \in M$, where

$$[X, Y]_\rho = X \circ Y - \rho(|X|, |Y|)Y \circ X.$$

Theorem 2.2.[6] *If the algebra A is ρ-commutative, then the curvature of any connection ∇ has the following properties:*

(1) A-linearity: $R_{aX,Y}(m) = aR_{X,Y}$;
(2) $R_{X,Y}$ is right A-linear: $R_{X,Y}(ma) = R_{X,Y}(m)a$;
(3) $R_{X,Y}$ is left A-linear: $R_{X,Y}(am) = \rho(|X| + |Y|, |a|)R_{X,Y}(m)$;
(4) R is a ρ-symmetric map: $R_{X,Y} = -\rho(|X|, |Y|)R_{Y,X}$;

for any $a \in A_{|a|}$, $m \in M$, $X, Y \in \rho$ -Der$A$.

In the case where the bimodule M is ρ-Der$A$ then the *torsion* of the connection ∇ is the map

$$T_\nabla : (\rho\text{-Der}A) \times (\rho\text{-Der}A) \to \rho\text{-Der}A$$

defined by

$$T_\nabla(X, Y) = [\nabla_X Y, \nabla_Y X]_\rho - [X, Y]_\rho$$

for any homogeneous $X, Y \in \rho$-Der$A$.

Remark 2.1. If the group G is $\mathbb{Z}_2$ and the cocycle is from example 2 then A is a superalgebra. In this case we obtain the same definition of linear connections as in Ref. 22.

Remark 2.2. The noncommutative geometry of ρ-algebras may be viewed as a natural generalization of fermionic differential calculus.

2.5. *Distributions*

Let A be a ρ-algebra and $(\Omega(A), d)$ a ρ-differential calculus over A.

Definition 2.6. A distribution $\mathcal{D}$ in the ρ-algebra A over the ρ -differential calculus $(\Omega(A), d)$ is an A-sub-bimodule $\mathcal{D}$ of $\Omega(A)$.

The distribution $\mathcal{D}$ is globally integrable if the is a ρ -subalgebra B of A such that $\mathcal{D}$ is the space generated by AdB and $(dB)A$.

Remark 2.3. Let us assume that A is generated as algebra by n homogeneous coordinates $x_1, x_2, \ldots, x_n$ and the ρ-differential calculus $(\Omega(A), d)$ by the differentials $dx_1, dx_2, \ldots, dx_n$ with some relations between them. In this case any globally integrable distribution $\mathcal{D}$ is generated by a subset of p elements, denoted by I of $\{1, \ldots, N\}$, such that $\mathcal{D}$ is generated by $x_j y_i$ and $y_i x_j$ for any $j \in \{1, \ldots, N\}$ and $i \in I$. Thus we say that the distribution $\mathcal{D}$ has the dimension p. For other examples, see Refs. 6,9–11.

Definition 2.7. We say that the distribution $\mathcal{D}$ over the ρ-differential calculus $(\Omega(A), d)$ is parallel with respect to the connection ∇: $\rho\text{-Der}A \to End(\Omega A)$ if

$$\nabla_X(m) = 0 \quad \text{for any } X \in \rho\text{-Der}A \text{ and for any } m \in \mathcal{D}.$$

3. Applications to the matrix algebra

In this section we apply the geometrical objects defined in the previous section to the particular case of the matrix algebra $M_n(\mathbb{C})$.

3.1. *Derivations*

We denote by $\rho\text{-Der}M_n(\mathbb{C})$ the set of ρ-derivations of the algebra $M_n(\mathbb{C})$, and it is generated by the elements $\frac{\partial}{\partial p^{\alpha_1}}$, $\frac{\partial}{\partial q^{\alpha_2}}$, with $\alpha = (\alpha_1, \alpha_2) \in G$, which acts on the basis $\{p^{\alpha_1} q^{\alpha_2} | (\alpha_1, \alpha_2) \in G\}$ like partial derivatives,

$$\frac{\partial}{\partial p^k}(p^{\alpha_1} q^{\alpha_2}) = \frac{\alpha_1}{k} p^{\alpha_1 - k} q^{\alpha_2} \text{ and } \frac{\partial}{\partial p^k}(q^{\alpha_2}) = 0 \text{ of } G\text{-degree } (-k, 0) \quad (3.1)$$

and

$$\frac{\partial}{\partial q^k}(q^{\alpha_2} p^{\alpha_1}) = \frac{\alpha_2}{k} q^{\alpha_2 - k} p^{\alpha_1} \text{ and } \frac{\partial}{\partial q^k}(p^{\alpha_1}) = 0 \text{ of } G\text{-degree } (0, -k) \quad (3.2)$$

for any $(\alpha_1, \alpha_2) \in G$. Remark that the first relation from (3.2) is equivalent with

$$\frac{\partial}{\partial q^k}(p^{\alpha_1} q^{\alpha_2}) = \frac{\alpha_2}{k} \varepsilon^{\alpha_1 k} p^{\alpha_1} q^{\alpha_2 - k} \tag{3.3}$$

From a simple calculus we obtain that the applications from the equations (3.1) and (3.2) are ρ-derivations. It follows that ρ- Der$M_n(\mathbb{C})$ is a $M_n(\mathbb{C})$-bimodule generated by $2n-1$ elements and the ρ-bracket of the ρ-derivations is zero, i.e., $[\frac{\partial}{\partial p^{k_1}}, \frac{\partial}{\partial q^{k_2}}] = 0$. Then any $X \in \rho\text{-}DerM_n(\mathbb{C})$ is given by the relation

$$X = \sum_{\alpha=(\alpha_1,\alpha_2)\in G} (\frac{\partial}{\partial p^{\alpha_1}} X^{\alpha_1} + \frac{\partial}{\partial q^{\alpha_2}} X^{\alpha_2}), \tag{3.4}$$

where X^{α_1}, $X^{\alpha_2} \in M_n(\mathbb{C})$. We use the compact form

$$X = \sum_{\alpha \in G} \partial_\alpha X^\alpha. \tag{3.5}$$

to write the derivation in (3.4).

3.2. *The algebra of forms of* $M_n(\mathbb{C})$

In this section we use the construction of the algebra of forms of a ρ-commutative algebra in Ref. 3 to introduce our construction of the algebra of forms of the algebra $M_n(\mathbb{C})$. Thus we obtain a new differential calculus on the matrix algebra.

We denote by $\Omega^p(M_n(\mathbb{C}))$ the space of $p-$ forms and

$$\Omega(M_n(\mathbb{C})) = \bigoplus_{p\in\mathbb{Z}} \Omega^p(M_n(\mathbb{C}))$$

the algebra of forms of $M_n(\mathbb{C})$.

The bimodule $\Omega^1(M_n(\mathbb{C}))$ is also free of rank $2n-1$ with the basis dual to the basis $\{\partial_\alpha \mid \alpha \in G\} := \left\{\frac{\partial}{\partial p^i}, \frac{\partial}{\partial q^j} \mid i,j = 1,\ldots,n\right\}$ of the bimodule ρ-Der$(M_n(\mathbb{C}))$. The basis of $\Omega^1(M_n(\mathbb{C}))$ is $\{d_\alpha \mid \alpha \in G\} := \left\{d_{p^i},\ d_{q^j} \mid i,j = 1,\ldots,n\right\}$ with the relations

$$d_{p^i}(\frac{\partial}{\partial p^j}) = 0 \text{ for } i \neq j,\ d_{p^i}(\frac{\partial}{\partial p^i}) = 1 \text{ and } d_{p^i}(\frac{\partial}{\partial q^j}) = 0, \tag{3.6}$$

$$d_{q^i}(\frac{\partial}{\partial q^j}) = 0 \text{ for } i \neq j,\ d_{p^i}(\frac{\partial}{\partial p^i}) = 1 \text{ and } d_{q^i}(\frac{\partial}{\partial p^j}) = 0. \tag{3.7}$$

For a simpler writing, the relations (3.6) and (3.7) can be written in the following compact form

$$d_\alpha(\partial_\beta) = 0 \text{ for } \alpha \neq \beta, \text{ and } d_\alpha(\partial_\alpha) = 1. \tag{3.8}$$

Remark that the $G-$degree of the 1-form d_{p^k} is $\left|d_{p^k}\right| = (k,0)$ and that of d_{q^k} is $\left|d_{q^k}\right| = (0,k)$.

An arbitrary 1-form α_1 can be written as

$$\alpha_1 = \sum_{\alpha\in G} d_\alpha A_\alpha := \sum_{i=1}^{n} d_{p^i} A_{p^i} + \sum_{j=1}^{n} d_{q^j} A_{q^j}, \tag{3.9}$$

where $A_{p^i} = \alpha_1(\frac{\partial}{\partial p^i}) \in M_n(\mathbb{C})$ and $A_{q^j} = \alpha_1(\frac{\partial}{\partial q^j}) \in M_n(\mathbb{C})$, for $i,j = 1,\dots,n$, or using the compact form we have: $A_\alpha = \alpha_1(\partial_\alpha) \in M_n(\mathbb{C})$, for $\alpha \in G$.

Because $\Omega^1(M_n(\mathbb{C}))$ is of finite rank n^2-1, $\Omega^p(M_n(\mathbb{C}))$ is the pth exterior power of $\Omega^1(M_n(\mathbb{C}))$ in the sense of $M_n(\mathbb{C})-$ modules and is also free, of rank $\left(p, n^2-1\right)$. An arbitrary $p-$form α_p can be written as

$$\alpha_p = \frac{1}{p!}(-1)^{\frac{p(p-1)}{2}} \sum_{i_1,\dots,i_p=1}^{p} d_{\alpha_{i_1}} \wedge \dots \wedge d_{\alpha_{i_{kp}}} A_{i_1\dots i_p},$$

with

$$A_{i_1\dots i_p} = \alpha_p(\partial_{\alpha_{i_1}},\dots,\partial_{\alpha_{i_p}}) \in M_n(\mathbb{C}).$$

From these considerations we see that the algebra $\Omega(M_n(\mathbb{C}))$ is generated by the elements p^i, q^j for $i,j = 1,\dots,n$ and their differentials d_{p^i}, d_{q^j}, for $i,j = 1,\dots,n$ with the relations

$$\begin{aligned} p^i q^j &= \varepsilon^{ij} q^j p^i, \quad p^i p^j = p^j p^i, \\ d_{p^i} d_{q^j} &= -\varepsilon^{ij} d_{q^j} d_{p^i}, \quad d_{p^i} d_{p^j} = d_{p^j} d_{p^i} \end{aligned}$$

and

$$p^i d_{q^j} = \varepsilon^{ij} d_{q^j} p^i, \quad q^i d_{p^j} = \varepsilon^{-ij} d_{p^j} q^i, \quad d_{p^i} p^j = p^j d_{p^i}, \quad q^i d_{q^j} = d_{q^j} q^i.$$

3.3. *The algebra of universal differential forms of* $M_n(\mathbb{C})$

In this paragraph we present our construction of the algebra of universal differential forms of $M_n(\mathbb{C})$, using the construction from the Subsection 2.2.

Let $\alpha = (\alpha_1,\alpha_2) \in G = \mathbb{Z}_n \times \mathbb{Z}_n$ an arbitrary element. $\Omega^1_\alpha M_n(\mathbb{C})$ is the $M_n(\mathbb{C})$-bimodule generated by the elements adb, with $a,b \in M_n(\mathbb{C})$ which satisfies the properties

(1) $d(a+b) = da + db$,
(2) $d(ab) = (da)b + \rho(\alpha,|a|)adb$,
(3) $d1 = 0$, for any $a,b \in M_n(\mathbb{C})$, where 1 is the unit of $M_n(\mathbb{C})$.

By a simple computation we obtain the following result.

Proposition 3.1. *One has*

(1) $p^k dp = (dp)p^k$ *and* $q^l dq = (dq)q^l$,
(2) $dp^k = \varepsilon^{\alpha}_{(k,0)} dp$,
(3) $dp^s = \varepsilon^{\alpha}_{(0,s)} dp$,
(4) $d(p^k q^s) = \varepsilon^{\alpha}_{(k,0)} p^{k-1}(dp)q^s + \varepsilon^{-\alpha_2}\varepsilon^{\alpha}_{(0,s)} p^k q^{s-1} dq$,

where $\varepsilon^{\alpha}_{(0,0)} = 0$, $\varepsilon^{\alpha}_{(k,0)} = 1 + \varepsilon^{-\alpha_2} + \varepsilon^{-2\alpha_2} + \cdots + \varepsilon^{-(k-1)\alpha_2}$ *for* $k \in \{1, \ldots, n-1\}$ *and* $\varepsilon^{\alpha}_{(0,s)} = 1 + \varepsilon^{-\alpha_1} + \varepsilon^{-2\alpha_1} + \cdots + \varepsilon^{-(s-1)\alpha_1}$ *for* $s \in \{1, \ldots, n-1\}$.

The structure of the $M_n(\mathbb{C})$-bimodule $\Omega^1_\alpha M_n(\mathbb{C})$ is given in the following theorem.

Theorem 3.1. $\Omega^1_\alpha M_n(\mathbb{C})$ *is generated by the elements* p^i, q^j, dp^k, dq^s, $i, j, k, s \in \{0, \ldots, n-1\}$ *with the relations*

(1) $p^k q^s = \varepsilon^{ks} q^s p^k$,
(2) $p^k dp^l = (dp^l)p^k$ *and* $q^s dq^l = (dq^l)q^s$,
(3) $dp^k = \varepsilon^{\alpha}_{(k,0)} p^{k-1} dp$ *and* $dq^s = \varepsilon^{\alpha}_{(0,s)} q^{s-1} dq$
(4) $d(p^k q^s) = \varepsilon^{\alpha}_{(k,0)} \varepsilon^s p^{k-1} q^s (dp) + \varepsilon^{-\alpha_2}\varepsilon^{\alpha}_{(0,s)} p^k q^{s-1} dq$,

for any $k, l, s \in G$.

The $M_n(\mathbb{C})$-bimodule $\Omega^k_\alpha M_n(\mathbb{C})$ is again free and an arbitrary element $\omega_k \in \Omega^k_\alpha M_n(\mathbb{C})$ can be written as

$$\omega^k = \sum_{l+s=k} A_{l+s}(dp)^l (dq)^s,$$

where $A_{l,s} \in M_n(\mathbb{C})$.

From these considerations we obtain the following theorem which gives the structure of the algebra $\Omega_\alpha M_n(\mathbb{C})$.

Theorem 3.2. *The algebra* $\Omega_\alpha M_n(\mathbb{C})$ *is generated by the elements* $p^i, q^j, (dp)^k := P^k, (dq)^s := Q^s$, $i, j \in \{0, \ldots, n-1\}$, $k, s \in \mathbb{Z}$ *with the relations*

(1) $p^i q^j = \varepsilon^{ij} q^j p^i$, $P^k Q^s = (-1)^{ks}\varepsilon^{ks} Q^s P^k$,
(2) $p^k P^s = P^s p^k$, $q^k Q^s = Q^s q^k$,
(3) $p^k Q^s = \varepsilon^{ks} Q^s p^k$, $q^k P^s = \varepsilon^{-ks} P^s q^k$.

3.4. *Tensors*

In this subsection we give the tensor components in the matrix algebra.

Let T be the ρ -tensor algebra of $M_n(\mathbb{C})$. The module $T^{\otimes_\rho^p}$ is generated by $d\alpha_{i_1} \otimes_\rho \cdots \otimes_\rho d\alpha_{i_p}$, with $\alpha_{i_1}, \ldots, \alpha_{i_p} \in G$. Specifically, any element $T \in T^{\otimes_\rho^p}$ can be written in terms of the elements of the basis as

$$T = \sum_{i_1,\ldots,i_p \in G} d\alpha_{i_1} \otimes_\rho \cdots \otimes_\rho d\alpha_{i_p} T_{\alpha_{i_1}\ldots\alpha_{i_p}},$$

where

$$T_{\alpha_{i_1}\ldots\alpha_{i_p}} = T\left(\partial_{\alpha_{i_1}}, \ldots, \partial\alpha_{i_p}\right) \times \prod_{k=1}^{p-1} \rho\Big(\sum_{j=k+1}^{p} |x_{\alpha_{i_j}}|, |x_{\alpha_{i_k}}| \Big).$$

3.5. *Linear connections on* $M_n(\mathbb{C})$

Next we introduce linear connections on the algebra $M_n(\mathbb{C})$. A linear connection on $M_n(\mathbb{C})$ is a linear map

$$\nabla : \rho\text{-Der}M_n(\mathbb{C}) \to End(\rho\text{- Der}M_n(\mathbb{C}))$$
$$\nabla_X : (\rho\text{-Der}M_n(\mathbb{C}))_* \to (\rho\text{-Der}M_n(\mathbb{C}))_{*+|X|}$$

satisfying the relations from the Definition 2.5. Any linear connection is well defined if the *connections coefficients* are given on the basis $\{\partial_\alpha | \alpha \in G\}$, that is,

$$\partial_\sigma \Gamma^\sigma_{\alpha,\beta} = \nabla_{\partial_\alpha} \partial_\beta$$

for any $\alpha, \beta \in G$.

The *curvature* R of the connection ∇ is given by the *curvature coefficients:* $R^\sigma_{\alpha,\beta,\tau}$

$$\partial_\sigma R^\sigma_{\alpha,\beta,\tau} = [\nabla_{\partial_\alpha}, \nabla_{\partial_\beta}](\partial_\tau) - \nabla_{[\partial_\alpha,\partial_\beta]}(\partial_\tau).$$

A simple computation shows that

$$R^\sigma_{\alpha,\beta,\tau} = \partial_\alpha(\Gamma^\sigma_{\beta,\tau}) - \rho(\alpha, \left|\Gamma^\mu_{\beta,\tau}\right|)\Gamma^\sigma_{\alpha,\mu} - \rho(\alpha,\beta)(\partial_\beta \Gamma^\sigma_{\alpha,\tau} - \rho(\beta, \left|\Gamma^\mu_{\beta,\sigma}\right|)\Gamma^\sigma_{\beta,\mu})$$

for any $\alpha, \beta, \tau, \sigma \in G$.

The torsion of the connection ∇ is well defined by the *torsion coefficients*

$$T(\partial_\alpha, \partial_\beta) = \partial_\sigma T^\sigma_{\alpha,\beta}$$

and the relations between connections coefficients and the torsion coefficients are

$$T^\sigma_{\alpha,\beta} = \Gamma^\sigma_{\alpha,\beta} - \rho(\alpha,\beta)\Gamma^\sigma_{\beta,\alpha}.$$

3.5.1. *Linear connections on* $\Omega^1_\alpha(M_n(\mathbb{C}))$

Any linear connection ∇ on the $M_n(\mathbb{C})$-bimodule $\Omega^1_\alpha(M_n(\mathbb{C}))$ is given by the connection coefficients thus (using the compact formula)

$$\nabla_{\partial_\beta} d_\alpha p = \Gamma^{p,p}_\beta d_\alpha p + \Gamma^{p,q}_\beta d_\alpha q,$$

Γ^p_β, $\Gamma^q_\beta \in M_n(\mathbb{C})$.

For example we have

$$\nabla_{\frac{\partial}{\partial p^i}}(d_\alpha p) = \Gamma^{p,p}_i d_\alpha p + \Gamma^{p,q}_i d_\alpha q$$

and

$$\begin{aligned}\nabla_{\frac{\partial}{\partial p^i}}\left(p^k d_\alpha p\right) &= \frac{\partial}{\partial p^i}\left(p^k\right) d_\alpha p + \rho\left((-i,0),(k,0)\right) p^k \nabla_{\frac{\partial}{\partial p^i}}(d_\alpha p)\\ &= \frac{k}{i} p^{k-i} d_\alpha p + p^k \Gamma^{p,p}_i d_\alpha p + \Gamma^{p,q}_i d_\alpha q.\end{aligned}$$

3.6. *Distributions*

In this subsection we introduce distributions on the matrix algebra $M_n(\mathbb{C})$ over the differential calculi $\Omega(M_n(\mathbb{C}))$ and $\Omega_\alpha(M_n(\mathbb{C}))$. In each of these situations we give characterizations of globally integrable distributions and globally integrable distributions parallel with respect to a connection ∇ on $\Omega^1(M_n(\mathbb{C}))$ and $\Omega^1_\alpha(M_n(\mathbb{C}))$.

3.6.1. *Distributions on* $\Omega(M_n(\mathbb{C}))$

From the Definition 2.6 a distribution $\mathcal{D}$ on $\Omega(M_n(\mathbb{C}))$ is a $M_n(\mathbb{C})$ ρ-subbimodule of $\Omega(M_n(\mathbb{C}))$. The distribution $\mathcal{D}$ is globally integrable if there is a subspace B of $M_n(\mathbb{C})$ such that $\mathcal{D}$ is generated by $M_n(\mathbb{C})d(B)$, so the determination of these kind of distributions is reduced to the determination of subalgebras from $M_n(\mathbb{C})$.

Let $D_n = \{k \in \mathbb{N} \text{ such that } k|n\}$ be the set of all natural divisors of n. Then for any subalgebra B of $M_n(\mathbb{C})$ there are $k, s \in D_n$ such that B is generated by the set $\left\{p^{k\cdot i} q^{s\cdot j},\ i,j \in \mathbb{Z}\right\}$. Consequently we have the following result.

Proposition 3.2. *For any globally integrable distribution* $\mathcal{D}$ *of* $\Omega(M_n(\mathbb{C}))$ *there are* $k, s \in D_n$ *such that* $\mathcal{D}$ *is generated by the elements* p^i, q^j *for* $i,j = 1,\ldots,n$ *and the differentials* $d_{p^{i\cdot k}}$, $d_{q^{j\cdot s}}$, *for* $i,j = 1,\ldots,n$.

Remark 3.1. Without any confusion the previous proposition may be written using the compact form (3.5) and (3.8): For any globally integrable

distribution $\mathcal{D}$ of $\Omega(M_n(\mathbb{C}))$ there is a subgroup H of G such that $\mathcal{D}$ is generated by the elements $a_\alpha db_\beta$, with a_α, $b_\beta \in M_n(\mathbb{C})$ with $\alpha \in G$ and $\beta \in H$.

Remark 3.2. If $\mathcal{D}$ is a globally integrable distribution of $\Omega(M_n(\mathbb{C}))$ of the dimension p, then p is a divisor of n^2.

It is obvious that a linear connection ∇ on the $M_n(\mathbb{C})$ -bimodule $\Omega^1(M_n(\mathbb{C}))$ is given by its connection coefficients, again denoted by $\Gamma^\sigma_{\alpha,\beta} \in M_n(\mathbb{C})$, and these are given by the equation

$$\nabla_{\partial_\alpha} d_\beta = \Gamma^\sigma_{\alpha,\beta} d_\sigma,$$

for any $\alpha, \beta \in G$.

Proposition 3.3. *Any globally integrable and parallel distribution $\mathcal{D}$ with respect to a connection $\nabla : \rho\text{-}DerM_n(\mathbb{C}) \to End(\Omega^1(M_n(\mathbb{C})))$ of dimension p is given by the equations*

$$\Gamma^\sigma_{\alpha,\beta} = 0,$$

for a subgroup H of G and for any $\sigma, \alpha \in G$, $\beta \in H$.

3.6.2. *Distributions on $\Omega_\alpha(M_n(\mathbb{C}))$*

Let $\alpha \in G$. Any distribution $\mathcal{D}$ on $\Omega_\alpha(M_n(\mathbb{C}))$ is a $M_n(\mathbb{C})$ ρ -sub-bimodule of $\Omega_\alpha(M_n(\mathbb{C}))$.

Using the structure of $\Omega_\alpha(M_n(\mathbb{C}))$ (Proposition 3.2) we have that any globally integrable distribution $\mathcal{D}$ on $\Omega_\alpha(M_n(\mathbb{C}))$ is one of the subalgebras $M_n(\mathbb{C})$, $M_n(\mathbb{C})d_\alpha p$, $M_n(\mathbb{C})d_\alpha q$ and $\Omega_\alpha(M_n(\mathbb{C}))$, consequently any globally integrable distribution on $\Omega_\alpha(M_n(\mathbb{C}))$ has the dimension 0, 1 or 2.

Any globally integrable and parallel distribution $\mathcal{D}$ with respect to a connection $\nabla : \rho\text{-Der}M_n(\mathbb{C}) \to End(\Omega^1_\alpha(M_n(\mathbb{C})))$ of dimension 1 is given by the equations

$$\Gamma^{p,p}_\beta = \Gamma^{p,q}_\beta = 0$$

if $\mathcal{D}$ is $M_n(\mathbb{C})d_\alpha p$ and

$$\Gamma^{q,p}_\beta = \Gamma^{q,q}_\beta = 0$$

if it is $M_n(\mathbb{C})d_\alpha q$, for any $\beta \in G$

Conclusions and remarks. In this paper we introduce the principal notions from the (noncommutative) geometry as differential calculi, tensors, linear connections and distributions to the matrix algebra $M_n(\mathbb{C})$ using

methods of ρ-algebras. We note that the tensors and connections open a way to introduce metrics and Levi-Civita connections on $M_n(\mathbb{C})$.

The general theory of $\rho-$differential calculi and of linear connections over $\rho-$algebras offers many new possibilities to study some noncommutative spaces (which may be quantum spaces), related to physics (which are ρ-commutative algebras): the quantum hyperplane, the quantum torus, the quaternionic algebra, etc.

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SELF-ADJOINTNESS VIA PARTIAL HARDY-LIKE INEQUALITIES *

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Distinguished selfadjoint extensions of operators which are not semibounded can be deduced from the positivity of the Schur Complement (as a quadratic form). In practical applications this amounts to proving a Hardy-like inequality. Particular cases are Dirac-Coulomb operators where distinguished selfadjoint extensions are obtained for the optimal range of coupling constants.

Keywords: Relativistic quantum mechanics, Dirac operator, self-adjoint operator, self-adjoint extension, Schur complement.

1. Introduction

In Ref. 4 we defined distinguished self-adjoint extensions of Dirac-Coulomb operators in the optimal range for the coupling constant. This was done by using a Hardy-like inequality which allowed the extension of one component of the operator by using the Friedrichs extension. Then, the remaining component could be extended by choosing the right domain for the whole operator. The method of proof used simple arguments of distributional differentiation. This work was the sequel of a series of papers where distinguished self-adjoint extensions of Dirac-Coulomb like operators were

defined by different methods almost in the optimal range, without reaching the limit case (see Refs. 6,7,9,10,12–14).

Here we present an abstract version of the method introduced in Ref. 4. We believe that this will clarify the precise structure and hypotheses necessary to define distinguished self-adjoint extensions by this method.

The main idea in our method is that Hardy-like inequalities are fundamental to define distinguished (physically relevant) self-adjoint extensions *even* for operators that are not bounded below.

We are going to apply our method to operators H defined on $\mathcal{D}_0^2$, where $\mathcal{D}_0$ is some dense subspace of a Hilbert space $\mathcal{H}_0$. The general structure taken into account here is:

$$H = \begin{pmatrix} P & Q \\ T & -S \end{pmatrix}, \tag{1.1}$$

where all the above operators satisfy $Q = T^*$, $P = P^*$, $S = S^*$ and $S \geq c_1 I > 0$. Moreover we assume that P, Q, S, , T, $S^{-1}T$ and $QS^{-1}T$ send $\mathcal{D}_0$ into $\mathcal{H}_0$.

In the Dirac-Coulomb case our choice was $\mathcal{H}_0 = L^2(\mathbb{R}^3, \mathbb{C}^2)$ and

$$P = V + 2 - \gamma,\ Q = T = -i\sigma \cdot \nabla,\ S = \gamma - V\,,$$

where V is a potential bounded from above satisfying

$$\sup_{x \neq 0} |x||V(x)| \leq 1\,. \tag{1.2}$$

Moreover, σ_i, $i = 1, 2, 3$, are the Pauli matrices (see Ref. 4) and γ is a constant slightly above $\max_{\mathbb{R}^3} V(x)$. For $\mathcal{D}_0$ we chose $C_c^\infty(\mathbb{R}^3, \mathbb{C}^2)$. Note that in our paper Ref. 4, where we deal with Dirac-Coulomb like operators, there is an omission. We forgot to specify the conditions on the potential V so that $QS^{-1}T$ is a symmetric operator on $C_c^\infty(\mathbb{R}^3, \mathbb{C}^2)$. The natural condition is that each component of

$$(\gamma - V)^{-2} \nabla V$$

is locally square integrable. This is easily seen to be true for the Coulomb-type potentials.

In the general context of the operator H, as defined in (1.1), our main assumption is that there exists a constant $c_2 > 0$ such that for all $u \in \mathcal{D}_0$,

$$q_{c_2}(u, u) := \big((S + c_2)^{-1} Tu, Tu\big) + \big((P - c_2)u, u\big) \geq 0\,. \tag{1.3}$$

Note that since $\frac{d}{d\alpha} q_\alpha(u, u) \leq -(u, u)$, (1.3) implies in fact that for all $0 \leq \alpha \leq c_2$ and for all $u \in \mathcal{D}_0$,

$$q_\alpha(u, u) := \big((S + \alpha)^{-1} Tu, Tu\big) + \big((P - \alpha)u, u\big) \geq 0\,. \tag{1.4}$$

Another consequence of assumption (1.3) is that the quadratic form

$$q_0(u,u) = \big(S^{-1}Tu, Tu\big) + \big(Pu, u\big)\,, \tag{1.5}$$

defined for $u \in \mathcal{D}_0$, is positive definite:

$$q_0(u,u) = \big(S^{-1}Tu, Tu\big) + \big(Pu, u\big) \geq c_2(u,u).$$

Note that the operator $P + QS^{-1}T$ which is associated with the quadratic form q_0 is actually the Schur complement of $-S$. Note also that by our assumptions on P, Q, $T\,S$ and by (1.3), for any $0 \leq \alpha \leq c_2$, q_α is the quadratic form associated with a positive symmetric operator. Therefore (by Thm. X.23 in Ref. 8), it is closable and we denote its closure by $\widehat{q}_\alpha$ and its form domain, which is easily seen to be independent of α (see Ref. 4) by $\mathcal{H}_{+1}$. Our main result states the following:

Theorem 1.1. *Assume the above hypotheses on the operators P, Q, T, S and* (1.3)*. Then there is a unique self-adjoint extension of H such that the domain of the operator is contained in $\mathcal{H}_{+1} \times \mathcal{H}_0$.*

Remark 1.1. Note that what this theorem says that "in some sense" the Schur complement of $-S$ is positive, and therefore has a natural self-adjoint extension, then one can define a distinguished self-adjoint extension of the operator H which is unique among those whose domain is contained in the form domain of the Schur complement of $-S$ times $\mathcal{H}_0$.

2. Intermediate results and proofs

We denote by R the unique selfadjoint operator associated with $\widehat{q}_0$: For all $u \in D(R) \subset \mathcal{H}_{+1}$,

$$\widehat{q}_0(u,u) = (u, Ru)\ .$$

R is an isometric isomorphism from $\mathcal{H}_{+1}$ to its dual $\mathcal{H}_{-1}$. Using the second representation theorem in Ref. 5, Theorem 2.23, we know that $\mathcal{H}_{+1}$ is the operator domain of $R^{1/2}$, and

$$\widehat{q}_0(u,u) = (R^{1/2}u, R^{1/2}u)\ ,$$

for all $u \in \mathcal{H}_{+1}$.

Definition 2.1. We define the domain $\mathcal{D}$ of H as the collection of all pairs $u \in \mathcal{H}_{+1}$, $v \in \mathcal{H}_0$ such that

$$Pu + Qv\ , \quad Tu - Sv \in\ \mathcal{H}_0\ . \tag{2.1}$$

The meaning of these two expressions is in the weak (distributional) sense, i.e., the linear functional $(P\eta, u) + (Q^*\eta, v)$, which is defined for all test functions $\eta \in \mathcal{D}_0$, extends uniquely to a bounded linear functional on $\mathcal{H}_0$. Likewise the same for $(-S\eta, v) + (T^*\eta, v)$.

On the domain $\mathcal{D}$, we define the operator H as

$$H\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} Pu + Qv \\ Tu - Sv \end{pmatrix}.$$

Note that for all vectors $(u, v) \in \mathcal{D}$ the expected total energy is finite.

The following two results are important in the proof of Theorem 1.1.

Proposition 2.1. *Under the assumptions of Theorem 1.1*

$$\mathcal{H}_{+1} \subset \left\{ u \in \mathcal{H}_0 \,:\, S^{-1}Tu \in \mathcal{H}_0 \right\}, \tag{2.2}$$

where the embedding holds in the continuous sense. Therefore, we have the 'scale of spaces' $\mathcal{H}_{+1} \subset \mathcal{H}_0 \subset \mathcal{H}_{-1}$.

Proof. Choose $c_2 \geq \alpha > 0$. Since $S \geq c_1 I$, we have for all $0 < \delta \leq \frac{c_1\alpha}{c_1+\alpha}$

$$S^{-1} - (S + \alpha)^{-1} \geq \delta\, S^{-2},$$

and so, for all $u \in \mathcal{D}_0$,

$$\begin{aligned} q_0(u, u) &\geq q_\alpha(u, u) + \alpha\,(u, u) + \delta\,(S^{-1}Tu, S^{-1}Tu) \\ &\geq \delta\,(u, u) + \delta\,(S^{-1}Tu, S^{-1}Tu)\ . \end{aligned}$$

The proof can be finished by density arguments. □

Lemma 2.1. *For any F in $\mathcal{H}_0$,*

$$QS^{-1}F \in \mathcal{H}_{-1}\ .$$

Proof. By our assumptions on H and by Proposition 2.1, for every $\eta \in \mathcal{D}_0$,

$$\left|(S^{-1}T\eta,\, F)\right| \leq \delta^{-1/2}\, \|\eta\|_{\mathcal{H}_{+1}}\, \|F\|_2\ .$$

Hence, the linear functional

$$\eta \to (Q^*\eta, S^{-1}F)$$

extends uniquely to a bounded linear functional on $\mathcal{H}_{+1}$. □

Proof of Theorem 1.1. We shall prove Theorem 1.1 by showing that H is symmetric and a bijection from its domain $\mathcal{D}$ onto $\mathcal{H}_0$. To prove the

symmetry we have to show that for both pairs (u, v), $(\tilde{u}, \tilde{v})$ in the domain $\mathcal{D}$,

$$\left(H \begin{pmatrix} u \\ v \end{pmatrix}, \begin{pmatrix} \tilde{u} \\ \tilde{v} \end{pmatrix} \right) = (Pu + Qv,\, \tilde{u}) + (Tu - Sv,\, \tilde{v})$$

equals

$$(u,\, P\tilde{u} + Q\tilde{v}) + (v,\, T\tilde{u} - S\tilde{v}) = \left(\begin{pmatrix} u \\ v \end{pmatrix}, H \begin{pmatrix} \tilde{u} \\ \tilde{v} \end{pmatrix} \right).$$

First, note that since (u, v) is in the domain,

$$S(v - S^{-1}Tu) \in \mathcal{H}_0) \ . \tag{2.3}$$

We now claim that

$$(Pu + Qv,\, \tilde{u}) = (Ru, \tilde{u}) + (\, S(v - S^{-1}Tu),\, S^{-1}T\tilde{u}\,) .$$

Note that each term makes sense. The one on the left, by definition of the domain and the first on the right, because both $u, \tilde{u}$ are in $\mathcal{H}_{+1}$. The second term on the right side makes sense because of (2.3) above and Proposition 2.1. Moreover both sides coincide for $\tilde{u}$ chosen to be a test function and both are continuous in $\tilde{u}$ with respect to the $\mathcal{H}_{+1}$ -norm. Hence the two expressions coincide on the domain. Thus we get that

$$\left(H \begin{pmatrix} u \\ v \end{pmatrix}, \begin{pmatrix} \tilde{u} \\ \tilde{v} \end{pmatrix} \right)$$

equals

$$(Ru, \tilde{u}) - (\, S(v - S^{-1}Tu),\, \tilde{v} - S^{-1}T\tilde{u}\,) ,$$

an expression which is symmetric in (u, v) and $(\tilde{u}, \tilde{v})$. To show that the operator is onto, pick any F_1, F_2 in $\mathcal{H}_0$. Since R is an isomorphism, there exists a unique u in $\mathcal{H}_{+1}$ such that

$$Ru = F_1 + QS^{-1}F_2 \ . \tag{2.4}$$

Indeed, F_1 is in $\mathcal{H}_0$ and therefore in $\mathcal{H}_{-1}$. Moreover the second term is also in $\mathcal{H}_{-1}$ by Lemma 2.1.

Now define v by

$$v = S^{-1}(Tu - F_2) , \tag{2.5}$$

which by Proposition 2.1 is in $\mathcal{H}_0$.

Now for any test function η we have that

$$\begin{aligned} &(P\eta,\, u) + (Q^*\eta,\, v) = (P\eta,\, u) + (T\eta,\, v) \\ &= (P\eta,\, u) + (\, T\eta,\, S^{-1}Tu) + (T\eta,\, (v - S^{-1}Tu)\,) \end{aligned}$$

which equals

$$(\eta, Ru) + (T\eta,\, (v - S^{-1}Tu) = (\eta, F_1)$$

This holds for all test functions η, but since F_1 is in $\mathcal{H}_0$, the functional $\eta \to (P\eta,\, u) + (T\eta,\, v)$ extends uniquely to a linear continuous functional on $\mathcal{H}_0$ which implies that

$$Pu + Qv = F_1 \ .$$

Hence (u, v) is in the domain $\mathcal{D}$ and the operator H applied to (u, v) yields (F_1, F_2).

Let us now prove the injectivity of H. Assuming that

$$H\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{2.6}$$

we find by (2.4) and (2.5),

$$v = S^{-1}Tu \ , \qquad Ru = 0 \, .$$

Since R is an isomorphism, this implies that $u = v = 0$.

It remains to show the uniqueness part in our theorem. By the bijectivity result proved above, for all $\binom{F_1}{F_2} \in {\mathcal{H}_0}^2$, there exists a unique pair $(\hat{u}\,, \hat{v}) \in \mathcal{H}_{+1} \times \mathcal{H}_0$ such that $H\binom{u}{v} = \binom{F_1}{F_2}$. Let us now pick any other self-adjoint extension with domain $\mathcal{D}'$ included in $\mathcal{H}_{+1} \times \mathcal{H}_0$. Then for all $(u, v) \in \mathcal{D}'$, $H\binom{u}{v}$ belongs to ${\mathcal{H}_0}^2$. Hence there exist a unique pair $(\hat{u}\,, \hat{v}) \in \mathcal{H}_{+1} \times \mathcal{H}_0$ such that $H\binom{\hat{u}}{\hat{v}} = H\binom{u}{v}$. But, by the above considerations on injectivity, $u = \hat{u}$ and $v = \hat{v}$. Therefore, $\mathcal{D}' \subset \mathcal{D}$ and so necessarily, $\mathcal{D}' = \mathcal{D}$. □

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INTERLACED DENSE POINT AND ABSOLUTELY CONTINUOUS SPECTRA FOR HAMILTONIANS WITH CONCENTRIC-SHELL SINGULAR INTERACTIONS

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We analyze the spectrum of the generalized Schrödinger operator in $L^2(\mathbb{R}^\nu)$, $\nu \geq 2$, with a general local, rotationally invariant singular interaction supported by an infinite family of concentric, equidistantly spaced spheres. It is shown that the essential spectrum consists of interlaced segments of the dense point and absolutely continuous character, and that the relation of their lengths at high energies depends on the choice of the interaction parameters; generically the p.p. component is asymptotically dominant. We also show that for $\nu = 2$ there is an infinite family of eigenvalues below the lowest band.

Keywords: Schrödinger operators, singular interactions, absolutely continuous spectrum, dense pure point spectrum

1. Introduction

Quantum systems with the spectrum consisting of components of a different nature attract attention from different points of view. Probably the most important among them concerns random potentials in higher dimensions — a demonstration of existence of a mobility edge is one of the hardest questions of the present mathematical physics. At the same time, a study of specific non-random systems can reveal various types of spectral behaviour which differ from the generic type.

An interesting example among these refers to the situation where the spectrum is composed of interlacing intervals of the dense point and abso-

lutely continuous character. A way to construct such models using radially periodic potentials was proposed in Ref. 10 since at large distances in such a system the radial and angular variables "almost decompose" locally and the radial part behaves thus essentially as one-dimensional there are spectral intervals where the particle can propagate, with the gaps between them filled densely by localized states.

To be specific consider, e.g., the operator $\mathsf{t} = -\mathsf{d}^2/\mathsf{d}x^2 + q(x)$ on $L^2(\mathbb{R})$ with q bounded and periodic. By the standard Floquet analysis the spectrum of t is purely absolutely continuous consisting of a family of bands, $\sigma(\mathsf{t}) = \bigcup_{k=0}^{N}[E_{2k}, E_{2k+1}]$, corresponding to a strictly increasing, generically infinite sequence $\{E_k\}_{k=0}^{N}$. Suppose now that the potential is mirror-symmetric, $q(x) = q(-x)$, and consider the operator

$$\mathsf{T} = -\triangle + q(|x|)$$

on $L^2(\mathbb{R}^\nu)$, $\nu \geq 2$. It was shown in Ref. 10 that the essential spectrum of T covers the half-line $[E_0, \infty)$, being absolutely continuous in the spectral bands of t and dense pure point in the gaps (E_{2k-1}, E_{2k}), $k = 1, \ldots N$.

The well-known properties of one-dimensional Schrödinger operators tell us that the dense point segments in this example shrink with increasing energy at a rate determined by the regularity of the potential. If we replace the bounded q by a family of δ interactions, the segment lengths tend instead to a positive constant, see Ref. 5. Nevertheless, the absolutely continuous component still dominates the spectrum at high energies.

The aim of this paper is to investigate a similar model in which a family of concentric, equally spaced spheres supports generalized point interactions with identical parameters. We will demonstrate that the interlaced spectral character persists and, depending on the choice of the parameters, each of the components may dominate in the high-energy limit, or neither of them. Specifically, the ratio of the adjacent *pp* and *ac* spectral segments, $(E_{2k} - E_{2k-1})/(E_{2k+1} - E_{2k})$, has three possible types of behaviour, namely like $\mathcal{O}(k^\mu)$ with $\mu = 0, \pm 1$. What is more, in the generic case we have $\mu = 1$ so the dense point part dominates, which is a picture very different from the mobility-edge situation mentioned in the opening. Apart from this main result, we are going to show that the interesting result about existence of the so-called "Welsh eigenvalues" in the two-dimensional case[1,11,14] also extends to the situation with the generalized point interactions.

2. The model

As we have said, we are going to investigate generalized Schrödinger operators in $\mathbb{R}^\nu$, $\nu \geq 2$, with spherically symmetric singular interactions on concentric spheres, the radii of which are supposed to be $R_n = nd + d/2$, $n \in \mathbb{N}$. It is important that the system is radially periodic, hence the interactions on all the spheres are assumed to be the same. In view of the spherical symmetry we may employ the partial-wave decomposition: the isometry $\mathsf{U} : L^2((0,\infty), r^{\nu-1}dr) \to L^2(0,\infty)$ defined by $\mathsf{U}f(r) = r^{\frac{\nu-1}{2}} f(r)$ allows us to write $L^2(R^\nu) = \bigoplus_{l\in\mathbb{N}_0} \mathsf{U}^{-1}L^2(0,\infty) \otimes S_l$, where S_l is the l-th eigenspace of the Laplace-Bertrami operator on the unit sphere. The operator we are interested in can be then written as

$$\mathsf{H}_\Lambda := \bigoplus_l \mathsf{U}^{-1}\mathsf{H}_{\Lambda,l}\mathsf{U} \otimes \mathsf{I}_l, \tag{2.1}$$

where I_l is the identity operator on S_l and the l-th partial wave operators

$$\mathsf{H}_{\Lambda,l} := -\frac{d^2}{d\,r^2} + \frac{1}{r^2}\left[\frac{(\nu-1)(\nu-3)}{4} + l(l+\nu-2)\right] \tag{2.2}$$

are determined by the boundary conditions[a] at the singular points R_n,

$$\begin{pmatrix} f(R_n+) \\ f'(R_n+) \end{pmatrix} = e^{i\chi} \begin{pmatrix} \gamma & \beta \\ \alpha & \delta \end{pmatrix} \begin{pmatrix} f(R_n-) \\ f'(R_n-) \end{pmatrix}; \tag{2.3}$$

in the transfer matrix $\Lambda := e^{i\chi}\begin{pmatrix} \gamma & \beta \\ \alpha & \delta \end{pmatrix}$ the parameters $\alpha, \beta, \gamma, \delta$ are real and satisfy the condition $\alpha\beta - \gamma\delta = -1$. In other words, the domain of the selfadjoint operator $\mathsf{H}_{\Lambda,l}$ is

$$\begin{aligned} D(\mathsf{H}_{\Lambda,l}) = \Big\{ & f \in L^2(0,\infty) :\ f,\, f' \in AC_{\mathrm{loc}}\big((0,\infty)\setminus \cup_n\{R_n\}\big); \\ & -f'' + \tfrac{1}{r^2}\left[\tfrac{(\nu-1)(\nu-3)}{4} + l(l+\nu-2)\right] f \in L^2(0,\infty); \\ & F(R_n+) = \Lambda F(R_n-)\Big\}, \end{aligned} \tag{2.4}$$

where the last equation is a shorthand for the boundary conditions (2.3). If the dimension $\nu \leq 3$ we have to add a condition for the behaviour of $f \in D(\mathsf{H}_l)$ at the origin: for $\nu = 2$, $l = 0$ we assume that $\lim_{r\to 0+}[\sqrt{r}\ln r]^{-1} f(r) = 0$, and for $\nu = 3$, $l = 0$ we replace it by $f(0+) = 0$. Since the generalized point interaction is kept fixed, we will mostly drop the symbol Λ in the following.

[a] For relations of these conditions to the other standard parametrization of the generalized point interaction, $(U-I)F(R_n) + i(U+I)F'(R_n) = 0$, see Ref. 4

3. Generalized Kronig-Penney model

As in the regular case the structure of the spectrum is determined by the underlying one-dimensional Kronig-Penney model. We need its generalized form where the Hamiltonian acts as the one dimensional Laplacian except at the interaction sites, $x_n := nd + d/2$, $n \in \mathbb{Z}$, where the wave functions satisfy boundary conditions analogous to (2.3). To be explicit we consider the four-parameter family of self-adjoint operators

$$\begin{aligned} \mathsf{h}_\Lambda f &:= -f'', \\ D(\mathsf{h}_\Lambda) &= \left\{ f \in \mathcal{H}^{2,2}\big(\mathbb{R} \setminus \cup_n \{x_n\}\big) : \; F(x_n+) = \Lambda F(x_n-) \right\} \end{aligned} \tag{3.1}$$

where the matrix Λ has been introduced in the previous section (without loss of generality we may assume $\chi = 0$ because it is easy to see that operators differing by the value of χ are isospectral). Spectral properties of this model were investigated in Refs. 3,6 where it was shown that the following three possibilities occur:

(i) *the δ-type:* $\beta = 0$ and $\gamma = \delta = 1$. In this case the gap width is asymptotically constant; it behaves like $2|\alpha|d^{-1} + \mathcal{O}(n^{-1})$ as the band index $n \to \infty$. This is the standard Kronig-Penney model.

(ii) *the intermediate type:* $\beta = 0$ and $|\gamma + \delta| > 2$. Now the quotient of the band width to the adjacent gap width is asymptotically constant behaving as $\arcsin(2|\delta + \gamma|^{-1}) / \arccos(2|\delta + \gamma|^{-1}) + \mathcal{O}(n^{-1})$.

(iii) *the δ'-type:* the generic case, $\beta \neq 0$. In this case the band width is asymptotically constant; it behaves like $8|\beta d|^{-1} + \mathcal{O}(n^{-1})$ as $n \to \infty$.

Recall that these types of spectral behaviour correspond to high-energy properties of a single generalized point interaction as manifested through the scattering, resonances,[4] etc.

There is one more difference from standard Floquet theory which we want to emphasize. It is well known [17, Thm 12.7, p. 188] that in the regular case the spectral edge E_0 corresponds to a symmetric eigenfunction. In the singular case this is no longer true; one can check easily the following claim.

Proposition 3.1. *Let u be an α-periodic solution of the equation $-u'' = E_0 u$ on $(-d/2, d/2)$ with $U(x_n+) = \Lambda U(x_n-)$, where $E_0 := \inf \sigma(\mathsf{h}_\Lambda)$. Then u is periodic for $\beta \geq 0$ and antiperiodic for $\beta < 0$.*

To finish the discussion of the one-dimensional comparison operator, let us state three auxiliary results which will be needed in the next section.

Lemma 3.1. *There is a constant $C > 0$ such that for every function u in the domain of the operator h_Λ it holds that*

$$\|u'\| \le C(\|\mathsf{h}_\Lambda u\| + \|u\|)\,. \tag{3.2}$$

Proof. We employ Redheffer's inequality[13] which states that

$$\int_a^b |u'(x)|^2\,\mathsf{d}x \le C'\left(\int_a^b |u''(x)|^2\,\mathsf{d}x + \int_a^b |u(x)|^2\,\mathsf{d}x\right)$$

holds for any u twice differentiable in an interval $[a,\, b]$ and some $C' > 0$; then we get an inequality similar to (3.2) for the squares of the norms by summing up these inequalities with $a = x_n$, $b = x_{n+1}$, and the sought result with $C = 2C'$ follows easily. □

Lemma 3.2. *The set of functions from $D(\mathsf{h}_\Lambda)$ with a compact support is a core of the operator h_Λ.*

Proof. To a given $u \in D(\mathsf{h}_\Lambda)$ and $\varepsilon > 0$ we will construct an approximation function $u_\varepsilon \in D(\mathsf{h}_\Lambda)$ which is compactly supported to the right, i.e., it satisfies $\sup \operatorname{supp} u_\varepsilon < \infty$, and

$$\int_{\mathbb{R}} \big(|u - u_\varepsilon|^2 + |u'' - u_\varepsilon''|^2\big)(t)\,\mathsf{d}t \le \varepsilon\,.$$

Given $x \in \mathbb{R}$ and $d > 0$ we can employ for a function $v \in \mathcal{H}^{2,2}(x, x+d)$ the Sobolev embedding,

$$\begin{aligned} |v(x)|^2 + |v'(x)|^2 &\le \sup_{t\in[x,\,x+d]} |v(t)|^2 + |v'(t)|^2 \\ &\le C_1 \int_x^{x+d} (|v|^2 + |v''|^2)(t)\,\mathsf{d}t \end{aligned}$$

with a constant C_1 which depends on d but not on x. Let us take next a pair of functions, $\phi_i \in C^\infty(0,d)$, $i = 1, 2$, such that they satisfy $\phi_1(0) = \phi_2'(0) = 1$ and $\phi_1'(0) = \phi_2(0) = \phi_i(d) = \phi_i'(d) = 0$. Denote by M_i the maximum of $|\phi_i(t)|^2 + |\phi_i''(t)|^2$ and put $M := \max\{M_1,\, M_2\}$; then it holds

$$\int_0^d (|a\phi_1 + b\phi_2|^2 + |a\phi_1'' + b\phi_2''|^2)(t)\,\mathsf{d}t \le 2Md(a^2 + b^2).$$

In view of the assumption made about the function u we can find n such that $\int_{x_n}^{\infty}(|u|^2+|u''|^2)(t)\mathsf{d}t \le \tilde{\varepsilon} := \varepsilon/(2+8MdC_1)$ and define

$$u_\varepsilon(x) := \begin{cases} u(x) & \text{if} \quad x \le x_n \\ u(x_n+)\phi_1(x) + u'(x_n+)\phi_2(x) & \text{if} \quad x \in (x_n,\, x_n+d) \\ 0 & \text{if} \quad x \ge x_n+d \end{cases}$$

Then u_ε belongs to $D(\mathsf{h}_\Lambda)$ being compactly supported to the right and

$$\begin{aligned} \int_{\mathbb{R}} (|u-u_\varepsilon|^2 + |u''-u_\varepsilon''|^2)(t)\,\mathsf{d}t &\le 2\int_{x_n}^{\infty} (|u|^2+|u''|^2+|u_\varepsilon|^2+|u_\varepsilon''|^2)(t)\,\mathsf{d}t \\ &\le 2\int_{x_n}^{\infty} (|u|^2+|u''|^2)(t)\,\mathsf{d}t + 8Md(|u(x_n)|^2+|u'(x_n)|^2) \\ &\le (2+8MdC_1)\int_{x_n}^{\infty} (|u|^2+|u''|^2)(t)\,\mathsf{d}t \le (2+8MdC_1)\tilde{\varepsilon} = \varepsilon\,. \end{aligned}$$

Furthermore, one can take this function u_ε and perform on it the analogous construction to get the support compact on the left, arriving in this way at a compactly supported $\tilde{u}_\varepsilon$ such that

$$\int_{\mathbb{R}} \big(|u-\tilde{u}_\varepsilon|^2 + |u''-\tilde{u}_\varepsilon''|^2\big)(t)\,\mathsf{d}t \le 2\varepsilon\,,$$

and since ε was arbitrary by assumption the lemma is proved. □

The last lemma is a simple observation, which is however the main tool for conversion of the proofs in the regular case to their singular counterparts.

Lemma 3.3. *Let $u,\, v \in D(\mathsf{h}_\Lambda)$, then the Wronskian*

$$W[\bar{u},\, v](x) := \bar{u}(x)v'(x) - \bar{u}'(x)v(x) \tag{3.3}$$

is a continuous function of x on the whole real axis.

Proof. The condition $\alpha\beta-\gamma\delta=-1$ for the transfer matrix Λ is equivalent to $\Lambda^*\sigma_2\Lambda=\sigma_2$, where σ_2 is the second Pauli matrix.[3] Then we have

$$\begin{aligned} W[\bar{u},\, v](x_n+) &= iU^*(x_n+)\sigma_2 V(x_n+) = i(\Lambda U(x_n-))^*\sigma_2\Lambda V(x_n-) \\ &= iU^*(x_n-)\sigma_2 V(x_n-) = W[\bar{u},\, v](x_n-)\,, \end{aligned}$$

which concludes the proof. □

The way in which we are going to employ this result is the following. Suppose we have *real-valued* functions u_0, v_0, u which are $\mathcal{H}^{2,\,2}$ away from the points x_n and satisfy the boundary conditions (2.3) at them. Let, in addition, $W[u_0,\, v_0]$ be nonzero – in the applications below this will be true as

u_0, v_0 will be linearly independent generalized eigenfunctions of h_Λ – then by the lemma the vector function

$$y = \begin{bmatrix} u_0 & v_0 \\ u_0' & v_0' \end{bmatrix}^{-1} \begin{pmatrix} u \\ u' \end{pmatrix} = W[u_0, v_0]^{-1} \begin{pmatrix} v_0' u - v_0 u' \\ -u_0' u + u_0 u' \end{pmatrix} \tag{3.4}$$

is continuous everywhere including the points x_n.

4. The essential spectrum

Now we are going to demonstrate the spectral properties of H_Λ announced in the introduction. We follow the ideology used in the regular case,[9,10] localizing first the essential spectrum and finding afterwards the subsets where it is absolutely continuous. In view of the partial wave decomposition (2.1) it is natural to start with the partial wave operators H_l.

The essential spectrum is stable under a rank one perturbation, hence adding the Dirichlet boundary condition at a point $a > 0$ to each of the operators H_l, h_Λ we do not change their essential spectrum. Moreover, multiplication by Cx^{-2} is a relatively compact operator on $L^2(a, \infty)$, thus the essential spectra of the said operators coincide,

$$\sigma_{ess}(\mathsf{H}_l) = \sigma_{ess}(\mathsf{h}_\Lambda). \tag{4.1}$$

With this prerequisite we can pass to our first main result.

Theorem 4.1. *The essential spectrum of the operator (2.1) is equal to*

$$\sigma_{ess}(\mathsf{H}_\Lambda) = [\inf \sigma_{ess}(\mathsf{h}_\Lambda), \infty)\,. \tag{4.2}$$

The idea of the proof is the same as in Ref. 9: First we check that $\inf \sigma_{ess}(\mathsf{H}_\Lambda)$ cannot be smaller than $\inf \sigma_{ess}(\mathsf{h}_\Lambda)$, after that we show that $\sigma_{ess}(\mathsf{H}_\Lambda)$ contains the whole interval $[\inf \sigma_{ess}(\mathsf{h}_\Lambda), \infty)$.

Proposition 4.1. *Under the assumptions stated we have*

$$\inf \sigma_{ess}(\mathsf{H}_\Lambda) \geq \inf \sigma_{ess}(\mathsf{h}_\Lambda)\,. \tag{4.3}$$

Proof. If $\nu > 2$ we infer from equations (4.1), (4.4) that

$$\inf \sigma_{ess}(\mathsf{H}_\Lambda) \geq \inf_l \inf \sigma(\mathsf{H}_l) = \inf \sigma_{ess}(\mathsf{h}_\Lambda)\,;$$

notice that with the exception of the case $\nu = 2$, $l = 0$ the centrifugal term in the partial waves operators (2.2) is strictly positive, and consequently, the mini-max principle implies

$$\inf \sigma(\mathsf{H}_l) \geq \inf \sigma(\mathsf{h}_\Lambda) = \inf \sigma_{ess}(\mathsf{H}_l) \geq \inf \sigma(\mathsf{H}_l). \tag{4.4}$$

For $\nu = 2$ the argument works again, we have just to be a little more cautious: for the operator $\mathsf{A} := \bigoplus_{l\neq 0} \mathsf{U}^{-1}\mathsf{H}_l\mathsf{U}\otimes\mathsf{I}_l$ the above reasoning yields $\inf\sigma_{ess}(\mathsf{A}) \geq \inf\sigma_{ess}(\mathsf{h}_\Lambda)$ and the proposition follows from the equation

$$\inf\sigma_{ess}((\mathsf{U}^{-1}\mathsf{H}_0\mathsf{U}\otimes\mathsf{I}_0)\oplus\mathsf{A}) = \min(\inf\sigma_{ess}(\mathsf{H}_0),\, \inf\sigma_{ess}(\mathsf{A})). \qquad \square$$

Proposition 4.2. $\sigma_{ess}(\mathsf{H}_\Lambda) \supset [\inf\sigma_{ess}(\mathsf{h}_\Lambda), \infty]$.

Proof. The idea is to employ Weyl criterion. Let $\lambda_0 \in \sigma_{ess}(h_\Lambda)$ and $\lambda > 0$, then we have to show that for every $\varepsilon > 0$ there exists a nonzero function

$$\phi \in D(\mathsf{H}_\Lambda) \quad \text{satisfying} \quad \|(\mathsf{H}_\Lambda - \lambda_0 - \lambda)\phi\| \leq \varepsilon\|\phi\|.$$

Basic properties of the essential spectrum together with Lemma 3.2 provide us with a compactly supported $u \in D(\mathsf{h}_\Lambda)$ such that $\|u'' - \lambda_0 u\| \leq \frac{1}{2}\varepsilon$. In view of the periodicity we may suppose that $supp\, u \subset (0,\, L)$. Next we are going to estimate λ by the repulsive centrifugal potential in a suitably chosen partial wave. Putting $l_R := [\sqrt{\lambda R}\,]$ we have

$$\frac{1}{r^2}\left[\frac{(\nu-1)(\nu-3)}{4} + l_R(l_R+\nu-2)\right] = \lambda + \mathcal{O}(R^{-1}) \quad \text{for} \quad r \in [R,\, R+L]$$

as $R \to \infty$, hence choosing R large enough one can achieve that

$$\sup_{r\in[R,\,R+L]} \left|\frac{1}{r^2}\left[\frac{(\nu-1)(\nu-3)}{4} + l_R(l_R+\nu-2)\right] - \lambda\right| \leq \frac{1}{2}\varepsilon\,.$$

Next we employ the partial wave decomposition, considering a unit vector $Y \in S_{l_{n_\varepsilon}}$ and putting $\phi(x) := \mathsf{U}^{-1}u(|x|-R)Y(x/|x|)$. It holds obviously $\phi \in D(\mathsf{H}_\Lambda)$, $\|\phi\| = \|u(\cdot - R)\|$, and[b]

$$\begin{aligned}
&\|\mathsf{H}_\Lambda\phi - (\lambda_0+\lambda)\phi\| = \|\mathsf{H}_{l_R}u(r-R) - (\lambda_0+\lambda)u(r-R)\| \\
&\quad \leq \|u''(r-R) - \lambda_0 u(r-R)\| \\
&\quad + \left\|\left(\frac{1}{r^2}\left[\frac{(\nu-1)(\nu-3)}{4} + l_R(l_R+\nu-2)\right] - \lambda\right)u(r-R)\right\| \leq \varepsilon\|\phi\|,
\end{aligned}$$

which concludes the proof. $\square$

Once the essential spectrum is localized, we can turn to its continuous component. In view of the decomposition (2.1) we have to describe the continuous spectrum in each partial wave and the results for H_Λ will immediately follow; recall that the essential spectrum of H_l consists of the

[b]For the sake of simplicity we allow ourselves the licence to write $\|f\| \equiv \|f(\cdot)\| = \|f(r)\|$ in the following formula.

bands of the underlying one-dimensional operator h_Λ. Our strategy is to prove that the transfer matrix — defined in the appendix, Sec. 5 below — is bounded inside the bands, which implies that the spectrum remains absolutely continuous.[8,16] The following claim is a simple adaptation of Lemma 2 from Ref. 10 to the singular case.

Lemma 4.1. *Let (a, b) be the interior of a band of the operator h_Λ in $L_2(\mathbb{R})$. Let further $K \subset (a, b)$ be a compact subinterval, $c \in \mathbb{R}$, and $x_0 > 0$. Then there is a number $C > 0$ such that for every $\lambda \in K$ any solution u of*

$$-u'' + \frac{c}{r^2} u = \lambda u, \quad u \in D(\mathsf{h}_\Lambda) \tag{4.5}$$

with the normalization

$$|u(x_0)|^2 + |u'(x_0)|^2 = 1 \tag{4.6}$$

satisfies in (x_0, ∞) the inequality

$$|u(x)|^2 + |u'(x)|^2 \le C\,. \tag{4.7}$$

Proof. For a fixed $\lambda \in K$ the equation $\mathsf{h}_\Lambda w = \lambda w$ has two real-valued, linearly independent solutions, $u_0 = u_0(\cdot, \lambda)$ and $v_0 = v_0(\cdot, \lambda)$, such that u_0, $v_0 \in D(\mathsf{h}_\Lambda)$ and the functions $|u_0|$, $|u_0'|$, $|v_0|$, $|v_0'|$ are periodic, bounded, and continuous with respect to λ, cf. Ref. 17). Without loss of generality we may assume that the determinant of the matrix

$$Y = \begin{bmatrix} u_0 & v_0 \\ u_0' & v_0' \end{bmatrix}$$

equals one; note that u_0, v_0 are real-valued and hence $\det Y$ is continuous at the singular points in view of Lemma 3.3. It is also nonzero, hence to any solution u of (4.5) we can define the function

$$y := Y^{-1} \begin{bmatrix} u \\ u' \end{bmatrix}$$

which satisfies

$$y' = Ay \quad \text{on every interval} \quad (na, (n+1)a), \tag{4.8}$$

where the the matrix A is given by

$$A := -\frac{c}{x^2} \begin{bmatrix} u_0 v_0 & v_0^2 \\ -u_0^2 & -u_0 v_0 \end{bmatrix},$$

being integrable away from zero. By a straightforward calculation we get

$$y = \begin{bmatrix} v_0' u - v_0 u' \\ -u_0' u + u_0 u' \end{bmatrix}$$

and using Lemma 3.3 again we infer that y is continuous at the singular points. Consequently,

$$y(x) = \exp\left\{ \int_{x_0}^{x} A(t)\, \mathrm{d}t \right\} y(x_0)$$

is a solution of (4.8) and following Ref. 10 we arrive at the estimates

$$\frac{1}{2}(|y|^2)' \le |(y,\, y')| \le \|A\| |y|^2$$

which further yield

$$|y(x)|^2 \le |y(x_0)|^2 \exp\left\{ 2 \int_{x_0}^{x} \|A\|(t)\, \mathrm{d}t \right\} \le |Y^{-1}(x_0)|^2 \exp\left\{ 2 \int_{x_0}^{\infty} \|A\|(t)\, \mathrm{d}t \right\}$$

for $x \ge x_0$ and every solution of (4.5) with the normalization (4.6). From

$$\begin{bmatrix} u(x) \\ u'(x) \end{bmatrix} = Y(x) Y^{-1}(x_0) \begin{bmatrix} u(x_0) \\ u'(x_0) \end{bmatrix} + \int_{x_0}^{x} Y(x) A(t) y(t) \mathrm{d}t$$

we then infer that the function $|u(\cdot)|^2 + |u'(\cdot)|^2$ is bounded in the interval (x_0, ∞) which we set out to prove. □

Now we are ready to describe the essential spectrum of H_Λ.

Theorem 4.2. *For H_Λ defined by (2.1) the following is true:*

(i) For any gap $(E_{2k-1},\, E_{2k})$ in the essential spectrum of h_Λ,
  (a) H_Λ has no continuous spectrum in $(E_{2k-1},\, E_{2k})$, and
  (b) the point spectrum of H_Λ is dense in $(E_{2k-1},\, E_{2k})$.

(ii) On any compact K contained in the interior of a band of h_Λ the spectrum of H_Λ is purely absolutely continuous.

Proof. (i) By (4.1), none of the operators H_l, $l = 0, 1, 2, \ldots$ has a continuous spectrum in $(E_{2k-1},\, E_{2k})$, hence H_Λ has no continuous spectrum in this interval either. On the other hand, the entire interval $(E_{2k-1},\, E_{2k})$ is contained in the essential spectrum of H_Λ; it follows that the spectrum of H_Λ in $(E_{2k-1},\, E_{2k})$ consists solely of eigenvalues which are necessarily

dense in that interval.
(ii) The claim follows from the previous lemma and Refs. 8,16. To make the article self-contained we prove in the appendix a weaker result which still guarantees the absolute continuity of the spectrum in the bands in our singular case. □

Remark 4.1. The distribution of eigenvalues of the operators partial wave H_l in the gaps of the underlying one-dimensional operator was studied in Refs. 2,12 Specifically, let $q(\cdot)$ be a periodic function and $(a,\, b)$ an interval inside a gap of the operator $-\frac{d^2}{dx^2}+q(x)$, then there is a numerical evidence[2] for the conjecture that the number of eigenvalues of the operator $-\frac{d^2}{dx^2}+q(x)+\frac{c}{x^2}$ in the said interval is proportional to $\sqrt{c}$. A similar question could be asked in the singular case but we do not address it here.

5. The discrete spectrum

Recall that with the exception of the case $\nu = 2$, $l = 0$ the centrifugal term in the partial waves operators (2.2) is strictly positive, hence by the mini-max principle there is no discrete spectrum below E_0. On the other hand, in the two-dimensional case Brown et al. noticed that regular radially periodic potentials give rise to bound states[1] which they named to honor the place where the observation was made. Subsequently Schmidt[14] proved that there are infinitely many such eigenvalues of the operator H_0 below $\inf\sigma_{\mathrm{ess}}(\mathsf{H}_\Lambda)$. Our aim is to show that this result persists for singular sphere interactions considered here.

Theorem 5.1. *Let $\nu = 2$, then except of the free case the operator H_Λ has infinitely many eigenvalues in $(-\infty, E_0)$, where $E_0 := \inf\sigma_{\mathrm{ess}}(\mathsf{H}_\Lambda)$.*

Proof. The argument is again similar to that of the regular case,[15] hence we limit ourselves to just sketching it. First of all, it is clear that we have to investigate the spectrum of $\mathsf{H}_{\Lambda,0}$.

Let u, v be linearly independent real-valued solutions of the equation $\mathsf{h}_\Lambda z = E_0 z$, where u is (anti)periodic — cf. Proposition 3.1. — satisfying $W[u,\, v] = 1$. We will search for the solution of $\mathsf{H}_0 y \equiv -y'' - \frac{1}{4r^2}y = E_0 y$, we are interested in, using a Prüfer-type Ansatz, namely

$$\begin{pmatrix} y \\ y' \end{pmatrix} = \begin{pmatrix} u & v \\ u' & v' \end{pmatrix} a \begin{pmatrix} \sin\gamma \\ -\cos\gamma \end{pmatrix},$$

where a is a positive function and γ is chosen continuous recalling Lemma 3.3 and eq. (3.4). It is demonstrated in Ref. 15 that the function

$\gamma(\cdot)$ and the standard Prüfer variable $\theta(\cdot)$, appearing in

$$\begin{pmatrix} y \\ y' \end{pmatrix} = \rho \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix},$$

are up to a constant asymptotically equal to each other as $r \to \infty$. According to Corollary 5.1 there are then infinitely many eigenvalues below E_0 if θ, and therefore also γ, is unbounded from below.

Now a straightforward computation yields

$$\gamma' = -\frac{1}{4r^2}(u\sin\gamma - v\cos\gamma)^2 = -\frac{1}{4}\,\cos^2\gamma\, u^2\Big(\frac{1}{r}\tan\gamma - \frac{v}{r\,u}\Big)^2.$$

Furthermore, the Kepler transformation given by the relation $\tan\phi = (r^{-1}\tan\gamma - r^{-1}v/u)$ satisfies $\gamma(r) = \phi(r) + \mathcal{O}(1)$ as $r \to \infty$, and

$$\begin{aligned}\phi' &= \frac{1}{r}\Big(-\sin\phi\cos\phi - \frac{1}{4}u^2\sin^2\phi - \frac{1}{u^2}\cos^2\phi\Big) \\ &= -\frac{1}{2r}\left(\frac{1}{u^2} + \frac{1}{4}u^2 + \sin 2\phi + \Big(\frac{1}{u^2} - \frac{1}{4}u^2\Big)\cos 2\phi\right) \qquad (5.1)\end{aligned}$$

holds on $\mathbb{R} \setminus \cup_n\{r_n\}$ with the discontinuity

$$\tan\phi(r_n+) - \tan\phi(r_n-) = -\frac{1}{r_n}\frac{\beta}{u(r_n+)u(r_n-)}, \qquad (5.2)$$

where β is the parameter appearing in (2.3). A direct analysis of the equation (5.1) shows that $\phi' \le 0$, and owing to (5.2) and Proposition 3.1 the corresponding discontinuity is strictly negative for $\beta \neq 0$. Hence ϕ is decreasing and there is a limit $L = \lim_{r\to\infty}\phi(r)$. Suppose that L is finite. Then the condition $|\int_0^\infty \phi'(t)\,\mathrm{d}t| < \infty$ gives

$$\frac{1}{u^2(r)} + \frac{1}{4}u^2(r) + \sin 2\phi(r) + \left(\frac{1}{u^2(r)} - \frac{1}{4}u^2(r)\right)\cos 2\phi(r) \to 0 \quad \text{as} \quad r \to \infty \qquad (5.3)$$

and, as u is (anti)-periodic and ϕ tends to a constant, we infer that u^2 is constant also, not only asymptotically but everywhere. With the exception of the free case this may happen only for pure repulsive δ' interaction, $\beta > 0$, $\alpha = 0$, $\gamma = \delta = 1$. To finish the proof we employ eq. (5.3) again and observe that $L \neq \pi/2 \,(\mathrm{mod}\,\pi)$ holds necessarily. We thus find a monotonous sequence of points r_n such that $\phi(r_n-) < \frac{\pi}{2}\left(1 + \left[\frac{2L}{\pi}\right]\right)$, where $[\cdot]$ is the integer part. Since ϕ is monotonous we have $\phi(r_n\pm) \ge L$, hence all these points belong to the same branch of the tan function. Summing then the

discontinuities (5.2) we get

$$\begin{aligned}\tan\phi(r_N+) - \tan\phi(r_n-) \;&\le \sum_{i=n}^{N} \tan\phi(r_i+) - \tan\phi(r_i-) \\ &= -\sum_{i=n}^{N} \frac{1}{r_i} \frac{\beta}{u(r_i+)u(r_i-)}\,,\end{aligned}$$

where the right-hand side diverges as $N \to \infty$ for any $\beta > 0$, while the left-hand side tends to a finite number $\tan(L) - \tan\phi(r_n-)$. Hence L can be finite for the free Hamiltonian only, which was to be demonstrated. □

Appendix A: Continuous spectra for one dimensional Schrödinger operators with singular interactions

In this appendix we consider Schrödinger operators on a half-line,

$$(\mathsf{H}u)(x) = -u''(x) + V(x)u(x) \tag{5.1}$$

$$u(0) = 0, \quad U(x_n+) = \Lambda U(x_n-), \tag{5.2}$$

where we suppose that the condition

$$\int_K^\infty |u'|^2 \le \beta \int_K^\infty (|\mathsf{H}u|^2 + |u|^2), \tag{5.3}$$

holds for some β, $K > 0$ and every $u \in D(\mathsf{H})$. This is obviously the case of operators $\mathsf{H}_{\lambda,l}$, where in the dimension $\nu > 2$ we may put $K = 0$, while for $\nu = 2$ we have to choose $K > 0$.

Given a solution u of $\mathsf{H}u = Eu$ we define the transfer matrix $\mathsf{T}(E, x, y)$ at energy E by

$$\mathsf{T}(E, x, y) \begin{pmatrix} u'(y) \\ u(y) \end{pmatrix} = \begin{pmatrix} u'(x) \\ u(x) \end{pmatrix}. \tag{5.4}$$

Our purpose is to prove the following result.

Theorem 5.2. *Let $\mathsf{T}(E, x, y)$ be bounded on S. Then for every interval $(E_1, E_2) \subset S$ we have $\rho_{ac}((E_1, E_2)) > 0$ and $\rho_{sc}((E_1, E_2)) = 0$, where ρ denotes the spectral measure associated with the operator H.*

Following Ref. 16 we employ the theory of Weyl m-functions. For $E \in C_+ = \{z, \operatorname{Im} z > 0\}$, there is a unique solution $u_+(x, E)$ of $\mathsf{H}u_+(x, E) = Eu_+(x, E)$ with $u_+ \in L^2$ at infinity, which is normalized by $u_+(0, E) = 1$. We define the m-function by

$$m_+(E) = u'_+(0, E)\,;$$

the spectral measure ρ is then related to it by

$$\mathsf{d}\rho(E) = \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \operatorname{Im} m_+(E + i\varepsilon)\,,$$

where the imaginary part at the right-hand side can be expressed as

$$\operatorname{Im} m_+(E) = \operatorname{Im} E \int_0^\infty |u_+(x,\, E)|^2 \mathsf{d}x. \tag{5.5}$$

It is known, see Ref. 16 and references therein, that

$$\operatorname{supp} \rho_{sc} = \left\{ E :\, \lim_{\varepsilon \downarrow 0} \operatorname{Im} m_+(E + i\varepsilon) = \infty \right\},$$

while $\mathsf{d}\rho_{ac}(E) = \frac{1}{\pi} \operatorname{Im} m_+(E + i0)\, \mathsf{d}E$. Theorem 5.2 is then an immediate consequence of the following result.

Theorem 5.3. *If* $\mathsf{T}(E,\, x,\, y)$ *be bounded as above and* $E \in (E_1,\, E_2)$*, then*

$$\liminf \operatorname{Im} m_+(E + i0) > 0 \quad \text{and} \quad \limsup \operatorname{Im} m_+(E + i0) < \infty\,.$$

Proof. For $x \neq x_n$ we have the relations

$$\frac{\mathsf{d}\mathsf{T}(E,\, x,\, y)}{\mathsf{d}x} = \begin{pmatrix} 0 & V(x) - E \\ 1 & 0 \end{pmatrix} \mathsf{T}(E,\, x,\, y),$$

$$\frac{\mathsf{d}}{\mathsf{d}y} \left(\mathsf{T}(E_1,\, x,\, y) \mathsf{T}(E_2,\, y,\, x) \right) = (E_1 - E_2) \mathsf{T}(E_1,\, x,\, y) \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \mathsf{T}(E_2,\, y,\, x).$$

It is straightforward to verify that $\mathsf{T}(E_1,\, x,\, y)\mathsf{T}(E_2,\, y,\, x)$ is continuous at singular points with respect to y and hence

$$1 - \mathsf{T}(E_1,\, x,\, 0)\mathsf{T}(E_2,\, 0,\, x) = \int_0^x (E_1 - E_2) \mathsf{T}(E_1,\, x,\, y) \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \mathsf{T}(E_2,\, y,\, x) \mathsf{d}y.$$

Now we put $E_1 = E$, $E_2 = E + i\varepsilon$ and multiply by $\mathsf{T}(E + i\varepsilon,\, x,\, 0)$ from the right to get the formula

$$\mathsf{T}(E + i\varepsilon,\, x,\, 0) = \mathsf{T}(E,\, x,\, 0) - (i\varepsilon) \int_0^x \mathsf{T}(E,\, x,\, y) \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \mathsf{T}(E + i\varepsilon,\, y,\, 0) \mathsf{d}y.$$

By assumption we have $\|\mathsf{T}(E,\, x,\, y)\| \leq C$, and therefore

$$\|\mathsf{T}(E + i\varepsilon,\, x,\, 0)\| \leq C + \varepsilon \int_0^x C \|\mathsf{T}(E + i\varepsilon,\, y,\, 0)\| \mathsf{d}y\,,$$

so by an iteration we get

$$\|\mathsf{T}(E + i\varepsilon,\, x,\, 0)\| \leq C e^{\varepsilon C x}.$$

Note that $\det \mathsf{T} = 1$ so $\|\mathsf{T}\| = \|\mathsf{T}^{-1}\|$. Putting now $\gamma = ((E+1)^2\beta^2 + 1)^{-1}$ and using the condition (5.3) we get

$$\begin{aligned}\int_0^\infty |u(x)|^2 \mathrm{d}x &\geq \gamma \int_K^\infty (|u(x)|^2 + |u'(x)|^2)\mathrm{d}x \\ &\geq C^{-2}\gamma(1+|m_+|^2)\int_K^\infty e^{-2\varepsilon C x}\mathrm{d}x\,,\end{aligned}$$

hence by (5.5) we infer that

$$\operatorname{Im} m_+ \geq \frac{1}{2}C^{-3}\gamma(1+|m_+|^2)\,.$$

From here the first claim follows immediately, and since

$$2C^3\gamma^{-1} \geq \frac{1+|m_+|^2}{\operatorname{Im} m_+} \geq |m_+|\,,$$

we get also the remaining part. □

Appendix B: Oscillation theory for singular potentials

In the case of point interactions the classical oscillation theory fails due to the discontinuity of the wave functions. Nevertheless, we can employ the continuity of the Wronskian and formulate the oscillation theory using the approach of relative oscillations.[7] The aim of this appendix is to present briefly the basic theorems; since the claims are the same as in the regular case we follow closely the above mentioned article. The same applies to the proofs which are again closely similar to those in the regular case; to observe the volume limit set for these proceedings contribution we refrain from presenting them.

We consider Schrödinger-type operators on $L^2(l_-, l_+)$ with the singular interactions at the points $x_n \in (l_-, l_+)$, $n \in M \subset \mathbb{N}$ which act as

$$\mathsf{T}u(x) = -u''(x) + q(x)u(x),$$

with a real-valued potential $q \in L^1_{\mathrm{loc}}(l_-, l_+)$ and the domain

$$\begin{aligned}D(\mathsf{T}) = \Big\{ u,\, u' \in AC_{\mathrm{loc}}\Big((l_-, l_+) \setminus \bigcup_{n\in M}\{x_n\}\Big) \,:\, \\ \mathsf{T}u \in L^2_{\mathrm{loc}}(l_-, l_+) \quad \text{and} \quad U(x_n+) = \Lambda_n U(x_n-)\Big\}\,.\end{aligned}$$

Such an operator is obviously symmetric. Denote by H an arbitrary self-adjoint extension of it satisfying either

(a) T is limit point in at least one endpoint, or
(b) H is defined by separated boundary conditions.

By $\psi_\pm(E, x)$ we denote the real-valued solutions of the equation $\mathsf{T}\psi_\pm(E, x) = E\psi_\pm(E, x)$, which satisfy the boundary conditions defining H at the points $l_\pm$, respectively. Note that such solutions may not exist, the theorems given below implicitly assume their existence. In particular, their existence is guaranteed for energies E outside the essential spectrum. Moreover, in view of the analyticity in the spectral parameter we may use the oscillation theory also at the edges of the essential spectrum.

The first theorem to follow provides the basic oscillation result, while the corollary of the second one is the result used in Section 5. By $W_0(u_1, u_2)$ we denote the number of zeros of the Wronskian $W[u_1, u_2](x)$ in the open interval (l_-, l_+), and given $E_1 < E_2$, we put $N_0(E_1, E_2) = \dim \mathrm{Ran}\mathsf{P}_{(E_1, E_2)}$, where P is the spectral measure of the self-adjoint operator H; we note that $N_0(E_1, E_2)$ may even be infinite. In particular, in case of the pure point spectrum $N_0(E_1, E_2)$ simply denotes the number of eigenvalues in the interval (E_1, E_2).

Theorem 5.4. *Suppose that $E_1 < E_2$ and put $u_1 = \psi_-(E_1)$, $u_2 = \psi_+(E_2)$. Then $W_0(u_1, u_2) = N_0(E_1, E_2)$.*

Theorem 5.5. *Let $E_1 < E_2$. Assume that either $u_1 = \psi_+(E_1)$ or $u_1 = \psi_-(E_1)$ holds, and similarly either $u_2 = \psi_+(E_2)$ or $u_2 = \psi_-(E_2)$. Then $W_0(u_1, u_2) \le N_0(E_1, E_2)$.*

Next we introduce Prüfer variables ρ_i, θ_i defined by

$$\begin{pmatrix} u_i(x) \\ u_i'(x) \end{pmatrix} = \rho_i(x) \begin{pmatrix} \cos\theta_i(x) \\ \sin\theta_i(x) \end{pmatrix},$$

where ρ_i is chosen positive and θ_i is uniquely determined by its boundary value and the requirement that θ_i is continuous on $(l_-, l_+) \setminus \bigcup_{n\in M}\{x_n\}$ while its discontinuity at the sites x_n of the point interactions satisfies $|\theta_i(x_n+) - \theta_i(x_n-)| = 0 \,(\mathrm{mod}\,\pi)$.

Corollary 5.1. *Suppose that E_1 is the edge of the essential spectrum, and $u_1 = \psi_-(E_1)$ or $u_1 = \psi_+(E_1)$. Then H has infinitely many eigenvalues below E_1 if $\theta_1(\cdot)$ is unbounded.*

Proof. In analogy with the regular case the function θ_2 corresponding to $u_2 = \psi_\pm(E)$ is bounded for negative E large enough. This implies that

$|\theta_2 - \theta_1| \to \infty$ and since $W[u_1, u_2](x) = \rho_1(x)\rho_2(x)\sin(\theta_2(x) - \theta_1(x))$ we get $W_0(u_1, u_2) = \infty$. Hence Theorem 5.5. completes the proof. □

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POINTWISE EXISTENCE OF THE LYAPUNOV EXPONENT FOR A QUASI-PERIODIC EQUATION

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In this note, we discuss the point-wise existence of the Lyapunov exponent for the ergodic family $\psi(n+1)+\psi(n-1)=2\lambda e^{i\pi\omega/2}\sin(\pi(n\omega+\theta))\psi(n)$, $n\in\mathbb{Z}$. Here, $\lambda>1$ is a fixed coupling constant, $\omega\in(0,1)$ is a fixed frequency, and $\theta\in[0,1)$ is the ergodic parameter numbering the equations. This is actually the Almost Mathieu equation with zero spectral parameter (and complex coupling constant). This model is related to various self-adjoint models via a cocycle representation. The existence of the Lyapunov exponent and the behavior of the solution can be described quite explicitly.

Keywords: Lyapunov exponent, quasi-periodic equation, ergodic family, Almost Methiew operator

1. Introduction

1.1. *Quasi-periodic finite difference equations*

Consider the finite difference Schrödinger equation

$$(H_\theta\psi)(n)=\psi(n+1)+\psi(n-1)+v(n\omega+\theta)\psi(n)=E\psi(n), \qquad (1.1)$$

where $v:\mathbb{R}\to\mathbb{R}$ is continuous and periodic, $v(x+1)=v(x)$, $0<\omega<1$ and $0\le\theta<1$. When $\omega\notin\mathbb{Q}$, the mapping $n\mapsto v(n\omega+\theta)$ is quasi-periodic.

The spectral theory of such quasi-periodic equations is very rich, and the study has generated a vast literature; among the authors are A. Avila, Y. Avron, J. Bellissard, J. Bourgain, V. Buslaev, V. Chulaevsky, D. Damanik, E. Dinaburg, H. Eliasson, A. F., B. Helffer, M. Hermann,

S. Jitomirskaya, F. K., R. Krikorian, Y. Last, L.Pastur, J. Puig, M. Shubin, B. Simon, Y. Sina¨ i, J. Sjöstrand, S. Sorets, T. Spencer, M. Wilkinson and many others (see e.g. Ref. 9 for a recent survey).

Speaking about intriguing spectral phenomena, one can mention for example that:

- For such equations, the spectral nature depends on the "number theoretical" properties of the frequency ω;

and that one expects that:

- Typically such equations exhibit Cantorian spectrum;
- $\sigma_{pp}(H_\theta)$, the singular continuous spectrum, is topologically typical.

This has been well understood only for a few models, most prominently, for the almost Mathieu equation when $v(x) = 2\lambda\cos(x)$).

1.2. *Lyapunov exponent*

One of the central objects of the spectral study of the quasi-periodic equations is the Lyapunov exponent. Recall its definition. Equation (1.1) can be rewritten as

$$\begin{pmatrix}\psi(n+1)\\ \psi(n)\end{pmatrix} = M(n\omega+\theta)\begin{pmatrix}\psi(n)\\ \psi(n-1)\end{pmatrix}, \quad M(x) = \begin{pmatrix}E-v(x) & -1\\ 1 & 0\end{pmatrix}. \tag{1.2}$$

So the large n behavior of solutions to (1.1) can be characterized by the limits (when they exist) :

$$\gamma^+(E,\theta) = \lim_{n\to+\infty}\frac{1}{n}\log\|M((n-1)\omega+\theta)\cdots M(\theta+\omega)\,M(\theta)\| \tag{1.3}$$

$$\gamma^-(E,\theta) = \lim_{n\to+\infty}\frac{1}{n}\log\|M^{-1}(\theta-n\omega)\cdots M^{-1}(\theta-2\omega)\,M^{-1}(\theta-\omega)\| \tag{1.4}$$

Furstenberg and Kesten have proved (see Ref. 2)

Theorem 1.1. *Fix E. For almost every θ, these limits exist, coincide and do not depend on θ.*

For energies E such that the limits exist, coincide and do not depend on θ, their common value is called the *Lyapunov exponent*; we denote it by $\gamma(E)$.

We are interested in the pointwise (in both E and θ) existence of the limits $\gamma^+(E,\theta)$ and $\gamma^-(E,\theta)$. We call them the *right* and *left* Lyapunov exponents. Speaking about the pointwise existence of the Lyapunov exponent

itself, we say that it does not exist for a pair (E, θ) when either at least one of $\gamma^{\pm}(E, \theta)$ does not exist or both of them exist, but at least one of them differs from $\gamma(E)$.

1.3. *Lyapunov exponents and the spectrum*

For $\omega \notin \mathbb{Q}$, one has the following theorem by Ishii - Pastur - Kotani.[2]

Theorem 1.2. *The absolutely continuous spectrum, $\sigma_{ac}(H_\theta)$, is the essential closure of the set of energies where the Lyapunov exponent vanishes.*

This theorem immediately implies (see Ref. 2)

Corollary 1.1. *If $\gamma(E)$ is positive on I, an interval, then the spectrum in I (if any) is singular, $\sigma \cap I \subset \sigma_s$.*

As, in general, singular continuous spectrum can be present, in this statement, one cannot replace σ_s, the singular spectrum, with σ_{pp}, the pure point spectrum. One may ask if it is possible to characterize the singular continuous spectrum in terms of the Lyapunov exponent. Consider equation (1.1) on the interval $E \in I$ where $\gamma(E) > 0$. Almost surely, for a given θ, the Lyapunov exponents exist a priori only almost everywhere in E. Denote by I_{Lyapunov} the subset of I where $\gamma^+(E, \theta)$ and $\gamma^-(E, \theta)$ both exist and are positive. For $E \in I_{\text{Lyapunov}}$, the solutions to (1.1) have to increase or decrease exponentially (see, e.g., Ref. 2). This implies that the singular continuous component of the spectral measure vanishes on I_{Lyapunov}. So, it can be positive only on $I \setminus I_{\text{Lyapunov}}$. And, the latter must happen if the spectrum on I is singular continuous.

1.4. *B. Simon's example*

We now recall an example by B.Simon showing that, for quasi-periodic operators, one can find singular continuous spectrum on an interval where the Lyapunov exponent is positive.

Consider the Almost Mathieu equation, i.e., equation (1.1) with $v(\theta) = 2\lambda \cos\theta$.

For this equation, by Herman's theorem,[7] $\gamma(E) \geq \log \lambda$. We assume that $\lambda > 1$. Then, $\gamma(E)$ is positive for all E, and the spectrum is singular.

Let the frequency ω be such that, for some infinite sequence $(p_m, q_m) \in \mathbb{N} \times \mathbb{N}^*$,

$$\left| \omega - \frac{p_m}{q_m} \right| \leq m^{-q_m}.$$

Such Liouvillean frequencies are topologically typical but of zero measure.

One has

Theorem 1.3.[2] *Under the above conditions, there are no eigenvalues and the spectrum is purely singular continuous.*

Note that this result is a consequence of a theorem by A. Gordon (see Ref. 4,5) which roughly says that when the quasi-periodic potential can be super-exponentially well approximated by periodic potentials, the equation (1.1) does not admit any decreasing solutions.

Note that actually, in the case of the almost Mathieu equation, Gordon's result implies that any of its solution ϕ satisfies the inequality

$$\overline{\lim}_{m\to\infty} \max\left(\, \phi(\pm q_m), \phi(\pm 2q_m)\,\right) \geq \frac{1}{2}\phi(0),$$
$$\phi(n) = (|\psi(n+1)|^2 + |\psi(n)|^2)^{1/2}.$$

This means that the corresponding generalized eigenfunctions have to have infinitely many humps located at some of the points $\pm q_m$, $\pm 2q_m$, $m \in \mathbb{N}$. These humps prevent the solutions from being square summable.

1.5. *Non-trivial model problem*

In the present note, we concentrate on the model equation

$$\psi(n+1) + \psi(n-1) = \lambda v_0(n\omega + \theta)\ \psi(n), \quad n \in \mathbb{Z}, \tag{1.5}$$
$$v_0(\theta) = 2\, e^{i\pi\omega/2} \sin(\pi\theta), \tag{1.6}$$

where $0 < \omega < 1$ is an irrational frequency, $1 < \lambda$ is a coupling constant, and θ is the ergodic parameter. Actually, up to a shift in θ, this is an Almost Mathieu equation with the spectral parameter equal to zero.

We study this equation for the following reasons:

(1) A large part of analysis is quite simple whereas (we believe that) to carry it out one has to use a non trivial renormalization procedure;
(2) The techniques developed in this study can be generalized to the case of real analytic potentials v;
(3) This model is related to various self-adjoint models via a cocycle representation (see Ref. 3), e.g., it comes up naturally when studying the spectral properties of the equation

$$-\psi''(t) + \alpha \sum_{l\geq 0} \delta\left(\, l(l-1)/2 + l\phi_1 + \phi_2 \,-\, t\,\right)\ \psi(t) = E\psi(t).$$

For the model equation (1.5), our ultimate goal is to describe the set of θ for which the Lyapunov exponent exists or does not exist and to describe the solutions both when the Lyapunov exponent exists and does not exist.

We concentrate on the case of frequencies complementary to the frequencies occurring Simon's example. And, in the case when the Lyapunov exponent does not exist, this leads to a new scenario for the behavior of solutions of (1.1).

Our main tool is the the *monodromization* renormalization method introduced by V. Buslaev - A. Fedotov originally for the semi-classical study of the geometry of the spectrum of one dimensional finite difference almost periodic equations, see Ref. 1. The idea was to construct Weyl solutions outside the spectrum but, at each step of the renormalization, closer to spectrum so as to uncover smaller and smaller gaps in the spectrum. Now, essentially, we use it to study the solutions of the model equation on the spectrum.

2. Existence of the Lyapunov exponent for the model equation

We now formulate our results on the pointwise existence of the right Lyapunov exponent $\gamma^+(\theta)$ for the model equation (1.5); as we have set the energy parameter, to a fixed value, we omit it in the Lyapunov exponents. The right Lyapunov exponent is defined by the formula (1.3) with

$$M(x) = \begin{pmatrix} \lambda v_0(\theta) & -1 \\ 1 & 0 \end{pmatrix}, \tag{2.1}$$

where v_0 is given by (1.6). Note that for $\gamma^-(\theta)$, the left Lyapunov exponent, one has similar results.

2.1. *Main result*

Here, we formulate a sufficient condition for the existence of the Lyapunov exponent. Therefore, we need to introduce some notations. For $L = 0, 1, 2 \ldots$, define

$$\omega_{L+1} = \left\{ \frac{1}{\omega_L} \right\}, \quad \omega_0 = \omega.$$

where $\{a\}$ is the fractional part of $a \in \mathbb{R}$, and

$$\lambda_{L+1} = \lambda_L^{\frac{1}{\omega_L}}, \quad \lambda_0 = \lambda$$

Remark 2.1. The numbers $\{\omega_l\}_{l=1}^{\infty}$ are related to the continued fraction expansion of ω:

$$\omega = \frac{1}{a_1+\omega_1} = \frac{1}{a_1+\frac{1}{a_2+\omega_2}} = \frac{1}{a_1+\frac{1}{a_2+\frac{1}{a_3+\omega_3}}} =$$
$$\ldots = \frac{1}{a_1+\frac{1}{a_2+\frac{1}{a_3+\frac{1}{a_4+\ldots}}}}$$

where $a_1, a_2, a_3 \ldots \in \mathbb{N}$ are the elements of the continuous fraction for ω. It is well known that, for any $l \in N$, one has $\omega_l\omega_{l+1} \leq 1/2$. This implies that the numbers λ_l increase super-exponentially.

Furthermore, for a given $\omega \in (0,1) \setminus \mathbb{Q}$ and $s \in (0,1)$, define the following sequence

$$s_L = \left\{\frac{s_{L-1}}{\omega_{L-1}}\right\}, \quad s_0 = s. \tag{2.2}$$

One has

Lemma 2.1. *If $s = k_0 + \omega_0 l_0$, where k_0, $l_0 \in \mathbb{Z}$, then:*

- *For all L, one has $s_L = k_L + \omega_L l_L$ with k_L, $l_L \in \mathbb{Z}$;*
- *if $k_0 > 0$, then the sequence $(k_{2L})_{L\geq 0}$ is monotonically decreasing until it vanishes and then it stays constant equal to 0;*
- *Let $k_0 > 0$ and L be the first number for which $k_{2L} = 0$, then*

$$k_0\omega_0\omega_1\ldots\omega_{2L-1} \leq 2.$$

For a given $L \in \mathbb{N}$, define $K(2L,\omega)$ being the maximal k_0 such that $k_{2L} = 0$ and set $K(2L-1,\omega) = K(2L,\omega)$. Now, we are ready to discuss the Lyapunov exponent. We have

Theorem 2.1. *Pick $\lambda > 1$ and $\omega \in (0,1)$ irrational. Assume that there exists a function $M : \mathbb{N} \to \mathbb{N}$ such that $M(L) < L$ and that, for $L \to \infty$,*

$$\begin{aligned} &\omega_{M(L)}\omega_{M(L)+1}\ldots\omega_{L-1} \to 0 \qquad\qquad \textit{and} \\ &\lambda_{M(L)}\omega_{M(L)}\omega_{M(L)+1}\ldots\omega_L \to \infty. \end{aligned} \tag{2.3}$$

For a given $0 \leq \theta \leq 1$, the Lyapunov exponent $\gamma^+(\theta)$ for equation (1.5) exists if, for all sufficiently large L, one has:

$$|\theta - k - l\omega_0| \geq \omega_0\omega_1\ldots\omega_{M(L)-1}e^{-\frac{1}{\omega_0\omega_1\cdots\omega_{M(L)-1}}}, \tag{2.4}$$

for all $k, l \in \mathbb{Z}$ *such that* $0 \leq k + l\omega_0 \leq 1$ *and*

$$K(M(L), \omega) < k \leq K(\tilde{L}, \omega), \qquad \tilde{L} = \begin{cases} L & \text{if } L \text{ is even,} \\ L+1 & \text{otherwise.} \end{cases} \tag{2.5}$$

Furthermore, when $\gamma^+(\theta)$ *exits, it is equal to* $\log \lambda$.

One also has a similar statement on the pointwise existence of the left Lyapunov exponent γ^-. Note that for γ^- to exist, θ has to avoid neighborhoods of the points $k+l\omega_0$ with negative k. Now, turn to a discussion of the results given in Theorem 2.1.

2.2. *Admissible frequencies*

Denote by Ω the set of $\omega \in (0,1)$ satisfying the conditions of Theorem 2.1

2.2.1. *The measure of* Ω

Khinchin's famous result (see e.g. Ref 8) on the geometric means of the products of the elements of the continued fractions implies

Lemma 2.2. mes $\Omega = 1$.

Proof. Let $\{a_l\}$ be the elements of the continued fraction for ω. By Khinchin, for almost all ω, one has $\lim_{L\to\infty} (a_1 a_2 \dots a_L)^{\frac{1}{L}} = C$, where $C = 2,6...$ is a universal constant. Pick $l \in \mathbb{N}$. One has $\frac{1}{2a_l} < \omega_{l-1} < \frac{1}{a_l}$. Therefore, for almost all frequencies ω,

$$\overline{\lim}_{L\to\infty} (\omega_0\omega_1 \dots \omega_{L-1})^{\frac{1}{L}} \leq \frac{1}{C}, \qquad \underline{\lim}_{L\to\infty} (\omega_0\omega_1 \dots \omega_{L-1})^{\frac{1}{L}} \geq \frac{1}{2C}.$$

Such ω belong to Ω: in (2.3) one can take $M(L) = [L/2]$. □

2.2.2. *Liouvillean numbers in* Ω

Recall that an irrational number ω is called Liouvillean if, for any $n \in \mathbb{N}$, there are infinitely many $(p, q) \in \mathbb{Z} \times \mathbb{N}$ such that

$$\left| \omega - \frac{p}{q} \right| \leq \frac{1}{q^n}.$$

(see e.g. Ref. 8). One has

Lemma 2.3. *The set* Ω *contains Liouvillean numbers satisfying*

$$\left| \omega - \frac{p}{q} \right| \leq \frac{1}{q\lambda^{cq}}, \qquad c = c(\omega) > 0, \tag{2.6}$$

for infinitely many $(p, q) \in \mathbb{Z} \times \mathbb{N}$.

Proof. We construct a Liouvillean $\omega \in \Omega$ by choosing inductively $(a_l)_{l\geq 1}$, the elements of its continued fraction. Therefore, we pick $a_1 \geq 1$ large and, for all $L \geq 1$, we choose a_{L+1} so that

$$\frac{1}{2}\, a_{L+1} \leq (a_1 a_2 \dots a_L)^{-1} \lambda^{a_1 a_2 \dots a_L} \leq a_{L+1}. \tag{2.7}$$

We now check that such an ω belongs to Ω. Therefore, we check that one has (2.3) for $M(l) = l-1$. As $\lambda > 1$, the sequence $(a_l)_l$ is quickly increasing, and so

$$\omega_{l-1} \to 0, \quad l \to \infty. \tag{2.8}$$

Furthermore, as, for all $l \geq 0$, one has $\omega_l = (a_{l+1} + \omega_{l+1})^{-1}$, we get

$$\omega_{l-1}\omega_l\lambda_{l-1} > \frac{1}{4a_l a_{l+1}}\, \lambda^{a_1 a_2 \dots a_l} \geq \frac{a_1 a_2 \dots a_{l-1}}{8}.$$

This implies that

$$\lambda_{l-1}\omega_{l-1}\omega_l \to \infty,$$

and so $\omega \in \Omega$. Now, let us check that ω satisfies (2.6) (and, thus, is a Liouville number). Consider $\left(\frac{p_l}{q_l}\right)$, the sequence of the best approximates for ω. Recall that (see e.g. Ref. 8), for all $l \in \mathbb{N}$,

$$\left|\omega - \frac{p_l}{q_l}\right| \leq \frac{1}{a_{l+1} q_l^2}, \tag{2.9}$$

$$q_{l+1} = a_{l+1} q_l + q_{l-1}, \qquad q_1 = a_1, \quad q_0 = 1. \tag{2.10}$$

The relations (2.10) imply that

$$a_l a_l \dots a_2 a_1 < q_l < P\, a_l \dots a_2 a_1, \quad P = \prod_{l=1}^{\infty} \left(1 + \frac{1}{a_l a_{l+1}}\right); \tag{2.11}$$

the product P converges as the sequence $(a_l)_l$ is quickly increasing. Relations (2.11) and (2.7) imply that $a_{l+1} \geq q_l^{-1}\, \lambda^{q_l/P}$. This and (2.9) imply (2.6). □

2.3. *The set of "bad" phases*

For given $\lambda > 1$ and $\omega \in \Omega$, denote by Θ the set of phases θ not satisfying (2.4) for infinetly many L. One has

Lemma 2.4. *The set Θ is topologically typical (countable intersection of dense open sets) and, under the condition*

$$\sum_{L>0}^{\infty} \left(\lambda_{M(L)}\omega_{M(L)}\omega_{M(L)+1}\dots\omega_L\right)^{-1} < \infty \tag{2.12}$$

(which is stronger than (2.3)), it has zero Lebesgue measure.

Proof. For a given $L > 0$, denote the set of θ not verifying (2.4) by Θ_L. Then

$$\Theta = \bigcap_{N\geq 0} \bigcup_{L\geq N} \Theta_L. \tag{2.13}$$

Thus, Θ is a countable intersection of open sets. As ω is irrational, the points $\theta_{k,l} = k + \omega_0 l$ $(k, l \in \mathbb{Z},\ k \geq 0)$ are dense in the interval $(0, 1)$. So, to complete the proof of the first property of Θ, it suffices to show that the set $\bigcup_{L\leq N} \Theta_L$ contains all the points $\theta_{k,l}$ with k sufficiently large. But, this follows from (2.5) and the inequality $M(L) < l$. Finally note that, by (2.4),

$$\begin{aligned} \operatorname{mes}\Theta_L &\leq \frac{1}{\omega}\, K(L)\omega_0\omega_1\dots\omega_{M(L)-1}\lambda_M(L)^{-1} \\ &\leq \frac{2}{\omega}\, \left(\lambda_M(L)\omega_{M(L)}\dots\omega_{L-1}\omega_L\right)^{-1}. \end{aligned}$$

Under the condition (2.12), this implies that the Lebesgue measure of Θ is zero. □

2.4. *Heuristics and the statement of Theorem 2.1*

Let us now describe some heuristics "explaining" Theorem 2.1. Consider a continuous version of equation (1.5)

$$\phi(s+\omega) + \phi(s-\omega) = \lambda v_0(s)\ \phi(s), \quad s \in \mathbb{R}. \tag{2.14}$$

If ϕ satisfies this equation, then the formula $\psi(n) = \phi(n\omega + \theta),\ \ n \in \mathbb{Z}$, defines a solution to (1.5).

If $\lambda >> 1$, then one can expect that, on a fixed compact interval, equation (2.14) has an exponentially increasing solution ϕ^+ with the leading term ϕ_0^+ satisfying the equation

$$\phi_0^+(s+\omega) = \lambda v_0(s)\ \phi_0^+(s), \quad s \in \mathbb{R}. \tag{2.15}$$

For the last equation, one can easily construct a solution ϕ_0^+ that is analytic and has no zeros in the band $0 < \operatorname{re} s < 1+\omega$. One can extend this solution analytically to the left of this band using equation (2.15). As v_0 vanishes at integers, ϕ_0^+ has zeros at all the points of the form $s_{k,l} = k + l\omega$ where k, $l > 0$ are integers.

If there is a true solution to (2.14) with the leading term ϕ_0^+, then (1.5) has a solution ψ^+ with the leading term $\phi_0^+(n\omega + \theta)$. Furthermore, if $\theta \in (0,1)$ admits the representation $\theta = k_0 - l_0\omega$ with some positive integers k_0 and l_0, then, at least for sufficiently large λ, the leading term of ψ^+ increases exponentially on the "interval" where $-\frac{k_0}{\omega} + l_0 < n < l_0 + 1$ and then vanishes at the points $n = l_0 + 1$, $l_0 + 2, \ldots$.

The equality $\theta = k_0 - l_0\omega$ can be interpreted as a quantization condition: when this condition is satisfied, the solution ψ^+ that is exponentially growing up to the point $n = l_0$, at this point, changes to the exponential decay.

So, it is natural to expect that the solution ψ^+ keeps growing up to the infinity if θ is "far enough" from all the points of the form $k_0 - l_0\omega$ with positive integers k_0 and l_0. Hence, the right Lyapunov exponent should exist.

3. Non-existence of the Lyapunov exponent

Theorem 2.1 is rather rough in the sense that the sizes of the "secure intervals" that θ has to avoid for the Lyapunov exponent to exist (see (2.4)) are too big. This is actually due to the fact that, under the conditions of Theorem 2.1, one has much more than the existence of Lyapunov exponent. Roughly, under these conditions, for each L large enough, equation (1.5) has solutions that, locally, on intervals of length of order $(\omega_0\omega_1 \ldots \omega_{M(L)-1})^{-1}$, can have complicated behavior whereas globally, on the interval $0 < k < \mathcal{K}$ of length of order $(\omega_0\omega_1 \ldots \omega_L)^{-1}$, they are nicely exponentially increasing.

Our method also allows a precise description of the set of θ where the Lyapunov exponent does not exist. The structure of this set is quite complicated; in the present note, we only describe it for frequencies in $\Omega_1 \subset \Omega$, the set of ω satisfying the conditions

$$\omega_L \to 0, \quad \text{and} \quad \lambda_{L-1}\omega_{L-1}\omega_L \to \infty \tag{3.1}$$

instead of (2.3). One has the following two statements:

Theorem 3.1. *Pick $\lambda > 1$. Let $\omega \in \Omega_1$. For a $0 < \theta < 1$, define the sequence $\{s_L\}$ by (2.2) with $s_0 = \theta$. Assume that there is a positive constant*

c such that for infinitely many even positive integers L one has

$$\text{dist}\,(\,s_{L-1}\,,\,\omega_{L-1}\cdot\mathbb{N}\,)\le\omega_{L-1}\,\lambda_L^{-c}\quad\text{and}\quad s_{L-1}\ge c.$$

Then, the right Lyapunov exponent $\gamma^+(\theta)$ does not exist.

and

Theorem 3.2. *Pick $\lambda>1$. Let $\omega\in\Omega_1$. For a $0<\theta<1$, define the sequence $\{s_L\}$ by (2.2) with $s_0=\theta$. Assume that there is a positive constants c and N such that for infinitely many odd positive integers L one has*

$$\text{dist}\,(\,s_L\,,\,\omega_L\cdot\mathbb{N}\,)\le\lambda_L^{-c},\quad s_{L-1}\le 1-c,\quad\text{and}\quad s_L\le\omega_L\,N.$$

Then, the right Lyapunov exponent $\gamma^+(\theta)$ does not exist.

The above two theorems are sharp: in the case of $\omega\in\Omega_1$, if the Lyapunov exponent does not exist, then θ satisfies the conditions of one of the them.

As for the behavior of the solutions, in both cases, roughly, we find that, for infinitely many L, even if we forget of the complicated local behavior of the solutions on the intervals of the length of order $(\omega_0\omega_1\dots\omega_{M(L)-1})^{-1}$, one can see that globally, on the interval $0<k<\mathcal{K}$ of the length of order $(\omega_0\omega_1\dots\omega_L)^{-1}$, the solutions change from exponential growth to the exponential decay. For example, in the case of Theorem 3.2, there exists solutions that, at first, are globally exponentially increasing then are globally exponentially decaying, the length of the interval of increase and the interval of decrease being of the same order. Here we use the word globally to refer to the fact that this exponential growth or decay happens at a large scale.

4. The main ideas of the proof

As we have mentioned in the introduction, the main tool of the proof is the *monodromization* renormalization method. The new idea is that one can consider the infinite sequence of the almost periodic equations arising in the course of the monodromization as a sequence of equations describing a given solution of the input equation on larger and larger intervals, the ratio of their length being determined by the continued fraction of the frequency.

Now, the renormalization formulas can be written in the form

$$\begin{aligned}&M(\theta+(k-1)\omega)\dots M(\theta+\omega)\,M(\theta)\\&\quad\sim\Psi(\{k\omega+\theta\})\,[\,M_1(\theta_1-\omega_1)\,M_1(\theta-2\omega_1)\dots M_1(\theta-k_1\omega_1)\,]^t\;\Psi^{-1}(\theta).\end{aligned}\tag{4.1}$$

Here, "$\sim$" means "equal up to a sign",

- $M(\theta) = \begin{pmatrix} 2\lambda \sin(\pi\theta) & -e^{-i\pi\theta} \\ e^{i\pi\theta} & 0 \end{pmatrix}$; the second order difference equation (2.14), the continuous analog of (1.5), is equivalent to the first order matrix difference equation

$$\Psi(s+\omega) = M(s)\Psi(s), \quad s \in \mathbb{R}; \tag{4.2}$$

- Ψ is a fundamental solution to (4.2), i.e., such that $\Psi(s) \in SL(2,\mathbb{C})$ for all s;
- ^{t} denotes the transposition;
- M_1 is a monodromy matrix corresponding to this solution, i.e., the matrix defined by $\Psi(s+1) = \Psi(s)M_1^t(s/\omega)$.

The new constants ω_1, θ_1 and the number k_1 are defined by

$$\omega_1 = \{\, 1/\omega \,\}, \quad \theta_1 = \{\, \theta/\omega \,\}, \quad k_1 = [\, \theta + k\omega \,].$$

And, as usual $\{a\}$ and $[a]$ denote the fractional and the integer part of $a \in \mathbb{R}$.

Formula (4.1) relates the study of the matrix product $M(\theta + (k-1)\omega) \dots M(\theta+\omega)\, M(\theta)$ to that of a similar product: the monodromy matrix M_1 is unimodular and, as the matrix M, it is 1 anti-periodic. One can apply the same renormalization formula for the new matrix product and so on. It is easy to check that after a finite number of renormalizations, one gets a matrix product containing at most ... one matrix. This feature recalls the renormalization of the quadratic exponential sums carried out by Hardy and Littlewood (see Ref.3,6).

At each step of the monodromization, one has to study similar difference equations $\Psi_L(s+\omega_k) = M_L(s)\Psi_L(s)$, $L = 0, 1, 2, \dots$. One needs to have a good enough control of their solutions but only on one fixed compact interval namely $[0, 1]$.

For our model, one can choose the fundamental solutions so that all the matrices M_L have the same functional structure, and the numbers (λ_L) are the successive coupling constants in these equations.

For $\lambda = \lambda_0 > 1$, the sequence $(\lambda_L)_L$ tends to infinity very rapidly; this enables an effective asymptotic analysis of the successive equations. For general almost periodic equations, one finds an analogous effect at least when the coupling constant in the input equation is large enough.

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RECENT ADVANCES ABOUT LOCALIZATION IN CONTINUUM RANDOM SCHRÖDINGER OPERATORS WITH AN EXTENSION TO UNDERLYING DELONNE SETS

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We review recent results on the universal occurrence of Anderson localization in continuum random Schrödinger operators, namely localization for any non trivial underlying probability measure. We extend known results to the case where impurities are located on Delone sets. We also recall the recent localization result for Poisson Hamiltonian. A discussion on the Wegner estimate is provided with a comparison between the "usual" estimate and the one derived through Sperner's type argument and (anti)concentration bounds.

1. Setup and results

1.1. *Setup and results for the Anderson model*

In this note, we consider random Schrödinger operators on $\mathrm{L}^2(\mathbb{R}^d)$ of the type

$$H_{D,\boldsymbol{\omega}} = H_{\boldsymbol{\omega}} := -\Delta + V_{\boldsymbol{\omega}}, \tag{1.1}$$

where Δ is the d-dimensional Laplacian operator, and $V_{\boldsymbol{\omega}}$ is an Anderson-type random potential,

$$V_{\boldsymbol{\omega}}(x) := \sum_{\zeta\in D} \omega_\zeta \, u(x-\zeta),$$

where

(I) the single site potential u is a nonnegative bounded measurable function on $\mathbb{R}^d$ with compact support, uniformly bounded away from zero in a

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neighborhood of the origin, more precisely,

$$u_-\chi_{\Lambda_{\delta_-}(0)} \leq u \leq u_+\chi_{\Lambda_{\delta_+}(0)} \quad \text{for some constants } u_\pm, \delta_\pm \in]0,\infty[; \tag{1.2}$$

(II) D is a periodic lattice.

(III) $\boldsymbol{\omega} = \{\omega_\zeta\}_{\zeta\in D}$ is a family of independent identically distributed random variables, whose common probability distribution μ is non-degenerate with bounded support, and satisfies

$$\{0,1\} \in \operatorname{supp}\mu \subset [0,1]. \tag{1.3}$$

To fix notations, the set of realizations of the random variables $\{\omega_\zeta\}_{\zeta\in D}$ is denoted by $\Omega = \Omega_D = [0,1]^D$; $\mathcal{F}$ denotes the σ-algebra generated by the coordinate functions, and $\mathbb{P} = \mathbb{P}_D = \otimes_{\zeta\in D}\,\mu$ is the product measure of the common probability distribution μ of the random variables $\boldsymbol{\omega} = \boldsymbol{\omega}_D = \{\omega_\zeta\}_{\zeta\in D}$. In other words, we work with the probability space $(\Omega, \mathcal{F}, \mathbb{P}) = \bigotimes_{\zeta\in D}\big([0,1], \mathcal{B}_{[0,1]}, \mu\big)$, where $\mathcal{B}_{[0,1]}$ is the Borel σ-algebra on $[0,1]$. A set $\mathcal{E} \in \mathcal{F}$ will be called an event.

Under assumption (II), that is if D is a lattice, $H_{\boldsymbol{\omega}}$ is a D-ergodic family of random self-adjoint operators. It follows from standard results (cf. Refs. 41,56) that there exists fixed subsets Σ, $\Sigma_{\rm pp}$, $\Sigma_{\rm ac}$ and $\Sigma_{\rm sc}$ of $\mathbb{R}$ so that the spectrum $\sigma(H_{\boldsymbol{\omega}})$ of $H_{\boldsymbol{\omega}}$, as well as its pure point, absolutely continuous, and singular continuous components, are equal to these fixed sets with probability one.

We shall take advantage of this review to extend some results to the more general setting

(II') $\exists\, 0 < r \leq R < \infty$, s.t. D is a (r,R)-Delone set, that is for any cubes Λ_r, Λ_R of respective sizes r, R, $|D \cap \Lambda_r| \leq 1$ and $|D \cap \Lambda_R| \geq 1$.

Recall that a lattice is a particular case of a Delone set.

With condition (1.3), the family of operators $H_{\boldsymbol{\omega}}$ is "normalized", so that, by the Borel-Cantelli lemma, assuming (I), (II'), (III),

$$\text{for } \mathbb{P}\text{a.e.}\boldsymbol{\omega},\ \sigma(H_{\boldsymbol{\omega}}) = [0,+\infty[. \tag{1.4}$$

Instead of Condition (III) above we may consider the more general situation:

(III') $\exists\, 0 \leq a < b < \infty$ s.t. $\{a,b\} \subset \operatorname{supp}\mu \subset [a,b]$.

Assuming (III'), the operator H_ω may be rewritten as

$$H_{\boldsymbol{\omega}} = -\Delta + V_0 + \sum_{\zeta\in D} \omega'_\zeta u'_\zeta$$

with

$$V_0 = a \sum_{\zeta \in D} u_\zeta,\ \omega'_\zeta = \frac{\omega_\zeta - a}{b-a},\ \text{and}\ u'_\zeta = (b-a)u_\zeta \geq 0.$$

The picture (1.4) is lost. The infimum of the spectrum is shifted by a constant $E_0 = \inf \sigma(-\Delta + V_0)$, which becomes the almost sure infimum of the spectrum. If (II) and (III) hold, then by ergodicity there exists a set $\Sigma \subset [E_0, \infty[$ that is the almost sure spectrum of H_ω. If we only assume (II'), then this picture is lost.

It will be convenient to work with the sup norm in $\mathbb{R}^d$,

$$\|x\| := \max\{|x_1|, |x_2|, \ldots, |x_d|\} \quad \text{for} \quad x = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d.$$

Then

$$\Lambda_L(x) := \left\{y \in \mathbb{R}^d;\ \|y - x\| < \tfrac{L}{2}\right\} = x + \left]-\frac{L}{2}, \frac{L}{2}\right[^d$$

denotes the (open) box of side L centered at $x \in \mathbb{R}^d$. By a box Λ_L we mean a box $\Lambda_L(x)$ for some $x \in \mathbb{R}^d$. Given a set B, we write χ_B for its characteristic function. By χ_x we denote the characteristic function of the unit box centered at $x \in \mathbb{R}^d$, i.e., $\chi_x := \chi_{\Lambda_1(x)}$.

We prove localization at the bottom of the spectrum for the Anderson Hamiltonian without any extra hypotheses. We actually prove stronger versions of Anderson localization (pure point spectrum with exponentially decaying eigenfunctions) and dynamical localization (no spreading of wave packets under the time evolution).

Theorem 1.1. *Let $H_{\boldsymbol{\omega}}$ be an Anderson Hamiltonian on $\mathrm{L}^2(\mathbb{R}^d)$ as above with hypotheses (I), (II), (III'). Then there exists $E_0 = E_0(d, u_\pm, \delta_\pm, \mu) > 0$ such that $H_{\boldsymbol{\omega}}$ exhibits Anderson localization as well as dynamical localization in the energy interval $[0, E_0]$. More precisely:*

- *(Anderson localization) There exists $m = m(d, V_{\mathrm{per}}, u_\pm, \delta_\pm) > 0$ such that the following holds with probability one:*
  - *$H_{\boldsymbol{\omega}}$ has pure point spectrum in $[0, E_0]$.*
  - *If ϕ is an eigenfunction of $H_{\boldsymbol{\omega}}$ with eigenvalue $E \in [0, E_0]$, then ϕ is exponentially localized with rate of decay m, more precisely,*

$$\|\chi_x \phi\| \leq C_{\boldsymbol{\omega},\phi}\, e^{-m|x|} \qquad \text{for all} \quad x \in \mathbb{R}^d. \tag{1.5}$$

  - *The eigenvalues of $H_{\boldsymbol{\omega}}$ in $[0, E_0]$ have finite multiplicity.*

- *(Dynamical localization) For all* $s < \frac{3}{8}d$ *we have*

$$\mathbb{E}\left\{\sup_{t\in\mathbb{R}}\left\|\langle x\rangle^{\frac{m}{2}}e^{-itH_\omega}\chi_{[0,E_0]}(H_\omega)\chi_0\right\|_2^{\frac{2s}{m}}\right\}<\infty \quad \textit{for all } m\geq 1. \quad (1.6)$$

The full proof of Theorem 1.1 is presented in Ref. 35. In particular it combines the multiscale analysis of Bourgain and Kenig[7] together with the concentration bound of Ref. 3. This yields Anderson localization (using Ref. 33 for finite multiplicity). To get dynamical localization, one builds on ideas that are by now standard and that come from Refs. 1,18,19,27,28,32, 33.

1.2. *Extension to underlying Delone sets*

The following theorem extends known results, in particular Theorem 11 in Ref. 8, where the regularity of the random variable is assumed.

Theorem 1.2. *Conclusions of Theorem 1.1 hold under conditions (I), (II'), (III). Constants then also depend on* r, R.

Remark 1.1. So far, the general case that would consist in assuming (II') and (III') is out of reach for the multiscale analysis cannot be started with current methods. Indeed if D is not a lattice, both the argument we provide in Section 3 and the Lifshtiz tails approach (e.g. Refs. 45,46,56) fail when the bottom of the spectrum is not zero.

Remark 1.2 (The Bernoulli case). *If the random variables* ω_ζ *are Bernoulli, taking values* $0, 1$ *(so that hypothesis (III) holds), then for a given configuration* $\boldsymbol{\omega}$*, the Hamiltonian reads, with* $D(\boldsymbol{\omega}) := \{\zeta \in D, \omega_\zeta = 1\}$,

$$H_{\boldsymbol{\omega}} = -\Delta + \sum_{\zeta\in D(\boldsymbol{\omega})} u_\zeta. \quad (1.7)$$

One may wonder what can be said about sets $\mathcal{D}(\boldsymbol{\omega})$*'s for which localization is proved. It is clear that they are not* (r, R)*-Delone sets anymore (otherwise the spectrum would not start at zero). However it is interesting to note that as a by product of the proof,* $\mathcal{D}(\boldsymbol{\omega})$ *is relatively dense in the following weak sense: for any* $\varepsilon > 0$*, for any* $x \in \mathbb{R}^d$,

$$\lim_{L\to\infty} L^{-(d-\varepsilon)}|\Lambda_L(x)\cap D(\boldsymbol{\omega})| = +\infty.$$

This observation follows from the existence of free sites, at any scale large enough, which associated value can be turned to 1 *at the end of the multiscale analysis, ensuring the presence of the point.*

Instead of considering just one underlying Delone set, one may want to look at a family of such sets. A common way of "randomizing" D is to consider the complete metric space given by the closure, with respect to the Delone topology, e.g., Ref. 50, of all its translates:

$$\mathcal{D} = \overline{\{x + D, x \in \mathbb{R}^d\}}.$$

Provided D has finite complexity, e.g., Ref. 50, such a set possesses a Haar measure that we shall denote by ν. It is then possible to consider "thinned" or "coloured" Delone sets $D^{\boldsymbol{\omega}} := (D, \boldsymbol{\omega}_D)$ on $\mathcal{D}$, and to construct the associated Schrödinger operator, which amounts, for any $D \in \mathcal{D}$, to consider the model $H_{D^{\boldsymbol{\omega}}} = H_{D,\boldsymbol{\omega}_D}$ described in (1.1). The probabilistic structure of such a colouring of $\mathcal{D}$ is well described in Ref. 53, elaborating on Ref. 39 who considered Bernoulli colourings on Penrose tilings. In particular the overall probability measure $d\hat{\mathbb{P}}(D^{\boldsymbol{\omega}})$ can be decomposed as $d\nu(D) \times d\mathbb{P}_D(\boldsymbol{\omega})$ [53, Theorem 3.5]. In particular, this enables one to first perform a conditionning with respect to the Delone variable and conduct the analysis with the random variables.

Since the event of $\{\sigma_c(H_{D,\boldsymbol{\omega}}) = \emptyset\}$ is $\hat{\mathbb{P}}$-measurable, the following statement follows from Theorem 1.2 along the same lines as in Ref. 3.

Corollary 1.1. *Assume D has finite local complexity. There exists $E(\mu) > 0$, such that, for $\hat{\mathbb{P}}$ a.e. $\boldsymbol{\omega}$, $H_{D^{\boldsymbol{\omega}}}$ exhibits spectral localization in $[0, E(\mu)]$, that is pure point spectrum.*

Remark 1.3. Extension of Corollary 1.1's result to the localization picture described in Theorem 1.1 and Theorem 1.2 requires a carefull treatment of measurability, since, one has to make sure that events considered throughout the multiscale analysis are jointly measurable in ν and $\mathbb{P}$, perform the conditionning and do the multiscale analysis. It is very likely that this can be done along the lines of Ref. 35.

For pure Delone sets, that is with no random colouring, the situation is much more delicate. One can nevertheless show for large dense sets of Delone sets that localization holds.[37]

1.3. *The Poisson model*

Writing the (Bernoulli-)Hamiltonian in the form (1.7) is reminiscent to cases where the randomness is introduced by the location of the impurities, rather than by their amplitudes as in the Anderson model. A popular model of such a Schrödinger operator with impurities located at random is given by the

Poisson Schrödinger operator, where single site potentials are centered at points obtained through a Poisson point process of a given intensity. While localization in any dimension is expected for many years for this model, at least since the proof of Lifshitz tails provided by Donskher and Varadhan in 1975,[20] a rigorous proof of this phenomena has recently been obtained in Refs. 29,30 for repulsive potentials and Ref. 31 for attractive potential. We review this result in the sequel. Note however that localization in dimension one was known to hold by the work of Stolz.[57]

Let us note that another model obtained by randomizing the location of impurities is also of interest: the random displacement model. Only partial results are known for this model: localization in dimension 1,[10,17] and an asymptotics result (of semi-classical type) in higher dimensions.[43] Other models of interest have been studied, such as potentials given by Gaussian random variables, see Refs. 51,58.

The Poisson Hamiltonian is the random Schrödinger operator on $\mathrm{L}^2(\mathbb{R}^d)$ given by

$$H_X = -\Delta + V_X, \quad \text{with} \quad V_X(x) = \sum_{\zeta \in X} u(x-\zeta),$$

where the single-site potential u is a nonnegative C^1 function on $\mathbb{R}^d$ with compact support satisfying (1.2), and V_X is a Poisson random potential, that is, X is a Poisson process on $\mathbb{R}^d$ with density $\varrho > 0$. Thus the configuration X is a random countable subset of $\mathbb{R}^d$, and, letting $N_X(A)$ denote the number of points of X in the Borel set $A \subset \mathbb{R}^d$, each $N_X(A)$ is a Poisson random variable with mean $\varrho|A|$ (i.e., $\mathbb{P}_\varrho\{N_X(A) = k\} = (\varrho|A|)^k (k!)^{-1} \mathrm{e}^{-\varrho|A|}$ for $k = 0, 1, 2, \dots$), and the random variables $\{N_X(A_j)\}_{j=1}^n$ are independent for disjoint Borel sets $\{A_j\}_{j=1}^n$. We will denote by $(\mathcal{X}, \mathbb{P}_\varrho)$ the underlying probability space for the Poisson process with density ϱ.

Note that H_X is an ergodic (with respect to translations in $\mathbb{R}^d$) random self-adjoint operator. It follows that the spectrum of H_X is the same for $\mathbb{P}_\varrho$-a.e. X, as well as the decomposition of the spectrum into pure point, absolutely continuous, and singular continuous spectra. For u as above we actually get $\sigma(H_X) = [0, +\infty[$ for $\mathbb{P}_\varrho$-a.e. X.[41]

Theorem 1.3.[30] *Given $\varrho > 0$, there exists $E_0 = E_0(\varrho) > 0$ and $m = m(\rho) > 0$, such that conclusions of Theorem 1.1 hold on $[0, E_0]$.*

2. A bit of history and the Wegner estimate

2.1. *Some history*

In the one-dimensional case the continuous Anderson Hamiltonian has been long known to exhibit spectral localization in the whole real line for any non-degenerate μ, i.e., when the random potential is not constant.[17,38,49]

In the multidimensional case, localization at the bottom of the spectrum is already known at great, but nevertheless not all-inclusive, generality; cf. Refs. 7,47,56 and references therein. First proofs of this result are due to Combes Hislop[11] and Klopp,[44] assuming that the single site probability distribution μ is absolutely continuous with bounded density. The result relies on a multiscale analysis argument "à la" Fröhlich Spencer[26] and adapted from Ref. 21's discrete version; it took more time and a lot of efforts to carry the Aizenman Molchanov approach of fractional moments[4] over the continuum,[2] still under the regularity assumption on μ.

The absolute continuity condition of μ can be relaxed to Hölder continuity of μ, both in the approach based on the multiscale analysis, and in the one based on the fractional moment method. The basis in the former case is an improved analysis of the Wegner estimate, which was first noticed by Stollmann in Ref. 55. Important improvements in Wegner estimates with (not too) singular continuous measures μ have then been successively obtained in Refs. 12,15,16,36,40 until the recent optimal form due to Combes Hislop and Klopp;[13] all theses improved forms provide in particular some continuity property of the integrated density of states.

However, techniques relying on the regularity of μ seem to reach their limit with log-Hölder continuity. In particular, until recently the Bernoulli random potential had been beyond the reach of analysis in more than one dimension. For that extreme case, i.e., of $H_{\boldsymbol{\omega}}$ with $\mu\{1\} = \mu\{0\} = \frac{1}{2}$, localization at the bottom of the spectrum was recently proven by Bourgain and Kenig.[7]

In Ref. 7, the Wegner estimate is obtained along the lines of (an elaborated version of) the multiscale analysis, scale by scale, through a combination of a quantitative unique continuation principle together with a lemma due to Sperner.[54] Although it definitely requires some technical care, it is quite clear from the analysis of Ref. 7 that the result extends to any measure for which a Sperner's type argument is valid. See for an illustration of this point the note Ref. 34, where μ is a uniform measure on some Cantor set (μ turns to be log log-Hölder continuous in this example).

Localization was thus proved for the two extreme cases: μ regular enough

and μ Bernoulli, and with two different proofs, none of which applying directly to the other case. Our motivation was then to find a single proof for any non degenerated measure, and thus unifying these two extreme results. A key step, the concentration bound extending the Sperner's Lemma estimate used by Bourgain and Kenig, was obtained in Ref. 3. The full technical details of the extension of the multiscale analysis of Ref. 7 are provided in Ref. 35.

2.2. *The Wegner estimate*

It is easy to understand (or at least to get a hint of) why regularity of the distribution might help for a proof of a Wegner type estimate. But let us first describe what a Wegner type estimate is and what it is good for. The multiscale analysis deals with resolvents of the random Hamiltonians, restricted to finite volume cubes. The aim of the game is to show that such kernels of finite volume resolvents decay exponentially with a good probability. Before showing that resolvents decay exponentially, it sounds reasonable to make sure that their norm is not too big, namely at most sub-exponentially big (so that it does not destroy the exponential decay that has already been obtained from previous scales).

To fix notations, consider a scale L, $H_{L,\boldsymbol{\omega}}$ a suitable restriction of $H_{\boldsymbol{\omega}}$ to a cube Λ_L of side L with Dirichlet boundary condition, and $R_{L,\boldsymbol{\omega}}(z)$ its resolvent (that is now a compact operator). The spectrum of $H_{L,\boldsymbol{\omega}}$ is thus discrete and given $E \in \sigma(H_{\boldsymbol{\omega}}) = [0, +\infty[$ we want to investigate the size of $\|R_{L,\boldsymbol{\omega}}(E)\|$ and show it is $\leq e^{L^{1-\delta}}$, $\delta > 0$, with probability at least $1 - L^{-p}$, for some $p > 0$ (note that $\|R_{L,\boldsymbol{\omega}}(E)\|$ may be infinite, namely when $E \in \sigma(H_{L,\boldsymbol{\omega}})$, but typically, this should happen for a set of $\boldsymbol{\omega}$'s of small measure. This amounts to analyze the probability that $\mathrm{dist}(E, \sigma(H_{L,\boldsymbol{\omega}})) \geq e^{-L^{1-\delta}}$.

The strong form of the Wegner estimate reads as follows:[13] there exists $C_W < \infty$, such that for η small enough and L large enough,

$$\mathbb{P}(\mathrm{dist}(E, \sigma(H_{L,\boldsymbol{\omega}})) < \eta) \leq C_W Q_{\omega_0}(2\eta) L^d,$$

where $Q_{\omega_0}(\eta)$ is the (Levy) concentration function of the random variable ω_0 (or equivalently the modulus of continuity of its measure μ), that is,

$$Q_{\omega_0}(\eta) = \sup_{x \in \mathbb{R}} \mathbb{P}(\omega_0 \in [x, x + \eta[) = \sup_{x \in \mathbb{R}} \mu([x, x + \eta[). \tag{2.1}$$

It is worth pointing out that (2.2) is an a priori estimate that is independent of the existence of localized states. Applying (2.2) with $\eta = e^{-L^{1-\delta}}$ obviously leads to the needed estimate. A weaker version, corresponding

to the approach of Bourgain Kenig, reads as follows. Let S be a subset of $D \cap \Lambda_L$, and $\omega_S = (\omega_\zeta)_{\zeta \in S}$. There exists $C_W < \infty$ and $\delta_0 > 0$ s.t., for suitable events $F_{L,\boldsymbol{\omega},S} \subset \mathcal{F}$ coming from the multiscale analysis, for L large enough, $\delta, \varepsilon > 0$ small enough,

$$\mathbb{P}_S(\mathrm{dist}(E, \sigma(H_{L,\boldsymbol{\omega}})) < e^{-L^{1-\delta}}; F_{L,\boldsymbol{\omega},S}) \leq L^{\varepsilon} Q_Z(2e^{-L^{1-\delta}}), \tag{2.2}$$

where $\mathbb{P}_S = \bigotimes_{\zeta \in S} \mu$ is the restriction of $\mathbb{P}$ to S, $Z = \Phi(\omega_S)$ is a random variable such that for any ω_S, for any $v_\zeta \geq \delta_0$,

$$\Phi(\omega_S + v_\zeta) - \Phi(\omega_S) > 2e^{-L^{1-\delta}}. \tag{2.3}$$

In practice, Φ is an eigenvalue of the finite volume operator, and property (2.3) follows from a quantitative unique continuation principle. Note that unlike what happens in the strong form, it is a only collective effect of the random variables ω_ζ, $\zeta \in S$, that provides some decay. The best universal bound is the following concentration bound (as proven in Ref. 3, see Theorem 2.1 below)

$$Q_Z(2e^{-L^{1-\delta}}) \leq C|S|^{-\frac{1}{2}}.$$

In practice, $|S| = L^{\frac{3}{4}d-}$, so that the probability in (2.2) amounts to $L^{-\frac{3}{8}d+}$. We shall discuss this point in the next subsection.

One way to understand this difference between regular and singular measures is to consider a purely discrete diagonal model, i.e. where $H_{L,\boldsymbol{\omega}} = V_{L,\boldsymbol{\omega}}$ is a diagonal matrix, with entries labelled by $n = 0, 1, \cdots, N = |\Lambda \cap D|$. Since the eigenvalues are exactly the ω_n's, the distance between E and the spectrum of this diagonal matrix is exactly $\inf_n |E - \omega_n|$. As a consequence

$$\mathbb{P}(\mathrm{dist}(E, \sigma(H_{L,\boldsymbol{\omega}})) < \eta) \leq N\mu(]E - \eta, E + \eta[) \leq Q_{\omega_0}(2\eta)N. \tag{2.4}$$

Note that it is the concentration of a single random variable that enters (2.4). Assume now the measure μ is singular, say Bernoulli with even probability $\frac{1}{2}$, then as soon as $]E - \eta, E + \eta[$ contains an atom of μ, a single ω_n is enough to spoil the picture: we get $\mathbb{P}((\mathrm{dist}(E, \sigma(H_{L,\boldsymbol{\omega}})) < \eta) \geq \frac{1}{2}$ and the situation is desperate! This simple example tell us that 1) some correlation between the eigenvalues is needed (in particular note that if $\Phi(\omega_S) = \omega_1$, then (2.3) fails) and it is the Laplacian and the unique quantitative principle that shall provide this; 2) it is by a collective effect that $\mathbb{P}((\mathrm{dist}(E, \sigma(H_{L,\boldsymbol{\omega}})) < \eta)$ has a chance to be small, and this is typically what Sperner's theorem provides.

2.3. *Antichains, Sperner's lemma and Ref. 3's concentration bound*

The configuration space $\{0,1\}^N$ for a collection of Bernoulli random variables $\boldsymbol{\eta} = \{\eta_1, \dots, \eta_N\}$ is partially ordered by the relation defined by:

$$\boldsymbol{\eta} \prec \boldsymbol{\eta}' \quad \Longleftrightarrow \qquad \text{for all } \; i \in \{1, ..., N\} : \quad \eta_i \leq \eta_i' \,. \tag{2.5}$$

A set $\mathcal{A} \subset \{0,1\}^N$ is said to be an *antichain* if it does not contain any pair of configurations which are comparable in the sense of "$\prec$". The original Sperner's Lemma[54] states that for any such set: $|\mathcal{A}| \leq \binom{N}{[\frac{N}{2}]}$. An immediate computation using Stirling formula shows that the latter is bounded by $C2^N/\sqrt{N}$. A more general result is the LYM inequality for antichains (e.g. Ref. 5):

$$\sum_{\boldsymbol{\eta} \in \mathcal{A}} \frac{1}{\binom{N}{|\boldsymbol{\eta}|}} \;\leq\; 1 \,, \tag{2.6}$$

where $|\boldsymbol{\eta}| = \sum \eta_j$. The LYM inequality has the following probabilistic implication. If $\{\eta_j\}$ are independent copies of a Bernoulli random variable η with probabilities $(1-p, p)$, then for any antichain $\mathcal{A} \subset \{0,1\}^N$:

$$\mathbb{P}\left(\{\boldsymbol{\eta} \in \mathcal{A}\}\right) \;\leq\; \frac{2\sqrt{2}}{\sigma_\eta \sqrt{N}}, \tag{2.7}$$

where $\boldsymbol{\eta} = (\eta_1, \dots, \eta_N)$, $\sigma_\eta = \sqrt{pq}$ is the standard deviation of η. The same bound extends to antichains on larger alphabet: $\{0, 1, \cdots, k\}^N$ with $k \geq 1$ for equidistributed weights[5] as well as for general weights[22,23] (more than an upper bound, an asymptotics as N goes to ∞ is proven in those cases). An extension of (2.7) to independent Bernoulli variables, but no necessarily identically distributed is proven in Ref. 3.

Such bounds on probability of antichains find their natural generalization in the following theorem, that deals with arbitrary non degenerate random variables and that is proved in Ref. 3.

Theorem 2.1. *Let $\boldsymbol{X} = (X_1, \dots, X_N)$ be a collection of independent random variables whose distributions satisfy, for all $j \in \{1, ..., N\}$:*

$$\mathbb{P}\left(\{X_j \leq x_-\}\right) \geq p_- \quad \textit{and} \quad \mathbb{P}\left(\{X_j > x_+\}\right) > p_+ \tag{2.8}$$

at some $p_\pm > 0$ and $x_- < x_+$, and $\Phi : \mathbb{R}^N \mapsto \mathbb{R}$ a function such that for some $\varepsilon > 0$

$$\Phi(\boldsymbol{u} + v\boldsymbol{e}_j) - \Phi(\boldsymbol{u}) \;>\; \varepsilon \tag{2.9}$$

for all $v \geq x_+ - x_-$*, all* $\boldsymbol{u} \in \mathbb{R}^N$*, and* $j = 1, \ldots, N$*, with* $\boldsymbol{e}_j$ *the unit vector in the* j*-direction. Then, the random variable* Z*, defined by* $Z = \Phi(\boldsymbol{X})$*, obeys the concentration bound*

$$Q_Z(\varepsilon) \;\leq\; \frac{4}{\sqrt{N}} \sqrt{\frac{1}{p_+} + \frac{1}{p_-}}\,. \tag{2.10}$$

If the random variables are Bernoulli then the link between Theorem 2.1 and Sperner's theory of antichains is quite obvious. Indeed, let $\varepsilon, \varepsilon'$ be two comparable realizations of $(X_1, \cdots, X_n)$, say $\varepsilon_j \leq \varepsilon'_j$ for all $j = 1, \cdots, N$. Then by (2.9), $\Phi(\varepsilon)$ and $\Phi(\varepsilon')$ cannot both belong to a given interval of length ε. In other words, for any given $x \in \mathbb{R}$, realizations of $Z = \Phi(X_1, \cdots, X_n)$ that fall into $[x, x + \varepsilon[$ belong to an antichain; (2.7) above then yields (2.10).

It remains to extend such a reasoning to arbitrary non degenerate random variables, and not just Bernoulli. This is achieved by taking advantage of a Bernoulli decomposition of random variables described in Ref. 3. This decomposition enables us to rewrite each variable as (in law) $X_i = F_i(t_i) + \delta_i(t_i)\varepsilon_i$, where F_i, δ_i are measurable functions, t_i is a random variable on $]0, 1[$ with uniform distribution, ε_i is a Bernoulli random variable independent of t_i. Moreover it is shown in Ref. 3 that under condition (2.8), $\mathbb{P}_{t_i}(\delta_i(t_i) \geq x_+ - x_-) \geq p_- + p_+$. A large deviation argument enables us to restrict ourselves to the latter case, that is where $\delta_i(t_i) \geq x_+ - x_-$ for all $i = 1, \cdots, N$. We are thus left with Bernoulli variables for which (2.9) applies (since $\delta_i(t_i) \geq x_+ - x_-$); as before (2.7) finishes the proof.

The Bernoulli decomposition we used here found also an application to random matrices theory.[9]

3. Proof of Theorem 1.2

With Theorem 2.1 in hands, the Bourgain-Kenig multiscale analysis can be conducted in the same way as in Ref. 35, provided we can start the algorithm and make sure the density condition on the so called "free sites" is satisfied at all scales. Both points will be clear from the construction we give in Section 3.2 below. It is indeed enough to show that with a sufficiently good probability, the bottom of the spectrum of finite volume operators is lifted up, uniformly with respect to the random variables attached to a set $S \subset D$ s.t. $|S \cap \Lambda| = C_R|\Lambda|$ for some $C_R < \infty$ (actually, $C_R = (2R)^{-d}$).

3.1. *Finite volume operators*

Given a box $\Lambda = \Lambda_L(x)$ in $\mathbb{R}^d$, we denote by $\hat{\Lambda}$ the subcube $\Lambda_{L-\delta_+}(x)$ (recall (1.2)). We then define finite volume operators as follows:

$$H_{\boldsymbol{\omega},\Lambda} := -\Delta_\Lambda + V_{\boldsymbol{\omega},\Lambda} \quad \text{on} \quad \mathcal{L}^2(\Lambda), \tag{3.1}$$

where Δ_Λ is the Laplacian on Λ with Dirichlet boundary condition, and

$$V_{\boldsymbol{\omega},\Lambda} = \sum_{\zeta \in D \cap \hat{\Lambda}} \omega_\zeta u_\zeta.$$

Since we are using Dirichlet boundary condition, we always have $\inf \sigma(H_{\boldsymbol{\omega},\Lambda}) > 0$.

The multiscale analysis estimates probabilities of desired properties of finite volume resolvents at energies $E \in \mathbb{R}$. As in Refs. 6,7,31, these properties include 'free sites'. Given a box Λ, a subset $S \subset \hat{\Lambda}$, and $\mathbf{t}_S = \{t_\zeta\}_{\zeta \in S} \in [0,1]^S$, we set

$$H_{\boldsymbol{\omega},\mathbf{t}_S,\Lambda} := H_{0,\Lambda} + V_{\boldsymbol{\omega},\mathbf{t}_S,\Lambda} \quad \text{on} \quad \mathcal{L}^2(\Lambda), \tag{3.2}$$

where $V_{\boldsymbol{\omega},\mathbf{t}_S,\Lambda} = \chi_\Lambda V_{\boldsymbol{\omega}_\Lambda,\mathbf{t}_S}$ with

$$V_{\boldsymbol{\omega}_\Lambda,\mathbf{t}_S}(x) := V_{\boldsymbol{\omega}_{\Lambda\setminus S}}(x) + V_{\mathbf{t}_S}(x) = \sum_{\zeta \in \hat{\Lambda}\setminus S} \omega_\zeta \, u_\zeta(x-\zeta) + \sum_{\zeta \in S} t_\zeta \, u_\zeta(x-\zeta). \tag{3.3}$$

$R_{\boldsymbol{\omega},\mathbf{t}_S,\Lambda}(z)$ will denote the corresponding finite volume resolvent.

3.2. *Proof of Theorem 1.2*

Given an energy E, to start the multiscale analysis we will need, as in Refs. 6,7,31, an *a priori* estimate on the probability that a box Λ_L is 'good' with an adequate supply of free sites, for some sufficiently large scale L. The multiscale analysis will then show that such a probabilistic estimate also holds at all large scales.

To prove the needed initial estimate, it is enough to prove that a spectral gap occurs above 0 for finite volume operators with a good probability. This is the purpose of the next proposition.

Proposition 3.1. *Fix $p > 0$ and $0 < \varepsilon \leq 1$. There exists a scale $\tilde{L} = \tilde{L}(d, q, u_-, \delta_-, \mu, p, \varepsilon)$, such that for all scales $L \geq \tilde{L}$ and all $x \in \mathbb{R}^d$ we have*

$$\mathbb{P}\left\{ H_{\boldsymbol{\omega},\mathbf{t}_S,\Lambda_L(x)} \geq CR^{-2d-2}(\log L)^{-\frac{2}{d}} \text{ for all } \mathbf{t}_S \in [0,1]^S \right\} \geq 1 - L^{-pd}, \tag{3.4}$$

where $S \subset \Lambda$, $|S| = (2R)^{-d}|\Lambda|$.

Proof. By definition of D being a (r,R)-Delone set, for any $j \in \mathbb{Z}^d$, there exists a point such that $\zeta_j \in D \cap \Lambda_R(j)$ (if ζ_j is not unique, we select one). We define the set $\Upsilon_R \subset D$ to be the collection of these ζ_j's, and we further define Υ_R^0 as the subcollection corresponding respectively to points ζ_j with $j \in (2\mathbb{Z})^d$. Note that $|\Upsilon_R \cap \Lambda| = R^{-d}|\Lambda|$, and $|\Upsilon_R^0 \cap \Lambda| = (2R)^{-d}|\Lambda|$. We set $S = \Upsilon_R^0 \cap \Lambda$.

We further set

$$V_{\Upsilon_R^0,\boldsymbol{\omega}} := \sum_{\zeta_j \in \Upsilon_R^0} \omega_{\zeta_j} u_{\zeta_j}$$

Clearly, for any $\boldsymbol{\omega}$,

$$V_{\boldsymbol{\omega}} \geq \sum_{\zeta_j \in \Upsilon_R} \omega_{\zeta_j} u_{\zeta_j} = V_{\Upsilon_R^0,\boldsymbol{\omega}} + \sum_{\zeta_j \in \Upsilon_R \setminus \Upsilon_R^0} \omega_{\zeta_j} u_{\zeta_j}$$

Going to finite volumes, the same inequality holds with $\boldsymbol{\omega}$ replaced by $\boldsymbol{\omega}_\Lambda$.

We now follow Refs. 7,30,35. Setting $K > 10\delta_-$, $\Lambda = \Lambda_L$, It follows from the lower bound in (1.2) that there exists a constant $c_{u,d} > 0$ such that

$$\overline{V}_{\Upsilon_R^0,\boldsymbol{\omega}_\Lambda}(x) := \frac{1}{(2RK)^d} \int_{\Lambda_{2RK}(0)} \mathrm{d}a\, V_{\boldsymbol{\omega}_\Lambda}(x-a) \geq \frac{c_{u,d}}{(2R)^d}\, Y_{\boldsymbol{\omega},\Lambda} \chi_\Lambda(x), \quad (3.5)$$

where

$$Y_{\boldsymbol{\omega},\Lambda} := \min_{\xi \in \widetilde{\Lambda}} \frac{1}{K^d} \sum_{\zeta \in \widetilde{\Lambda_{\frac{K}{3}}(\xi)}} \omega_\zeta \,.$$

It follows from standard estimates (e.g., Proposition 3.3.1 in Ref. 59) that, with $\bar{\mu}$ the mean of the probability measure μ, we have, for some $A_\mu > 0$,

$$\mathbb{P}\left\{ \frac{1}{K^d} \sum_{\zeta \in \widetilde{\Lambda_{\frac{K}{3}}(\xi)}} \omega_\zeta \leq \frac{\bar{\mu}}{2} \right\} \leq \mathrm{e}^{-A_\mu K^d}. \quad (3.6)$$

It follows from (3.5) and (3.6) that. with $c'_{u,d} = \frac{c_{u,d}}{2}$,

$$\mathbb{P}\left\{ \overline{V}_{\boldsymbol{\omega}_\Lambda} > c'_{u,d}(2R)^{-d} \bar{\mu} \chi_\Lambda \right\} \geq 1 - L^d \mathrm{e}^{-A_\mu K^d}, \quad (3.7)$$

and thus, we have for the "free sites Hamiltonian" with

$$S = (D \setminus \Upsilon_R^0) \cap \Lambda, \quad (3.8)$$

(recall (3.2)-(3.3)), with probability $\geq 1 - L^d \mathrm{e}^{-A_\mu K^d}$, uniformly in $\mathbf{t}_S$,

$$\overline{H}_{\boldsymbol{\omega},\Lambda,\mathbf{t}_S} := -\Delta_\Lambda + V_{\boldsymbol{\omega}_\Lambda,\mathbf{t}_S} + \overline{V}_{\Upsilon_R^0,\boldsymbol{\omega}_\Lambda} \geq c'_{u,d}(2R)^{-d}\bar{\mu} \quad \text{on} \quad \mathcal{L}^2(\Lambda). \quad (3.9)$$

Thus, if $\varphi \in C_c^\infty(\Lambda)$ with $\|\varphi\| = 1$, we have

$$\begin{aligned}
&\langle \varphi, H_{\boldsymbol{\omega},\Lambda,\mathbf{t}_S}\varphi\rangle_\Lambda = \langle \varphi, \overline{H}_{\boldsymbol{\omega},\Lambda,\mathbf{t}_S}\varphi\rangle_\Lambda + \left\langle \varphi, \left(V_{\Upsilon^0_R,\boldsymbol{\omega}_\Lambda} - \overline{V}_{\Upsilon^0_R,\boldsymbol{\omega}_\Lambda}\right)\varphi\right\rangle_\Lambda \\
&\geq c'_{u,d}(2R)^{-d}\bar{\mu} + \left\langle \varphi, \left(V_{\Upsilon^0_R,\boldsymbol{\omega}_\Lambda} - \overline{V}_{\Upsilon^0_R,\boldsymbol{\omega}_\Lambda}\right)\varphi\right\rangle_{\mathbb{R}^d} \\
&\geq \frac{c'_{u,d}}{(2R)^d}\bar{\mu} + \left\langle \varphi, V_{\Upsilon^0_R,\boldsymbol{\omega}_\Lambda}\varphi\right\rangle_{\mathbb{R}^d} - \frac{1}{(2RK)^d}\int\limits_{\Lambda_{2RK}(0)} \mathrm{d}a\ \langle \varphi(\cdot + a), V_{\boldsymbol{\omega}_\Lambda}\varphi(\cdot + a)\rangle \\
&\geq \frac{c'_{u,d}}{(2R)^d}\bar{\mu} - \frac{1}{(2RK)^d}\times \\
&\quad \times \int\limits_{\Lambda_{2RK}(0)} \mathrm{d}a\ \left|\left\langle \varphi, V_{\Upsilon^0_R,\boldsymbol{\omega}_\Lambda}\varphi\right\rangle - \left\langle \varphi(\cdot + a), V_{\Upsilon^0_R,\boldsymbol{\omega}_\Lambda}\varphi(\cdot + a)\right\rangle\right| \\
&\geq \frac{c'_{u,d}}{(2R)^d}\bar{\mu} - 2c'_u KR\,\|\nabla_\Lambda\varphi\|_\Lambda \geq c'_{u,d}\,\bar{\mu} - 2c'_u KR\,\langle \varphi, H_{\boldsymbol{\omega},\Lambda}\varphi\rangle_\Lambda^{\frac{1}{2}},
\end{aligned}$$

where we used

$$\|\varphi(\cdot + a) - \varphi\|_{\mathbb{R}^d} = \left\|(\mathrm{e}^{a\cdot\nabla} - 1)\varphi\right\|_{\mathbb{R}^d} \leq |a|\,\|\nabla\varphi\|_{\mathbb{R}^d} = |a|\,\|\nabla_\Lambda\varphi\|_\Lambda .$$

It follows that there is $\tilde{K}_{u,d} > 0$, such that for $K > \tilde{K}_{u,d}$ we have, uniformly in $\mathbf{t}_S$,

$$\langle \varphi, H_{\boldsymbol{\omega},\Lambda,\mathbf{t}_S}\varphi\rangle_\Lambda \geq c''_{u,d}\,\frac{\bar{\mu}^2}{R^{2d+2}K^2}.$$

Since this holds for all $\varphi \in C_c^\infty(\Lambda)$ with $\|\varphi\| = 1$, we have, from (3.7), uniformly in $\mathbf{t}_S$,

$$H_{\boldsymbol{\omega},\Lambda,\mathbf{t}_S} \geq c''_{u,d}\,\frac{\bar{\mu}^2}{R^{2d+2}K^2} \quad \text{on } \mathcal{L}^2(\Lambda), \tag{3.10}$$

with probability $\geq 1 - L^d\mathrm{e}^{-A_\mu K^d}$. Given $p > 0$, we take $K = \left(\frac{(p+1)d}{A_\mu}\log L\right)^{\frac{1}{d}}$ and get uniformly in $\mathbf{t}_S$,

$$\mathbb{P}\left\{H_{\boldsymbol{\omega},\Lambda_L,\mathbf{t}_S} \geq C_{u,\mu,d,p}R^{-(2d+2)}\,(\log L)^{-\frac{2}{d}}\right\} > 1 - L^{-pd},$$

for $L \geq \tilde{L}_{u,\mu,d,p}$, where $C_{u,\mu,d,p} > 0$ is an appropriate constant. □

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THE THERMODYNAMIC LIMIT OF QUANTUM COULOMB SYSTEMS: A NEW APPROACH*

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We present recent works[15,16] on the thermodynamic limit of quantum Coulomb systems. We provide a general method which allows to show the existence of the limit for many different systems.

1. Introduction

Ordinary matter is composed of electrons (negatively charged) and nuclei (positively charged) interacting via Coulomb forces. The potential between two particles of charges z and z' located at x and x' in $\mathbb{R}^3$ is

$$\frac{zz'}{|x-x'|}.$$

There are two difficulties which occur when trying to describe systems composed of electrons and nuclei. Both have to do with the physical problem of *stability* of quantum systems.

The first is due to the singularity of $1/|x|$ at 0: it is necessary to explain why a particle will not rush to a particle of the opposite charge. One of the first major triumphs of the theory of quantum mechanics is the explanation it gives of the stability of the hydrogen atom (and the complete description of its spectrum) and of other microscopic quantum Coulomb systems, via the uncertainty principle. Stability means that the total energy of the considered system cannot be arbitrarily negative. If there was no such lower bound to the energy it would be possible in principle to extract an infinite amount of energy. One often refers to this kind of stability as *stability of the first kind*.[19,20] If we denote by $E(N)$ the ground state energy of the system under consideration, for N particles stability of the first kind can be written

$$E(N) > -\infty. \tag{1.1}$$

In proving (1.1) for Coulomb systems, a major role is played by the uncertainty principle which for nonrelativistic systems is mathematically expressed by the critical Sobolev embedding $H^1(\mathbb{R}^3) \hookrightarrow L^6(\mathbb{R}^3)$. The latter allows to prove Kato's inequality

$$\forall \varepsilon > 0, \qquad \frac{1}{|x|} \leq \varepsilon(-\Delta) + \frac{1}{\varepsilon},$$

which means that the Coulomb potential is controlled by the kinetic energy.

The second issue concerns the slow decay of $1/|x|$ at infinity and this has to do with the macroscopic behavior of quantum Coulomb systems. It is indeed necessary to explain how a very large number of electrons and nuclei can stay bounded together to form macroscopic systems, although each particle interacts with a lot of other charged particles due to the long tail of the Coulomb interaction potential. Whereas the stability of atoms was an early triumph of quantum mechanics it, surprisingly, took nearly forty years before the question of stability of everyday macroscopic objects was even raised (see Fisher and Ruelle[11]). A rigorous answer to the question came shortly thereafter in what came to be known as the Theorem on Stability of Matter proved first by Dyson and Lenard.[8]

The main question is how the lowest possible energy $E(N)$ appearing in (1.1) depends on the (macroscopic) number N of particles in the object. More precisely, one is interested in proving a behavior of the form

$$E(N) \sim_{N\to\infty} \bar{e}N. \tag{1.2}$$

This behavior as the number of particles grows is mandatory to explain why matter does not collapse or explode in the thermodynamic limit. Assume that (1.2) does not hold and that for instance $E(N) \sim_{N\to\infty} cN^p$ with $p \neq 1$. Then $|E(2N) - 2E(N)|$ becomes very large as $N \gg 1$. Depending on p and the sign of the constant c, a very large amount of energy will be either released when two identical systems are put together, or necessary to assemble them. The constant $\bar{e}$ in (1.2) is the energy per particle.

Stability of Matter is itself a necessary first step towards a proof of (1.2) as it can be expressed by the lower bound

$$E(N) \geq -\kappa N. \tag{1.3}$$

Put differently, the lowest possible energy calculated per particle cannot be arbitrarily negative as the number of particles increases. This is also often referred to as *stability of the second kind*.[19,20]

A maybe more intuitive notion of stability would be to ask for the volume occupied by a macroscopic object (in its ground state). Usually this volume is proportional to the number of particles N. Denoting by Ω a domain in $\mathbb{R}^3$ which is occupied by the system under consideration and by $E(\Omega)$ its (lowest possible) energy, (1.2) then reads

$$E(\Omega) \sim_{|\Omega|\to\infty} \bar{e}|\Omega| \tag{1.4}$$

where $|\Omega|$ is the volume of Ω. Stability of the second kind is expressed as

$$E(\Omega) \geq -\kappa|\Omega|. \tag{1.5}$$

Instead of the ground state energy, one can similarly consider the free energy $F(\Omega, \beta, \mu)$ at temperature $T = 1/\beta$ and chemical potential μ. One is then interested in proving the equivalent of (1.4)

$$F(\Omega, \beta, \mu) \sim_{|\Omega|\to\infty} \bar{f}(\beta, \mu)|\Omega| \tag{1.6}$$

where $\bar{f}(\beta, \mu)$ is the free energy per unit volume.

Large quantum Coulomb systems have been the object of an important investigation in the last decades and many techniques have been developed. A result like (1.3) (or equivalently (1.5)) was first proved for quantum electrons and nuclei by Dyson and Lenard.[8] After the original proof by Dyson and Lenard several other proofs were given. Lieb and Thirring[27] in particular presented an elegant and simple proof relying on an uncertainty principle for fermions. The different techniques and results concerning stability of matter were reviewed in several articles.[19–21,29,33]

It is very important that the negatively charged particles (the electrons) are fermions. It was discovered by Dyson[7] that the Pauli exclusion principle is essential for Coulomb systems: charged bosons are alone not stable because their ground state energy satisfies $E(N) \sim -CN^{7/5}$, as was proved later.[4,26,32]

A result like (1.2) (or equivalently (1.4)) was first proved by Lieb and Lebowitz[22] for a system containing electrons and nuclei both considered as quantum particles, hence invariant by rotation. Later Fefferman gave a different proof[9] for the case where the nuclei are classical particles placed on a lattice, a system which is not invariant by rotation.

In a recent work,[15,16] we provide a new insight in the study of the thermodynamic limit of quantum systems, by giving a general proof of (1.4) or (1.6) which can be applied to many different quantum systems including those studied by Lieb and Lebowitz[22] or Fefferman,[9] and others which were not considered before. Our goal was to identify the main general physical properties of the free energy which are sufficient to prove the existence of the thermodynamic limit. However, for the sake of simplicity we will essentially address the crystal case in this paper and we refer to our works[15,16] for a detailed study of the other cases.

In proving the existence of the thermodynamic limit of Coulomb quantum systems, the most difficult task is to quantify *screening*. Screening means that matter is arranged in such a way that it is essentially locally neutral, hence the electrostatic potential created by any subsystem decays much faster than expected. This effect is the main reason of the stability of ordinary matter but it is very subtle in the framework of quantum mechanics because the particles are by essence delocalized. In our approach, we shall heavily rely on an electrostatic inequality which was proved by Graf and Schenker[12,13] and which serves as a way to quantify screening. It was itself inspired by previous works of Conlon, Lieb and Yau,[4,5] for systems interacting with the Yukawa potential. Fefferman used a similar idea in his study of the crystal case.[9]

Like in previous works, our method consists in first showing the existence of the limit (1.6) for a specific domain $\triangle$ which is dilated (and possibly rotated and translated). Usually $\triangle$ is chosen to be a ball, a cube or a tetrahedron. In the applications[16] we always choose a tetrahedron as we shall use the Graf-Schenker inequality[13] which holds for this type of domains. The second step consists in showing the existence of the limit (1.6) for any (reasonable) sequence of domains $\{\Omega_n\}$ such that $|\Omega_n| \to \infty$. This is important as in principle the limit could depend on the chosen sequence,

a fact that we want to exclude for our systems. We shall specify later what a "reasonable" sequence is. Essentially some properties will be needed to ensure that boundary effects always stay negligible.

It is to be noticed that our method (relying on the Graf-Schenker inequality) is primarily devoted to the study of quantum systems interacting through Coulomb forces. It might be applicable to other interactions but we shall not address this question here.

Proving a result like (1.4) or (1.6) is only a first step in the study of the thermodynamic limit of Coulomb quantum systems. An interesting open problem is to prove the convergence of *states* (or for instance of all k-body density matrices) and not only of energy levels. For the crystal case, convergence of the charge density or of the first order density matrix was proved for simplified models from Density Functional Theory or from Hartree-Fock theory.[3,25] A result of this type was also proved for the Hartree-Fock approximation of no-photon Quantum Electrodynamics.[14]

Another (related) open question is to determine the next order in the asymptotics of the energy in the presence of local perturbations. Assume for instance that the crystal possesses a local defect modelled by a local potential V and denote the ground state energy in the domain Ω by $E^V(\Omega)$. Since V is local, it does not contribute to the energy in the first order of the thermodynamic limit. One is then interested in proving a behavior like $E^V(\Omega) = E^0(\Omega) + f(V) + o(1)_{|\Omega|\to\infty}$. Such a result was recently proved for the *reduced* Hartree-Fock model of the crystal with the exchange term neglected.[2] This includes an identification of the function $f(V)$. This program was also tackled for the Hartree-Fock model (with exchange term) of no-photon Quantum Electrodynamics.[14]

The present paper is organized as follows. In the next section we introduce the model for the crystal and state our main theorem. In Section 3, we briefly describe two other quantum systems which we can treat using our method. Section 4 is devoted to the presentation of our new approach, in a quite general setting, together with hints on how it can be applied to the crystal case.

2. The Crystal Case

For simplicity, we put identical nuclei of charge $+1$ on each site of $\mathbb{Z}^3$. The results below can be generalized to any periodic system. Let Ω be a bounded

open set of $\mathbb{R}^3$ and define the N-body Hamiltonian in Ω by

$$H_\Omega^N := \sum_{i=1}^N -\frac{\Delta_{x_i}}{2} + V_\Omega(x_1, ..., x_N),$$

where

$$V_\Omega(x) = \sum_{i=1}^N \sum_{R\in\mathbb{Z}^3\cap\Omega} \frac{-1}{|R-x_i|} + \frac{1}{2}\sum_{1\le i\neq j\le N} \frac{1}{|x_i-x_j|} + \frac{1}{2}\sum_{R\neq R'\in\mathbb{Z}^3\cap\Omega} \frac{1}{|R-R'|}.$$

Here $-\Delta$ is the *Dirichlet Laplacian* on Ω (we could as well consider another boundary condition). The Hamiltonian H_Ω^N acts on N-body fermionic wavefunctions $\Psi(x_1, .., x_N) \in \bigwedge_1^N L^2(\Omega)$. Stability of the first kind states that the spectrum of H_Ω^N is bounded from below:

$$E_\Omega^N = \inf_{\substack{\Psi\in\bigwedge_1^N H_0^1(\Omega),\\ \|\Psi\|_{L^2}=1}} \left\langle \Psi, H_\Omega^N \Psi\right\rangle = \inf \sigma_{\bigwedge_1^N L^2(\Omega)}(H_\Omega^N) > -\infty.$$

We may define the ground state energy in Ω by

$$E(\Omega) := \inf_{N\ge 0} E_\Omega^N. \tag{2.1}$$

It is more convenient to express (2.1) in a grand canonical formalism. We define the (electronic) Fock space as

$$\mathcal{F}_\Omega := \mathbb{C} \oplus \bigoplus_{N\ge 1} \bigwedge_1^N L^2(\Omega).$$

The grand canonical Hamiltonian is then given by $H_\Omega := \bigoplus_{N\ge 0} H_\Omega^N$ with the convention that $H_\Omega^0 = (1/2)\sum_{R\neq R'\in\mathbb{Z}^3\cap\Omega} |R-R'|^{-1} \in \mathbb{C}$. The number operator reads $\mathcal{N} := \bigoplus_{N\ge 0} N$. It is then straightforward to check that

$$E(\Omega) = \inf \sigma_{\mathcal{F}_\Omega}(H_\Omega) = \inf_{\substack{\Gamma\in\mathcal{B}(\mathcal{F}_\Omega),\ \Gamma^*=\Gamma,\\ 0\le\Gamma\le 1,\ \mathrm{tr}_{\mathcal{F}_\Omega}(\Gamma)=1.}} \mathrm{tr}_{\mathcal{F}_\Omega}\left(H_\Omega\Gamma\right).$$

The free energy at temperature $1/\beta$ and chemical potential $\mu \in \mathbb{R}$ is defined by

$$\begin{aligned} F(\Omega,\beta,\mu) &:= \inf_{\substack{\Gamma\in\mathcal{B}(\mathcal{F}_\Omega),\ \Gamma^*=\Gamma,\\ 0\le\Gamma\le 1,\ \mathrm{tr}_{\mathcal{F}_\Omega}(\Gamma)=1.}} \left(\mathrm{tr}_{\mathcal{F}_\Omega}((H_\Omega-\mu\mathcal{N})\Gamma) + \frac{1}{\beta}\mathrm{tr}_{\mathcal{F}_\Omega}(\Gamma\log\Gamma)\right) \\ &= -\frac{1}{\beta}\log \mathrm{tr}_{\mathcal{F}_\Omega}\left[e^{-\beta(H_\Omega-\mu\mathcal{N})}\right]. \end{aligned} \tag{2.2}$$

As explained in Introduction, our purpose is to prove that

$$E(\Omega) \sim_{|\Omega|\to\infty} \bar{e}|\Omega| \quad \text{and} \quad F(\Omega,\beta,\mu) \sim_{|\Omega|\to\infty} \bar{f}(\beta,\mu)|\Omega| \tag{2.3}$$

in an appropriate sense. The first important property of E and F is the stability of matter.

Theorem 2.1 (Stability of Matter[16]). *There exists a constant C such that the following holds:*

$$E(\Omega) \geq -C|\Omega|, \qquad F(\Omega,\beta,\mu) \geq -C\left(1+\beta^{-5/2}+\max(0,\mu)^{5/2}\right)|\Omega|$$

for any bounded open set $\Omega \subset \mathbb{R}^3$ and any $\beta > 0$, $\mu \in \mathbb{R}$.

Sketch of the proof. The first step is to use an inequality for classical systems due to Baxter,[1] improved later by Lieb and Yau,[28] and which allows to bound the full N-body Coulomb potential by a one-body potential:

$$V(x_1,...,x_N) \geq -\sum_{i=1}^{N} \frac{3/2+\sqrt{2}}{\delta(x_i)} \tag{2.4}$$

where $\delta(x) = \inf_{R\in\mathbb{Z}^3}|x-R|$ is the distance to the closest nucleus. Hence we have the lower bound

$$H_\Omega^N \geq \sum_{i=1}^{N}\left(-\frac{\Delta_{x_i}}{2} - \frac{3/2+\sqrt{2}}{\delta(x_i)}\right).$$

Next we split the kinetic energy in two parts and we use the uncertainty principle to show that on $L^2(\Omega)$

$$-\frac{\Delta}{4} - \frac{3/2+\sqrt{2}}{\delta(x)} \geq -C.$$

In proving this lower bound, one uses the Sobolev inequality in a small ball around each nucleus, exploiting the fact that the nuclei are fixed and separated by a distance at least one to each other. The proof of the stability of matter for systems with classical nuclei whose position is unknown is more difficult and it uses the improved version of (2.4) contained in the paper by Lieb and Yau,[28] as explained in our work.[16] This shows

$$H_\Omega^N \geq \sum_{i=1}^{N}\left(-\frac{\Delta_{x_i}}{4} - C\right) \quad \text{hence} \quad H_\Omega \geq -\frac{1}{4}\sum_i \Delta_i - C\mathcal{N} \tag{2.5}$$

on $L^2(\Omega)$ and $\mathcal{F}_\Omega$ respectively. The last step is to use the Lieb-Thirring inequality[27] which states that

$$\left\langle \sum_{i=1}^{N}(-\Delta_{x_i})\,\Psi,\Psi\right\rangle \geq C_{\mathrm{LT}}\int_\Omega \rho_\Psi(x)^{5/3}dx \tag{2.6}$$

for all $N \geq 1$ and all N-body fermionic wavefunction $\Psi \in \bigwedge_1^N L^2(\Omega)$. The density of charge ρ_Ψ is as usual defined by $\rho_\Psi(x) = N \int_{\Omega^{N-1}} |\Psi(x,y)|^2 dy$. Using the fact that $\int_\Omega \rho_\Psi = N$ and Hölder's inequality, (2.6) yields on the Fock space $\mathcal{F}_\Omega$

$$\sum_i (-\Delta_{x_i}) \geq C_{\rm LT} |\Omega|^{-2/3} \mathcal{N}^{5/3}. \tag{2.7}$$

Hence we obtain $H_\Omega \geq (C_{\rm LT}/4)|\Omega|^{-2/3}\mathcal{N}^{5/3} - C\mathcal{N}$ which, when optimized over N, gives the result for the ground state energy.

For the free energy, we use (2.5), (2.7) and Peierls' inequality[30,34] to get

$$F(\beta,\mu,\Omega) \geq -\frac{1}{\beta} \log {\rm tr}_{\mathcal{F}} \left(e^{-\beta \sum_i (-\Delta_i)/4} \right) - C(1+\mu_+^{5/2})|\Omega|.$$

The first term of the r.h.s. is the free energy of a free-electron gas which is bounded below by $-C(1+\beta^{-5/2})|\Omega|$ in the thermodynamic limit.[16] □

In order to state our main result, we need the

Definition 2.1 (Regular sets in $\mathbb{R}^3$). *Let be $a > 0$ and $\varepsilon > 0$. We say that a bounded open set $\Omega \subseteq \mathbb{R}^3$ has* an a-regular boundary in the sense of Fisher *if, denoting by $\partial\Omega = \overline{\Omega} \setminus \Omega$ the boundary of Ω,*

$$\forall t \in [0,1], \qquad \left| \left\{ x \in \mathbb{R}^3 \mid {\rm d}(x, \partial\Omega) \leq |\Omega|^{1/3} t \right\} \right| \leq |\Omega|\, a\, t. \tag{2.8}$$

*We say that a bounded open set $\Omega \subseteq \mathbb{R}^3$ satisfies the ε-*cone property *if for any $x \in \Omega$ there is a unit vector $a_x \in \mathbb{R}^3$ such that*

$$\{ y \in \mathbb{R}^3 \mid (x-y)\cdot a_x > (1-\varepsilon^2)|x-y|,\ |x-y| < \varepsilon \} \subseteq \Omega.$$

We denote by $\mathcal{R}_{a,\varepsilon}$ the set of all $\Omega \subseteq \mathbb{R}^3$ which have an a-regular boundary and such that both Ω and $\mathbb{R}^3 \setminus \Omega$ satisfy the ε-cone property.

Note that any open convex set is in $\mathcal{R}_{a,\varepsilon}$ for some $a > 0$ large enough and $\varepsilon > 0$ small enough.[15] We may state our main

Theorem 2.2 (Thermodynamic Limit for the Crystal[16]). *There exist $\bar{e} \in \mathbb{R}$ and a function $\bar{f} : (0,\infty) \times \mathbb{R} \to \mathbb{R}$ such that the following holds: for any sequence $\{\Omega_n\}_{n\geq 1} \subseteq \mathcal{R}_{a,\varepsilon}$ of domains with $|\Omega_n| \to \infty$, $|\Omega_n|^{-1/3}{\rm diam}(\Omega_n) \leq C$, $a \geq a_0 > 0$ and $0 < \varepsilon \leq \varepsilon_0$*

$$\lim_{n\to\infty} \frac{E(\Omega_n)}{|\Omega_n|} = \bar{e}, \qquad \lim_{n\to\infty} \frac{F(\Omega_n,\beta,\mu)}{|\Omega_n|} = \bar{f}(\beta,\mu). \tag{2.9}$$

Moreover $\bar{f}$ takes the form $\bar{f}(\beta,\mu) = \varphi(\beta) - \mu$.

Remark 2.1. We know from [22, Appendix A p. 385] and [10, Lemma 1] that if each set Ω_n of the considered sequence is connected, then automatically $|\Omega_n|^{-1/3}\mathrm{diam}(\Omega_n) \leq C$.

A very similar result was proved by C. Fefferman.[9] Our result is more general: we allow any sequence Ω_n tending to infinity and which is regular in the sense that $\{\Omega_n\}_{n\geq 1} \subseteq \mathcal{R}_{a,\varepsilon}$. In Fefferman's paper,[9] $\Omega_n = \ell_n(\Omega + x_n)$ where $\ell_n \to \infty$, Ω is a fixed convex open set and x_n is any sequence in $\mathbb{R}^3$. These sets are always in $\mathcal{R}_{a,\varepsilon}$ for some $a, \varepsilon > 0$.

In our work[16] a result even more general than Theorem 2.2 is shown: we are able to prove the existence of the same thermodynamic limit if the crystal is *locally perturbed* (for instance finitely many nuclei are moved or their charge is changed). A similar result can also be proved for the Hartree-Fock model.

3. Other models

Our approach[15,16] is general and it can be applied to a variety of models, not only the crystal case. We quickly mention two such examples. It is interesting to note that for these other models, we do not need the cone property and we can weaken the assumptions on the regularity of the boundary by replacing t on the r.h.s. of (2.8) by any t^p, $0 < p \leq 1$. Details may be found in our article.[16] Roughly speaking, when the system is "rigid" like for the crystal (the nuclei are fixed), the proof is more complicated and more assumptions are needed on the sequence of domains to avoid undesirable boundary effects.

3.1. *Quantum particles in a periodic magnetic field*

Define the magnetic kinetic energy $T(A) = (-i\nabla + A(x))^2$ where $B = \nabla \times A$ is periodic (for instance constant) and $A \in L^2_{\mathrm{loc}}(\mathbb{R}^3)$. Next, consider the Hamiltonian

$$H_\Omega^{N,K} := \sum_{i=1}^{N} T(A)_{x_i} + \sum_{k=1}^{K} T(A)_{R_k} + V(x,R),$$

$$V(x,R) = \sum_{i,k} \frac{-z}{|R_k - x_i|} + \frac{1}{2}\sum_{i\neq j} \frac{1}{|x_i - x_j|} + \frac{1}{2}\sum_{k\neq k'} \frac{z^2}{|R_k - R_{k'}|}.$$

The ground state energy is this time defined as

$$E'(\Omega) := \inf_{N,K\geq 0} \inf \sigma_{\bigwedge_1^N L^2(\Omega)\otimes S \bigotimes_1^K L^2(\Omega)} \left(H_\Omega^{N,K}\right).$$

We do not precise the symmetry S of the particles of charge z which can be bosons or fermions. A formula similar to (2.2) may be used for the free energy on the (electronic and nucleic) Fock space. We prove in our paper[16] a result similar to Theorem 2.2 for this model. Lieb and Lebowitz already proved it in the seminal paper Ref. 22 when $A \equiv 0$. They used as an essential tool the rotation-invariance of the system to obtain screening. When $A \neq 0$ the system is no more invariant by rotations and their method cannot be applied.

3.2. *Classical nuclei with optimized position*

For all $R \subset \Omega$, $\#R < \infty$, let us define

$$H_\Omega^{N,R} := \sum_{i=1}^{N} -\frac{\Delta_{x_i}}{2} + V(x,R)$$

and the associated ground state energy by

$$E''(\Omega) := \inf_{N\geq 0} \inf_{\substack{R\subset\Omega,\\ \#R<\infty}} \inf \sigma_{\bigwedge_1^N L^2(\mathbb{R}^3)} \left(H_\Omega^{N,R}\right).$$

We could as well optimize the charges in $[0,z]$ of the nuclei without changing the energy.[6,16] However, the free energy itself is not the same when the charges of the nuclei are optimized or not.[16]

Surprisingly, to our knowledge the existence of the thermodynamic limit for this model was unknown. A result similar to Theorem 2.2 is proved in our paper[16] for E''.

4. A general method

In this section, we give the main ideas of our new approach which allows to prove Theorem 2.2 and its counterparts for the other models quoted before.

4.1. *Screening via the Graf-Schenker inequality*

As mentioned in the introduction, an important step is to quantify screening. For quantum nuclei without a magnetic field ($A \equiv 0$), Lieb and Lebowitz used[22] the following method (see Figure 1). First they took a big ball B which they packed with several small balls B_k of different size. In each of these balls, they took the (neutral) ground state of the corresponding ball. As the system is invariant under rotations, they can freely rotate each ground state. Averaging over rotations of all the small balls, they reduced the computation of the interaction between them to that of classical

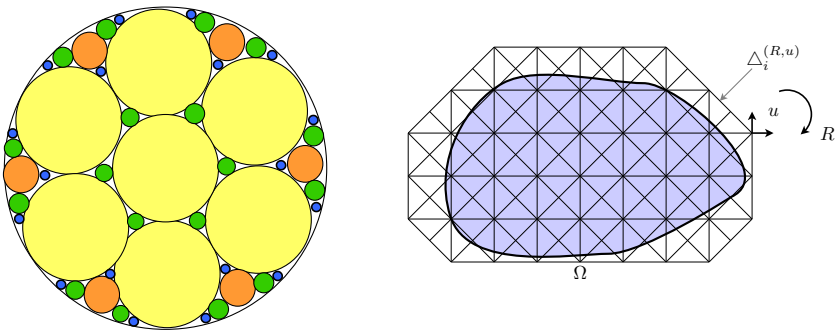

Fig. 1. A comparison between the original method of Lieb and Lebowitz[22] (left) and our method based on the Graf-Schenker inequality[13,15,16] (right).

pointwise particles located at the center of the balls, by Newton's theorem. As each subsystem is neutral, this interaction vanishes. This proves *a fortiori* that there exists an adequate rotation of each system in each little ball such that the total interaction between them cancels. Choosing this configuration, they could build a test function whose energy is just the sum of the small energies, proving an estimate of the form $E(B) \leq \sum_k E(B_k)$. This inequality can be used to prove the limit for balls. Clearly this trick can only be used for rotation-invariant systems.

Note in the Lieb-Lebowitz proof, a domain (the big ball) is split in several *fixed subdomains* and an average is done *over rotations of the states* in each small domain. This yields an *upper bound* to the energy. The Graf-Schenker inequality is kind of dual to the above method (see Figure 1). This time a domain Ω is split in several subdomains by using a tiling of the space $\mathbb{R}^3$. But the system is frozen in the state of the big domain Ω and the average is done *over the position of the tiling*. This yields a *lower bound* to the energy of the form $E(\Omega) \geq \sum_k E(\Delta_i^{(r,u)} \cap \Omega) + \text{errors}$, where $\Delta_i^{(r,u)}$ are the tetrahedrons which make up the (translated and rotated) tiling.

The Graf-Schenker inequality was inspired by previous works of Conlon, Lieb and Yau.[4,5] It is an estimate on the Coulomb energy of classical particles. The proof of Fefferman in the crystal case[9] was also based on a *lower bound* on the free energy in a big set and an average over translations of a covering of this set (the method was reexplained later in details by Hugues[17]). Fefferman[9] uses a covering with balls and cubes of different size. The lower bound depends on the number of balls contained in the big domain and of the form of the kinetic energy which is used to control error terms.

Let $G = \mathbb{R}^3 \rtimes SO_3(\mathbb{R})$ be the group of translations and rotations acting on $\mathbb{R}^3$, and denote by $d\lambda(g)$ its Haar measure.

Lemma 4.1 (Graf-Schenker inequality[13]). *Let $\triangle$ be a simplex in $\mathbb{R}^3$. There exists a constant C such that for any $N \in \mathbb{N}$, $z_1, ..., z_N \in \mathbb{R}$, $x_i \in \mathbb{R}^3$ and any $\ell > 0$,*

$$\sum_{1\leq i<j\leq N} \frac{z_i z_j}{|x_i - x_j|} \geq \int_G \frac{d\lambda(g)}{|\ell\triangle|} \sum_{1\leq i<j\leq N} \frac{z_i z_j \mathbb{1}_{g\ell\triangle}(x_i)\mathbb{1}_{g\ell\triangle}(x_j)}{|x_i - x_j|} - \frac{C}{\ell}\sum_{i=1}^N z_i^2. \tag{4.1}$$

In the previous theorem it is not assumed that $\triangle$ yields a tiling of $\mathbb{R}^3$. Up to an error which scales like ℓ, (4.1) says that the total Coulomb energy can be bounded from below by the Coulomb energy (per unit volume) of the particles which are in the (dilated) simplex $g\ell\triangle$, averaged over all translations and rotations g of this simplex.

Because of the above inequality, simplices play a specific role in the study of Coulomb systems. Hence proving the existence of the thermodynamic limit for simplices first is natural (as it was natural to consider balls in the Lieb-Lebowitz case due to the invariance by rotation). In the next section we give an abstract setting for proving the existence of the limit when an inequality of the form (4.1) holds true.

4.2. *An abstract result*

In this section we consider an abstract energy $E : \Omega \in \mathcal{M} \mapsto E(\Omega) \in \mathbb{R}$ defined on the set $\mathcal{M}$ of all bounded open subsets of $\mathbb{R}^3$ and we give sufficient conditions for the existence of the thermodynamic limit. In the application, E will be either the ground state energy, or the free energy of the system under consideration.

We fix a reference set $\triangle \in \mathcal{R}_{a,\varepsilon}$ which is only assumed to be a bounded open convex set in $\mathbb{R}^3$ (it need not be a simplex for this section), such that $0 \in \triangle$. Here $a, \varepsilon > 0$ are fixed. We assume that the energy E satisfies the following five assumptions:

(A1) *(Normalization).* $E(\emptyset) = 0$.

(A2) *(Stability).* $\forall \Omega \in \mathcal{M}$, $E(\Omega) \geq -\kappa|\Omega|$.

(A3) *(Translation Invariance).* $\forall \Omega \in \mathcal{R}_{a,\varepsilon}$, $\forall z \in \mathbb{Z}^3$, $E(\Omega + z) = E(\Omega)$.

(A4) *(Continuity).* $\forall \Omega \in \mathcal{R}_{a,\varepsilon}, \Omega' \in \mathcal{R}_{a',\varepsilon'}$ with $\Omega' \subseteq \Omega$ and $\mathrm{d}(\partial\Omega, \partial\Omega') > \delta$,

$$E(\Omega) \leq E(\Omega') + \kappa|\Omega \setminus \Omega'| + |\Omega|\alpha(|\Omega|).$$

(A5) *(Subaverage Property).* For all $\Omega \in \mathcal{M}$, we have

$$E(\Omega) \geq \frac{1-\alpha(\ell)}{|\ell\triangle|} \int_G E\big(\Omega \cap g \cdot (\ell\triangle)\big)\, d\lambda(g) - |\Omega|_{\mathrm{r}}\, \alpha(\ell) \tag{4.2}$$

where $|\Omega|_{\mathrm{r}} := \inf\{|\tilde{\Omega}|,\ \Omega \subseteq \tilde{\Omega},\ \tilde{\Omega} \in \mathcal{R}_{a,\varepsilon}\}$ is the regularized volume of Ω.

In the assumptions above α is a fixed function which tends to 0 at infinity and δ, a', ε' are fixed positive constants. In our work,[15] an even more general setting is provided. First **(A3)** can be replaced by a much weaker assumption but we do not detail this here. Also a generic class of regular sets $\mathcal{R}$ is considered instead of $\mathcal{R}_{a,\varepsilon}$. This is because for instance the cone property is only needed for the crystal case and it is not at all necessary in other models, hence the concept of regularity depends on the application.

Notice **(A4)** essentially says that a small decrease of Ω will not increase too much the energy. A similar property was used and proved in the crystal case by Fefferman [9, Lemma 2]. Taking $\Omega' = \emptyset$ and using **(A1)**, property **(A4)** in particular implies that for any regular set $\Omega \in \mathcal{R}_{a,\varepsilon}$, $E(\Omega) \leq C|\Omega|$. However this upper bound need not be true for all $\Omega \in \mathcal{M}$. We give a sketch of the proof of the following result in Section 4.5.

Theorem 4.1 (Abstract Thermodynamic Limit for $\triangle$[15]).
*Assume $E : \mathcal{M} \to \mathbb{R}$ satisfies the above properties **(A1)–(A5)** for some open convex set $\triangle \in \mathcal{R}_{a,\varepsilon}$ with $0 \in \triangle$. There exists $\bar{e} \in \mathbb{R}$ such that $e_\ell(g) = |\ell\triangle|^{-1} E\big(g\ell\triangle\big)$ converges uniformly towards $\bar{e}$ for $g \in G = \mathbb{R}^3 \rtimes SO(3)$ and as $\ell \to \infty$. Additionally, the limit $\bar{e}$ does not depend on the set $\triangle$*[a].

4.3. *Idea of the proof of (A1)–(A5) for the crystal*

Before switching to the abstract case of a general sequence $\{\Omega_n\}$, we give an idea of the proof of **(A1)**–**(A5)** in the crystal case. We apply the theory of the previous section to both the ground state energy and the free energy of the crystal which were defined in Section 2. First **(A1)** and **(A3)** are obvious. Property **(A2)** is the stability of matter as stated in Theorem 2.1. On the other hand **(A5)** is essentially the Graf-Schenker inequality (4.1), up to some localization issues of the kinetic energy which essentially have already been delt with by Graf and Schenker.[13]

For the crystal the most difficult property is **(A4)**. The difficulty arises from the fact that this is a very rigid system. For the two other examples

[a]This means if all the assumptions are true for another set $\triangle'$ then one must have $\bar{e}' = \bar{e}$.

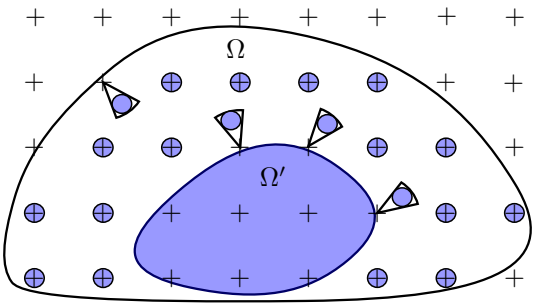

Fig. 2. Idea of the proof of **(A4)** for the crystal.

mentioned in Section 3, **(A4)** is obvious, the energy being nonincreasing: $E(\Omega) \leq E(\Omega')$. This is because we can simply choose a ground state of Ω' as a test for Ω and take the vacuum in $\Omega \setminus \Omega'$. In the crystal case we always have nuclei in $\Omega \setminus \Omega'$ and if we do not put any electron to screen them, they will create an enormous electrostatic energy.

The idea of the proof of **(A4)** for the crystal is displayed in Figure 2. We build a test state in Ω by considering the ground state in Ω', and placing one radial electron in a ball of fixed size on top of each nucleus ouside Ω'. By Newton's theorem, the electrostatic potential out of the support of the electron will vanish, hence the energy will simply be $E(\Omega')$ plus the sum of the kinetic energies of the electrons, which is bounded above by a constant times $|\Omega \setminus \Omega'|$ for regular domains. The only problem is that we cannot put an electron on top of the nuclei which are too close to the boundary of Ω or of Ω'. For these nuclei, using the cone property we can place the ball aside and create a dipole. The difficult task is then to compute a bound on the total interaction between the dipoles and the ground state in Ω'. We prove[16] that it is $o(|\Omega|)$, using a specific version of stability of matter.

4.4. *General domains and strong subadditivity of entropy*

In the previous two subsections, we have presented our abstract theory giving the thermodynamic limit of special sequences built upon the reference set $\triangle$, and we have explained how to apply it to the crystal case. For all regular domain sequences we can only get from **(A5)** a bound of the form

$$\liminf_{n\to\infty} \frac{E(\Omega_n)}{|\Omega_n|} \geq \bar{e}.$$

In order to get the upper bound, we use a big simplex $L_n\triangle$ of the same size as Ω_n and a tiling made with simplices of size $\ell_n \ll L_n$, as shown in Figure

3. We use the ground state of the big simplex $L_n\triangle$ to build a test state in Ω_n, hence giving the appropriate upper bound. To this end, we need some localization features, hence more assumptions in the general theory.

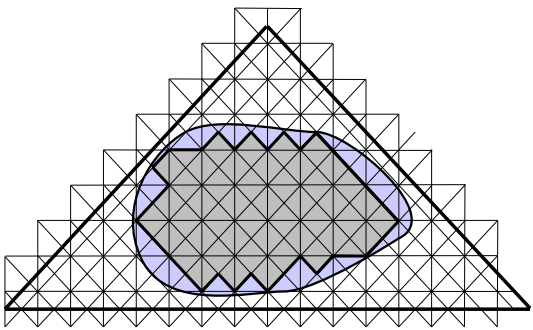

Fig. 3. Proof for general sequences $\{\Omega_n\}$.

It is sufficient[15] to assume that

(*i*) $\triangle$ can be used to build a tiling of $\mathbb{R}^3$;

(*ii*) the free energy is essentially "two-body"[b] such that we may write the total energy $E(L_n\triangle)$ as the sum of the energies of the small sets of the tiling, plus the interaction between them and the relative entropy;

(*iii*) the entropy is strongly subadditive.

This is summarized in the following assumption. We assume that Γ is a subgroup of G yielding a tiling of $\mathbb{R}^3$ by means of $\triangle$, i.e. $\overline{\cup_{\mu\in\Gamma}\mu\triangle} = \mathbb{R}^3$ and $\mu\triangle \cap \nu\triangle = \emptyset$ for $\mu \neq \nu$.

(A6) *(Two-body decomposition).* For all L and ℓ we can find $g \in G$ and maps $E_g : \Gamma \to \mathbb{R}$, $I_g : \Gamma \times \Gamma \to \mathbb{R}$, $s_g : \{\mathcal{P} : \mathcal{P} \subseteq \Gamma\} \to \mathbb{R}$ such that

- $E_g(\mu) = I_g(\mu, \nu) = 0$ if $\ell g\mu\triangle \cap (L\triangle) = \emptyset$;
- $E(L\triangle) \geq \sum_{\mu\in\Gamma} E_g(\mu) + \frac{1}{2} \sum_{\substack{\mu,\nu\in\Gamma \\ \mu\neq\nu}} I_g(\mu, \nu) - s_g(\Gamma) - |L\triangle|\alpha(\ell)$;
- For all $\mathcal{P} \subseteq \Gamma$ and $A_\mathcal{P} = L\triangle \cap \bigcup_{\mu\in\mathcal{P}} \ell g\mu\triangle$

$$E(A_\mathcal{P}) \leq \sum_{\mu\in\mathcal{P}} E_g(\mu) + \frac{1}{2} \sum_{\substack{\mu,\nu\in\mathcal{P} \\ \mu\neq\nu}} I_g(\mu, \nu) - s_g(\mathcal{P}) + |A_\mathcal{P}|\alpha(\ell);$$

[b] We could as well assume that the energy is k-body with $k < \infty$ but this would complicate the assumptions further more.

- *(Strong subadditivity).* for any disjoint subsets $\mathcal{P}_1$, $\mathcal{P}_2$, $\mathcal{P}_3 \subseteq \Gamma$

$$s_g(\mathcal{P}_1 \cup \mathcal{P}_2 \cup \mathcal{P}_3) + s_g(\mathcal{P}_2) \leq s_g(\mathcal{P}_1 \cup \mathcal{P}_2) + s_g(\mathcal{P}_2 \cup \mathcal{P}_3);$$

- *(Subaverage property).* $\displaystyle\int_{G/\Gamma} dg \sum_{\substack{\mu,\nu\in\Gamma \\ \mu\neq\nu}} I_g(\mu,\nu) \geq -|L\triangle|\alpha(\ell).$

In the applications[c] the previous quantities are interpreted as follows: $E_g(\mathcal{P})$ is the free energy in the union $A_{\mathcal{P}} = (L\triangle) \cap \cup_{\mu\in\mathcal{P}} \ell g\mu\triangle$, $I_g(\mu,\nu)$ is the interaction energy between the simplices $\ell g\mu\triangle$ and $\ell g\nu\triangle$, and $s_g(\mathcal{P})$ is the difference between the entropy of $A_{\mathcal{P}}$ and the sum of the entropies of $\ell g\mu\triangle$ with $\mu \in \mathcal{P}$.

Conjectured by Lanford and Robinson[18] the strong subadditivity (SSA) of the entropy in the quantum mechanical case was proved by Lieb and Ruskai.[23,24] The fact that SSA is very important in the thermodynamic limit was remarked by Robinson and Ruelle[31] and others.[34] In a forthcoming article[15] we prove the following

Theorem 4.2 (Abstract Limit for general domains[15]). *Assume $E : \mathcal{M} \to \mathbb{R}$ satisfies the properties **(A1)–(A6)** for some open convex polyhedron $\triangle \in \mathcal{R}_{a,\varepsilon}$ with $0 \in \triangle$, yielding a tiling of $\mathbb{R}^3$. Then we have for all sequences $\{\Omega_n\} \subset \mathcal{R}_{a,\varepsilon}$ with $|\Omega_n| \to \infty$ and $|\Omega_n|^{-1/3}\mathrm{diam}(\Omega_n) \leq C$,*

$$\lim_{n\to\infty} \frac{E(\Omega_n)}{|\Omega_n|} = \bar{e},$$

where $\bar{e}$ is the limit obtained in Theorem 4.1.

The proof of Theorem 4.2 is based on a careful estimate of the energy and the interaction energies of boundary terms, ie. of the sets $\ell g\mu\triangle$ which intersect the boundary of the big set $L\triangle$. The application to the crystal is not much more difficult than for Theorem 4.1. Indeed in the paper of Graf and Schenker,[13] (4.1) was expressed using a tiling of $\mathbb{R}^3$ and the last subaverage property of **(A6)** essentially follows from their ideas.[13] Strong subadditivity of the entropy is usually expressed via partial traces. A generalization in the setting of localization in Fock space is detailed in our article.[16]

[c]Due to some localization issues of the kinetic energy, it is often needed that the sets of the tiling slightly overlap. See[15] for a generalization in this direction.

4.5. *Proof of Theorem 4.1*

Denote as in the Theorem $e_\ell(g) = E(g\ell\triangle)|\ell\triangle|^{-1}$. Notice that **(A2)**, **(A4)** with $\Omega' = \emptyset$, and **(A1)** imply that e_ℓ is uniformly bounded on G. Also we have by **(A3)** $e_\ell(u+z, R) = e_\ell(u, R)$ for all $(u, R) \in \mathbb{R}^3 \times SO_3(\mathbb{R})$, $z \in \mathbb{Z}^3$, i.e. e_ℓ is periodic with respect to translations. Hence it suffices to prove the theorem for $g = (u, R) \in [0,1]^3 \times SO_3(\mathbb{R})$.

Next we take $\bar{g} \in G$, $L \gg \ell$ and apply **(A5)** with $\Omega = \bar{g}L\triangle$. We get

$$e_L(\bar{g}) \geq \frac{1-\alpha(\ell)}{|L\triangle|} \int_G \frac{E(\bar{g}L\triangle \cap g\ell\triangle)}{|\ell\triangle|} dg - \alpha(\ell).$$

Let us introduce the set $\mathcal{Z}$ of points $z \in \mathbb{Z}^3$ such that $R\ell\triangle + u + z \subset \bar{g}L\triangle$ for all $u \in [0,1]^3$ and all $R \in SO_3(\mathbb{R})$. We also define $\partial\mathcal{Z}$ as the set of points $z \in \mathbb{Z}^3$ such that $(R\ell\triangle + u + z) \cap \bar{g}L\triangle \neq \emptyset$ for some $(u, R) \in [0,1]^3 \times SO_3(\mathbb{R})$ but $z \notin \mathcal{Z}$. We obtain using **(A1)** and **(A3)**

$$\begin{aligned}\int_G \frac{E(\bar{g}L\triangle \cap g\ell\triangle)}{|\ell\triangle|} dg &= \sum_{z\in\mathbb{Z}^3} \int_{[0,1]^3} du \int_{SO_3(\mathbb{R})} dR \frac{E(\bar{g}L\triangle \cap (R\ell\triangle + u + z))}{|\ell\triangle|} \\ &= \sum_{z\in\partial\mathcal{Z}} \int_{[0,1]^3} du \int_{SO_3(\mathbb{R})} dR \frac{E(\bar{g}L\triangle \cap (R\ell\triangle + u + z))}{|\ell\triangle|} \\ &\quad + (\#\mathcal{Z}) \int_{[0,1]^3} du \int_{SO_3(\mathbb{R})} dR\, e_\ell(u, R).\end{aligned}$$

Using the stability property **(A2)**, we infer

$$\frac{E(\bar{g}L\triangle \cap (R\ell\triangle + u + z))}{|\ell\triangle|} \geq -\kappa \frac{|\bar{g}L\triangle \cap (R\ell\triangle + u + z)|}{|\ell\triangle|} \geq -\kappa.$$

Hence

$$\int_G \frac{E(\bar{g}L\triangle \cap g\ell\triangle)}{|\ell\triangle|} dg \geq (\#\mathcal{Z}) \int_{[0,1]^3\times SO_3(\mathbb{R})} e_\ell(g)\, dg + \kappa(\#\partial\mathcal{Z}).$$

As $\triangle$ has an a-regular boundary, it can be seen that $(\#\partial\mathcal{Z}) \leq CL^2\ell$ and $\#\mathcal{Z} = |L\triangle| + O(L^2\ell)$. Using again that e_ℓ is bounded, we eventually obtain the estimate

$$e_L(\bar{g}) \geq \int_{[0,1]^3\times SO_3(\mathbb{R})} e_\ell(g)\, dg - C(\alpha(\ell) + \ell/L)$$

for some constant C. It is then an easy exercise to prove that

$$\lim_{\ell\to\infty} \inf_G e_\ell = \lim_{\ell\to\infty} \int_{[0,1]^3\times SO_3(\mathbb{R})} e_\ell := \bar{e}$$

and finally that $e_\ell \to \bar{e}$ in $L^1([0,1]^3 \times SO_3(\mathbb{R}))$.

The last step consists in proving the uniform convergence, using **(A4)**. Fix some small $\eta > 0$. As $0 \in \triangle$ and $\triangle$ is convex, we have $(1-\eta)\triangle \subset \triangle$. More precisely, there exists an $r > 0$ and a neighborhood W of the identity in $SO_3(\mathbb{R})$ such that $R(1-\eta)\triangle + u \subset \triangle$ for all $(u, R) \in A := B(0, r) \times W \subset G$. We have that $g\ell(1-\eta)\triangle \subset \ell\triangle$ for all $g \in A_\ell := B(0, r\ell) \times W$, hence in particular for all $g \in A$. Now we fix some $\bar{g} \in G$ and apply **(A4)** with $\Omega = \bar{g}\ell\triangle$ and $\Omega' = \bar{g}g\ell(1-\eta)\triangle$, we get

$$E(\bar{g}\ell\triangle) \leq E(\bar{g}g\ell(1-\eta)\triangle) + C|\ell\triangle|\eta + o(|\ell\triangle|).$$

Integrating over $g \in A$ and dividing by $|\ell\triangle|$ we infer

$$e_\ell(\bar{g}) \leq \frac{1}{|\bar{g}A|} \int_{\bar{g}A} e_{(1-\eta)\ell}(g)\, dg + C\eta + o(1)_{\ell\to\infty}.$$

First we pass to the limit as $\ell \to \infty$ using that $e_\ell \to \bar{e}$ in $L^1(G)$ and $|A| \neq 0$. Then we take $\eta \to 0$ and get $\limsup_{\ell\to\infty} \sup_{\bar{g}\in G} e_\ell(\bar{g}) \leq \bar{e}$. This ends the proof of Theorem 4.1.

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SPECTRAL PROPERTIES OF THE BCS GAP EQUATION OF SUPERFLUIDITY*

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We present a review of recent work on the mathematical aspects of the BCS gap equation, covering our results of Ref. 9 as well our recent joint work with Hamza and Solovej[8] and with Frank and Naboko,[6] respectively. In addition, we mention some related new results.

1. Introduction

In this paper we shall describe our recent mathematical study[6,8,9] of one of the current hot topics in condensed matter physics, namely ultra cold fermionic gases consisting of neutral spin-$\frac{1}{2}$ atoms. The kinetic energy of these atoms is described by the non-relativistic Schrödinger operator, and their interaction by a pair potential λV with λ being a coupling parameter. As experimentalists are nowadays able to vary the inter-atomic potentials, the form of λV in actual physical systems can be quite general; see the recent reviews in Refs. 5 and 4. Our primary goal concerns the study of the *superfluid phases* of such systems. According to Bardeen, Cooper and Schrieffer[2] (BCS) the superfluid state is characterized by the existence of a non-trivial solution of the *gap equation*

$$\Delta(p) = -\frac{\lambda}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{V}(p-q) \frac{\Delta(q)}{E(q)} \tilde{\alpha} n h \frac{E(q)}{2T}\, dq \tag{1.1}$$

at some temperature $T \geq 0$, with $E(p) = \sqrt{(p^2-\mu)^2 + |\Delta(p)|^2}$. Here, $\mu > 0$ is the chemical potential and $\hat{V}(p) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} V(x) e^{-ipx} dx$ denotes the Fourier transform of V. The function $\Delta(p)$ is the order parameter and represents the wavefunction of the *Cooper pairs*. Despite the fact that the BCS equation (1.1) is highly non-linear, we shall show in Theorem 2.1 (see also [8, Thm 1]) that the existence of a non-trivial solution to (1.1) at some temperature T is equivalent to the fact that a certain *linear operator*, given in (2.3) below, has a negative eigenvalue. For $T = 0$ this operator is given by $|-\Delta - \mu| + \lambda V$. This rather astonishing possibility of reducing a non-linear to a linear problem allows for a more thorough mathematical study. Using spectral-theoretic methods, we are able to give a precise characterization of the class of potentials leading to a non-trivial solution for (1.1). In particular, in Theorem 2.2 (see also [6, Thm 1]) we prove that for all interaction potentials that create a negative eigenvalue of the effective potential on the Fermi sphere (see (2.6) below; a sufficient condition for this property is that $\int_{\mathbb{R}^3} V(x)dx < 0$), there exists a *critical temperature* $T_c(\lambda V) > 0$ such that (1.1) has a non-trivial (i.e., not identically vanishing) solution for all $T < T_c(\lambda V)$, whereas there is no such solution for $T \geq T_c(\lambda V)$. Additionally, we shall determine in Theorem 2.2 the precise asymptotic behavior of $T_c(\lambda V)$ in the small coupling limit. We extend this result in Theorem 2.3 (see also [9, Thm 1]) and give a derivation of the critical temperature T_c valid to *second order* Born approximation. More precisely, we shall show that

$$T_c = \mu \frac{8e^{\gamma-2}}{\pi} e^{\pi/(2\sqrt{\mu} b_\mu)} \tag{1.2}$$

where $\gamma \approx 0.577$ denotes Euler's constant, and where $b_\mu < 0$ is an effective scattering length. To first order in the Born approximation, b_μ is related to the scattering amplitude of particles with momenta on the Fermi sphere, but to second order the expression is more complicated. The precise formula is given in Eq. (2.11) below. For interaction potentials that decay fast enough at large distances, we shall show that b_μ reduces to the usual *scattering length* a_0 of the interaction potential in the low density limit, i.e., for small μ. Our formula thus represents a *generalization* of a well-known formula in the physics literature.[7,13]

In the case of zero temperature, the function $E(p)$ in (1.1) describes an effective energy-momentum relation for quasi particles, and

$$\Xi := \inf_p E(p) = \inf_p \sqrt{(p^2-\mu)^2 + |\Delta(p)|^2}$$

is called the *energy gap* of the system. It is of major importance for applications, such as the classification of different types of superfluids. In fact, Ξ is the spectral gap of the corresponding second quantized BCS Hamiltonian. (See Refs. 2 and 12 or the appendix in Ref. 8.)

An important problem is the classification of potentials V for which $\Xi > 0$. This questions turns out to be intimately related to the continuity of the momentum distribution $\gamma(p)$, which will be introduced in the next section. In the normal (i.e., not superfluid) state, $\Delta = 0$ and γ is a step function at $T = 0$, namely $\gamma(p) = \theta(|p| - \sqrt{\mu})$. According to the picture presented in standard textbooks the appearance of a superfluid phase softens this step function and $\gamma(p)$ becomes continuous. We are going to prove in this paper that if $V(x)|x| \in L^{6/5}$ and $\int V < 0$ then indeed both strict positivity of $\Xi > 0$ and continuity γ hold. It remains an open problem to find examples of potentials such that the gap vanishes in cases where a superfluid phase occurs.

One of the difficulties involved in evaluating Ξ is the potential nonuniqueness of the solution of the BCS gap equation. For interaction potentials that have nonpositive Fourier transform, however, we shall show that the BCS pair wavefunction *is* unique, and has zero angular momentum. In this case, we shall prove in Theorem 2.5 (see also [9, Thm. 2]) similar results for Ξ as for the critical temperature. It turns out that, at least up to second order Born approximation,

$$\Xi = T_c \frac{\pi}{e^\gamma} \tag{1.3}$$

in this case. This equality is valid for any density, i.e., for any value of the chemical potential μ. In particular, Ξ has exactly the same exponential dependence on the interaction potential, described by b_μ, as the critical temperature T_c.

2. Preliminaries and main results

We consider a gas of spin 1/2 fermions at temperature $T \geq 0$ and chemical potential $\mu > 0$, interacting via a local two-body interaction potential of the form $2\lambda V(x)$. Here, $\lambda > 0$ is a coupling parameter, and the factor 2 is introduced for convenience. We assume that V is real-valued and has some mild regularity properties, namely $V \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$. In the BCS approximation, the system is described by the *BCS functional* $\mathcal{F}_T$, derived by Leggett in his seminal paper,[11] based on the original work of BCS.[2] The

BCS functional $\mathcal{F}_T$ is related to the *pressure* of the system and is given by

$$\mathcal{F}_T(\gamma,\alpha) = \int (p^2-\mu)\gamma(p)dp + \int |\alpha(x)|^2 V(x)dx - TS(\gamma,\alpha), \qquad (2.1)$$

where the entropy S is

$$S(\gamma,\alpha) = -\int \mathrm{Tr}_{\mathbb{C}^2}\left[\Gamma(p)\log\Gamma(p)\right]dp, \qquad \Gamma(p) = \begin{pmatrix} \gamma(p) & \hat{\alpha}(p) \\ \hat{\alpha}(p) & 1-\gamma(p) \end{pmatrix}.$$

The functions $\gamma(p)$ and $\hat{\alpha}(p)$ are interpreted as the momentum distribution and the Cooper pair wave function, respectively. The satisfy the matrix constraint $0 \leq \Gamma(p) \leq 1$ for all $p \in \mathbb{R}^3$. In terms of the BCS functional the occurrence of superfluidity is described by minimizers with $\alpha \neq 0$. We remark that in the case of the Hubbard-model this functional was studied in Ref. 1.

For an arbitrary temperature $0 \leq T < \infty$ the BCS gap equation, which is the Euler-Lagrange equation associated with the functional $\mathcal{F}_T$, reads

$$\Delta(p) = -\frac{\lambda}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{V}(p-q)\frac{\Delta(q)}{E(q)}\tilde{\alpha}nh\frac{E(q)}{2T}\,dq, \qquad (2.2)$$

where $E(p) = \sqrt{(p^2-\mu)^2 + |\Delta(p)|^2}$. The order parameter Δ is related to the expectation value of the Cooper pairs α via $2\alpha(p) = \Delta(p)/E(p)$. We present in the following a thorough mathematical study of this equation. In order to do so, we shall not attack the equation (2.2) directly, but exploit the fact that α is a critical point of the semi-bounded functional $\mathcal{F}_T$.

The key to our studies is the observation in Ref. 8 that the existence of a non-trivial solution to the *non-linear* equation (2.2) can be reduced to a *linear* criterion, which can be formulated as follows.

Theorem 2.1 ([8, Theorem 1]). *Let $V \in L^{3/2}$, $\mu \in \mathbb{R}$, and $\infty > T \geq 0$. Define*

$$K_{T,\mu} = (p^2-\mu)\frac{e^{(p^2-\mu)/T}+1}{e^{(p^2-\mu)/T}-1}\,.$$

Then the non-linear BCS equation (2.2) *has a non-trivial solution if and only if the linear operator*

$$K_{T,\mu} + \lambda V\,, \qquad (2.3)$$

acting on $L^2(\mathbb{R}^3)$, has at least one negative eigenvalue.

Hence we are able to relate a non-linear problem to a linear problem which is much easier to handle. The operator $K_{T,\mu}$ is understood as a multiplication operator in momentum space. In the limit $T \to 0$ this operator reduces to $|-\Delta-\mu| + \lambda V$.

2.1. *The critical temperature*

Theorem 2.1 enables a precise definition of the critical temperature, by

$$T_c(\lambda V) := \inf\{T \,|K_{T,\mu} + \lambda V \geq 0\}. \tag{2.4}$$

The symbol $K_{T,\mu}(p)$ is point-wise monotone in T. This implies that for any potential V, there is a critical temperature $0 \leq T_c(\lambda V) < \infty$ that separates two phases, a *superfluid* phase for $0 \leq T < T_c(\lambda V)$ from a *normal* phase for $T_c(\lambda V) \leq T < \infty$. Note that $T_c(\lambda V) = 0$ means that there is no superfluid phase for λV. Using the linear criterion (2.4) we can classify the potentials for which $T_c(\lambda V) > 0$, and simultaneously we can evaluate the asymptotic behavior of $T_c(\lambda V)$ in the limit of small λ. This can be done by spectral theoretical methods. Applying the Birman-Schwinger principle one observes that the critical temperature T_c can be characterized by the fact that the compact operator

$$\lambda(\operatorname{sgn} V)|V|^{1/2} K_{T_c,\mu}^{-1} |V|^{1/2} \tag{2.5}$$

has -1 as its lowest eigenvalue. This operator is singular for $T_c \to 0$, and the key observation is that its singular part is represented by the operator $\lambda \ln(1/T_c)\mathcal{V}_\mu$, where $\mathcal{V}_\mu : L^2(\Omega_\mu) \mapsto L^2(\Omega_\mu)$ is given by

$$\big(\mathcal{V}_\mu u\big)(p) = \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{\mu}} \int_{\Omega_\mu} \hat{V}(p-q) u(q)\, d\omega(q)\,. \tag{2.6}$$

Here, Ω_μ denotes the 2-sphere with radius $\sqrt{\mu}$, and $d\omega$ denotes Lebesgue measure on Ω_μ. We note that the operator $\mathcal{V}_\mu$ has appeared already earlier in the literature.[3,10]

Our analysis here is somewhat similar in spirit to the one concerning the lowest eigenvalue of the Schrödinger operator $p^2 + \lambda V$ in *two* space dimensions.[14] This latter case is considerably simpler, however, as p^2 has a unique minimum at $p = 0$, whereas $K_{T,\mu}(p)$ takes its minimal value on the Fermi sphere $p^2 = \mu$, meaning that its minimum is highly degenerate. Hence, in our case, the problem is reduced to analyzing a map from the L^2 functions on the Fermi sphere Ω_μ (of radius $\sqrt{\mu}$) to itself. Let us denote the lowest eigenvalue of $\mathcal{V}_\mu$ as

$$e_\mu(V) := \inf \operatorname{spec} \mathcal{V}_\mu\,.$$

Whenever this eigenvalue is negative then the critical temperature is non zero for *all* $\lambda > 0$, and we can evaluate its asymptotics. Moreover, the converse is "almost" true:

Theorem 2.2 ([6, Theorem 1]). *Let $V \in L^{3/2}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$ be real-valued, and let $\lambda > 0$.*

(i) Assume that $e_\mu(V) < 0$. Then $T_c(\lambda V)$ is non-zero for all $\lambda > 0$, and

$$\lim_{\lambda \to 0} \lambda \ln \frac{\mu}{T_c(\lambda V)} = -\frac{1}{e_\mu(V)}\,. \tag{2.7}$$

(ii) Assume that $e_\mu(V) = 0$. If $T_c(\lambda V)$ is non-zero, then $\ln(\mu/T_c(\lambda V)) \geq c\lambda^{-2}$ for some $c > 0$ and small λ.

(iii) If there exists an $\varepsilon > 0$ such that $e_\mu(V - \epsilon|V|) = 0$, then $T_c(\lambda V) = 0$ for small enough λ.

As we see, the occurrence of superfluidity as well as the asymptotic behavior of $T_c(\lambda V)$ is governed by $e_\mu(V)$. A sufficient condition for $e_\mu(V)$ to be negative is $\int V < 0$. But one can easily find other examples. Eq. (2.7) shows that the critical temperature behaves like $T_c(\lambda V) \sim \mu e^{1/(\lambda e_\mu(V))}$. In other words it is exponentially small in the coupling.

In the following, we shall derive the second order correction, i.e., we will compute the constant in front of the exponentially small term in T_c. For this purpose, we define an operator $\mathcal{W}_\mu$ on $L^2(\Omega_\mu)$ via its quadratic form

$$\langle u|\mathcal{W}_\mu|u\rangle = \int_0^\infty d|p| \left(\frac{|p|^2}{\big||p|^2 - \mu\big|} \left[\int_{\mathbb{S}^2} d\Omega \left(|\hat\varphi(p)|^2 - |\hat\varphi(\sqrt{\mu}p/|p|)|^2 \right) \right] + \int_{\mathbb{S}^2} d\Omega\, |\hat\varphi(\sqrt{\mu}p/|p|)|^2 \right). \tag{2.8}$$

Here, $\hat\varphi(p) = (2\pi)^{-3/2} \int_{\Omega_\mu} \hat V(p-q) u(q) d\omega(q)$, and $(|p|, \Omega) \in \mathbb{R}_+ \times \mathbb{S}^2$ denote spherical coordinates for $p \in \mathbb{R}^3$. We note that since $V \in L^1(\mathbb{R}^3)$, $\int_{\mathbb{S}^2} d\Omega\, |\hat\varphi(p)|^2$ is Lipschitz continuous in $|p|$ for any $u \in L^2(\mathbb{R}^3)$, and hence the radial integration is well-defined, even in the vicinity of $p^2 = \mu$. In fact the operator $\mathcal{W}_\mu$ can be shown to be Hilbert-Schmidt class, see [9, Section 3].

For $\lambda > 0$, let

$$\mathcal{B}_\mu = \lambda \frac{\pi}{2\sqrt{\mu}} \mathcal{V}_\mu - \lambda^2 \frac{\pi}{2\mu} \mathcal{W}_\mu\,, \tag{2.9}$$

and let $b_\mu(\lambda)$ denote its ground state energy,

$$b_\mu(\lambda) = \inf \operatorname{spec} \mathcal{B}_\mu\,. \tag{2.10}$$

We note that if $e_\mu < 0$, then also $b_\mu(\lambda) < 0$ for small λ. In fact, if the eigenfunction corresponding to the lowest eigenvalue e_μ of $\mathcal{V}_\mu$ is unique and

equals $u \in L^2(\Omega_\mu)$, then

$$b_\mu(\lambda) = \langle u|\mathcal{B}_\mu|u\rangle + O(\lambda^3) = \lambda \frac{\pi e_\mu}{2\sqrt{\mu}} - \lambda^2 \frac{\pi \langle u|\mathcal{W}_\mu|u\rangle}{2\mu} + O(\lambda^3)\,. \tag{2.11}$$

In the degenerate case, this formula holds if one chooses u to be the eigenfunction of $\mathcal{V}_\mu$ that yields the largest value $\langle u|\mathcal{W}_\mu|u\rangle$ among all such (normalized) eigenfunctions.

With the aid of $b_\mu(\lambda)$, we can now recover the next order of the critical temperature for small λ.

Theorem 2.3 ([9, Theorem 1]). *Let $V \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$ and let $\mu > 0$. Assume that $e_\mu = \inf \operatorname{spec} \mathcal{V}_\mu < 0$, and let $b_\mu(\lambda)$ be defined in (2.10). Then the critical temperature T_c for the BCS equation is strictly positive and satisfies*

$$\lim_{\lambda\to 0} \left(\ln\left(\frac{\mu}{T_c}\right) + \frac{\pi}{2\sqrt{\mu}\, b_\mu(\lambda)} \right) = 2 - \gamma - \ln(8/\pi)\,. \tag{2.12}$$

Here, $\gamma \approx 0.577$ denotes Euler's constant.

The Theorem says that, for small λ,

$$T_c \sim \mu \frac{8e^{\gamma-2}}{\pi} e^{\pi/(2\sqrt{\mu} b_\mu(\lambda))}\,. \tag{2.13}$$

Note that $b_\mu(\lambda)$ can be interpreted as a (renormalized) effective scattering length of $2\lambda V(x)$ (in second order Born approximation) for particles with momenta on the Fermi sphere. In fact, if V is *radial* and $\int_{\mathbb{R}^3} V(x)dx < 0$, it is not difficult to see that for small enough μ the (unique) eigenfunction corresponding to the lowest eigenvalue e_μ of $\mathcal{V}_\mu$ is the constant function $u(p) = (4\pi\mu)^{-1/2}$. (See [6, Section 2.1].) For this u, we have

$$\lim_{\mu\to 0} \langle u|\mathcal{B}_\mu|u\rangle = (\lambda/4\pi) \int_{\mathbb{R}^3} V(x)dx - (\lambda/4\pi)^2 \int_{\mathbb{R}^6} \frac{V(x)V(y)}{|x-y|} dxdy \equiv a_0(\lambda)\,.$$

Here, $a_0(\lambda)$ equals the *scattering length* of $2\lambda V$ in second order Born approximation. Assuming additionally that $V(x)|x| \in L^1$ and bearing in mind that $b_\mu(\lambda) = \langle u|\mathcal{B}_\mu|u\rangle + O(\lambda^3)$ for small enough μ, we can, in fact, estimate the difference between $b_\mu(\lambda)$ and $a_0(\lambda)$. Namely we prove in [9, Proposition 1] that

$$\lim_{\mu\to 0} \frac{1}{\sqrt{\mu}} \left(\frac{1}{\langle u|\mathcal{B}_\mu|u\rangle} - \frac{1}{a_0(\lambda)} \right) = 0\,.$$

This yields the approximation

$$T_c \approx \mu \frac{8e^{\gamma-2}}{\pi} e^{\pi/(2\sqrt{\mu} a_0(\lambda))}$$

in the limit of small λ *and* small μ. This expression is well-known in the physics literature.[7,13] We point out, however, that our formula (2.13) is much more general since it holds for any value of $\mu > 0$.

2.2. *Energy Gap at Zero Temperature*

Consider now the zero temperature case $T = 0$. In this case, it is natural to formulate a functional depending only on α instead of γ and α. In fact, for $T = 0$ the optimal choice of $\gamma(p)$ in $\mathcal{F}_T$ for given $\hat{\alpha}(p)$ is clearly

$$\gamma(p) = \begin{cases} \frac{1}{2}(1 + \sqrt{1 - 4|\hat{\alpha}(p)|^2}) \text{ for } p^2 < \mu \\ \frac{1}{2}(1 - \sqrt{1 - 4|\hat{\alpha}(p)|^2}) \text{ for } p^2 > \mu \end{cases} . \tag{2.14}$$

Subtracting an unimportant constant, this leads to the *zero temperature BCS functional*

$$\mathcal{F}_0(\alpha) = \frac{1}{2} \int_{\mathbb{R}^3} |p^2 - \mu| \left(1 - \sqrt{1 - 4|\hat{\alpha}(p)|^2}\right) dp + \lambda \int_{\mathbb{R}^3} V(x)|\alpha(x)|^2 \, dx \, . \tag{2.15}$$

The variational equation satisfied by a minimizer of (2.15) is then

$$\Delta(p) = -\frac{\lambda}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{V}(p - q) \frac{\Delta(q)}{E(q)} \, dq \, , \tag{2.16}$$

with $\Delta(p) = 2E(p)\hat{\alpha}(p)$. This is simply the BCS equation (2.2) at $T = 0$. For a solution Δ, the *energy gap* Ξ is defined as

$$\Xi = \inf_p E(p) = \inf_p \sqrt{(p^2 - \mu)^2 + |\Delta(p)|^2} \, . \tag{2.17}$$

It has the interpretation of an energy gap in the corresponding second-quantized BCS Hamiltonian (see, e.g., Ref. 12 or the appendix in Ref. 8.)

A priori, the fact that the order parameter Δ is non vanishing does not imply that $\Xi > 0$. Strict positivity of Ξ turns out to be related to the continuity of the corresponding γ in (2.14). In fact, we are going to prove in Lemma 5.1 that if V decays fast enough, i.e., $V(x)|x| \in L^{6/5}(\mathbb{R}^3)$, the two properties, $\Xi > 0$ and $\gamma(p)$ continuous, are equivalent. Both properties hold true under the assumption that $\int V < 0$:

Theorem 2.4. *Let $V \in L^{3/2} \cap L^1$, with $V(x)|x| \in L^{6/5}(\mathbb{R}^3)$ and $\int V = (2\pi)^{3/2}\hat{V}(0) < 0$. Let α be a minimizer of the BCS functional. Then Ξ defined in (2.17) is strictly positive, and the corresponding momentum distribution γ in (2.14) is continuous.*

One of the difficulties involved in evaluating Ξ is the potential non-uniqueness of minimizers of (2.15), and hence non-uniqueness of solutions

of the BCS gap equation (2.16). The gap Ξ may depend on the choice of Δ in this case. For potentials V with non-positive Fourier transform, however, we can prove the uniqueness of Δ and, in addition, we are able to derive the precise asymptotic of Ξ as $\lambda \to 0$.

In the following we will restrict our attention to radial potentials V with non-positive Fourier transform. We also assume that $\hat{V}(0) = (2\pi)^{-3/2} \int V(x)dx < 0$. It is easy to see that $e_\mu = \inf \operatorname{spec} \mathcal{V}_\mu < 0$ in this case, and that the (unique) eigenfunction corresponding to this lowest eigenvalue of $\mathcal{V}_\mu$ is the constant function.

In particular we have the following asymptotic behavior of the energy gap Ξ as $\lambda \to 0$.

Theorem 2.5 ([9, Theorem 2]). *Assume that $V \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$ is radial, with $\hat{V}(p) \leq 0$ and $\hat{V}(0) < 0$. Then there is a unique minimizer (up to a constant phase) of the BCS functional (2.15) at $T = 0$. The corresponding energy gap, $\Xi = \inf_p \sqrt{(p^2 - \mu)^2 + |\Delta(p)|^2}$, is strictly positive, and satisfies*

$$\lim_{\lambda \to 0} \left(\ln \left(\frac{\mu}{\Xi} \right) + \frac{\pi}{2\sqrt{\mu}\, b_\mu(\lambda)} \right) = 2 - \ln(8)\,. \tag{2.18}$$

Here, $b_\mu(\lambda)$ be defined in (2.10).

The Theorem says that, for small λ,

$$\Xi \sim \mu \frac{8}{e^2} e^{\pi/(2\sqrt{\mu} b_\mu(\lambda))}\,.$$

In particular, in combination with Theorem 2.3, we obtain the *universal ratio*

$$\lim_{\lambda \to 0} \frac{\Xi}{T_c} = \frac{\pi}{e^\gamma} \approx 1.7639\,.$$

That is, the ratio of the energy gap Ξ and the critical temperature T_c tends to a universal constant as $\lambda \to 0$, independently of V and μ. This property has been observed before for the original BCS model with rank one interaction,[2,12] and in the low density limit for more general interactions[7] under additional assumptions. Our analysis shows that it is valid in full generality at small coupling $\lambda \ll 1$.

3. Sketch of the proof of Theorem 2.1

The backbone of our analysis is the linear criterion in Theorem 2.1. As a first step towards its proof, one has to prove that the functional $\mathcal{F}_T(\gamma, \alpha)$

in (2.1) attains a minimum on the set

$$\mathcal{D} = \{(\gamma,\alpha)\,|\,\gamma \in L^1(\mathbb{R}^3,(1+p^2)dp), \alpha \in H^1(\mathbb{R}^3), 0 \leq \gamma \leq 1, |\hat{\alpha}|^2 \leq \gamma(1-\gamma)\}.$$

This can be done by proving lower semi-continuity of $\mathcal{F}_T$ on $\mathcal{D}$. See [8, Prop. 1] for details. Theorem 2.1 is then a direct consequence of the equivalence of the following three statements [8, Theorem 1]:

(i) The normal state $(\gamma_0, 0)$, with $\gamma_0 = [e^{(p^2-\mu)/T}+1]^{-1}$ being the Fermi-Dirac distribution, is unstable under pair formation, i.e.,

$$\inf_{(\gamma,\alpha)\in\mathcal{D}} \mathcal{F}_T(\gamma,\alpha) < \mathcal{F}_T(\gamma_0,0)\,.$$

(ii) There exists a pair $(\gamma,\alpha) \in \mathcal{D}$, with $\alpha \neq 0$, such that

$$\Delta(p) = \frac{p^2-\mu}{\frac{1}{2}-\gamma(p)}\hat{\alpha}(p) \tag{3.1}$$

satisfies the BCS gap equation (2.2).

(iii) The linear operator $K_{T,\mu}+V$ has at least one negative eigenvalue.

The proof of the equivalence of these three statement consists of the following steps. First, it is straightforward to show that (i) $\Rightarrow$ (ii). By evaluating the stationary equations in both variables, γ and α, one shows that the combination (3.1) satisfies the BCS equation (2.2).

To show that (iii) $\Rightarrow$ (i), first note that $(\gamma_0, 0)$ is the minimizer of $\mathcal{F}_T$ in the case $V = 0$. Consequently $\frac{d}{dt}\mathcal{F}_T(\gamma_0, tg)|_{t=0} = 0$ for general g. Moreover, a simple calculation shows that

$$\frac{d^2}{dt^2}\mathcal{F}(\gamma_0,tg)_{t=0} = 2\langle g|K_{T,\mu}+\lambda V|g\rangle\,.$$

If $K_{T,\mu}+\lambda V$ has a negative eigenvalue, we thus see that $\mathcal{F}(\gamma_0,tg) < \mathcal{F}_T(\gamma_0,0)$ for small t and an appropriate choice of g.

The hardest part in showing the equivalence of the three statements is to show that (ii) $\Rightarrow$ (iii). Given a pair $(\tilde{\gamma},\tilde{\alpha})$ such that the corresponding Δ in (3.1) satisfies the BCS equation (2.2), we note that if $\hat{\alpha} = m(p)\hat{\tilde{\alpha}}(p)$ and $\gamma(p) = 1/2 + m(p)(\gamma(p)-1/2)$, the pair (γ,α) yields the same Δ and hence also satisfies (2.2). Moreover, with the choice

$$m(p) = \frac{p^2-\mu}{\frac{1}{2}-\tilde{\gamma}(p)}\frac{\tilde{\alpha}nh\frac{E(p)}{2T}}{2E(p)}$$

(where $E(p) = \sqrt{(p^2-\mu)^2 + |\Delta(p)|^2}$), the new pair (γ, α) satisfies additionally

$$\frac{2E(p)}{\tilde{\alpha} n h \frac{E(p)}{2T}} = \frac{p^2-\mu}{\frac{1}{2} - \gamma(p)} \tag{3.2}$$

$$\frac{\lambda}{(2\pi)^3} \int \hat{V}(p-q)\hat{\alpha}(q)dq = -\frac{p^2-\mu}{\frac{1}{2}-\gamma}\hat{\alpha}(p)\,. \tag{3.3}$$

Note that in the case $V = 0$, i.e., $\Delta = 0$, the equation (3.2) reduces to

$$2K_{T,\mu}(p) = \frac{p^2-\mu}{\frac{1}{2}-\gamma_0}.$$

Using this fact, together with (3.3), we thus obtain

$$\langle \alpha | K_{T,\mu} + \lambda V | \alpha \rangle = \frac{1}{2} \left\langle \alpha \left| \frac{p^2-\mu}{\frac{1}{2}-\gamma_0} - \frac{p^2-\mu}{\frac{1}{2}-\gamma} \right| \alpha \right\rangle . \tag{3.4}$$

Using the definition of $E(p)$ and the strict monotonicity of the function $x \mapsto x/\tilde{\alpha} n h \frac{x}{2T}$ for $x \geq 0$, we infer from (3.2) that

$$\frac{p^2-\mu}{\frac{1}{2}-\gamma_0} \leq \frac{p^2-\mu}{\frac{1}{2}-\gamma}\,,$$

with strict the inequality on the set where $\Delta \neq 0$. Consequently, the expression (3.4) is strictly negative. Hence $K_{T,\mu} + \lambda V$ has a negative eigenvalue. This shows that (ii) implies (iii).

4. Proof of Theorems 2.2 and 2.3

For a (not necessarily sign-definite) potential $V(x)$ let us use the notation

$$V(x)^{1/2} = (\operatorname{sgn} V(x))|V(x)|^{1/2}\,.$$

From our definition of the critical temperature T_c it follows immediately that for $T = T_c$ the operator $K_{T,\mu} + \lambda V$ has and eigenvalue 0 and no negative eigenvalue. If ψ is the corresponding eigenvector, one can rewrite the eigenvalue equation in the form

$$-\psi = \lambda K_{T,\mu}^{-1} V \psi.$$

Multiplying this equation by $V^{1/2}(x)$, one obtains an eigenvalue equation for $\varphi = V^{1/2}\psi$. This argument works in both directions and is called the Birman-Schwinger principle (see [6, Lemma 1]). In particular it tells us that

the critical temperature T_c is determined by the fact that for this value of T the smallest eigenvalue of

$$B_T = \lambda V^{1/2} K_{T,\mu}^{-1} |V|^{1/2} \tag{4.1}$$

equals -1. Note that although B_T is not self-adjoint, it has real spectrum.

Let $\mathfrak{F} : L^1(\mathbb{R}^3) \to L^2(\Omega_\mu)$ denote the (bounded) operator which maps $\psi \in L^1(\mathbb{R}^3)$ to the Fourier transform of ψ, restricted to the sphere Ω_μ. Since $V \in L^1(\mathbb{R}^3)$, multiplication by $|V|^{1/2}$ is a bounded operator from $L^2(\mathbb{R}^3)$ to $L^1(\mathbb{R}^3)$, and hence $\mathfrak{F}|V|^{1/2}$ is a bounded operator from $L^2(\mathbb{R}^3)$ to $L^2(\Omega_\mu)$. Let

$$m_\mu(T) = \max\left\{ \frac{1}{4\pi\mu} \int_{\mathbb{R}^3} \left(\frac{1}{K_{T,\mu}(p)} - \frac{1}{p^2} \right) dp \, , 0 \right\} ,$$

and let

$$M_T = K_{T,\mu}^{-1} - m_\mu(T) \mathfrak{F}^* \mathfrak{F} \, . \tag{4.2}$$

As in [6, Lemma 2] one can show that $V^{1/2} M_T |V|^{1/2}$ is a Hilbert-Schmidt operator on $L^2(\mathbb{R}^3)$, and its Hilbert Schmidt norm is bounded uniformly in T. In particular, the singular part of B_T as $T \to 0$ is entirely determined by $V^{1/2} \mathfrak{F}^* \mathfrak{F} |V|^{1/2}$.

Since $V^{1/2} M_T |V|^{1/2}$ is uniformly bounded, we can choose λ small enough such that $1 + \lambda V^{1/2} M_T |V|^{1/2}$ is invertible, and we can then write $1 + B_T$ as

$$\begin{aligned} 1 + B_T &= 1 + \lambda V^{1/2} \left(m_\mu(T) \mathfrak{F}^* \mathfrak{F} + M_T \right) |V|^{1/2} \qquad (4.3) \\ &= \left(1 + \lambda V^{1/2} M_T |V|^{1/2} \right) \left(1 + \frac{\lambda m_\mu(T)}{1 + \lambda V^{1/2} M_T |V|^{1/2}} V^{1/2} \mathfrak{F}^* \mathfrak{F} |V|^{1/2} \right) . \end{aligned}$$

Then B_T having an eigenvalue -1 is equivalent to

$$\frac{\lambda m_\mu(T)}{1 + \lambda V^{1/2} M_T |V|^{1/2}} V^{1/2} \mathfrak{F}^* \mathfrak{F} |V|^{1/2} \tag{4.4}$$

having an eigenvalue -1. The operator in (4.4) is isospectral to the selfadjoint operator

$$\mathfrak{F} |V|^{1/2} \frac{\lambda m_\mu(T)}{1 + \lambda V^{1/2} M_T |V|^{1/2}} V^{1/2} \mathfrak{F}^* \, , \tag{4.5}$$

acting on $L^2(\Omega_\mu)$.

At $T = T_c$, -1 is the smallest eigenvalue of B_T, hence (4.4) and (4.5) have an eigenvalue -1 for this value of T. Moreover, we can conclude that -1 is actually the *smallest* eigenvalue of (4.4) and (4.5) in this case. For, if

there were an eigenvalue less then -1, we could increase T and, by continuity, find some $T > T_c$ for which there is an eigenvalue -1. Using (4.3), this would contradict the fact that B_T has no eigenvalue -1 for $T > T_c$.

Consequently, the equation for the critical temperature can be written as

$$\lambda m_\mu(T_c) \inf \operatorname{spec} \mathfrak{F}|V|^{1/2} \frac{1}{1+\lambda V^{1/2} M_{T_c} |V|^{1/2}} V^{1/2} \mathfrak{F}^* = -1\,. \tag{4.6}$$

This equation is the starting point for the proof of Theorems 2.2 and 2.3.

Proof of Theorem 2.2. Up to first order in λ the equation (4.6) reads

$$\lambda m_\mu(T_c) \inf \operatorname{spec} \mathfrak{F}[V - \lambda V M_{T_c} V + O(\lambda^2)]\mathfrak{F}^* = -1\,, \tag{4.7}$$

where the error term $O(\lambda^2)$ is uniformly bounded in T_c. Note that $\mathfrak{F}V\mathfrak{F}^* = \sqrt{\mu}\,\mathcal{V}_\mu$ defined in (2.6). Assume now that $e_\mu = \inf \operatorname{spec} \mathcal{V}_\mu$ is strictly negative. Since $V^{1/2} M_{T_c} V^{1/2}$ is uniformly bounded, it follows immediately that

$$\lim_{\lambda \to 0} \lambda m_\mu(T_c) = -\frac{1}{\inf \operatorname{spec} \mathfrak{F} V \mathfrak{F}^*} = -\frac{1}{\sqrt{\mu}\, e_\mu}\,.$$

Together with the asymptotic behavior $m_\mu(T) \sim \mu^{-1/2} \ln(\mu/T)$ as $T \to 0$, this implies the leading order behavior of $\ln(\mu/T_c)$ as $\lambda \to 0$ and proves the statement in (i).

In order to see (ii) it suffices to realize that, in the case $\mathfrak{F}V\mathfrak{F}^* \geq 0$, Eq. (4.7) yields $m_{T_c} \geq \text{const}\,/\lambda^2$.

The statement (iii) is a consequence of the fact that

$$\mathfrak{F}|V|^{1/2} \frac{1}{1+\lambda V^{1/2} M_{T_c} |V|^{1/2}} V^{1/2} \mathfrak{F}^* \geq \mathfrak{F}[V - \text{const}\,\lambda |V|]\mathfrak{F}^* \geq 0,$$

for λ small enough. We refer to Ref. 6 for details. □

Proof of Theorem 2.3. To obtain the next order, we use Eq. (4.7) and employ first order perturbation theory. Since $\mathfrak{F}V\mathfrak{F}^*$ is compact and $\inf \operatorname{spec} \mathfrak{F}V\mathfrak{F}^* < 0$ by assumption, first order perturbation theory implies that

$$m_\mu(T_c) = \frac{-1}{\lambda \langle u|\mathfrak{F}V\mathfrak{F}^*|u\rangle - \lambda^2 \langle u|\mathfrak{F}V M_{T_c} V\mathfrak{F}^*|u\rangle + O(\lambda^3)}\,, \tag{4.8}$$

where u is the (normalized) eigenfunction corresponding to the lowest eigenvalue of $\mathfrak{F}V\mathfrak{F}^*$. (In case of degeneracy, one has to the choose the u that minimizes the λ^2 term in the denominator of (4.8) among all such eigenfunctions.)

Eq. (4.8) is an implicit equation for T_c. Since $\mathfrak{F}VM_TV\mathfrak{F}^*$ is uniformly bounded and $T_c \to 0$ as $\lambda \to 0$, we have to evaluate the limit of $\langle u|\mathfrak{F}VM_TV\mathfrak{F}^*|u\rangle$ as $T \to 0$. To this aim, let $\varphi = V\mathfrak{F}^*u$. Then

$$\begin{aligned}&\langle u|\mathfrak{F}VM_TV\mathfrak{F}^*|u\rangle\\ &= \int_{\mathbb{R}^3} \frac{1}{K_{T,\mu}(p)} |\hat\varphi(p)|^2\, dp - m_\mu(T) \int_{\Omega_\mu} |\hat\varphi(p)|^2\, d\omega(p) \qquad (4.9)\\ &= \int_{\mathbb{R}^3} \left(\frac{1}{K_{T,\mu}(p)} \left[|\hat\varphi(p)|^2 - |\hat\varphi(\sqrt{\mu}p/|p|)|^2 \right] + \frac{1}{p^2} |\hat\varphi(\sqrt{\mu}p/|p|)|^2 \right) dp\,.\end{aligned}$$

Recall that $K_{T,\mu}(p)$ converges to $|p^2 - \mu|$ as $T \to 0$. Using the Lipschitz continuity of the spherical average of $|\hat\varphi(p)|^2$ (see [9, Equ. (29)]) it is easy to see that

$$\lim_{T\to 0} \langle u|\mathfrak{F}VM_TV\mathfrak{F}^*|u\rangle = \langle u|\mathcal{W}_\mu|u\rangle\,, \qquad (4.10)$$

with $\mathcal{W}_\mu$ defined in (2.8). In particular, combining (4.8) and (4.10), we have thus shown that

$$\lim_{\lambda\to 0} \left(m_\mu(T_c) + \frac{1}{\inf \text{ spec } \left(\lambda\sqrt{\mu}\,\mathcal{V}_\mu - \lambda^2 \mathcal{W}_\mu\right)} \right) = 0\,. \qquad (4.11)$$

The statement follows by using the asymptotic behavior ([9, Lemma 1])

$$m_\mu(T) = \frac{1}{\sqrt{\mu}} \left(\ln \frac{\mu}{T} + \gamma - 2 + \ln \frac{8}{\pi} + o(1) \right) \qquad (4.12)$$

in the limit of small T, where $\gamma \approx 0.5772$ is Euler's constant. □

5. Proof of Theorems 2.4 and 2.5

5.1. *Sufficient condition for* $\Xi > 0$

If $e_\mu(V) < 0$ we know that the BCS equation (2.16) has a solution, meaning the system shows a superfluid phase for $T = 0$. This is not sufficient, however, to guarantee the existence of a positive gap $\Xi > 0$ nor the continuity of the momentum distribution γ. Unlike the case of the critical temperature, we lack a linear criterion which allows a precise characterization of potentials V giving rise to a strictly positive gap. We are, however, able to derive sufficient conditions, namely a fast enough decay of V. Under such assumptions one can show the equivalence of the positivity of Ξ and the continuity of γ. Both hold true if additionally $\int V < 0$. It remains an open problem to find examples for V such that $e_\mu < 0$ but $\Xi = 0$.

Lemma 5.1. *Assume that $V \in L^{3/2}$ and that $V(x)|x| \in L^{6/5}(\mathbb{R}^3)$. Then $\Xi > 0$ if and only if γ is continuous.*

Proof. It is easy to deduce[8] from the BCS equation (2.16) that $\hat{\alpha}$ is in $C^0(\mathbb{R}^3)$. Because of (2.14) the continuity of γ is equivalent to the fact that $|\hat{\alpha}| \equiv 1/4$ on the Fermi Ω_μ. From the relation $\Delta(p) = 2E(p)\hat{\alpha}(p)$ one obtains

$$|\hat{\alpha}(p)|^2 = \frac{1}{4}\frac{1}{\sqrt{\frac{(p^2-\mu)^2}{|\Delta(p)|^2}+1}}\,, \tag{5.1}$$

and we can conclude that $|\hat{\alpha}|^2 = 1/4$ on the Fermi surface if and only if $\Delta(p)$ does not vanish on Ω_μ. Namely, suppose that Δ vanishes at some p' on the Fermi surface. Since $\alpha \in H^1(\mathbb{R}^3)$ we see that $\alpha \in L^2(\mathbb{R}^3) \cap L^6(\mathbb{R}^3)$ and hence, together with $V(x)|x| \in L^{6/5}$, Hölder's inequality implies that $\check{\Delta}(x)|x| = V(x)\alpha(x)|x| \in L^1(\mathbb{R}^3)$. We thus infer that $\Delta(p)$ is Lipschitz continuous, meaning that $\Delta(p)$ cannot decay slower to 0 than linear. Hence there is a δ such that $\lim_{p\to p'} \frac{(p^2-\mu)^2}{|\Delta(p)|^2} \geq \delta$ and $|\alpha(p')|^2 \leq \frac{1}{4}\frac{1}{\sqrt{\delta+1}} < \frac{1}{4}$. □

Proof of Theorem 2.4. Let α be a global minimizer of the BCS functional $\mathcal{F}_0$. Then for any $\hat{g} \in C_0^\infty(\mathbb{R}^3)$ such that $|\hat{\alpha} + \epsilon\hat{g}| \leq 1/2$ for ϵ small enough,

$$\frac{d^2}{d\epsilon^2}\mathcal{F}(\alpha+\epsilon g)\bigg|_{\epsilon=0} \geq 0. \tag{5.2}$$

A straightforward calculation yields

$$\frac{d^2}{d\epsilon^2}\mathcal{F}(\alpha+\epsilon g)\bigg|_{\epsilon=0} = 2\langle g|E(-i\nabla)+\lambda V|g\rangle + 8\int \frac{|p^2-\mu|[\mathbb{R}e(\hat{\alpha}\bar{\hat{g}})]^2}{[1-4|\hat{\alpha}|^2]^{3/2}}. \tag{5.3}$$

Assume now that $\Xi = 0$. This means that Δ has to vanish at some point $p' \in \Omega_\mu$. Then there has to be an open neighborhood on Ω_μ on which Δ vanishes. In fact, according to the argument in the proof of Lemma 5.1 (Eq. (5.1) and Lipschitz continuity of Δ) there is a neighborhood $\mathcal{N}_\delta(p') \subset \mathbb{R}^3$ in the vicinity of p' where $|\hat{\alpha}|^2 < 1/4 - \delta$ for some $\delta > 0$, and hence Δ vanishes on $\mathcal{N}_\delta(p') \cap \Omega_\mu$. Note that Δ cannot vanish at one point on the Fermi surface since otherwise $|\hat{\alpha}| = 1/2$ except on one point, which contradicts the continuity of $\hat{\alpha}$.

We shall now construct an appropriate trial sequence $\hat{g}_n$, essentially supported in $\mathcal{N}_\delta$, such that

$$\lim_{n\to\infty}\left[\langle g_n|E(-i\nabla)|g_n\rangle + 8\int \frac{|p^2-\mu|[\mathbb{R}e(\hat{\alpha}\bar{\hat{g}_n})]^2}{[1-4|\hat{\alpha}|^2]^{3/2}}\right] = 0 \tag{5.4}$$

and

$$\lim_{n\to\infty}\langle g_n|V|g_n\rangle = \int_{\mathbb{R}^3} V(x)dx < 0\,. \tag{5.5}$$

This gives a contradiction to (5.2).

For the construction of g_n let $\psi_n \in L^2(\Omega_\mu)$ be supported in $\mathcal{N}_\delta(p') \cap \Omega_\mu$ such that $\psi_n(s) \to \delta(s-p')$ as $n \to \infty$. Choose also $f_n \in L^2(\mathbb{R}_+, t^2 dt)$ such that $f_n(t) \to \delta(\sqrt{\mu} - t)$, and let $\hat{g}_n(p) = \psi_n(s) f_n(|p|)$. Observe that on $\mathcal{N}(p')$, $E(p) = |p^2 - \mu|/\sqrt{1 - 4|\hat{\alpha}(p)|^2} \leq c|p^2 - \mu|$ for some constant c, and thus grows *linearly* in $|p|$ close to $\sqrt{\mu}$. Hence one easily sees that the problem here is equivalent to the existence of a negative eigenvalue of the relativistic operator $|p| + V$ in *one* dimension. Using the Birman-Schwinger principle, it is easy to see that the latter always has a negative eigenvalue if $\int V < 0$. □

5.2. *Proof of Theorem 2.5*

The energy gap of the system at zero temperature, $\Xi = \inf_p E(p)$, with

$$E(p) = |p^2 - \mu|/\sqrt{1 - 4|\hat{\alpha}(p)|^2} = \sqrt{|p^2 - \mu|^2 + |\Delta(p)|^2},$$

depends on the behavior of $|\Delta(p)|$ on the Fermi sphere. The function Δ is not unique, in general and need not be radial even in case V is radial.

Under the assumption that $\hat{V}$ is non-positive and $\hat{V}(0) < 0$, we shall argue in the following that the minimizer of the BCS functional (2.15) at $T = 0$ is unique [9, Lemma 3]. If, in addition, V is radial, this necessarily implies that also the minimizer has to be radial. Since $\hat{V} \leq 0$,

$$\int_{\mathbb{R}^6} \overline{\hat{\alpha}(p)} \hat{V}(p-q) \hat{\alpha}(q)\, dpdq \geq \int_{\mathbb{R}^6} |\hat{\alpha}(p)| \hat{V}(p-q) |\hat{\alpha}(q)|\, dpdq\,. \tag{5.6}$$

Hence, if $\hat{\alpha}(p)$ is a minimizer of $\mathcal{F}_0$, (2.15), so is $|\hat{\alpha}(p)|$.

Assume now there are two different minimizers $f \neq g$, both with non-negative Fourier transform. Since $t \to 1 - \sqrt{1-4t}$ is strictly convex for $0 \leq t \leq 1/2$ we see that $\psi = \frac{1}{\sqrt{2}} f + i \frac{1}{\sqrt{2}} g$, satisfies

$$\mathcal{F}_0(\psi) < \tfrac{1}{2}\mathcal{F}_0(f) + \tfrac{1}{2}\mathcal{F}_0(g)\,.$$

This is a contradiction to f, g being distinct minimizers, and hence $f = g$. In particular, the absolute value of a minimizer has to be unique. If $\hat{\alpha}$ is the unique non-negative minimizer, then one easily sees from the BCS equation (using $\int V < 0$) that $\hat{\alpha}$ is, in fact, strictly positive. Hence *any* minimizer is non-vanishing. But (5.6) is *strict* for non-vanishing functions, unless $\hat{\alpha}(p) = |\hat{\alpha}(p)| e^{i\kappa}$ for some constant $\kappa \in \mathbb{R}$.

To summarize, we have just argued that for $\hat{V} \leq 0$, $\hat{V}(0) < 0$ and V radial, the solution of the BCS equation is unique, up to a constant phase, and it is radially symmetric. This will enable us to apply the same methods

as we used for the critical temperature T_c in order to derive the asymptotic behavior of Ξ.

The variational equation (2.16) for the minimizer of $\mathcal{F}_0$ can be rewritten in terms of α as

$$\left(E(-i\nabla) + \lambda V(x)\right)\alpha(x) = 0. \tag{5.7}$$

That is, α is an eigenfunction of the pseudodifferential operator $E(-i\nabla) + \lambda V(x)$, with zero eigenvalue. Since $\hat{V} \leq 0$ and $\hat{\alpha}(p)$ is non-negative we can even conclude that α has to be the ground state.

Similarly to the proof of Theorem 2.3, we can now employ the Birman-Schwinger principle to conclude from (5.7) that $\phi_\lambda = V^{1/2}\alpha$ satisfies the eigenvalue equation

$$\lambda V^{1/2}\frac{1}{\sqrt{(p^2-\mu)^2 + |\Delta(p)|^2}}|V|^{1/2}\phi_\lambda = -\phi_\lambda\,. \tag{5.8}$$

Moreover, there are no eigenvalues smaller than -1 of the operator on the left side of (5.8).

Let

$$\widetilde{m}_\mu(\Delta) = \max\left\{\frac{1}{4\pi\mu}\int_{\mathbb{R}^3}\left(\frac{1}{\sqrt{(p^2-\mu)^2 + |\Delta(p)|^2}} - \frac{1}{p^2}\right)dp\,,\,0\right\}\,. \tag{5.9}$$

Similarly to (4.2), we split the operator in (5.8) as

$$V^{1/2}\frac{1}{E(-i\nabla)}|V|^{1/2} = \widetilde{m}_\mu(\Delta)V^{1/2}\mathfrak{F}^*\mathfrak{F}|V|^{1/2} + V^{1/2}M_\Delta|V|^{1/2}\,.$$

Again one shows that $V^{1/2}M_\Delta|V|^{1/2}$ is bounded in Hilbert-Schmidt norm, independently of Δ. Moreover, as in the proof of Theorem 2.3 (cf. Eqs. (4.3)–(4.5)), the fact that the lowest eigenvalue of $\lambda V^{1/2}E(-i\nabla)^{-1}|V|^{1/2}$ is -1 is, for small enough λ, equivalent to the fact that the selfadjoint operator on $L^2(\Omega_\mu)$

$$\mathfrak{F}|V|^{1/2}\frac{\lambda\widetilde{m}_\mu(\Delta)}{1+\lambda V^{1/2}M_\Delta|V|^{1/2}}V^{1/2}\mathfrak{F}^* \tag{5.10}$$

has -1 as its smallest eigenvalue. This implies that $\lim_{\lambda\to 0}\lambda\widetilde{m}_\mu(\Delta) = -1/(\sqrt{\mu}\,e_\mu)$ and hence, in particular, $\widetilde{m}_\mu(\Delta) \sim \lambda^{-1}$ as $\lambda \to 0$. The unique eigenfunction corresponding to the lowest eigenvalue $e_\mu < 0$ of $\mathcal{V}_\mu$ is, in fact, a positive function, and because of radial symmetry of V it is actually the constant function $u(p) = (4\pi\mu)^{-1/2}$.

We now give a precise characterization of $\Delta(p)$ for small λ.

Lemma 5.2. *Let $V \in L^1 \cap L^{3/2}$ be radial, with $\hat{V} \leq 0$ and $\hat{V}(0) < 0$, and let Δ be given in (2.16), with α the unique minimizer of the BCS functional (2.15). Then*

$$\Delta(p) = -f(\lambda) \left(\int_{\Omega_\mu} \hat{V}(p-q)\, d\omega(q) + \lambda \eta_\lambda(p) \right) \tag{5.11}$$

for some positive function $f(\lambda)$, with $\|\eta_\lambda\|_{L^\infty(\mathbb{R}^3)}$ bounded independently of λ.

Proof. Because of (5.8), $\mathfrak{F}|V|^{1/2}\phi_\lambda$ is the eigenfunction of (5.10) corresponding to the lowest eigenvalue -1. Note that because of radial symmetry, the constant function $u(p) = (4\pi\mu)^{-1/2}$ is an eigenfunction of (5.10). For small enough λ it has to be eigenfunction corresponding to the lowest eigenvalue (since it is the unique ground state of the compact operator $\mathfrak{F}V\mathfrak{F}^*$). We conclude that

$$\phi_\lambda = f(\lambda) \frac{1}{1 + \lambda V^{1/2} M_\Delta |V|^{1/2}} V^{1/2} \mathfrak{F}^* u = f(\lambda) \left(V^{1/2} \mathfrak{F}^* u + \lambda \xi_\lambda \right) \tag{5.12}$$

for some normalization constant $f(\lambda)$. Note that $\|\xi_\lambda\|_2$ uniformly bounded for small λ, since both $V^{1/2} M_\Delta |V|^{1/2}$ and $V^{1/2}\mathfrak{F}^*$ are bounded operators.

From (5.7) and the definition $\phi_\lambda = V^{1/2}\alpha$ we know that

$$\Delta(p) = 2E(p)\hat{\alpha}(p) = -2\lambda \widehat{V\alpha}(p) = -2\lambda \widehat{|V|^{1/2}\phi_\lambda}(p)\,.$$

In combination with (5.12) this implies that

$$\Delta(p) = -2\lambda f(\lambda) \left(\widehat{V\mathfrak{F}^* u}(p) + \lambda \widehat{\eta_\lambda}(p) \right)\,,$$

with $\eta_\lambda = |V|^{1/2}\xi_\lambda$. With $\|\widehat{\eta_\lambda}\|_\infty \leq (2\pi)^{-3/2}\|\eta_\lambda\|_1 \leq (2\pi)^{-3/2}\|V\|_1\|\xi_\lambda\|_2$ by Schwarz's inequality, we arrive at the statement of the Lemma. □

With the aid of Lemma 5.2 and Lipschitz continuity of $\int_{\Omega_\mu} \hat{V}(p-q)\, d\omega(q)$ (which follows from $V \in L^1(\mathbb{R}^3)$) it is not difficult to see that

$$\widetilde{m}_\mu(\Delta) = \frac{1}{\sqrt{\mu}} \left(\ln \frac{\mu}{\Delta(\sqrt{\mu})} - 2 + \ln 8 + o(1) \right) \tag{5.13}$$

as $\lambda \to 0$. From Eq. (5.10) we now conclude that

$$\widetilde{m}_\mu(\Delta) = \frac{1}{\lambda \langle u|\mathfrak{F}V\mathfrak{F}^*|u\rangle - \lambda^2 \langle u|\mathfrak{F}VM_\Delta V\mathfrak{F}^*|u\rangle + O(\lambda^3)}\,, \tag{5.14}$$

where $u(p) = (4\pi\mu)^{-1/2}$ is the normalized constant function on the sphere Ω_μ. Moreover, with $\varphi = V\mathfrak{F}^* u$,

$$\begin{aligned}\langle u|\mathfrak{F}VM_\Delta V\mathfrak{F}^*|u\rangle &= \int_{\mathbb{R}^3} \frac{1}{E(p)}|\hat\varphi(p)|^2\,dp - \widetilde{m}_\mu(\Delta)\int_{\Omega_\mu}|\hat\varphi(\sqrt{\mu}p/|p|)|^2\,d\omega(p)\\ &= \int_{\mathbb{R}^3}\left(\frac{1}{E(p)}\left[|\hat\varphi(p)|^2 - |\hat\varphi(\sqrt{\mu}p/|p|)|^2\right] + \frac{1}{p^2}|\hat\varphi(\sqrt{\mu}p/|p|)|^2\right)dp\,.\end{aligned}$$

Using Lemma 5.2 and the fact that $\lim_{\lambda\to 0} f(\lambda) = 0$, we conclude that

$$\lim_{\lambda\to 0}\langle u|\mathfrak{F}VM_\Delta V\mathfrak{F}^*|u\rangle = \langle u|\mathcal{W}_\mu|u\rangle\,, \tag{5.15}$$

with $\mathcal{W}_\mu$ defined in (2.8). (Compare with Eqs. (4.9) and (4.10).) In combination with (5.13) and (5.14) and the definition of $\mathcal{B}_\mu$ in (2.9), this proves that

$$\lim_{\lambda\to 0}\left(\ln\left(\frac{\mu}{\Delta(\sqrt{\mu})}\right) + \frac{\pi}{2\sqrt{\mu}\,\langle u|\mathcal{B}_\mu|u\rangle}\right) = 2 - \ln(8)\,.$$

The same holds true with $\langle u|\mathcal{B}_\mu|u\rangle$ replaced by $b_\mu(\lambda) = \inf \operatorname{spec}\mathcal{B}_\mu$, since under our assumptions on V the two quantities differ only by terms of order λ^3.

Now, by the definition of the energy gap Ξ in (2.17), $\Xi \leq \Delta(\sqrt{\mu})$. Moreover,

$$\Xi \geq \min_{|p^2-\mu|\leq\Xi}|\Delta(p)|\,,$$

from which it easily follows that $\Xi \geq \Delta(\sqrt{\mu})(1 - o(1))$, using Lemma 5.2. This proves Theorem 2.5.

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SPECTRAL GAPS FOR PERIODIC SCHRÖDINGER OPERATORS WITH HYPERSURFACE MAGNETIC WELLS

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We consider a periodic magnetic Schrödinger operator on a noncompact Riemannian manifold M such that $H^1(M,\mathbb{R}) = 0$ endowed with a properly discontinuous cocompact isometric action of a discrete group. We assume that there is no electric field and that the magnetic field has a periodic set of compact magnetic wells. We review a general scheme of a proof of existence of an arbitrary large number of gaps in the spectrum of such an operator in the semiclassical limit, which was suggested in our previous paper, and some applications of this scheme. Then we apply these methods to establish similar results in the case when the wells have regular hypersurface pieces.

Keywords: magnetic Schrödinger operator; magnetic well; spectral gaps; Riemannian manifolds; semiclassical limit; quasimodes

1. Introduction

Let M be a noncompact oriented manifold of dimension $n \geq 2$ equipped with a properly discontinuous action of a finitely generated, discrete group Γ such that M/Γ is compact. Suppose that $H^1(M,\mathbb{R}) = 0$, i.e., any closed 1-form on M is exact. Let g be a Γ-invariant Riemannian metric and $\mathbf{B}$ a real-valued Γ-invariant closed 2-form on M. Assume that $\mathbf{B}$ is exact and choose a real-valued 1-form $\mathbf{A}$ on M such that $d\mathbf{A} = \mathbf{B}$.

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Thus, one has a natural mapping

$$u \mapsto ih\,du + \mathbf{A}u$$

from $C_c^\infty(M)$ to the space $\Omega_c^1(M)$ of smooth, compactly supported one-forms on M. The Riemannian metric allows to define scalar products in these spaces and consider the adjoint operator

$$(ih\,d + \mathbf{A})^* : \Omega_c^1(M) \to C_c^\infty(M).$$

A Schrödinger operator with magnetic potential $\mathbf{A}$ is defined by the formula

$$H^h = (ih\,d + \mathbf{A})^*(ih\,d + \mathbf{A}).$$

Here $h > 0$ is a semiclassical parameter, which is assumed to be small.

Choose local coordinates $X = (X_1, \dots, X_n)$ on M. Write the 1-form $\mathbf{A}$ in these local coordinates as

$$\mathbf{A} = \sum_{j=1}^n A_j(X)\,dX_j,$$

the matrix of the Riemannian metric g as

$$g(X) = (g_{j\ell}(X))_{1\le j,\ell\le n}$$

and its inverse as

$$g(X)^{-1} = (g^{j\ell}(X))_{1\le j,\ell\le n}.$$

Denote $|g(X)| = \det(g(X))$. Then the magnetic field $\mathbf{B}$ is given by the following formula

$$\mathbf{B} = \sum_{j<k} B_{jk}\,dX_j \wedge dX_k, \quad B_{jk} = \frac{\partial A_k}{\partial X_j} - \frac{\partial A_j}{\partial X_k}.$$

Moreover, the operator H^h has the form

$$H^h = \frac{1}{\sqrt{|g(X)|}} \sum_{1\le j,\ell\le n} \left(ih\frac{\partial}{\partial X_j} + A_j(X)\right) \times \left[\sqrt{|g(X)|}g^{j\ell}(X)\left(ih\frac{\partial}{\partial X_\ell} + A_\ell(X)\right)\right].$$

For any $x \in M$, denote by $B(x)$ the anti-symmetric linear operator on the tangent space T_xM associated with the 2-form $\mathbf{B}$:

$$g_x(B(x)u, v) = \mathbf{B}_x(u, v), \quad u, v \in T_xM.$$

Recall that the intensity of the magnetic field is defined as

$$\mathrm{Tr}^+(B(x)) = \sum_{\substack{\lambda_j(x)>0 \\ i\lambda_j(x)\in\sigma(B(x))}} \lambda_j(x) = \frac{1}{2}\,\mathrm{Tr}([B^*(x)\cdot B(x)]^{1/2}).$$

It turns out that in many problems the function $x \mapsto h\cdot \mathrm{Tr}^+(B(x))$ can be considered as a magnetic analogue of the electric potential V in a Schrödinger operator $-h^2\Delta + V$.

We will also use the trace norm of $B(x)$:

$$|B(x)| = [\mathrm{Tr}(B^*(x)\cdot B(x))]^{1/2}.$$

It coincides with the norm of $B(x)$ with respect to the Riemannian metric on the space of linear operators on T_xM induced by the Riemannian metric g on M.

In this paper we will always assume that the magnetic field has a periodic set of compact potential wells. More precisely, put

$$b_0 = \min\{\mathrm{Tr}^+(B(x)) \,:\, x\in M\}$$

and assume that there exist a (connected) fundamental domain $\mathcal{F}$ and a constant $\epsilon_0 > 0$ such that

$$\mathrm{Tr}^+(B(x)) \geq b_0 + \epsilon_0, \quad x\in\partial\mathcal{F}. \tag{1.1}$$

For any $\epsilon_1 \leq \epsilon_0$, put

$$U_{\epsilon_1} = \{x\in\mathcal{F} \,:\, \mathrm{Tr}^+(B(x)) < b_0+\epsilon_1\}.$$

Thus U_{ϵ_1} is an open subset of $\mathcal{F}$ such that $U_{\epsilon_1}\cap\partial\mathcal{F} = \emptyset$ and, for $\epsilon_1 < \epsilon_0$, $\overline{U_{\epsilon_1}}$ is compact and included in the interior of $\mathcal{F}$. Any connected component of U_{ϵ_1} with $\epsilon_1 < \epsilon_0$ and also any of its translates under the action of an element of Γ can be understood as a magnetic well. These magnetic wells are separated by barriers, which are getting higher and higher when $h\to 0$ (in the semiclassical limit).

For any linear operator T in a Hilbert space, we will denote by $\sigma(T)$ its spectrum. By a gap in the spectrum of a self-adjoint operator T we will mean any connected component of the complement of $\sigma(T)$ in $\mathbb{R}$, that is, any maximal interval (a,b) such that

$$(a,b)\cap\sigma(T) = \emptyset\,.$$

The problem of existence of gaps in the spectra of second order periodic differential operators has been extensively studied recently. Some related

results on spectral gaps for periodic magnetic Schrödinger operators can be found for example in Refs. 1,4,5,14–22,24 (see also the references therein).

In this paper, we consider the magnetic Schrödinger operator H^h as an unbounded self-adjoint operator in the Hilbert space $L^2(M)$ and will study gaps in the spectrum of this operator, which are located below the top of potential barriers, that is, on the interval $[0, h(b_0 + \epsilon_0)]$. In this case, an important role is played by the tunneling effect, that is, by the possibility for the quantum particle described by the Hamiltonian H^h with such an energy to pass through a potential barrier. Using the semiclassical analysis of the tunneling effect, we showed in Ref. 4 that the spectrum of the magnetic Schrödinger operator H^h on the interval is localized in an exponentially small neighborhood of the spectrum of its Dirichlet realization inside the wells. This result reduces the investigation of gaps in the spectrum of the operator H^h to the study of the eigenvalue distribution for a "one-well" operator and leads us to suggest a general scheme of a proof of existence of spectral gaps in Ref. 5. We review this scheme and some of its applications in Sec. 2. Then, in Sec. 3, we will apply these methods to prove the existence of an arbitrary large number of gaps in the spectrum of the operator H^h, as $h \to 0$, under the assumption that $b_0 = 0$ and the zero set of $\mathbf{B}$ has regular codimension one pieces.

2. Quasimodes and spectral gaps

In this section, we review a general scheme of a proof of existence of gaps in the spectrum of the magnetic Schrödinger operator H^h on the interval $[0, h(b_0 + \epsilon_0)]$ and some of its applications obtained in Ref. 5.

2.1. *A general scheme*

For any domain W in M, denote by H^h_W the unbounded self-adjoint operator in the Hilbert space $L^2(W)$ defined by the operator H^h in $\overline{W}$ with Dirichlet boundary conditions. The operator H^h_W is generated by the quadratic form

$$u \mapsto q^h_W[u] := \int_W |(ih\,d + \mathbf{A})u|^2\,dx$$

with the domain

$$\mathrm{Dom}(q^h_W) = \{u \in L^2(W) : (ih\,d + \mathbf{A})u \in L^2\Omega^1(W), u\,|_{\partial W} = 0\},$$

where $L^2\Omega^1(W)$ denotes the Hilbert space of L^2 differential 1-forms on W, dx is the Riemannian volume form on M.

Assume now that the operator H^h satisfies the condition of Eq. (1.1). Fix $\epsilon_1 > 0$ and $\epsilon_2 > 0$ such that $\epsilon_1 < \epsilon_2 < \epsilon_0$, and consider the operator H_D^h associated with the domain $D = \overline{U_{\epsilon_2}}$. The operator H_D^h has discrete spectrum.

The following result is a slight generalization of Theorem 2.1 in Ref. 5, which is concerned with the case when N_h is independent of h. It permits to get a more precise information on the number of gaps as $h \to 0$.

Theorem 2.1. *Suppose that there exist $h_0 > 0$, $c > 0$, $M \geq 1$ and that, for $h \in (0, h_0]$, there exists N_h and a subset $\mu_0^h < \mu_1^h < \ldots < \mu_{N_h}^h$ of an interval $I(h) \subset [0, h(b_0 + \epsilon_1))$ such that*

$$\mu_j^h - \mu_{j-1}^h > ch^M, \quad j = 1, \ldots, N_h,$$
$$\operatorname{dist}(\mu_0^h, \partial I(h)) > ch^M, \quad \operatorname{dist}(\mu_{N_h}^h, \partial I(h)) > ch^M,$$

and, for each $j = 0, 1, \ldots, N_h$, there exists some non trivial $v_j^h \in C_c^\infty(D)$ such that

$$\|H_D^h v_j^h - \mu_j^h v_j^h\| \leq \frac{c}{3} h^M \|v_j^h\|.$$

Then there exists $h_1 \in (0, h_0]$ such that the spectrum of H^h on the interval $I(h)$ has at least N_h gaps for $h \in (0, h_1)$.

2.2. *A generic situation*

As a first application of Theorem 2.1, we show in Ref. 5 that the spectrum of the Schrödinger operator H^h, satisfying the assumption of Eq. (1.1), always has gaps (moreover, an arbitrarily large number of gaps) on the interval $[0, h(b_0+\epsilon_0)]$ in the semiclassical limit $h \to 0$. Under some additional generic assumption, this result was obtained in Ref. 4. Indeed, slightly modifying the arguments of Ref. 5, one can show the following theorem.

Theorem 2.2. *Under the assumption of Eq. (1.1), for any interval $[\alpha, \beta] \subset [b_0, b_0 + \epsilon_0]$ and for any natural N, there exists $h_0 > 0$ such that, for any $h \in (0, h_0]$, the spectrum of H^h in the interval $[h\alpha, h\beta]$ has at least N gaps.*

The proof of this theorem can be given by a straightforward repetition of the proof of Theorem 3.1 in Ref. 5 with the only difference that one should choose $\mu_0 < \mu_1 < \ldots < \mu_N$ in the interval (α, β) instead of $(b_0, b_0 + \epsilon_0)$.

Indeed, using Theorem 2.1 with N_h dependent on h and a continuous family of quasimodes constructed in the proof of Proposition 2.3 in Ref. 4, we can get an estimate for the number of gaps in the constant rank case. Denote by $[a]$ the integer part of a (the largest integer n satisfying $n \leq a$).

Theorem 2.3. *Under the assumption of Eq. (1.1), suppose that the rank of* $\mathbf{B}$ *is constant in an open set* $U \subset M$*. Then, for any interval* $[\alpha, \beta] \subset \mathrm{Tr}^+ B(U)$*, there exists* $h_0 > 0$ *and* $C > 0$ *such that, for any* $h \in (0, h_0]$*, the spectrum of* H^h *in the interval* $[h\alpha, h\beta]$ *has at least* $[Ch^{-1/3}]$ *gaps.*

2.3. *The case of discrete wells*

A more precise information on location and asymptotic behavior of gaps in the spectrum of the magnetic Schrödinger operator H^h, satisfying the assumption of Eq. (1.1), can be obtained, if we impose additional hypotheses on the bottoms of the magnetic wells. In this section, we consider a case when the bottom of the magnetic well contains zero-dimensional components, that is, isolated points, and, moreover, the magnetic field behaves regularly near these points. More precisely, we will assume that $b_0 = 0$ and that there is at least one zero x_0 of B such that, for some integer $k > 0$, there exists a positive constant C such that for all x in some neighborhood of x_0 the following estimate holds:

$$C^{-1} d(x, x_0)^k \leq |B(x)| \leq C d(x, x_0)^k \tag{2.1}$$

(here $d(x, y)$ denotes the geodesic distance between x and y). In this case, the important role is played by a differential operator $K^h_{\bar{x}_0}$ in $\mathbb{R}^n$, which is in some sense an approximation to the operator H^h near x_0. Recall its definition (see Ref. 7).

Let $\bar{x}_0$ be a zero of B. Choose local coordinates $f : U(\bar{x}_0) \to \mathbb{R}^n$ on M, defined in a sufficiently small neighborhood $U(\bar{x}_0)$ of $\bar{x}_0$. Suppose that $f(\bar{x}_0) = 0$, and the image $f(U(\bar{x}_0))$ is a ball $B(0, r)$ in $\mathbb{R}^n$ centered at the origin.

Write the 2-form $\mathbf{B}$ in these local coordinates as

$$\mathbf{B}(X) = \sum_{1 \leq \ell < m \leq n} b_{\ell m}(X)\, dX_\ell \wedge dX_m, \quad X = (X_1, \ldots, X_n) \in B(0, r).$$

Let $\mathbf{B}^0$ be the closed 2-form in $\mathbb{R}^n$ with polynomial components defined by the formula

$$\mathbf{B}^0(X) = \sum_{1 \leq \ell < m \leq n} \sum_{|\alpha| = k} \frac{X^\alpha}{\alpha!} \frac{\partial^\alpha b_{\ell m}}{\partial X^\alpha}(0)\, dX_\ell \wedge dX_m, \quad X \in \mathbb{R}^n.$$

One can find a 1-form $\mathbf{A}^0$ on $\mathbb{R}^n$ with polynomial components such that

$$d\mathbf{A}^0(X) = \mathbf{B}^0(X), \quad X \in \mathbb{R}^n.$$

Let $K^h_{\bar{x}_0}$ be the self-adjoint differential operator in $L^2(\mathbb{R}^n)$ with polynomial coefficients given by the formula

$$K^h_{\bar{x}_0} = (ih\,d + \mathbf{A}^0)^*(ih\,d + \mathbf{A}^0),$$

where the adjoints are taken with respect to the Hilbert structure in $L^2(\mathbb{R}^n)$ given by the flat Riemannian metric $(g_{\ell m}(0))$ in $\mathbb{R}^n$. If $\mathbf{A}^0$ is written as

$$\mathbf{A}^0 = A^0_1\,dX_1 + \ldots + A^0_n\,dX_n,$$

then $K^h_{\bar{x}_0}$ is given by the formula

$$K^h_{\bar{x}_0} = \sum_{1\le \ell,m\le n} g^{\ell m}(0)\left(ih\frac{\partial}{\partial X_\ell} + A^0_\ell(X)\right)\left(ih\frac{\partial}{\partial X_m} + A^0_m(X)\right).$$

The operators $K^h_{\bar{x}_0}$ have discrete spectrum (cf, for instance, Refs. 10 and 8). Using the simple dilation $X \mapsto h^{\frac{1}{k+2}}X$, one can show that the operator $K^h_{\bar{x}_0}$ is unitarily equivalent to $h^{\frac{2k+2}{k+2}}K^1_{\bar{x}_0}$. Thus, $h^{-\frac{2k+2}{k+2}}K^h_{\bar{x}_0}$ has discrete spectrum, independent of h.

Theorem 2.4.[5] *Suppose that the operator H^h satisfies the condition of Eq. (1.1) with some $\epsilon_0 > 0$ and that there exists a zero $\bar{x}_0$ of B, satisfying the assumption of Eq. (2.1) for some integer $k > 0$. Denote by $\lambda_1 < \lambda_2 < \lambda_3 < \ldots$ the eigenvalues of the operator $K^1_{\bar{x}_0}$ (not taking into account multiplicities). Then, for any natural N and any $C > \lambda_{N+1}$, there exists $h_0 > 0$ such that the spectrum of H^h in the interval $[0, Ch^{\frac{2k+2}{k+2}}]$ has at least N gaps for any $h \in (0, h_0)$.*

3. Hypersurface wells

In this section, we consider the case when $b_0 = 0$ and the zero set of the magnetic field has regular hypersurface parts. More precisely, suppose that there is an open subset U of $\mathcal{F}$ such that the zero set of $\mathbf{B}$ in U is a smooth oriented hypersurface S, and, moreover, there are constants $k \in \mathbb{N}$ and $C > 0$ such that for all $x \in U$ we have:

$$C^{-1}d(x,S)^k \le |B(x)| \le Cd(x,S)^k\,. \tag{3.1}$$

On compact manifolds, this model was introduced for the first time by Montgomery[23] and was further studied in Refs. 7, 25 and 3.

Let

$$\omega_{0.0} = i^*_S\mathbf{A}$$

be the closed one form on S induced by $\mathbf{A}$, where i_S is the embedding of S into M.

Denote by N the external unit normal vector to S and by $\tilde{N}$ an arbitrary extension of N to a smooth vector field on U.

Let $\omega_{0,1}$ be the smooth one form on S defined, for any vector field V on S, by the formula

$$\langle V, \omega_{0,1}\rangle(y) = \frac{1}{k!}\tilde{N}^k(\mathbf{B}(\tilde{N}, \tilde{V}))(y), \quad y \in S,$$

where $\tilde{V}$ is a C^∞ extension of V to U. By Eq. (3.1), it is easy to see that $\omega_{0,1}(x) \neq 0$ for any $x \in S$. Denote

$$\omega_{\min}(B) = \inf_{x\in S} |\omega_{0,1}(x)| > 0.$$

For any $\alpha \in \mathbb{R}$ and $\beta \in \mathbb{R}, \beta \neq 0$, consider the self-adjoint second order differential operator in $L^2(\mathbb{R})$ given by

$$Q(\alpha, \beta) = -\frac{d^2}{dt^2} + \left(\frac{1}{k+1}\beta t^{k+1} - \alpha\right)^2.$$

In the context of magnetic bottles, this family of operators (for $k = 1$) first appears in Ref. 23 (see also Ref. 7). Denote by $\lambda_0(\alpha, \beta)$ the bottom of the spectrum of the operator $Q(\alpha, \beta)$.

Let us recall some properties of $\lambda_0(\alpha, \beta)$, which were established in Refs. 23, 7 and 25. First of all, remark that $\lambda_0(\alpha, \beta)$ is a continuous function of $\alpha \in \mathbb{R}$ and $\beta \in \mathbb{R} \setminus \{0\}$. One can see by scaling that, for $\beta > 0$,

$$\lambda_0(\alpha, \beta) = \beta^{\frac{2}{k+2}} \lambda_0(\beta^{-\frac{1}{k+2}}\alpha, 1)\ . \tag{3.2}$$

A further discussion depends on k odd or k even.

When k is odd, $\lambda_0(\alpha, 1)$ tends to $+\infty$ as $\alpha \to -\infty$ by monotonicity. For analyzing its behavior as $\alpha \to +\infty$, it is suitable to do a dilation $t = \alpha^{\frac{1}{k+1}} s$, which leads to the analysis of

$$\alpha^2 \left(-h^2 \frac{d^2}{ds^2} + \left(\frac{s^{k+1}}{k+1} - 1\right)^2\right)$$

with $h = \alpha^{-(k+2)/(k+1)}$ small. One can use the semi-classical analysis (see Ref. 2 for the one-dimensional case and Refs. 26 and 11 for the multidimensional case) to show that

$$\lambda_0(\alpha, 1) \sim (k+1)^{\frac{2k}{k+1}} \alpha^{\frac{k}{k+1}}\ , \quad \text{as } \alpha \to +\infty\ .$$

In particular, we see that $\lambda_0(\alpha, 1)$ tends to $+\infty$.

When k is even, we have $\lambda_0(\alpha,1) = \lambda_0(-\alpha,1)$, and, therefore, it is sufficient to consider the case $\alpha \geq 0$. As $\alpha \to +\infty$, semi-classical analysis again shows that $\lambda_0(\alpha,1)$ tends to $+\infty$.

So in both cases, it is clear that the continuous function $\lambda_0(\alpha,1)$ is lower semi-bounded,

$$\hat{\nu} := \inf_{\alpha\in\mathbb{R}} \lambda_0(\alpha,1) > -\infty,$$

and there exists (at least one) $\alpha_{\min} \in \mathbb{R}$ such that $\lambda_0(\alpha,1)$ is minimal,

$$\lambda_0(\alpha_{\min},1) = \hat{\nu}.$$

For k odd, one can show that the minimum $\alpha_{\min}$ is strictly positive. One can indeed compute the derivative of $\lambda_0(\alpha,1)$ at $\alpha = 0$ and find that

$$\frac{\partial\lambda_0}{\partial\alpha}(0,1) < 0\ .$$

In the case $k = 1$, it has been shown that this minimum is unique (see Ref. 25). Numerical computations show (see Refs. 23 and 7) that, in this case, $\hat{\nu} \cong 0.5698$.

Theorem 3.1. *For any a and b such that*

$$\hat{\nu}\,\omega_{\min}(B)^{\frac{2}{k+2}} < a < b$$

and for any natural N, there exists $h_0 > 0$ such that, for any $h \in (0,h_0]$, the spectrum of H^h in the interval

$$[h^{\frac{2k+2}{k+2}}a, h^{\frac{2k+2}{k+2}}b]$$

has at least N gaps.

Proof. Let S and U as defined before (3.1) and g_0 be the Riemannian metric on S induced by g. Without loss of generality, we can assume that U coincides with an open tubular neighborhood of S and choose a diffeomorphism

$$\Theta : I \times S \to U,$$

where I is an open interval $(-\varepsilon_0,\varepsilon_0)$ with $\varepsilon_0 > 0$ small enough, such that $\Theta\big|_{\{0\}\times S} = \mathrm{id}$ and

$$(\Theta^* g - \tilde{g}_0)\big|_{\{0\}\times S} = 0,$$

where $\tilde{g}_0$ is a Riemannian metric on $I \times S$ given by

$$\tilde{g}_0 = dt^2 + g_0.$$

By adding to $\mathbf{A}$ the exact one form $d\phi$, where ϕ is the function satisfying

$$N(x)\phi(x) = -\langle N, \mathbf{A}\rangle(x), \quad x \in U,$$
$$\phi(x) = 0, \quad x \in S,$$

we may assume that

$$\langle N, \mathbf{A}\rangle(x) = 0, \quad x \in U.$$

As above, denote by H^h_D the unbounded self-adjoint operator in $L^2(D)$ given by the operator H^h in the domain $D = \overline{U}$ with Dirichlet boundary conditions.

For any $t \in \mathbb{R}$, let $P^h_S\left(\omega_{0,0} + \frac{1}{k+1}t^{k+1}\omega_{0,1}\right)$ be the formally self-adjoint operator in $L^2(S, dx_{g_0})$ defined by

$$P^h_S\left(\omega_{0,0} + \frac{1}{k+1}t^{k+1}\omega_{0,1}\right) = \left(ihd + \omega_{0,0} + \frac{1}{k+1}t^{k+1}\omega_{0,1}\right)^* \times \left(ihd + \omega_{0,0} + \frac{1}{k+1}t^{k+1}\omega_{0,1}\right).$$

Consider the self-adjoint operator $H^{h,0}$ in $L^2(\mathbb{R}\times S, dt\, dx_{g_0})$ defined by the formula

$$H^{h,0} = -h^2\frac{\partial^2}{\partial t^2} + P^h_S\left(\omega_{0,0} + \frac{1}{k+1}t^{k+1}\omega_{0,1}\right)$$

with Dirichlet boundary conditions. By Theorem 2.7 of Ref. 7, the operator $H^{h,0}$ has discrete spectrum. Moreover, it can be seen from the proof of this theorem that if $\lambda^0(h)$ is an approximate eigenvalue of $H^{h,0}$ with the corresponding approximate eigenfunction $w^h \in C^\infty_c(\mathbb{R}\times S)$ such that

$$\lambda^0(h) \le Dh^{(2k+2)/(k+2)}$$

and

$$\|(H^{h,0} - \lambda^0(h))w^h\| \le Ch^{(2k+3)/(k+2)}\|w^h\|,$$

then $\lambda^0(h)$ is an approximate eigenvalue of H^h_D with the corresponding approximate eigenfunction $v^h = (\Theta^{-1})^* w^h \in C^\infty_c(U)$,

$$\|(H^h_D - \lambda^0(h))v^h\| \le Ch^{(2k+3)/(k+2)}\|v^h\|.$$

So it remains to construct approximate eigenvalues of $H^{h,0}$.

Lemma 3.1. *For any $\lambda \ge \hat{\nu}\,\omega_{\min}(B)^{2/(k+2)}$, there exists $\Phi \in C^\infty_c(\mathbb{R}\times S)$ such that*

$$\|(H^{h,0} - \lambda h^{\frac{2k+2}{k+2}})\Phi\| \le Ch^{\frac{6k+8}{3(k+2)}}\|\Phi\|.$$

Proof. Take $x_1 \in S$ such that $|\omega_{0,1}(x_1)| = \omega_{\min}(B)$. Consider $\alpha_1 \in \mathbb{R}$ such that $\lambda_0(\alpha_1, 1) = \lambda\omega_{\min}(B)^{-2/(k+2)} \geq \hat{\nu}$. Let $\psi \in L^2(\mathbb{R})$ be a normalized eigenfunction of $Q(\alpha_1, 1)$, corresponding to $\lambda_0(\alpha_1, 1)$,

$$\left[-\frac{d^2}{dt^2} + \left(\frac{1}{k+1}t^{k+1} - \alpha_1\right)^2\right]\psi(t) = \lambda\omega_{\min}(B)^{-\frac{2}{k+2}}\psi(t), \quad \|\psi\|_{L^2(\mathbb{R})} = 1.$$

For simplicity of notation, put $\alpha_B = \alpha_1\omega_{\min}(B)^{-\frac{k+1}{k+2}}h^{\frac{k+1}{k+2}}$. Then the function

$$\Psi(t) = \omega_{\min}(B)^{\frac{1}{2(k+2)}}h^{-\frac{1}{2(k+2)}}\psi(\omega_{\min}(B)^{\frac{1}{k+2}}h^{-\frac{1}{k+2}}t)$$

satisfies

$$\left(-h^2\frac{d^2}{dt^2} + \omega_{\min}(B)^2\left(\frac{1}{k+1}t^{k+1} - \alpha_B\right)^2\right)\Psi(t) = \lambda h^{\frac{2k+2}{k+2}}\Psi(t),$$
$$\|\Psi\|_{L^2(\mathbb{R})} = 1.$$

Take normal coordinates $f : U(x_1) \subset S \to \mathbb{R}^{n-1}$ on S defined in a neighborhood $U(x_1)$ of x_1, where $f(U(x_1)) = B(0, r)$ is a ball in $\mathbb{R}^{n-1}$ centered at the origin and $f(x_1) = 0$. Choose a function $\phi \in C^\infty(B(0, r))$ such that $d\phi = \omega_{0,0}$. Write $\omega_{0,1} = \sum_{j=1}^{n-1}\omega_j(s)\,ds_j$. Note that

$$\omega_{\min}(B) = \left(\sum_{j=1}^{n-1}|\omega_j(0)|^2\right)^{1/2}.$$

Consider the function $\Phi \in C^\infty(B(0, r) \times \mathbb{R})$ given by

$$\Phi(s,t) = ch^{-\beta/2(n-1)}\chi(s)\exp\left(-i\frac{\phi(s)}{h}\right)\exp\left(i\frac{\alpha_B}{h}\sum_{j=1}^{n-1}\omega_j(0)s_j\right)$$
$$\times\exp\left(-\frac{|s|^2}{2h^{2\beta}}\right)\Psi(t), \quad s \in B(0, r), \quad t \in \mathbb{R}, \tag{3.3}$$

with some β, where $\chi \in C_c^\infty(B(0, r))$ is a cut-off function and c is chosen in such a way that $\|\Phi\|_{L^2(S\times\mathbb{R})} = 1$.

Put

$$H^{h,1} = -h^2\frac{\partial^2}{\partial t^2} + P_S^h\left(\frac{1}{k+1}t^{k+1}\omega_{0,1} - \alpha_B\omega_{0,1}(0)\right),$$
$$E(s) = ch^{-\beta/2(n-1)}\chi(s)\exp\left(-\frac{|s|^2}{2h^{2\beta}}\right),$$
$$\Phi_1(s,t) = E(s)\Psi(t).$$

Then we have

$$H^{h,0}\Phi(s,t) = \exp\left(-i\frac{\phi(s)}{h}\right)\exp\left(i\frac{\alpha_B}{h}\sum_{j=1}^{n-1}\omega_j(0)s_j\right)H^{h,1}\Phi_1(s,t).$$

Next, we have

$$\begin{aligned}
&P_S^h\left(\frac{1}{k+1}t^{k+1}\omega_{0,1} - \alpha_B\omega_{0,1}(0)\right)\\
&= \sum_{j,\ell}\frac{1}{\sqrt{g_0}}\left(ih\frac{\partial}{\partial s_j} + \frac{1}{k+1}t^{k+1}\omega_j(s) - \alpha_B\omega_j(0)\right)\\
&\times\left(g_0^{j\ell}\sqrt{g_0}\left(ih\frac{\partial}{\partial s_\ell} + \frac{1}{k+1}t^{k+1}\omega_\ell(s) - \alpha_B\omega_\ell(0)\right)\right)\\
&= \sum_{j,\ell} g_0^{j\ell}\left(ih\frac{\partial}{\partial s_j} + \frac{1}{k+1}t^{k+1}\omega_j(s) - \alpha_B\omega_j(0)\right)\\
&\qquad\times\left(ih\frac{\partial}{\partial s_\ell} + \frac{1}{k+1}t^{k+1}\omega_\ell(s) - \alpha_B\omega_\ell(0)\right)\\
&+\sum_\ell ih\Gamma^\ell(s)\left(ih\frac{\partial}{\partial s_\ell} + \frac{1}{k+1}t^{k+1}\omega_\ell(s) - \alpha_B\omega_\ell(0)\right)\\
&= -h^2\sum_{j,\ell} g_0^{j\ell}\frac{\partial^2}{\partial s_j\partial s_\ell} + 2ih\sum_{j,\ell} g_0^{j\ell}\frac{1}{k+1}t^{k+1}\frac{\partial\omega_\ell}{\partial s_j}(s)\\
&\qquad+2ih\sum_{j,\ell} g_0^{j\ell}\left(\frac{1}{k+1}t^{k+1}\omega_\ell(s) - \alpha_B\omega_\ell(0)\right)\frac{\partial}{\partial s_j}\\
&\qquad+\sum_{j,\ell} g_0^{j\ell}\left(\frac{1}{k+1}t^{k+1}\omega_j(s) - \alpha_B\omega_j(0)\right)\\
&\times\left(\frac{1}{k+1}t^{k+1}\omega_\ell(s) - \alpha_B\omega_\ell(0)\right) - h^2\sum_\ell\Gamma^\ell(s)\frac{\partial}{\partial s_\ell}\\
&\qquad+ih\sum_\ell\Gamma^\ell(s)\left(\frac{1}{k+1}t^{k+1}\omega_\ell(s) - \alpha_B\omega_\ell(0)\right),
\end{aligned}$$

where

$$\Gamma^\ell = \sum_j\frac{1}{\sqrt{g_0}}\frac{\partial}{\partial s_j}\left(g_0^{j\ell}\sqrt{g_0}\right).$$

By a well-known property of normal coordinates, we have $\partial_j g_0^{\ell m}(0) = 0$. So we get $\Gamma^\ell(0) = 0$, and

$$g_0^{\ell m}(s) = \delta^{\ell m} + O(|s|^2), \quad \Gamma^\ell(s) = O(|s|), \quad s\to 0. \tag{3.4}$$

We get

$$\begin{aligned}
H^{h,1}\Phi_1(s,t) &= \lambda h^{\frac{2k+2}{k+2}}\Phi_1(s,t) - h^2\sum_{j,\ell} g_0^{j\ell}\frac{\partial^2 E}{\partial s_j \partial s_\ell}(s)\Psi(t) \\
&+2ih\sum_{j,\ell} g_0^{j\ell}\frac{1}{k+1}\frac{\partial \omega_\ell}{\partial s_j}E(s)t^{k+1}\Psi(t) \\
&+2ih\sum_{j,\ell} g_0^{j\ell}\frac{\partial E}{\partial s_j}(s)\left(\frac{1}{k+1}t^{k+1}\omega_\ell(s) - \alpha_B\omega_\ell(0)\right)\Psi(t) \\
&+R(s,t)\Phi_1(s,t) - h^2\sum_{\ell}\Gamma^\ell(s)\frac{\partial}{\partial s_\ell}E(s)\Psi(t) \\
&+ih\sum_{\ell}\Gamma^\ell(s)\left(\frac{1}{k+1}t^{k+1}\omega_\ell(s) - \alpha_B\omega_\ell(0)\right)E(s)\Psi(t),
\end{aligned}$$

where

$$\begin{aligned}
R(s,t) &= \sum_{j,\ell} g_0^{j\ell}\left(\frac{1}{k+1}t^{k+1}\omega_j(s) - \alpha_B\omega_j(0)\right)\times \\
&\times\left(\frac{1}{k+1}t^{k+1}\omega_\ell(s) - \alpha_B\omega_\ell(0)\right) - \omega_{\min}(B)^2\sum_j\left(\frac{1}{k+1}t^{k+1} - \alpha_B\right)^2 \\
&= \frac{1}{(k+1)^2}\left(\sum_{j,\ell} g_0^\ell(s)\omega_j(s)\omega_\ell(s) - \sum_j(\omega_j(0))^2\right)t^{2(k+1)} \\
&-\frac{2}{k+1}t^{k+1}\sum_j(\omega_j(s)-\omega_j(0))\alpha_B\omega_j(0) \\
&+O(|s|^2)\sum_j\left(\frac{1}{k+1}t^{k+1} - \alpha_B\right)^2.
\end{aligned}$$

We have

$$\||s|^m E(s)\| = \left(h^{-\beta(n-1)}\int_{\mathbb{R}^{n-1}}|s|^{2m}\exp\left(-\frac{|s|^2}{h^{2\beta}}\right)ds\right)^{1/2} = C_1 h^{\beta m}, \tag{3.5}$$

and, furthermore,

$$\||s|^m\frac{\partial E}{\partial s_j}(s)\| = C_2 h^{\beta(m-1)}, \quad \||s|^m\frac{\partial^2 E}{\partial s_j\partial s_\ell}(s)\| = C_3 h^{\beta(m-2)}. \tag{3.6}$$

We also have

$$\|t^{k+1}\Psi(t)\| \le C_4 h^{\frac{k+1}{k+2}}, \quad \|t^{2(k+1)}\Psi(t)\| \le C_5 h^{\frac{2k+2}{k+2}}. \tag{3.7}$$

Since $s = 0$ is a minimum of $|\omega_{0,1}(s)|^2$, we have

$$|\omega_{0,1}(s)|^2 - \omega_{\min}(B)^2 = \sum_{j,\ell} g_0^{j\ell}(s)\omega_j(s)\omega_\ell(s) - (\omega_j(0))^2 \le C_6|s|^2 \quad (3.8)$$

and

$$\left(\frac{\partial}{\partial s_r}|\omega_{0,1}|^2\right)(0) = 2\sum_j \frac{\partial \omega_j}{\partial s_r}(0)\omega_j(0) = 0,$$

which implies

$$\left|\sum_j (\omega_j(s) - \omega_j(0))\omega_j(0)\right| \le C_7|s|^2. \quad (3.9)$$

Using Eq. (3.4), Eq. (3.5), Eq. (3.6), Eq. (3.7), Eq. (3.8) and Eq. (3.9) and putting $\beta = \frac{1}{3(k+2)}$, one can easily get that

$$\|H^{h,0}\Phi - \lambda h^{\frac{2k+2}{k+2}}\Phi\| \le Ch^{\frac{6k+8}{3(k+2)}}. \qquad \square$$

Given a and b such that $\hat{\nu}\,\omega_{\min}(B)^{2/(k+2)} < a < b$ and some natural N, choose numbers $\nu_j, j = 0, \dots, N$, such that

$$a < \nu_0 < \nu_1 < \ldots < \nu_N < b.$$

By Lemma 3.1, for any $m = 0, 1, \dots, N$,

$$\mu_m^h = \nu_m h^{\frac{2k+2}{k+2}} \in [h^{(2k+2)/(k+2)}a, h^{(2k+2)/(k+2)}b]$$

is an approximate eigenvalue of the operator H_D^h: for some $\Phi_m^h \in C_c^\infty(D)$

$$\|(H^{h,0} - \mu_m^h)\Phi_m^h\| \le Ch^{\frac{6k+8}{3(k+2)}}\|\Phi_m^h\|.$$

Using Theorem 2.1 with $N_h = N$ independent of h, we complete the proof.

Remark 3.1. Using the methods of the proof of Theorem 3.1, one can construct a much larger (h-dependent) number of approximate eigenvalues of the operator H^h on the interval $[h^{(2k+2)/(k+2)}a, h^{(2k+2)/(k+2)}b]$ with some a and b such that $\hat{\nu}\,\omega_{\min}(B)^{2/(k+2)} < a < b$. Applying then Theorem 2.1 with N_h dependent on h, one can get the following theorem.

Theorem 3.2. *Under the assumptions of Theorem 3.1, for any a and b such that*

$$\hat{\nu}\,\omega_{\min}(B)^{\frac{2}{k+2}} < a < b,$$

there exist $h_0 > 0$ *and* $C > 0$ *such that, for any* $h \in (0, h_0]$, *the spectrum of* H^h *in the interval*

$$[h^{\frac{2k+2}{k+2}} a, h^{\frac{2k+2}{k+2}} b]$$

has at least $[Ch^{-\frac{2}{3(k+2)}}]$ *gaps.*

4. Concluding remarks

1. Suppose that the operator H^h satisfies the condition of Eq. (1.1) with some $\epsilon_0 > 0$, and that the zero set of the magnetic field $\mathbf{B}$ is a smooth oriented hypersurface S. Moreover, assume that there are constants $k \in \mathbb{N}$ and $C > 0$ such that for all x in a neighborhood of S we have:

$$C^{-1} d(x, S)^k \leq |B(x)| \leq C d(x, S)^k .$$

Note that these assumptions are stronger than the assumptions of Theorem 3.1.

It is interesting to determine the bottom $\lambda_0(H^h)$ of the spectrum of the operator H^h in $L^2(M)$. By Theorem 2.1 in Ref. 4 and Theorem 2.7 in Ref. 7, $\lambda_0(H^h)$ is asymptotically equal to the bottom $\lambda_0(H^{h,0})$ of the spectrum of the operator $H^{h,0}$. From the construction of approximate eigenvalues of $H^{h,0}$ given in Lemma 3.1, one can see that, in order to find $\lambda_0(H^{h,0})$, it is natural to consider a self-adjoint second order differential operator $P(\mathbf{v}, \mathbf{w})$, $\mathbf{v}, \mathbf{w} \in \mathbb{R}^{n-1}$, in $L^2(\mathbb{R})$ given by

$$P(\mathbf{v}, \mathbf{w}) = -\frac{d^2}{dt^2} + \left| \frac{1}{k+1} \mathbf{w} t^{k+1} - \mathbf{v} \right|^2$$

and minimize the bottom $\lambda_0(\mathbf{v}, \mathbf{w})$ of the spectrum of the operator $P(\mathbf{v}, \mathbf{w})$ over $\mathbf{v} \in \mathbb{R}^{n-1}$ and $\mathbf{w} \in K$, where $K = \{\omega_{0,1}(s) : s \in \bar{S}\}$ is a compact subset of $\mathbb{R}^{n-1} \setminus \{0\}$.

The identity

$$P(\mathbf{v}, \mathbf{w}) = \left(-\frac{d^2}{dt^2} + \left(\frac{1}{k+1} |\mathbf{w}| t^{k+1} - \frac{\mathbf{v} \cdot \mathbf{w}}{|\mathbf{w}|} \right)^2 \right) + \left| \mathbf{v} - \frac{\mathbf{v} \cdot \mathbf{w}}{|\mathbf{w}|^2} \mathbf{w} \right|^2$$

shows that, for determining the minimum of $\lambda_0(\mathbf{v}, \mathbf{w})$ over $\mathbf{v} \in \mathbb{R}^{n-1}$ and $\mathbf{w} \in K$, it is sufficient to assume that $\mathbf{v}$ is parallel to $\mathbf{w}$. For such $\mathbf{v}$ and $\mathbf{w}$, we obtain $P(\mathbf{v}, \mathbf{w}) = Q(\alpha, \beta)$ with $\alpha = \pm|\mathbf{v}|, \beta = |\mathbf{w}|$. By Eq. (3.2), it follows that, for determining the minimum of $\lambda_0(\alpha, \beta)$ over $\alpha \in \mathbb{R}$ and $\beta \in \{|\omega_{0,1}(s)| : s \in \bar{S}\}$, we should first minimize over β, that is, take $s_1 \in S$ such that

$$|\omega_{0,1}(s_1)| = \min\{|\omega_{0,1}(s)| : s \in \bar{S}\},$$

and then, for the minimal β, minimize over α.

This observation provides some explanations of our construction of approximate eigenvalues of the operator $H^{h,0}$ in Lemma 3.1, in particular, of our choice for the exponent in Eq. (3.3). It also motivates us to formulate the following conjecture:

Conjecture 4.1. *Under current assumptions, for the bottom $\lambda_0(H^h)$ of the spectrum of the operator H^h in $L^2(M)$, we have*

$$\lim_{h\to 0} h^{-\frac{2k+2}{k+2}} \lambda_0(H^h) = \hat{\nu}\, \omega_{\min}(B)^{\frac{2}{k+2}}.$$

Observe that a similar result was obtained by Pan and Kwek[25] for the bottom of the spectrum of the Neumann realization of the operator H^h in a bounded domain in the case $k = 1$.

2. In the setting of Sec. 3, one can assume that the function $|\omega_{0,1}(x)|$ has a non-degenerate minimum at some $x_1 \in S$. In some sense this is the "miniwells case" analyzed in Ref. 12 in comparison with the "uniform case" analyzed in Ref. 13, which in this setting was studied in Ref. 5. Then we can obtain a more precise information about gaps located near the bottom of the spectrum of H^h (see some relevant calculations in Ref. 3). This will be discussed elsewhere.

3. The results obtained in Sec. 3 and in the previous remark can be extended to the case $b_0 \neq 0$ (for the "miniwells case", see some relevant results in Ref. 9). We will consider these problems in a future publication (cf. Ref. 6).

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ASYMPTOTIC ENTANGLEMENT IN OPEN QUANTUM DYNAMICS

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In the framework of the theory of open systems based on completely positive quantum dynamical semigroups, we describe the behaviour of a bipartite system interacting with an environment in connection with the quantum entanglement. We solve in the asymptotic long-time regime the master equation for two independent harmonic oscillators interacting with an environment and give a description of the continuous-variable asymptotic entanglement in terms of the covariance matrix of the considered subsystem for an arbitrary Gaussian input state. Using Peres–Simon necessary and sufficient condition for separability of two-mode Gaussian states, we show that for certain classes of environments the initial state evolves asymptotically to an entangled equilibrium bipartite state, while for other values of the coefficients describing the environment, the asymptotic state is separable. We calculate also the logarithmic negativity characterizing the degree of entanglement of the asymptotic state.

Keywords: Open systems, Quantum entanglement, Nonseparable states

1. Introduction

The rapid development of the theory of quantum information, communication and computation has revived the interest in open quantum systems in relation, on one side, to their decohering properties and, on the other side, to their capacity of creating entanglement in multi-partite systems immersed in certain environments. Quantum entanglement represents the physical resource in quantum information science which is indispensable for the description and performance of such tasks like teleportation, superdense coding, quantum cryptography and quantum computation.[13] Therefore the generation, detection and manipulation of the entanglement continues to be presently a problem of intense investigation.

When two systems are immersed in an environment, then, besides and

at the same time with the quantum decoherence, the environment can also generate a quantum entanglement of the two systems and therefore an additional mechanism to correlate them.[1,2,5] In certain circumstances, the environment enhances entanglement and in others it suppresses the entanglement and the state describing the two systems becomes separable. The structure and properties of the environment may be such that not only the two systems become entangled, but also such that a certain amount of entanglement survives in the asymptotic long-time regime. The reason is that even if not directly coupled, the two systems immersed in the same environment can interact through the environment itself and it depends on how strong this indirect interaction is with respect to the quantum decoherence, whether entanglement can be generated at the beginning of the evolution and, in the case of an affirmative answer, if it can be maintained for a definite time or it survives indefinitely in time.[1]

In this work we study, in the framework of the theory of open quantum systems based on completely positive dynamical semigroups, the existence of the continuous variable asymptotic entanglement for a subsystem composed of two identical harmonic oscillators interacting with an environment. We are interested in discussing the correlation effect of the environment, therefore we assume that the two systems are independent, i.e., they do not interact directly. The initial state of the subsystem is taken of Gaussian form and the evolution under the quantum dynamical semigroup assures the preservation in time of the Gaussian form of the state. We only investigate here the asymptotic behaviour of the subsystem states. The time evolution of the entanglement, in particular the possibility of the so-called "entanglement sudden death", that is suppression of the entanglement at a certain finite moment of time, will be discussed in a future work.

The organizing of the paper is as follows. In Sect. 2 the notion of the quantum dynamical semigroup is defined using the concept of a completely positive map. Then we give the general form of the Markovian quantum mechanical master equation describing the evolution of open quantum systems. We mention the role of complete positivity in connection with the quantum entanglement of systems interacting with an external environment. In Sec. 3 we write the equations of motion in the Heisenberg picture for two independent harmonic oscillators interacting with a general environment. From these equations we derive in Sec. 4 the asymptotic values of the variances and covariances of the coordinates and momenta which enter the asymptotic covariance matrix. Then, by using the Peres-Simon necessary and sufficient condition for separability of two-mode Gaussian

states,[14,17] we investigate the behaviour of the environment induced entanglement in the limit of long times. We show that for certain classes of environments the initial state evolves asymptotically to an equilibrium state which is entangled, while for other values of the parameters describing the environment, the entanglement is suppressed and the asymptotic state is separable. The existence of the quantum correlations between the two systems in the asymptotic long-time regime is the result of the competition between entanglement and quantum decoherence. We calculate also the logarithmic negativity characterizing the degree of entanglement of the asymptotic state. Conclusions are given in Sec. 5.

2. Axiomatic theory of open quantum systems

The standard quantum mechanics is Hamiltonian. The time evolution of a closed physical system is given by a dynamical group U_t, uniquely determined by its generator H, which is the Hamiltonian operator of the system. The action of the dynamical group U_t on any density matrix ρ from the set $\mathcal{D}(\mathcal{H})$ of all density matrices in the Hilbert space $\mathcal{H}$ of the quantum system is defined by

$$\rho(t) = U_t(\rho) = e^{-\frac{i}{\hbar}Ht}\rho e^{\frac{i}{\hbar}Ht}$$

for all $t \in (-\infty, \infty)$. According to von Neumann, density operators $\rho \in \mathcal{D}(\mathcal{H})$ are trace class ($\mathrm{Tr}\rho < \infty$), self-adjoint ($\rho^\dagger = \rho$), positive ($\rho > 0$) operators with $\mathrm{Tr}\rho = 1$. All these properties are conserved by the time evolution defined by U_t.

In the case of open quantum systems, the time evolution Φ_t of the density operator $\rho(t) = \Phi_t(\rho)$ has to preserve the von Neumann conditions for all times. It follows that Φ_t must have the following properties:

(i) $\Phi_t(\lambda_1\rho_1 + \lambda_2\rho_2) = \lambda_1\Phi_t(\rho_1) + \lambda_2\Phi_t(\rho_2)$ for $\lambda_1, \lambda_2 \geq 0$, $\lambda_1 + \lambda_2 = 1$, i. e., Φ_t must preserve the convex structure of $\mathcal{D}(\mathcal{H})$,

(ii) $\Phi_t(\rho^\dagger) = \Phi_t(\rho)^\dagger$,

(iii) $\Phi_t(\rho) > 0$,

(iv) $\mathrm{Tr}\Phi_t(\rho) = 1$.

The time evolution U_t for closed systems must be a group $U_{t+s} = U_tU_s$. We have also $U_0(\rho) = \rho$ and $U_t(\rho) \to \rho$ in the trace norm when $t \to 0$. The dual group $\widetilde{U}_t$ acting on the observables $A \in \mathcal{B}(\mathcal{H})$, i.e., on the bounded operators on $\mathcal{H}$, is given by

$$\widetilde{U}_t(A) = e^{\frac{i}{\hbar}Ht}Ae^{-\frac{i}{\hbar}Ht}.$$

Then $\widetilde{U}_t(AB) = \widetilde{U}_t(A)\widetilde{U}_t(B)$ and $\widetilde{U}_t(I) = I$, where I is the identity operator on $\mathcal{H}$. Also, $\widetilde{U}_t(A) \to A$ ultraweakly when $t \to 0$ and $\widetilde{U}_t$ is an ultraweakly continuous mapping.[4,7,12] These mappings have a strong positivity property called complete positivity,

$$\sum_{i,j} B_i^\dagger \widetilde{U}_t(A_i^\dagger A_j) B_j \geq 0, \quad A_i, B_i \in \mathcal{B}(\mathcal{H}).$$

In the axiomatic approach to the description of the evolution of open quantum systems,[4,7,12] one supposes that the time evolution Φ_t of open systems is not very different from the time evolution of closed systems. The simplest dynamics Φ_t which introduces a preferred direction in time, characteristic for dissipative processes, is that in which the group condition is replaced by the semigroup condition[6,7,11]

$$\Phi_{t+s} = \Phi_t \Phi_s, \ t, s \geq 0.$$

The complete positivity condition has the form

$$\sum_{i,j} B_i^\dagger \widetilde{\Phi}_t(A_i^\dagger A_j) B_j \geq 0, \quad A_i, B_i \in \mathcal{B}(\mathcal{H}), \tag{2.1}$$

where $\widetilde{\Phi}_t$ denotes the dual of Φ_t acting on $\mathcal{B}(\mathcal{H})$ and is defined by the duality condition

$$\mathrm{Tr}(\Phi_t(\rho)A) = \mathrm{Tr}(\rho \widetilde{\Phi}_t(A)).$$

Then the conditions $\mathrm{Tr}\Phi_t(\rho) = 1$ and $\widetilde{\Phi}_t(I) = I$ are equivalent. Also the conditions $\widetilde{\Phi}_t(A) \to A$ ultraweakly when $t \to 0$ and $\Phi_t(\rho) \to \rho$ in the trace norm when $t \to 0$, are equivalent. For the semigroups with these properties and with a more weak property of positivity than Eq. (2.1), namely

$$A \geq 0 \to \widetilde{\Phi}_t(A) \geq 0,$$

it is well known that there exists a (generally unbounded) mapping $\widetilde{L}$ – the generator of $\widetilde{\Phi}_t$, and $\widetilde{\Phi}_t$ is uniquely determined by $\widetilde{L}$. The dual generator of the dual semigroup Φ_t is denoted by L,

$$\mathrm{Tr}(L(\rho)A) = \mathrm{Tr}(\rho \widetilde{L}(A)).$$

The evolution equations by which L and $\widetilde{L}$ determine uniquely Φ_t and $\widetilde{\Phi}_t$, respectively, are given in the Schrödinger and Heisenberg picture as

$$\frac{d\Phi_t(\rho)}{dt} = L(\Phi_t(\rho)) \tag{2.2}$$

and

$$\frac{d\widetilde{\Phi}_t(A)}{dt} = \widetilde{L}(\widetilde{\Phi}_t(A)). \tag{2.3}$$

These equations replace in the case of open systems the von Neumann-Liouville equations

$$\frac{dU_t(\rho)}{dt} = -\frac{i}{\hbar}[H, U_t(\rho)]$$

and

$$\frac{d\widetilde{U}_t(A)}{dt} = \frac{i}{\hbar}[H, \widetilde{U}_t(A)],$$

respectively. For applications, Eqs. (2.2) and (2.3) are only useful if the detailed structure of the generator $L(\widetilde{L})$ is known and can be related to the concrete properties of the open systems described by such equations. For the class of dynamical semigroups which are completely positive and norm continuous, the generator $\widetilde{L}$ is bounded. In many applications the generator is unbounded.

According to Lindblad,[12] the following argument can be used to justify the complete positivity of $\widetilde{\Phi}_t$: If the open system is extended in a trivial way to a larger system described in a Hilbert space $\mathcal{H} \otimes \mathcal{K}$ with the time evolution defined by

$$\widetilde{W}_t(A \otimes B) = \widetilde{\Phi}_t(A) \otimes B, \quad A \in \mathcal{B}(\mathcal{H}),\ B \in \mathcal{B}(\mathcal{K}),$$

then the positivity of the states of the compound system will be preserved by $\widetilde{W}_t$ only if $\widetilde{\Phi}_t$ is completely positive. With this observation a new equivalent definition of the complete positivity is obtained: $\widetilde{\Phi}_t$ is completely positive if $\widetilde{W}_t$ is positive for any finite dimensional Hilbert space $\mathcal{K}$. The physical meaning of complete positivity can mainly be understood in relation to the existence of entangled states, the typical example being given by a vector state with a singlet-like structure that cannot be written as a tensor product of vector states. Positivity property guarantees the physical consistency of evolving states of single systems, while complete positivity prevents inconsistencies in entangled composite systems; therefore the existence of entangled states makes the request of complete positivity necessary.[1]

A bounded mapping $\widetilde{L} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ which satisfies $\widetilde{L}(I) = 0$, $\widetilde{L}(A^\dagger) = \widetilde{L}(A)^\dagger$ and

$$\widetilde{L}(A^\dagger A) - \widetilde{L}(A^\dagger)A - A^\dagger \widetilde{L}(A) \geq 0$$

is called dissipative. The 2-positivity property of the completely positive mapping $\widetilde{\Phi}_t$,

$$\widetilde{\Phi}_t(A^\dagger A) \geq \widetilde{\Phi}_t(A^\dagger)\widetilde{\Phi}_t(A), \tag{2.4}$$

with equality at $t = 0$, implies that $\widetilde{L}$ is dissipative. Lindblad[12] has shown that conversely, the dissipativity of $\widetilde{L}$ implies that $\widetilde{\Phi}_t$ is 2-positive. $\widetilde{L}$ is called completely dissipative if all trivial extensions of $\widetilde{L}$ to a compound system described by $\mathcal{H} \otimes \mathcal{K}$ with any finite dimensional Hilbert space $\mathcal{K}$ are dissipative. Lindblad has also shown that there exists a one-to-one correspondence between the completely positive norm continuous semigroups $\widetilde{\Phi}_t$ and completely dissipative generators $\widetilde{L}$. The structural theorem of Lindblad gives the most general form of a completely dissipative mapping $\widetilde{L}$.[12]

Theorem 2.1. *$\widetilde{L}$ is completely dissipative and ultraweakly continuous if and only if it is of the form*

$$\widetilde{L}(A) = \frac{i}{\hbar}[H, A] + \frac{1}{2\hbar}\sum_j (V_j^\dagger [A, V_j] + [V_j^\dagger, A] V_j), \tag{2.5}$$

where $V_j,\ \sum_j V_j^\dagger V_j \in \mathcal{B}(\mathcal{H}),\ H \in \mathcal{B}(\mathcal{H})_{\text{s.a.}}$.

The dual generator on the state space (Schrödinger picture) is of the form

$$L(\rho) = -\frac{i}{\hbar}[H, \rho] + \frac{1}{2\hbar}\sum_j ([V_j \rho, V_j^\dagger] + [V_j, \rho V_j^\dagger]). \tag{2.6}$$

Eqs. (2.2) and (2.6) give the explicit form of the most general time-homogeneous quantum mechanical Markovian master equation with a bounded Liouville operator:[8,12,15]

$$\frac{d\Phi_t(\rho)}{dt} = -\frac{i}{\hbar}[H, \Phi_t(\rho)] + \frac{1}{2\hbar}\sum_j ([V_j \Phi_t(\rho), V_j^\dagger] + [V_j, \Phi_t(\rho) V_j^\dagger]).$$

The assumption of a semigroup dynamics is only applicable in the limit of weak coupling of the subsystem with its environment, i.e., for long relaxation times.[18] We mention that the majority of Markovian master equations found in the literature are of this form after some rearrangement of terms, even for unbounded generators. It is also an empirical fact for many physically interesting situations that the time evolutions Φ_t drive the system towards a unique final state $\rho(\infty) = \lim_{t\to\infty} \Phi_t(\rho(0))$ for all $\rho(0) \in \mathcal{D}(\mathcal{H})$.

The evolution equations of Lindblad are operator equations. In cases when these equations are exactly solvable, the solutions give complete information about the studied problem and determine completely the time evolution of the observables.

3. Equations of motion for two independent harmonic oscillators

We are interested in the generation of entanglement between two harmonic oscillators due to their interaction with the environment. Since the two harmonic oscillators interact with a common environment, there will be induced coupling between them, even if initially they are uncoupled. Thus, the master equation for the two harmonic oscillators must account for their mutual interaction by their coupling to the environment. We study the dynamics of the subsystem composed of two identical non-interacting (independent) oscillators in weak interaction with a large environment, so that their reduced time evolution can be described by a Markovian, completely positive quantum dynamical semigroup.

If $\widetilde{\Phi}_t$ is the dynamical semigroup describing the time evolution of the open quantum system in the Heisenberg picture, then the master equation has the following form for an operator A (see Eqs. (2.3), (2.5)):[8,12,15]

$$\frac{d\widetilde{\Phi}_t(A)}{dt} = \frac{i}{\hbar}[H, \widetilde{\Phi}_t(A)] + \frac{1}{2\hbar}\sum_j (V_j^\dagger[\widetilde{\Phi}_t(A), V_j] + [V_j^\dagger, \widetilde{\Phi}_t(A)]V_j). \quad (3.1)$$

Here, H denotes the Hamiltonian of the open system and $V_j, V_j^\dagger$, which are operators defined on the Hilbert space of H, model the interaction of the open system with the environment. Since we are interested in the set of Gaussian states, we introduce those quantum dynamical semigroups that preserve this set. Therefore H is taken to be a polynomial of second degree in the coordinates x, y and momenta p_x, p_y of the two quantum oscillators and $V_j, V_j^\dagger$ are taken polynomials of only first degree in these canonical observables. Then in the linear space spanned by the coordinates and momenta there exist only four linearly independent operators $V_{j=1,2,3,4}$,[16]

$$V_j = a_{xj}p_x + a_{yj}p_y + b_{xj}x + b_{yj}y,$$

where $a_{xj}, a_{yj}, b_{xj}, b_{yj} \in \mathbf{C}$. The Hamiltonian H of the two uncoupled identical harmonic oscillators of mass m and frequency ω is given by

$$H = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{m\omega^2}{2}(x^2 + y^2).$$

The fact that $\widetilde{\Phi}_t$ is a dynamical semigroup implies the positivity of the following matrix formed by the scalar products of the four vectors $\mathbf{a}_x, \mathbf{b}_x, \mathbf{a}_y, \mathbf{b}_y$, whose entries are the components $a_{xj}, b_{xj}, a_{yj}, b_{yj}$, respec-

tively,

$$\frac{1}{2}\hbar \begin{pmatrix} (\mathbf{a}_x\mathbf{a}_x) & (\mathbf{a}_x\mathbf{b}_x) & (\mathbf{a}_x\mathbf{a}_y) & (\mathbf{a}_x\mathbf{b}_y) \\ (\mathbf{b}_x\mathbf{a}_x) & (\mathbf{b}_x\mathbf{b}_x) & (\mathbf{b}_x\mathbf{a}_y) & (\mathbf{b}_x\mathbf{b}_y) \\ (\mathbf{a}_y\mathbf{a}_x) & (\mathbf{a}_y\mathbf{b}_x) & (\mathbf{a}_y\mathbf{a}_y) & (\mathbf{a}_y\mathbf{b}_y) \\ (\mathbf{b}_y\mathbf{a}_x) & (\mathbf{b}_y\mathbf{b}_x) & (\mathbf{b}_y\mathbf{a}_y) & (\mathbf{b}_y\mathbf{b}_y) \end{pmatrix}.$$

Its matrix elements have to be chosen appropriately to suit various physical models of the environment. For a quite general environment able to induce noise and damping effects, we take this matrix of the following form, where the coefficients $D_{xx}, D_{xp_x} \ldots$, and λ are real quantities, representing the diffusion coefficients and, respectively, the dissipation constant

$$\begin{pmatrix} D_{xx} & -D_{xp_x} - i\hbar\lambda/2 & D_{xy} & -D_{xp_y} \\ -D_{xp_x} + i\hbar\lambda/2 & D_{p_xp_x} & -D_{yp_x} & D_{p_xp_y} \\ D_{xy} & -D_{yp_x} & D_{yy} & -D_{yp_y} - i\hbar\lambda/2 \\ -D_{xp_y} & D_{p_xp_y} & -D_{yp_y} + i\hbar\lambda/2 & D_{p_yp_y} \end{pmatrix} \tag{3.2}$$

It follows that the principal minors of this matrix are positive or zero. From the Cauchy-Schwarz inequality the following relations for the coefficients defined in Eq. (3.2) hold (from now on we put, for simplicity, $\hbar = 1$),

$$D_{xx}D_{yy} - D_{xy}^2 \geq 0,\ D_{xx}D_{p_xp_x} - D_{xp_x}^2 \geq \frac{\lambda^2}{4},$$

$$D_{p_xp_x}D_{p_yp_y} - D_{p_xp_y}^2 \geq 0,\ D_{yy}D_{p_yp_y} - D_{yp_y}^2 \geq \frac{\lambda^2}{4},$$

$$D_{xx}D_{p_yp_y} - D_{xp_y}^2 \geq 0,\ D_{yy}D_{p_xp_x} - D_{yp_x}^2 \geq 0. \tag{3.3}$$

The matrix of the coefficients (3.2) can be conveniently written as

$$\begin{pmatrix} C_1 & C_3 \\ {C_3}^\dagger & C_2 \end{pmatrix}, \tag{3.4}$$

in terms of 2×2 matrices $C_1 = {C_1}^\dagger$, $C_2 = {C_2}^\dagger$ and C_3. This decomposition has a direct physical interpretation: The elements containing the diagonal contributions C_1 and C_2 represent diffusion and dissipation coefficients corresponding to the first, respectively the second, system in absence of the other, while the elements in C_3 represent environment generated couplings between the two, initially independent, oscillators.

The covariance of self-adjoint operators A_1 and A_2 can be written with the density operator ρ, describing the initial state of the quantum system, as follows,

$$\sigma_{A_1A_2}(t) = \frac{1}{2}\mathrm{Tr}(\rho\widetilde{\Phi}_t(A_1A_2 + A_2A_1)).$$

We introduce the following 4×4 covariance matrix:

$$\sigma(t) = \begin{pmatrix} \sigma_{xx} & \sigma_{xp_x} & \sigma_{xy} & \sigma_{xp_y} \\ \sigma_{xp_x} & \sigma_{p_xp_x} & \sigma_{yp_x} & \sigma_{p_xp_y} \\ \sigma_{xy} & \sigma_{yp_x} & \sigma_{yy} & \sigma_{yp_y} \\ \sigma_{xp_y} & \sigma_{p_xp_y} & \sigma_{yp_y} & \sigma_{p_yp_y} \end{pmatrix}. \tag{3.5}$$

By direct calculation we obtain[16]

$$\frac{d\sigma}{dt} = Y\sigma + \sigma Y^{\mathrm{T}} + 2D, \tag{3.6}$$

where

$$Y = \begin{pmatrix} -\lambda & 1/m & 0 & 0 \\ -m\omega^2 & -\lambda & 0 & 0 \\ 0 & 0 & -\lambda & 1/m \\ 0 & 0 & -m\omega^2 & -\lambda \end{pmatrix},$$

D is the matrix of the diffusion coefficients

$$D = \begin{pmatrix} D_{xx} & D_{xp_x} & D_{xy} & D_{xp_y} \\ D_{xp_x} & D_{p_xp_x} & D_{yp_x} & D_{p_xp_y} \\ D_{xy} & D_{yp_x} & D_{yy} & D_{yp_y} \\ D_{xp_y} & D_{p_xp_y} & D_{yp_y} & D_{p_yp_y} \end{pmatrix}$$

and T denotes the transposed matrix. Introducing the notation $\sigma(\infty) \equiv \lim_{t\to\infty} \sigma(t)$, the time-dependent solution of Eq. (3.6) is given by[16]

$$\sigma(t) = M(t)(\sigma(0) - \sigma(\infty))M^{\mathrm{T}}(t) + \sigma(\infty),$$

where $M(t) = \exp(tY)$. The matrix $M(t)$ has to fulfil the condition $\lim_{t\to\infty} M(t) = 0$. In order that this limit exists, Y must only have eigenvalues with negative real parts. The values at infinity are obtained from the equation[16]

$$Y\sigma(\infty) + \sigma(\infty)Y^{\mathrm{T}} = -2D. \tag{3.7}$$

4. Environment induced entanglement

The two-mode Gaussian state is entirely specified by its covariance matrix σ (3.5), which is a real, symmetric and positive matrix with the following block structure

$$\sigma = \begin{pmatrix} A & C \\ C^{\mathrm{T}} & B \end{pmatrix},$$

where A, B and C are 2×2 matrices. Their entries are correlations of the canonical operators x, y, p_x, p_y, A and B denote the symmetric covariance matrices for the individual reduced one-mode states, while the matrix C contains the cross-correlations between modes. The entries of the covariance matrix depend on Y and D and can be calculated from Eq. (3.7). To simplify the calculations, we shall consider environments for which the two diagonal submatrices in Eq. (3.4) are equal: $C_1 = C_2$, so that $D_{xx} = D_{yy}, D_{xp_x} = D_{yp_y}, D_{p_xp_x} = D_{p_yp_y}$. In addition, in the matrix C_3 we take $D_{xp_y} = D_{yp_x}$. Then both unimodal covariance matrices are equal, $A = B$ and the entanglement matrix C is symmetric. With the chosen coefficients, we obtain the following elements of the asymptotic entanglement matrix C:

$$\sigma_{xy}(\infty) = \frac{m^2(2\lambda^2+\omega^2)D_{xy} + 2m\lambda D_{xp_y} + D_{p_xp_y}}{2m^2\lambda(\lambda^2+\omega^2)},$$

$$\sigma_{xp_y}(\infty) = \sigma_{yp_x}(\infty) = \frac{-m^2\omega^2 D_{xy} + 2m\lambda D_{xp_y} + D_{p_xp_y}}{2m(\lambda^2+\omega^2)},$$

$$\sigma_{p_xp_y}(\infty) = \frac{m^2\omega^4 D_{xy} - 2m\omega^2\lambda D_{xp_y} + (2\lambda^2+\omega^2)D_{p_xp_y}}{2\lambda(\lambda^2+\omega^2)}$$

and of matrices A and B

$$\sigma_{xx}(\infty) = \sigma_{yy}(\infty) = \frac{m^2(2\lambda^2+\omega^2)D_{xx} + 2m\lambda D_{xp_x} + D_{p_xp_x}}{2m^2\lambda(\lambda^2+\omega^2)},$$

$$\sigma_{xp_x}(\infty) = \sigma_{yp_y}(\infty) = \frac{-m^2\omega^2 D_{xx} + 2m\lambda D_{xp_x} + D_{p_xp_x}}{2m(\lambda^2+\omega^2)}, \tag{4.1}$$

$$\sigma_{p_xp_x}(\infty) = \sigma_{p_yp_y}(\infty) = \frac{m^2\omega^4 D_{xx} - 2m\omega^2\lambda D_{xp_x} + (2\lambda^2+\omega^2)D_{p_xp_x}}{2\lambda(\lambda^2+\omega^2)}.$$

With these quantities we calculate the determinant of the entanglement matrix

$$\begin{aligned} \det C = \frac{1}{4\lambda^2(\lambda^2+\omega^2)} \times \\ \times[(m\omega^2 D_{xy} + \frac{1}{m}D_{p_xp_y})^2 + 4\lambda^2(D_{xy}D_{p_xp_y} - D_{xp_y}^2)]. \end{aligned} \tag{4.2}$$

It is very interesting that the general theory of open quantum systems allows couplings via the environment between uncoupled oscillators. According to the definitions of the environment parameters, the diffusion coefficients above can be different from zero and can simulate an interaction between the uncoupled oscillators. Indeed, the Gaussian states with $\det C \geq 0$ are separable states, but for $\det C < 0$, it may be possible that the asymptotic equilibrium states are entangled, as it will be shown in the following.

On general grounds, one expects that the effects of decoherence, counteracting entanglement production, be dominant in the long-time regime, so that no quantum correlation (entanglement) is expected to be left at infinity. Nevertheless, there are situations in which the environment allows the presence of entangled asymptotic equilibrium states. In order to investigate whether an external environment can actually entangle the two independent systems, we can use the partial transposition criterion:[14,17] A state is entangled if and only if the operation of partial transposition does not preserve its positivity. Simon[17] obtained the following necessary and sufficient criterion for separability, $S \geq 0$, where

$$\begin{aligned} S &\equiv \det A \det B \\ &+(\frac{1}{4} - |\det C|)^2 - \mathrm{Tr}[AJCJBJC^{\mathrm{T}}J] - \frac{1}{4}(\det A + \det B) \end{aligned} \tag{4.3}$$

and J is the 2×2 symplectic matrix

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

In order to analyze the possible persistence of the environment induced entanglement in the asymptotic long-time regime, we consider the environment characterized by the following values of its parameters: $m^2\omega^2 D_{xx} = D_{p_x p_x}$, $D_{xp_x} = 0$, $m^2\omega^2 D_{xy} = D_{p_x p_y}$. In this case the Simon expression (4.3) takes the form

$$S = \left(\frac{m^2\omega^2(D_{xx}^2 - D_{xy}^2)}{\lambda^2} + \frac{D_{xp_y}^2}{\lambda^2 + \omega^2} - \frac{1}{4} \right)^2 - 4\frac{m^2\omega^2 D_{xx}^2 D_{xp_y}^2}{\lambda^2(\lambda^2 + \omega^2)}. \tag{4.4}$$

There exists a large range of diffusion coefficients characterizing the environment (and fulfilling at the same time the constraints (3.3)) for which the expression (4.4) is negative, so that the asymptotic final state becomes entangled. Just to give an example, without compromising the general features of the system, we consider the particular case of $D_{xy} = 0$. Then we obtain that $S < 0$, i.e., the asymptotic final state is entangled, for the following range of values of the coefficient D_{xp_y} characterizing the environment,

$$\frac{m\omega D_{xx}}{\lambda} - \frac{1}{2} < \frac{D_{xp_y}}{\sqrt{\lambda^2 + \omega^2}} < \frac{m\omega D_{xx}}{\lambda} + \frac{1}{2},$$

where the coefficient D_{xx} satisfies the condition $m\omega D_{xx}/\lambda \geq 1/2$, equivalent with the unimodal uncertainty relation. If the coefficients do not fulfil the inequalities (4.5), then $S \geq 0$ and therefore the asymptotic final state of the considered bipartite system is separable.[9] These results show that,

irrespective of the initial conditions, we can obtain either an separable or an inseparable asymptotic entangled state, for a suitable choice of the diffusion and dissipation coefficients.

We apply the measure of entanglement based on negative eigenvalues of the partial transpose of the subsystem density matrix. For a Gaussian density operator, the negativity is completely defined by the symplectic spectrum of the partial transpose of the covariance matrix. The logarithmic negativity $E = -\frac{1}{2}\log_2[4f(\sigma)]$ determines the strength of entanglement for $E > 0$. If $E \leq 0$, then the state is separable. Here

$$f(\sigma) = \frac{1}{2}(\det A + \det B) - \det C - \sqrt{\left[\frac{1}{2}(\det A + \det B) - \det C\right]^2 - \det \sigma}. \tag{4.5}$$

In the considered particular case the logarithmic negativity is given by

$$E = -\log_2\left[2\left|\frac{m\omega D_{xx}}{\lambda} - \frac{D_{xp_y}}{\sqrt{\lambda^2+\omega^2}}\right|\right]. \tag{4.6}$$

This expression depends only on the diffusion and dissipation coefficients characterizing the environment and does not depend on the initial Gaussian state.[10] One can easily see that the double inequality (4.5), assuring the existence of entangled states ($S < 0$) is equivalent with the condition of the positivity of logarithmic negativity, $E > 0$. For $E > 0$, quantity E (4.6) simply gives a measure of the degree of entanglement contained in the particular asymptotic inseparable state determined by inequalities (4.5).

5. Summary

We have given a brief review of the theory of open quantum systems based on completely positive quantum dynamical semigroups and mentioned the necessity of the complete positivity for the existence of entangled states of systems interacting with an external environment. In the framework of this theory we investigated the existence of the asymptotic quantum entanglement for a subsystem composed of two uncoupled identical harmonic oscillators interacting with a common environment. By using the Peres-Simon necessary and sufficient criterion for separability of two-mode Gaussian states, we have shown that for certain classes of environments the initial state evolves asymptotically to an equilibrium state which is entangled, i.e., there exist non-local quantum correlations for the bipartite states of the two harmonic oscillator subsystem, while for other values of the coefficients describing the environment, the asymptotic state is separable. We determined

also the logarithmic negativity characterizing the degree of entanglement of the asymptotic state.

Due to the increased interest manifested towards the continuous variables approach[3] to quantum information theory, these results, in particular the possibility of maintaining a bipartite entanglement in a diffusive-dissipative environment for asymptotic long times, might be useful for applications in the field of quantum information processing and communication.

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REPEATED INTERACTIONS QUANTUM SYSTEMS: DETERMINISTIC AND RANDOM

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This paper gives an overview of recent results concerning the long time dynamics of repeated interaction quantum systems in a deterministic and random framework. We describe the non equilibrium steady states (NESS) such systems display and we present, as a macroscopic consequence, a second law of thermodynamics these NESS give rise to. We also explain in some details the analysis of products of certain random matrices underlying this dynamical problem.

Keywords: Non equilibrium quantum statistical mechanics, Repeated interaction quantum systems, Products of random matrices

1. Introduction and Model

A repeated interaction quantum system consists of a reference quantum subsystem $\mathcal{S}$ which interacts successively with the elements $\mathcal{E}_m$ of a chain $\mathcal{C} = \mathcal{E}_1 + \mathcal{E}_2 + \cdots$ of independent quantum systems. At each moment in time, $\mathcal{S}$ interacts precisely with one $\mathcal{E}_m$ (m increases as time does), while the other elements in the chain evolve freely according to their intrinsic dynamics. The complete evolution is described by the intrinsic dynamics of $\mathcal{S}$ and of all the $\mathcal{E}_m$, plus an interaction between $\mathcal{S}$ and $\mathcal{E}_m$, for each m. The latter is characterized by an interaction time $\tau_m > 0$, and an interaction operator V_m (acting on $\mathcal{S}$ and $\mathcal{E}_m$); during the time interval $[\tau_1 + \cdots + \tau_{m-1}, \tau_1 + \cdots + \tau_m)$, $\mathcal{S}$ is coupled to $\mathcal{E}_m$ only via V_m. Systems with this structure are important from a physical point of view, since they arise naturally as models for fundamental experiments on the interaction of matter with quantized radiation. As an example, the "One atom maser" provides an experimental setup in which the system $\mathcal{S}$ represents a mode of the electromagnetic field, whereas the elements $\mathcal{E}_k$ describe atoms injected in the cavity, one by one, which

interact with the field during their flight in the cavity. After they leave the cavity, the atoms encode some properties of the field which can be measured on these atoms.[14,16] For repeated interaction systems considered as *ideal*, i.e., such that all atoms are identical with identical interactions and times of flight through the cavity, corresponding mathematical analyses are provided in Refs. 7,17. To take into account the unavoidable fluctuations in the experiment setup used to study these repeated interaction systems, modelizations incorporating randomness have been proposed and studied in Refs. 8,9. With a different perspective, repeated quantum interaction models also appear naturally in the mathematical study of modelization of open quantum systems by means of quantum noises, see Ref. 4 and references therein. Any (continuous) master equation governing the dynamics of states on a system $\mathcal{S}$ can be viewed as the projection of a unitary evolution driving the system $\mathcal{S}$ and a field of quantum noises in interaction. It is shown in Ref. 4 how to recover such continuous models as some delicate limit of a discretization given by a repeated quantum interaction model. Let us finally mention Ref. 15 for results of a similar flavour in a somewhat different framework.

Our goal is to present the results of the papers Refs. 7,8 and Ref.9 on (random) repeated interaction quantum systems, which focus on the long time behaviour of these systems.

Let us describe the mathematical framework used to describe these quantum dynamical systems. According to the fundamental principles of quantum mechanics, states of the systems $\mathcal{S}$ and $\mathcal{E}_m$ are given by normalized vectors (or density matrices) on Hilbert spaces $\mathcal{H}_\mathcal{S}$ and $\mathcal{H}_{\mathcal{E}_m}$, respectively,[3,6a]. We assume that $\dim \mathcal{H}_\mathcal{S} < \infty$, while $\dim \mathcal{H}_{\mathcal{E}_m}$ may be infinite. Observables $A_\mathcal{S}$ and $A_{\mathcal{E}_m}$ of the systems $\mathcal{S}$ and $\mathcal{E}_m$ are bounded operators forming *von Neumann algebras* $\mathfrak{M}_\mathcal{S} \subset \mathcal{B}(\mathcal{H}_\mathcal{S})$ and $\mathfrak{M}_{\mathcal{E}_m} \subset \mathcal{B}(\mathcal{H}_{\mathcal{E}_m})$. They evolve according to the *Heisenberg dynamics* $\mathbb{R} \ni t \mapsto \alpha^t_\mathcal{S}(A_\mathcal{S})$ and $\mathbb{R} \ni t \mapsto \alpha^t_{\mathcal{E}_m}(A_{\mathcal{E}_m})$, where $\alpha^t_\mathcal{S}$ and $\alpha^t_{\mathcal{E}_m}$ are $*$-automorphism groups of $\mathfrak{M}_\mathcal{S}$ and $\mathfrak{M}_{\mathcal{E}_m}$, respectively, see e.g., Ref. 6. We now introduce distinguished *reference states*, given by vectors $\psi_\mathcal{S} \in \mathcal{H}_\mathcal{S}$ and $\psi_{\mathcal{E}_m} \in \mathcal{H}_{\mathcal{E}_m}$. Typical choices for $\psi_\mathcal{S}$, $\psi_{\mathcal{E}_m}$ are equilibrium (KMS) states for the dynamics $\alpha^t_\mathcal{S}$, $\alpha^t_{\mathcal{E}_m}$, at inverse temperatures $\beta_\mathcal{S}$, $\beta_{\mathcal{E}_m}$. The Hilbert space of states of the total system

[a]A normalized vector ψ defines a "pure" state $A \mapsto \langle \psi, A\psi\rangle = \mathrm{Tr}(\varrho_\psi A)$, where $\varrho_\psi = |\psi\rangle\langle\psi|$. A general "mixed" state is given by a density matrix $\varrho = \sum_{n\geq 1} p_n \varrho_{\psi_n}$, where the probabilities $p_n \geq 0$ sum up to one, and where the ψ_n are normalized vectors.

is the tensor product

$$\mathcal{H} = \mathcal{H}_{\mathcal{S}} \otimes \mathcal{H}_{\mathcal{C}},$$

where $\mathcal{H}_{\mathcal{C}} = \bigotimes_{m\geq 1} \mathcal{H}_{\mathcal{E}_m}$, and where the infinite product is taken with respect to $\psi_{\mathcal{C}} = \bigotimes_{m\geq 1} \psi_{\mathcal{E}_m}$. The non-interacting dynamics is the product of the individual dynamics, defined on the algebra $\mathfrak{M}_{\mathcal{S}} \bigotimes_{m\geq 1} \mathfrak{M}_{\mathcal{E}_m}$ by $\alpha^t_{\mathcal{S}} \bigotimes_{m\geq 1} \alpha^t_{\mathcal{E}_m}$. It will prove useful to consider the dynamics in the *Schrödinger picture*, i.e. as acting on vectors in $\mathcal{H}$. To do this, we first implement the dynamics via unitaries, satisfying

$$\alpha^t_{\#}(A_{\#}) = \mathrm{e}^{\mathrm{i}tL_{\#}} A_{\#} \mathrm{e}^{-\mathrm{i}tL_{\#}},\ t \in \mathbb{R}, \quad \text{and } L_{\#}\psi_{\#} = 0, \tag{1.1}$$

for any $A_{\#} \in \mathfrak{M}_{\#}$, where # stands for either $\mathcal{S}$ or $\mathcal{E}_m$. The self-adjoint operators $L_{\mathcal{S}}$ and $L_{\mathcal{E}_m}$, called *Liouville operators* or "positive temperature Hamiltonians", act on $\mathcal{H}_{\mathcal{S}}$ and $\mathcal{H}_{\mathcal{E}_m}$, respectively. The existence and uniqueness of $L_{\#}$ satisfying (1.1) is well known, under general assumptions on the reference states $\psi_{\#}$.[6] We require these states to be *cyclic* and *separating*. In particular, (1.1) holds if the reference states are equilibrium states. Let $\tau_m > 0$ and $V_m \in \mathfrak{M}_{\mathcal{S}} \otimes \mathfrak{M}_{\mathcal{E}_m}$ be the interaction time and interaction operator associated to $\mathcal{S}$ and $\mathcal{E}_m$. We define the (discrete) repeated interaction Schrödinger dynamics of a state vector $\phi \in \mathcal{H}$, for $m \geq 0$, by

$$U(m)\phi = \mathrm{e}^{-\mathrm{i}\widetilde{L}_m} \cdots \mathrm{e}^{-\mathrm{i}\widetilde{L}_2} \mathrm{e}^{-\mathrm{i}\widetilde{L}_1} \phi, \tag{1.2}$$

where

$$\widetilde{L}_k = \tau_k L_k + \tau_k \sum_{n\neq k} L_{\mathcal{E}_n} \tag{1.3}$$

describes the dynamics of the system during the time interval $[\tau_1 + \cdots + \tau_{k-1}, \tau_1 + \cdots + \tau_k)$, which corresponds to the time-step k of our discrete process. Hence L_k is

$$L_k = L_{\mathcal{S}} + L_{\mathcal{E}_k} + V_k, \tag{1.4}$$

acting on $\mathcal{H}_{\mathcal{S}} \otimes \mathcal{H}_{\mathcal{E}_k}$. We understand that the operator $L_{\mathcal{E}_n}$ in (1.3) acts nontrivially only on the n-th factor of the Hilbert space $\mathcal{H}_{\mathcal{C}}$ of the chain. As a general rule, we will ignore tensor products with the identity operator in the notation.

A state $\varrho(\cdot) = \mathrm{Tr}(\rho\,\cdot\,)$ given by density matrix ρ on $\mathcal{H}$ is called a *normal state*. Our goal is to understand the large-time asymptotics ($m \to \infty$) of expectations

$$\varrho\left(U(m)^* O U(m)\right) = \varrho(\alpha^m(O)), \tag{1.5}$$

for normal states ϱ and certain classes of observables O that we specify below. We denote the (random) repeated interaction dynamics by

$$\alpha^m(O) = U(m)^* O U(m). \tag{1.6}$$

1.1. *Van Hove Limit Type Results*

A first step towards understanding the dynamics of repeated interaction quantum systems reduced to the reference system $\mathcal{S}$ was performed in the work Ref. 2. This paper considers *Ideal Repeated Quantum Interaction Systems* which are characterized by identical elements $\mathcal{E}_k \equiv \mathcal{E}$ in the chain $\mathcal{C}$, constant interaction times $\tau_k \equiv \tau$ and identical interaction operators $V_k \equiv V \in \mathfrak{M}_\mathcal{S} \otimes \mathfrak{M}_\mathcal{E}$ between $\mathcal{S}$ and the elements $\mathcal{E}$ of the chain. In this setup, a Van Hove type analysis of the system is presented, in several regimes, to describe the dynamics of observables on $\mathcal{S}$ in terms of a Markovian evolution equation of Lindblad type. Informally, the simplest result of Ref. 2 reads as follows. Assume the interaction operator V is replaced by λV, where $\lambda > 0$ is a coupling constant, and let m, the number of interactions during the time $T = m\tau$, scale like $m \simeq t/\lambda^2$, where $0 \leq t < \infty$ and τ are fixed. Assume all elements of the chain are in a same thermal state at temperature β. Then, the weak coupling limit $\lambda \to 0$ of the evolution of any observable O acting on $\mathcal{S}$ obtained by tracing out the chain degrees of freedom from the evolution (1.6) satisfies, after removing a trivial free evolution, a continuous Lindblad type evolution equation in t. The temperature dependent generator is explicitely obtained from the interaction operator V and the free dynamics. The asymptotic regimes of the parameters (λ, τ) characterized by $\tau \to 0$ and $\tau\lambda^2 \leq 1$ are also covered in Ref. 2, giving rise to different Lindblad generators which all commute with the free Hamiltonian on $\mathcal{S}$. The critical situation, where $\tau \to 0$ with $\tau\lambda^2 = 1$ yields a quite general Lindblad generator, without any specific symmetry. In particular, it shows that any master equation driven by Lindblad operator, under reasonable assumptions, can be viewed as a Van Hove type limit of a certain explicit repeated interaction quantum system.

By contrast, the long time limit results obtained in Refs. 7–9 that we present here are obtained without rescaling any coupling constant or parameter, as is usually the case with master equation techniques. It is possible to do without these approximations, making use of the structure of repeated interaction systems only, as we now show.

2. Reduction to Products of Matrices

We first link the study of the dynamics to that of a product of reduced dynamics operators. In order to make the argument clearer, we only consider the expectation of an observable $A_{\mathcal{S}} \in \mathfrak{M}_{\mathcal{S}}$, and we take the initial state of the entire system to be given by the vector

$$\psi_0 = \psi_{\mathcal{S}} \otimes \psi_{\mathcal{C}}, \tag{2.1}$$

where the $\psi_{\mathcal{S}}$ and $\psi_{\mathcal{C}}$ are the reference states introduced above. We'll comment on the general case below. The expectation of $A_{\mathcal{S}}$ at the time-step m is

$$\langle \psi_0, \alpha^m(A_{\mathcal{S}})\psi_0 \rangle = \left\langle \psi_0, P\mathrm{e}^{\mathrm{i}\widetilde{L}_1} \cdots \mathrm{e}^{\mathrm{i}\widetilde{L}_m} A_{\mathcal{S}}\, \mathrm{e}^{-\mathrm{i}\widetilde{L}_m} \cdots \mathrm{e}^{-\mathrm{i}\widetilde{L}_1} P\psi_0 \right\rangle, \tag{2.2}$$

where we introduced

$$P = \mathbb{1}_{\mathcal{H}_{\mathcal{S}}} \bigotimes_{m\geq 1} P_{\psi_{\mathcal{E}_m}}, \tag{2.3}$$

the orthogonal projection onto $\mathcal{H}_{\mathcal{S}} \otimes \mathbb{C}\psi_{\mathcal{C}}$. A first important ingredient in our analysis is the use of *C-Liouvilleans* introduced in Ref. 11 , which are operators K_k defined by the properties

$$\mathrm{e}^{\mathrm{i}\widetilde{L}_k} A \mathrm{e}^{-\mathrm{i}\widetilde{L}_k} = \mathrm{e}^{\mathrm{i}K_k} A \mathrm{e}^{-\mathrm{i}K_k}, \tag{2.4}$$

$$K_k\, \psi_{\mathcal{S}} \otimes \psi_{\mathcal{C}} = 0, \tag{2.5}$$

where A in (2.4) is any observable of the total system. The identity (2.4) means that the operators K_k implement the same dynamics as the $\widetilde{L}_k$ whereas relation (2.5) selects a unique generator of the dynamics among all operators which satisfy (2.4). The existence of operators K_k satisfying (2.4) and (2.5) is rooted to the Tomita-Takesaki theory of von Neumann algebras, c.f. Ref. 11 and references therein. It turns out that the K_k are non-normal operators on $\mathcal{H}$, while the $\widetilde{L}_k$ are self-adjoint. Combining (2.4) with (2.2) we can write

$$\langle \psi_0, \alpha^m(A_{\mathcal{S}})\psi_0 \rangle = \left\langle \psi_0, P\mathrm{e}^{\mathrm{i}K_1} \cdots \mathrm{e}^{\mathrm{i}K_m} P A_{\mathcal{S}}\, \psi_0 \right\rangle. \tag{2.6}$$

A second important ingredient of our approach is to realize that the *independence* of the sub-systems $\mathcal{E}_m$ implies the relation

$$P\mathrm{e}^{\mathrm{i}K_1} \cdots \mathrm{e}^{\mathrm{i}K_m} P = P\mathrm{e}^{\mathrm{i}K_1} P \cdots P\mathrm{e}^{\mathrm{i}K_m} P. \tag{2.7}$$

Identifying $P\mathrm{e}^{\mathrm{i}K_k}P$ with an operator M_k on $\mathcal{H}_{\mathcal{S}}$, we thus obtain from (2.6) and (2.7),

$$\langle \psi_0, \alpha^m(A_{\mathcal{S}})\psi_0 \rangle = \langle \psi_{\mathcal{S}}, M_1 \cdots M_m A_{\mathcal{S}}\, \psi_{\mathcal{S}} \rangle. \tag{2.8}$$

It follows from (2.5) that $M_k\psi_{\mathcal{S}} = \psi_{\mathcal{S}}$, for all k, and, because the operators $M_k = P\mathrm{e}^{\mathrm{i}K_k}P$ implement a unitary dynamics, we show (Lemma 4.1) that the M_k are always contractions for some suitable norm $|||\cdot|||$ on $\mathbb{C}^d$. This motivates the following definition.

Definition 2.1. Given a vector $\psi_{\mathcal{S}} \in \mathbb{C}^d$ and a norm on $|||\cdot|||$ on $\mathbb{C}^d$, we call *Reduced Dynamics Operator* any matrix which is a contraction for $|||\cdot|||$ and leaves $\psi_{\mathcal{S}}$ invariant.

Remark 2.1. In case all couplings between $\mathcal{S}$ and $\mathcal{E}_k$ are absent, $V_k \equiv 0$, $M_k = e^{i\tau_k L_{\mathcal{S}}}$ is unitary and admits 1 as a degenerate eigenvalue.

We will come back on the properties of reduced dynamics operators (RDO's, for short) below. Let us emphasize here that the reduction process to product of RDO's is free from any approximation, so that the set of matrices $\{M_k = P\mathrm{e}^{\mathrm{i}K_k}P\}_{k\in\mathbb{N}}$ encodes the complete dynamics. In particular, we show, using the cyclicity and separability of the reference vectors $\psi_{\mathcal{S}}, \psi_{\mathcal{E}_k}$, that the evolution of any normal state, not only $\langle\psi_0, \cdot\,\psi_0\rangle$, can be understood completely in terms of the product of these RDO's.

We are now in a position to state our main results concerning the asymptotic dynamics of normal states ϱ acting on certain observables O. These result involve a spectral hypothesis which we introduce in the next definition.

Definition 2.2. Let $\mathcal{M}_{(E)}$ denote the set of reduced dynamics operators whose spectrum $\sigma(M)$ satisfies $\sigma(M) \cap \{z \in \mathbb{C} \mid |z| = 1\} = \{1\}$ and 1 is simple eigenvalue.

We shall denote by $P_{1,M}$ the spectral projector of a matrix M corresponding to the eigenvalue 1. As usual, if the eigenvalue 1 is simple, with corresponding normalized eigenvector $\psi_{\mathcal{S}}$, we shall write $P_{1,M} = |\psi_{\mathcal{S}}\rangle\langle\psi|$ for some ψ s.t. $\langle\psi|\psi_{\mathcal{S}}\rangle = 1$.

3. Results

3.1. *Ideal Repeated Interaction Quantum System*

We consider first the case of *Ideal Repeated Interaction Quantum Systems*, characterized by

$$\mathcal{E}_k = \mathcal{E},\ L_{\mathcal{E}_k} = L_{\mathcal{E}},\ V_k = V,\ \tau_k = \tau \quad \text{for all} \quad k \geq 1,$$
$$M_k = M, \quad \text{for all} \quad k \geq 1.$$

Theorem 3.1. *Let α^n be the repeated interaction dynamics determined by one RDO M. Suppose that $M \in \mathcal{M}_{(E)}$ so that $P_{1,M} = |\psi_{\mathcal{S}}\rangle\langle\psi|$. Then, for any $0 < \gamma < \inf_{z\in\sigma(M)\setminus\{1\}}(1-|z|)$, any normal state ϱ, and any $A_{\mathcal{S}} \in \mathfrak{M}_{\mathcal{S}}$,*

$$\varrho\,(\alpha^n(A_{\mathcal{S}})) = \langle\psi, A_{\mathcal{S}}\psi_{\mathcal{S}}\rangle + O(e^{-\gamma n}). \tag{3.1}$$

Remark 3.1. 1. The asymptotic state $\langle\psi|\cdot\psi_{\mathcal{S}}\rangle$ and the exponential decay rate γ are both determined by the spectral properties of the RDO M.

2. On concrete examples, the verification of the spectral assumption on M can be done by rigorous perturbation theory, see Ref. 7. It is reminiscent of a Fermi Golden Rule type condition on the efficiency of the coupling V, see the remark following the definiton of RDO's.

3. Other properties of ideal repeated interaction quantum systems are discussed in Ref. 7 , e.g. continuous time evolution and correlations.

For deterministic systems which are *not* ideal, the quantity $\varrho\,(\alpha^n(A_{\mathcal{S}}))$ keeps fluctuating as n increases, which, in general, forbids convergence, see Proposition 5.3. That's why we resort to ergodic limits in a random setup, as we now explain.

3.2. *Random Repeated Interaction Quantum System*

To allow a description of the effects of fluctuations on the dynamics of repeated interaction quantum systems, we consider the following setup.

Let $\omega \mapsto M(\omega)$ be a random matrix valued variable on $\mathbb{C}^d$ defined on a probability space $(\Omega, \mathcal{F}, \mathrm{p})$. We say that $M(\omega)$ is a *random reduced dynamics operator* (RRDO) if

(i) There exists a norm $|||\cdot|||$ on $\mathbb{C}^d$ such that, for all ω, $M(\omega)$ is a contraction on $\mathbb{C}^d$ for the norm $|||\cdot|||$.
(ii) There exists a vector $\psi_{\mathcal{S}}$, constant in ω, such that $M(\omega)\psi_{\mathcal{S}} = \psi_{\mathcal{S}}$, for all ω.

To an RRDO $\omega \mapsto M(\omega)$ on Ω is naturally associated a iid *random reduced dynamics process* (RRDP)

$$\overline{\omega} \mapsto M(\omega_1)\cdots M(\omega_n), \qquad \overline{\omega} \in \Omega^{\mathbb{N}^*}, \tag{3.2}$$

where we define in a standard fashion a probability measure $\mathrm{d}\mathbb{P}$ on $\Omega^{\mathbb{N}^*}$ by

$$\mathrm{d}\mathbb{P} = \mathbb{P}i_{j\geq 1}\mathrm{d}p_j, \quad \text{where} \quad \mathrm{d}p_j \equiv \mathrm{d}p, \text{ for all } \quad j \in \mathbb{N}^*.$$

We shall write the expectation of any random variable f as $\mathbb{E}[f]$.

Let us denote by $\alpha^n_{\overline{\omega}}$, $\overline{\omega} \in \Omega^{\mathbb{N}^*}$, the process obtained from (1.6), (2.8), where the $M_j = M(\omega_j)$ in (2.8) are iid random matrices. We call $\alpha^n_{\overline{\omega}}$ the random repeated interaction dynamics determined by the RRDO $M(\omega) = P\mathrm{e}^{\mathrm{i}K(\omega)}P$. It is the independence of the successive elements $\mathcal{E}_k$ of the chain $\mathcal{C}$ which motivates the assumption that the process (3.2) be iid.

Theorem 3.2. *Let $\alpha^n_{\overline{\omega}}$ be the random repeated interaction dynamics determined by an RRDO $M(\omega)$. Suppose that $\mathrm{p}(M(\omega) \in \mathcal{M}_{(E)}) > 0$. Then there exists a set $\overline{\Omega} \subset \Omega^{\mathbb{N}^*}$, s.t. $\mathbb{P}(\overline{\Omega}) = 1$, and s.t. for any $\overline{\omega} \in \overline{\Omega}$, any normal state ϱ and any $A_{\mathcal{S}} \in \mathfrak{M}_{\mathcal{S}}$,*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \varrho\left(\alpha^n_{\overline{\omega}}(A_{\mathcal{S}})\right) = \langle \theta, A_{\mathcal{S}}\psi_{\mathcal{S}}\rangle\,, \tag{3.3}$$

where $\theta = P^*_{1,\mathbb{E}[M]}\psi_{\mathcal{S}}$.

Remark 3.2. 1. Our setup allows us to treat systems having various sources of randomness. For example, random interactions or times of interactions, as well as random characteristics of the systems $\mathcal{E}_m$ and $\mathcal{S}$ such as random temperatures and dimensions of the $\mathcal{E}_m$ and of $\mathcal{S}$.

2. The asymptotic state $\langle \theta, \cdot\, \psi_{\mathcal{S}}\rangle$ is again determined by the spectral data of a matrix, the expectation $\mathbb{E}[M]$ of the RRDO $M(\omega)$. Actually, our hypotheses imply that $\mathbb{E}[M]$ belongs to $\mathcal{M}_{(E)}$, see below.

3. The explicit computation of the asymptotic state, in this Theorem and in the previous one, is in general difficult. Nevertheless, they can be reached by rigorous perturbation theory, see the examples in Refs. 7–9.

3.3. *Instantaneous Observables*

There are important physical observables that describe exchange processes between $\mathcal{S}$ and the chain $\mathcal{C}$ and, which, therefore, are not represented by operators that act just on $\mathcal{S}$. To take into account such phenomena, we consider the set of observables defined as follows.

Definition 3.1. The *instantaneous observables* of $\mathcal{S} + \mathcal{C}$ are of the form

$$O = A_{\mathcal{S}} \otimes_{j=-l}^{r} B^{(j)}_m, \tag{3.4}$$

where $A_{\mathcal{S}} \in \mathfrak{M}_{\mathcal{S}}$ and $B^{(j)}_m \in \mathfrak{M}_{\mathcal{E}_{m+j}}$.

Instantaneous observables can be viewed as a train of $l + r + 1$ observables, roughly centered at $\mathcal{E}_m$, which travel along the chain $\mathcal{C}$ with time.

Following the same steps as in Section 2, we arrive at the following expression for the evolution of the state ψ_0 acting on an instantaneous observable O at time m:

$$\langle \psi_0, \alpha^m(O)\psi_0 \rangle = \langle \psi_0, PM_1 \cdots M_{m-l-1} N_m(O) P\psi_0 \rangle \,. \tag{3.5}$$

Here again, P is the orthogonal projection onto $\mathcal{H}_{\mathcal{S}}$, along $\psi_{\mathcal{C}}$. The operator $N_m(O)$ acts on $\mathcal{H}_{\mathcal{S}}$ and has the expression (Proposition 2.4 in Ref. 9)

$$\begin{gathered} N_m(O)\psi_0 = \\ P\mathrm{e}^{\mathrm{i}\tau_{m-l}\widetilde{L}_{m-l}} \cdots \mathrm{e}^{\mathrm{i}\tau_m \widetilde{L}_m}(A_{\mathcal{S}} \otimes_{j=-l}^{r} B_m^{(j)}) \mathrm{e}^{-\mathrm{i}\tau_m \widetilde{L}_m} \cdots \mathrm{e}^{-\mathrm{i}\tau_{m-l}\widetilde{L}_{m-l}} \psi_0. \end{gathered} \tag{3.6}$$

We want to analyze the asymptotics $m \to \infty$ of (3.5), allowing for randomness in the system. We make the following assumptions on the random instantaneous observable:

(R1) The operators M_k are RRDO's, and we write the corresponding iid random matrices $M_k = M(\omega_k)$, $k = 1, 2, \cdots, .$

(R2) The random operator $N_m(O)$ is independent of the M_k with $1 \leq k \leq m-l-1$, and it has the form $N(\omega_{m-l}, \ldots, \omega_{m+r})$, where $N : \Omega^{r+l+1} \to \mathcal{B}(\mathbb{C}^d)$ is an operator valued random variable.

The operator M_k describes the effect of the random k-th interaction on $\mathcal{S}$, as before. The random variable N in (R2) does not depend on the time step m, which is a condition on the observables. It means that the nature of the quantities measured at time m are the same. For instance, the $B_m^{(j)}$ in (3.4) can represent the energy of $\mathcal{E}_{m+j}$, or the part of the interaction energy V_{m+j} belonging to $\mathcal{E}_{m+j}$, etc. Both assumptions are verified in a wide variety of physical systems: we may take random interaction times $\tau_k = \tau(\omega_k)$, random coupling operators $V_k = V(\omega_k)$, random energy levels of the $\mathcal{E}_k$ encoded in $L_{\mathcal{E}_k} = L_{\mathcal{E}}(\omega_k)$, random temperatures $\beta_{\mathcal{E}_k} = \beta_{\mathcal{E}}(\omega_k)$ of the initial states of $\mathcal{E}_k$, and so on.

The expectation value in any normal state of such instantaneous observables reaches an asymptotic value in the ergodic limit given in the next

Theorem 3.3. *Suppose that* $\mathrm{p}(M(\omega) \in \mathcal{M}_{(E)}) \neq 0$. *There exists a set* $\widetilde{\Omega} \subset \Omega^{\mathbb{N}^*}$ *of probability one s.t. for any* $\overline{\omega} \in \widetilde{\Omega}$, *for any instantaneous observable* O, *(3.4), and for any normal initial state* ϱ, *we have*

$$\lim_{\mu \to \infty} \frac{1}{\mu} \sum_{m=1}^{\mu} \varrho\big(\alpha_{\overline{\omega}}^m(O)\big) = \langle \theta, \mathbb{E}[N]\psi_{\mathcal{S}} \rangle \,, \quad \mathbb{E}[N] \in \mathfrak{M}_{\mathcal{S}}. \tag{3.7}$$

Remark 3.3. 1. The asymptotic state in which one computes the expectation (w.r.t the randomness) of N is the same as in Theorem 3.2, with $\theta = P^*_{1,\mathbb{E}[M]}\psi_{\mathcal{S}}$.

2. In case the system is deterministic and ideal, the same result holds, dropping the expectation on the randomness and taking $\theta = \psi$, as in Theorem 3.1, see Ref. 7.

3.4. *Energy and Entropy Fluxes*

Let us consider some macroscopic properties of the asymptotic state. The systems we consider may contain randomness, but we drop the variable $\overline{\omega}$ from the notation.

Since we deal with open systems, we cannot speak about its total energy; however, variations in total energy are often well defined. Using an argument of Ref. 7 one gets a formal expression for the total energy which is constant during all time-intervals $[\tau_{m-1}, \tau_m)$, and which undergoes a jump

$$j(m) := \alpha^m(V_{m+1} - V_m) \tag{3.8}$$

at time step m. Hence, the variation of the total energy between the instants 0 and m is then $\Delta E(m) = \sum_{k=1}^{m} j(k)$. The relative entropy of ϱ with respect to ϱ_0, two normal states on $\mathfrak{M}$, is denoted by $\mathrm{Ent}(\varrho|\varrho_0)$. Our definition of relative entropy differs from that given in Ref. 6 by a sign, so that in our case, $\mathrm{Ent}(\varrho|\varrho_0) \geq 0$. For a thermodynamic interpretation of entropy and its relation to energy, we assume for the next result that $\psi_{\mathcal{S}}$ is a $(\beta_{\mathcal{S}}, \alpha^t_{\mathcal{S}})$–KMS state on $\mathfrak{M}_{\mathcal{S}}$, and that the $\psi_{\mathcal{E}_m}$ are $(\beta_{\mathcal{E}_m}, \alpha^t_{\mathcal{E}_m})$–KMS state on $\mathfrak{M}_{\mathcal{E}_m}$, where $\beta_{\mathcal{S}}$ is the inverse temperature of $\mathcal{S}$, and $\beta_{\mathcal{E}_m}$ are random inverse temperatures of the $\mathcal{E}_m$. Let ϱ_0 be the state on $\mathfrak{M}$ determined by the vector $\psi_0 = \psi_{\mathcal{S}} \otimes \psi_{\mathcal{C}} = \psi_{\mathcal{S}} \bigotimes_m \psi_{\mathcal{E}_m}$. The change of relative entropy is denoted $\Delta S(m) := \mathrm{Ent}(\varrho \circ \alpha^m|\varrho_0) - \mathrm{Ent}(\varrho|\varrho_0)$. This quantity can be expressed in terms of the Liouvillean and interaction operators by means of a formula proved in Ref. 12.

One checks that both the energy variation and the entropy variations can be expressed as instantaneous observables, to which we can apply the results of the previous Section. Defining the asymptotic energy and entropy productions by the limits, if they exist,

$$\lim_{m\to\infty} \varrho\left(\frac{\Delta E(m}{m}\right) =: \mathrm{d}E_+ \quad \text{and} \quad \lim_{m\to\infty} \frac{\Delta S(m)}{m} =: \mathrm{d}S_+,$$

we obtain

Theorem 3.4 (2^{nd} **law of thermodynamics).** *Let ϱ be a normal state on $\mathfrak{M}$. Then*

$$\mathrm{d}E_+ = \big\langle \theta, \mathbb{E}\big[P(L_{\mathcal{S}} + V - \mathrm{e}^{\mathrm{i}\tau L}(L_{\mathcal{S}} + V)\mathrm{e}^{-\mathrm{i}\tau L})P\big]\psi_{\mathcal{S}}\big\rangle \quad a.s.$$
$$\mathrm{d}S_+ = \big\langle \theta, \mathbb{E}\big[\beta_{\mathcal{E}}\, P(L_{\mathcal{S}} + V - \mathrm{e}^{\mathrm{i}\tau L}(L_{\mathcal{S}} + V)\mathrm{e}^{-\mathrm{i}\tau L})P\big]\psi_{\mathcal{S}}\big\rangle \quad a.s.$$

The energy- and entropy productions $\mathrm{d}E_+$ and $\mathrm{d}S_+$ are independent of the initial state ϱ. If $\beta_{\mathcal{E}}$ is deterministic, i.e., $\overline{\omega}$-independent, then the system satisfies the second law of thermodynamics: $\mathrm{d}S_+ = \beta_{\mathcal{E}}\mathrm{d}E_+$.

Remark: There are explicit examples in which the entropy production can be obtained via rigorous perturbation theory and is proven to be strictly positive, a sure sign that the asymptotic state is a NESS, see Ref. 7 .

As motivated by (2.8), the theorems presented in this Sections all rely on the analysis of products of large numbers of (random) RDO's. The rest of this note is devoted to a presentation of some of the key features such products have.

4. Basic Properties of RDO's

Let us start with a result proved in Ref. 7 as Proposition 2.1.

Lemma 4.1. *Under our general assumptions, the set of matrices $\{M_j\}_{j\in\mathbb{N}^*}$ defined in* (2.8) *satisfy $M_j\psi_{\mathcal{S}} = \psi_{\mathcal{S}}$, for all $j \in \mathbb{N}^*$. Moreover, to any $\phi \in \mathcal{H}_{\mathcal{S}}$ there corresponds a unique $A \in \mathfrak{M}_{\mathcal{S}}$ such that $\phi = A\psi_{\mathcal{S}}$. $|||\phi||| := \|A\|_{\mathcal{B}(\mathcal{H}_{\mathcal{S}})}$ defines a norm on $\mathcal{H}_{\mathcal{S}}$, and as operators on $\mathcal{H}_{\mathcal{S}}$ endowed with this norm, the M_j are contractions for any $j \in \mathbb{N}^*$.*

Again, the fact that $\psi_{\mathcal{S}}$ is invariant under M_j is a consequence of (2.5) and their being contractions comes from the unitarity of the quantum evolution together with the finite dimension of $\mathcal{H}_{\mathcal{S}}$.

As a consequence of the equivalence of the norms $\|\cdot\|$ and $|||\cdot|||$, we get

Corollary 4.1. *We have $1 \in \sigma(M_j) \subset \{z \mid |z| = 1\}$ and*

$$\sup\{\|M_{j_n}M_{j_{n-1}}\cdots M_{j_1}\|,\ n \in \mathbb{N}^*,\ j_k \in \mathbb{N}^*\} = C_0 < \infty$$

Actually, if a set of operators satisfies the bound of the Corollary, it is always possible to construct a norm on $\mathbb{C}^d$ relative to which they are contractions, as proven in the next

Lemma 4.2. *Let $R = \{M_j \in M_d(\mathbb{C})\}_{j\in J}$, where J is any set of indices and $C(R) \geq 1$ such that*

$$\|M_{j_1} M_{j_2} \cdots M_{j_n}\| \leq C(R), \quad \textit{forall } \{j_i\}_{i=1,\cdots,n} \in J^n, \textit{ for all } \quad n \in \mathbb{N}. \tag{4.1}$$

Then, there exists a norm $|||\cdot|||$ on $\mathbb{C}^d$, which depends on R, relative to which the elements of R are contractions.

Proof. Let us define $T \subset M_d(\mathbb{C})$ by

$$T = \cup_{n\in\mathbb{N}} \cup_{(j_1,j_2,\cdots j_n)\in J^n} M_{j_1} M_{j_2} \cdots M_{j_n}. \tag{4.2}$$

Obviously $R \subset T$, but the identity matrix $\mathbb{I}$ does not necessarily belong to T. Moreover, the estimate (4.1) still holds if the M_{j_i}'s belong to T instead of R. For any $\varphi \in \mathbb{C}^d$ we set

$$|||\varphi||| = \sup_{M\in T\cup\mathbb{I}} \|M\varphi\| \geq \|\varphi\|, \tag{4.3}$$

which defines a *bona fide* norm. Then, for any vector φ and any element N of T we compute

$$|||N\varphi||| = \sup_{M\in T\cup\mathbb{I}} \|MN\varphi\| \leq \sup_{M\in T\cup\mathbb{I}} \|M\varphi\| = |||\varphi|||, \tag{4.4}$$

from which the result follows. □

Remark 4.1. If there exists a vector ψ_S invariant under all elements of R, it is invariant under all elements of T and satisfies $\|\psi_S\| = |||\psi_S||| = 1$.

5. Deterministic Results

In this section, we derive some algebraic formulae and some uniform bounds for later purposes. Since there is no probabilistic issue involved here, we shall therefore simply denote $M_j = M(\omega_j)$. We are concerned with the product

$$\Psi_n := M_1 \cdots M_n. \tag{5.1}$$

5.1. *Decomposition of the M_j*

With P_{1,M_j} the spectral projection of M_j for the eigenvalue 1 we define

$$\psi_j := P^*_{1,j}\psi_{\mathcal{S}}, \qquad P_j := |\psi_{\mathcal{S}}\rangle\langle\psi_j|. \tag{5.2}$$

Note that $\langle\psi_j|\psi_{\mathcal{S}}\rangle = 1$ so that P_j is a projection and, moreover, $M_j^*\psi_j = \psi_j$. We introduce the following decomposition of M_j

$$M_j := P_j + Q_j M_j Q_j, \quad \text{with} \quad Q_j = \mathbb{1} - P_j. \tag{5.3}$$

We denote the part of M_j in $Q_j\mathbb{C}^d$, by $M_{Q_j} := Q_j M_j Q_j$. It easily follows from these definitions that

$$P_j P_k = P_k, \;\; Q_j Q_k = Q_j, \tag{5.4}$$

$$Q_j P_k = 0, \quad P_k Q_j = P_k - P_j = Q_j - Q_k. \tag{5.5}$$

Remark 5.1. If 1 is a simple eigenvalue, $P_{1,M_j} = P_j$ and (5.3) is a (partial) spectral decomposition of M_j.

Proposition 5.1. *For any n,*

$$\Psi_n = |\psi_{\mathcal{S}}\rangle\langle\theta_n| + M_{Q_1}\cdots M_{Q_n}, \tag{5.6}$$

where

$$\theta_n = \psi_n + M^*_{Q_n}\psi_{n-1} + \cdots + M^*_{Q_n}\cdots M^*_{Q_2}\psi_1 \tag{5.7}$$

$$= M^*_n \cdots M^*_2 \psi_1 \tag{5.8}$$

and where $\langle\psi_{\mathcal{S}}, \theta_n\rangle = 1$.

Proof. Inserting the decomposition (5.3) into (5.1), and using (5.4), (5.5), we have

$$\Psi_n = \sum_{j=1}^{n} P_j M_{Q_{j+1}} \cdots M_{Q_n} + M_{Q_1}\cdots$$

Since $P_j = |\psi_{\mathcal{S}}\rangle\langle\psi_j|$, this proves (5.6) and (5.7). From (5.5), we obtain for any j, k,

$$M_{Q_j} M_{Q_k} = M_{Q_j} M_k = Q_j M_j M_k. \tag{5.9}$$

Hence, $\Psi_n = P_1 M_1 \cdots M_n + Q_1 M_1 \cdots M_n = |\psi_{\mathcal{S}}\rangle\langle M^*_n \cdots M^*_2 \psi_1| + M_{Q_1}\cdots M_{Q_n}$, which proves (5.8). □

5.2. *Uniform Bounds*

The operators M_j, and hence the product Ψ_n, are contractions on $\mathbb{C}^d$ for the norm $|||\cdot|||$. In order to study their asymptotic behaviour, we need some uniform bounds on the $P_j, Q_j, \ldots$ Recall that $\|\psi_{\mathcal{S}}\| = 1$.

Proposition 5.2. *Let C_0 be as in Corollary 4.1. Then, the following bounds hold*

(1) For any $n \in \mathbb{N}^*$, $\|\Psi_n\| \leq C_0$.
(2) For any $j \in \mathbb{N}^*$, $\|P_j\| = \|\psi_j\| \leq C_0$ and $\|Q_j\| \leq 1 + C_0$.
(3) $\sup\{\|M_{Q_{j_n}} M_{Q_{j_{n-1}}} \cdots M_{Q_{j_1}}\|, \; n \in \mathbb{N}^*, \, j_k \in \mathbb{N}^*\} \leq C_0(1 + C_0)$.

(4) For any $n \in \mathbb{N}^*$, $\|\theta_n\| \leq C_0^2$.

Proof. It is based on von Neumann's ergodic Theorem, which states that

$$P_{1,M_j} = \lim_{N\to\infty} \frac{1}{N} \sum_{k=0}^{N-1} M_j^k.$$

The first two estimate easily follow, whereas the third makes use of (5.9) to get $M_{Q_{j_n}} M_{Q_{j_{n-1}}} \cdots M_{Q_{j_1}} = Q_{j_n} M_{j_n} M_{j_{n-1}} \cdots M_{j_1}$, so that

$$\|M_{Q_{j_n}} M_{Q_{j_{n-1}}} \cdots M_{Q_{j_1}}\| \leq \|Q_{j_n}\| C_0 \leq C_0(1 + C_0).$$

Finally, (5.8) and the above estimates yield $\|\theta_n\| \leq C_0 \|\psi_1\| \leq C_0^2$. □

5.3. *Asymptotic Behaviour*

We now turn to the study of the asymptotic behaviour of Ψ_n, starting with the simpler case of *Ideal Repeated Interaction Quantum Systems*.

That means we assume

$$M_k = M, \quad \text{for all} \quad k \geq 1.$$

If 1 is a simple eigenvalue of M, then $P_{1,M} = |\psi_{\mathcal{S}}\rangle\langle\psi|$, for some ψ s.t. $\langle\psi|\psi_{\mathcal{S}}\rangle = 1$, and

$$\Psi_n = M^n = |\psi_{\mathcal{S}}\rangle\langle\psi| + M_Q^n$$

Further, if all other eigenvalues of M belong to the open unit disk, M_Q^n converges exponentially fast to zero as $n \to \infty$.

Consequently, denoting by $\mathrm{spr}(N)$ the spectral radius of $N \in M_d(\mathbb{C})$,

Lemma 5.1. *If the RDO* M *belongs to* $\mathcal{M}_{(E)}$,

$$\Psi_n = |\psi_{\mathcal{S}}\rangle\langle\psi| + O(e^{-\gamma n}),$$

for all $0 < \gamma < 1 - spr(M_Q)$.

Two things are used above, the decay of M_Q^n and the fact that $\theta_n = \psi$ is constant, see (5.6). The following result shows that in general, if one knows *a priori* that the products of M_{Q_j}'s in (5.6) goes to zero, Ψ_n converges if and only if $P_n = |\psi_{\mathcal{S}}\rangle\langle\psi_n|$, does.

Proposition 5.3. *Suppose that* $\lim_{n\to\infty} \sup\{\|M_{Q_{j_n}} \cdots M_{Q_{j_1}}\|, \ j_k \in \mathbb{N}^*\} = 0$. *Then* θ_n *converges if and only if* ψ_n *does. If they exist, these two limits coincide, and thus*

$$\lim_{n\to\infty} \Psi_n = |\psi_{\mathcal{S}}\rangle\langle\psi_\infty|,$$

where $\psi_\infty = \lim_{n\to\infty} \psi_n$. *Moreover,* $|\psi_{\mathcal{S}}\rangle\langle\psi_\infty|$ *is a projection.*

In general, we cannot expect pointwise convergence of the θ_n, but we can consider an ergodic average of θ_n instead. This is natural in terms of dynamical systems, a fluctuating system does not converge.

The previous convergence results relies on the decay of the product of operators M_{Q_j}. Conditions ensuring this are rather strong. However, Theorem 6.1 below shows that in the *random setting*, a similar exponential decay holds under rather weaker assumptions.

6. Random Framework

6.1. *Product of Random Matrices*

We now turn to the random setup in the framework of Section 3.2. For $M(\omega)$ an RRDO, with probability space $(\Omega, \mathcal{F}, \mathrm{p})$, we consider the RRDP on $\Omega^{\mathbb{N}^*}$ given by

$$\Psi_n(\overline{\omega}) := M(\omega_1)\cdots M(\omega_n), \qquad \overline{\omega} \in \Omega^{\mathbb{N}^*}.$$

We show that Ψ_n has a decomposition into an exponentially decaying part and a fluctuating part. Let $P_1(\omega)$ denote the spectral projection of $M(\omega)$ corresponding to the eigenvalue one ($\dim P_1(\omega) \geq 1$), and let $P_1^*(\omega)$ be its adjoint operator. Define

$$\psi(\omega) := P_1(\omega)^* \psi_{\mathcal{S}}, \tag{6.1}$$

and set

$$P(\omega) = |\psi_{\mathcal{S}}\rangle\langle\psi(\omega)|, \quad Q(\omega) = \mathbb{1} - P(\omega).$$

The vector $\psi(\omega)$ is normalized as $\langle\psi_{\mathcal{S}}, \psi(\omega)\rangle = 1$. We decompose $M(\omega)$ as

$$M(\omega) = P(\omega) + Q(\omega)M(\omega)Q(\omega) =: P(\omega) + M_Q(\omega). \tag{6.2}$$

Taking into account this decomposition, we obtain (c.f. Proposition 5.1)

$$\Psi_n(\overline{\omega}) := M(\omega_1)\cdots M(\omega_n) = |\psi_{\mathcal{S}}\rangle\langle\theta_n(\overline{\omega})| + M_Q(\omega_1)\cdots M_Q(\omega_n), \tag{6.3}$$

where $\theta_n(\overline{\omega})$ is the Markov process

$$\begin{aligned}\theta_n(\overline{\omega}) &= M^*(\omega_n)\cdots M^*(\omega_2)\psi(\omega_1) \\ &= \psi(\omega_n) + M_Q^*(\omega_n)\psi(\omega_{n-1}) + \cdots + M_Q^*(\omega_n)\cdots M_Q^*(\omega_2)\psi(\omega_1),\end{aligned} \tag{6.4}$$

a $M^*(\omega_j)$ being the adjoint operator of $M(\omega_j)$. We analyze the two parts in the r.h.s. of (6.3) separately.

Theorem 6.1 (Decaying process). *Let $M(\omega)$ be a random reduced dynamics operator. Suppose that* $\mathrm{p}(M(\omega) \in \mathcal{M}_{(E)}) > 0$. *Then there exist a set $\Omega_1 \subset \Omega^{\mathbb{N}^*}$ and constants $C, \alpha > 0$ s.t. $\mathbb{P}(\Omega_1) = 1$ and s.t. for any $\overline{\omega} \in \Omega_1$, there exists a random variable $n_0(\omega)$ s.t. for any $n \geq n_0(\overline{\omega})$,*

$$\|M_Q(\omega_1) \cdots M_Q(\omega_n)\| \leq C\mathrm{e}^{-\alpha n}, \tag{6.5}$$

and $\mathbb{E}[e^{\alpha n_0}] < \infty$. Moreover, $\mathbb{E}[M] \in \mathcal{M}_{(E)}$.

Remark 6.1. 1. The sole condition of M having an arbitrarily small, non-vanishing probability to be in $\mathcal{M}_{(E)}$ suffices to guarantee the exponential decay of the product in (6.5) and that $\mathbb{E}[M]$ belongs to $\mathcal{M}_{(E)}$.

2. Actually, $\mathbb{E}[M] \in \mathcal{M}_{(E)}$ is a consequence of $\mathrm{spr}(\mathbb{E}[M_Q]) < 1$, which comes as a by product of the proof of Theorem 6.1. From the identities

$$\mathbb{E}[M] = |\psi_{\mathcal{S}}\rangle\langle\mathbb{E}[\psi]| + \mathbb{E}[M_Q], \quad \langle\mathbb{E}[\psi]|\psi_{\mathcal{S}}\rangle = 1, \quad \mathbb{E}[M_Q]\psi_{\mathcal{S}} = 0, \tag{6.6}$$

which *do not* correspond to a (partial) spectral decomposition of $\mathbb{E}[M]$, and this estimate, we get

$$\begin{aligned}\mathbb{E}[M]^n = |\psi_{\mathcal{S}}\rangle\langle\, \mathbb{E}[\psi] + \mathbb{E}[M_Q]^*\mathbb{E}[\psi] + \cdots + \mathbb{E}[M_Q]^{*n-1}\mathbb{E}[\psi] \,| + \mathbb{E}[M_Q]^{*n} \\ \stackrel{n\to\infty}{\longrightarrow} |\psi_{\mathcal{S}}\rangle\langle(\mathbb{I} - \mathbb{E}[M_Q]^*)^{-1}\mathbb{E}[\psi]| \equiv P_{1,\mathbb{E}[M]}.\end{aligned} \tag{6.7}$$

3. Our choice (6.1) makes $\psi(\omega)$ an eigenvector of $M^*(\omega)$. Other choices of (measurable) $\psi(\omega)$ which are bounded in ω lead to different decompositions of $M(\omega)$, and can be useful as well. In particular, if $M(\omega)$ is a bistochastic matrix, $\psi(\omega)$ can be chosen as an $M^*(\omega)$-invariant vector which is independent of ω.

6.2. *A Law of Large Numbers*

We now turn to the asymptotics of the Markov process (6.5).

Theorem 6.2 (Fluctuating process). *Let $M(\omega)$ be a random reduced dynamics operator s.t. that* $\mathrm{p}(M(\omega) \in \mathcal{M}_{(E)}) > 0$. *There exists a set $\Omega_2 \subset \Omega^{\mathbb{N}^*}$ s.t. $\mathbb{P}(\Omega_2) = 1$ and, for all $\overline{\omega} \in \Omega_2$,*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \theta_n(\overline{\omega}) = \theta, \tag{6.8}$$

where

$$\theta = \lim_{n\to\infty} \mathbb{E}[\theta_n] = P^*_{1,\mathbb{E}[M]}\mathbb{E}[\psi] = P^*_{1,\mathbb{E}[M]}\psi_{\mathcal{S}}. \tag{6.9}$$

Remark 6.2. 1. The ergodic average limit of $\theta_n(\overline{\omega})$ does not depend on the particular choice of $\psi(\omega)$. This follows from the last equality in (6.9).

2. The second equality in (6.9) stems from

$$\mathbb{E}[\theta_n] = \sum_{k=0}^{n-1} (\mathbb{E}[M_Q])^k \mathbb{E}[\psi],$$

by independence, and which converges to $P^*_{1,\mathbb{E}[M]}\mathbb{E}[\psi]$ by (6.7). The third equality follows from (6.6).

3. Comments on the proof of these Theorems are provided below.

Combining Theorems 6.1 and 6.2 we immediately get the following result.

Theorem 6.3 (Ergodic theorem for RRDP). *Let $M(\omega)$ be a random reduced dynamics operator. Suppose* $\mathrm{p}(M(\omega) \in \mathcal{M}_{(E)}) > 0$. *Then there exists a set $\Omega_3 \subset \Omega^{\mathbb{N}^*}$ s.t. $\mathbb{P}(\Omega_3) = 1$ and, for all $\overline{\omega} \in \Omega_3$,*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} M(\omega_1) \cdots M(\omega_n) = |\psi_{\mathcal{S}}\rangle\langle\theta| = P_{1,\mathbb{E}[M]}. \tag{6.10}$$

Remark 6.3. 1. If one can choose $\psi(\omega) \equiv \psi$ to be independent of ω, then we have by (5.8) that $\theta_n(\overline{\omega}) = \psi$, for all $n, \overline{\omega}$. Thus, from (6.3)-(6.5), we get the stronger result $\lim_{n\to\infty} M(\omega_1) \cdots M(\omega_n) = |\psi_{\mathcal{S}}\rangle\langle\psi|$, a.s., exponentially fast.

2. This result can be viewed as a strong law of large numbers for the matrix valued process $\Psi_n(\overline{\omega}) = M(\omega_1) \cdots M(\omega_n)$.

Comments. The existence of (ergodic) limits of products of random operators is known for a long time and under very general conditions, see e.g., Refs. 5,13 . However, the explicit value of the limit depends on the detailed properties of the set of random matrices considered. The point of our analysis is thus the explicit determination of the limit (6.10) which is crucial for the applications to the dynamics of random repeated interaction quantum systems.

The more difficult part of this task is to prove Theorem 6.1. The idea consists in identifying matrices in the product $\Psi_n(\overline{\omega})$ which are equal (or close) to a fixed matrix M that belongs to $\mathcal{M}_{(E)}$. Consecutive products of M give an exponential decay, whereas products of other matrices are uniformly bounded. Then one shows that the density of long strings of consecutive M's in a typical sample is finite. Once this is done, a self-contained proof of Theorem 6.3, is not very hard to get[8] .

On the other hand, given Theorem 6.1 and the existence result of Ref.,[5] we can deduce Theorem 6.3 as follows. Let us state the result of Beck and Schwarz in our setup. Let T denote the usual shift operator on $\Omega^{\mathbb{N}^*}$ defined by $(T\overline{\omega})_j = \overline{\omega}_{j+1}$, $j = 1, 2, \cdots$.

Theorem 6.4 (Beck and Schwartz[5]). *Let $M(\omega)$ be a random reduced dynamics operator on Ω. Then there exists a matrix valued random variable $L(\overline{\omega})$ on $\Omega^{\mathbb{N}^*}$, s.t. $\mathbb{E}[\|L\|] < \infty$, which satisfies almost surely*

$$ginequation L(\overline{\omega}) = M(\omega_1)L(T\overline{\omega}), \tag{6.11}$$

where T is the shift operator, and

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} M(\omega_1) \cdots M(\omega_n) = L(\overline{\omega}). \tag{6.12}$$

Further assuming the hypotheses of Theorem 6.1, and making use of the decomposition (6.3), we get that L can be written as

$$L(\overline{\omega}) = |\Psi_{\mathcal{S}}\rangle\langle\theta(\overline{\omega})|,$$

for some random vector $\theta(\overline{\omega})$. Now, due to (6.11) and the fact that $\psi_{\mathcal{S}}$ is invariant, $\theta(\overline{\omega})$ satisfies

$$\theta(\overline{\omega}) = \theta(T\overline{\omega}) \quad \text{a.s.}$$

The shift being ergodic, we deduce that θ is constant a.s., so that

$$\theta(\overline{\omega}) = \mathbb{E}[\theta] \quad \text{a.s.}$$

which, in turn, thanks to Proposition 5.2 and Lebesgue dominated convergence Theorem, allows to get from (6.5)

$$\mathbb{E}[\theta] = \lim_{n\to\infty} \mathbb{E}[\theta_n] = P^*_{1,\mathbb{E}[M]}\Psi_{\mathcal{S}}.$$

6.3. *Limit in Law and Lyapunov Exponents*

We present here results for products "in reverse order" of the form $\Phi_n(\overline{\omega}) := M(\omega_n)\cdots M(\omega_1)$, which have the same law as $\Psi_n(\overline{\omega})$. They also yield information about the Lyapunov exponent of the process. The following results are standard, see e.g. Ref.1 . The limits

$$\Lambda_\Phi(\overline{\omega}) = \lim_{n\to\infty} (\Phi_n(\overline{\omega})^*\Phi_n(\overline{\omega}))^{1/2n} \quad \text{and} \quad \Lambda_\Psi(\overline{\omega}) = \lim_{n\to\infty} (\Psi_n(\overline{\omega})^*\Psi_n(\overline{\omega}))^{1/2n}$$

exist almost surely, the top Lyapunov exponent $\gamma_1(\overline{\omega})$ of $\Lambda_\Phi(\overline{\omega})$ coincides with that of $\Lambda_\Psi(\overline{\omega})$, it is constant a.s., and so is its multiplicity. It is in general difficult to prove that the multiplicity of $\gamma_1(\overline{\omega})$ is 1.

Theorem 6.5. *Suppose* $\mathrm{p}(M(\omega) \in \mathcal{M}_{(E)}) > 0$. *Then there exist* $\alpha > 0$, *a random vector*

$$\eta_\infty(\overline{\omega}) = \lim_{n\to\infty} \psi(\omega_1) + M_Q^*(\omega_1)\psi(\omega_2) + \cdots + M_Q^*(\omega_1)\cdots M_Q^*(\omega_{n-1})\psi(\omega_n)$$

and $\Omega_4 \subset \Omega^{\mathbb{N}^*}$ *with* $\mathbb{P}(\Omega_4) = 1$ *such that for any* $\overline{\omega} \in \Omega_4$ *and* $n \in \mathbb{N}^*$

$$\textit{ginequation}\left\|\Phi_n(\overline{\omega}) - |\psi_{\mathcal{S}}\rangle\langle\eta_\infty(\overline{\omega})|\right\| \leq C_{\overline{\omega}} e^{-\alpha n}, \quad \textit{for some} \quad C_{\overline{\omega}}. \tag{6.13}$$

As a consequence, for any $\overline{\omega} \in \Omega_4$, $\gamma_1(\overline{\omega})$ *is of multiplicity one.*

Comments. While the Theorems above on the convergence of asymptotic states give us the comfortable feeling provided by almost sure results, it is an important aspect of the theory to understand the fluctuations around the asymptotic state the system reaches almost surely. In our iid setup, the law of the product $\Psi_n(\overline{\omega})$ of RRDO's coincides with the law of $\Phi_n(\overline{\omega})$ which converges exponentially fast to $|\psi_{\mathcal{S}}\rangle\langle\eta_\infty(\overline{\omega})|$. Therefore, the fluctuations are encoded in the law of the random vector $\eta_\infty(\overline{\omega})$. It turns out it is quite difficult, in general, to get informations about this law. There are partial results only about certain aspects of the law of such random vectors in case they are obtained by means of matrices belonging to some subgroups of $Gl_d(\mathbb{R})$ satisfying certain irreducibility conditions, see e.g. Ref. 10. However, these results do not apply to our RRDO's.

6.4. *Generalization*

A generalization of the analysis performed for observables acting on $\mathcal{S}$ only described above allows to establish the following corresponding results when instantaneous observables are considered.

The asymptotics of the dynamics (3.5), in the random case, is encoded in the product

$$M(\omega_1)\cdots M(\omega_{m-l-1})N(\omega_{m-l},\ldots,\omega_{m+r}),$$

where $N : \Omega^{r+l+1} \to M_d(\mathbb{C})$ is given in assumption (R2).

Theorem 6.6 (Ergodic limit of infinite operator product). *Assume* $M(\omega)$ *is a RRDO and (R2) is satisfied. Suppose that* $\mathrm{p}(M(\omega) \in \mathcal{M}_{(E)}) \neq 0$. *Then* $\mathbb{E}[M] \in \mathcal{M}_{(E)}$. *Moreover, there exists a set* $\Omega_5 \subset \Omega^{\mathbb{N}^*}$ *of probability one s.t. for any* $\overline{\omega} = (\omega_n)_{n\in\mathbb{N}} \in \Omega_5$,

$$\lim_{\nu\to\infty} \frac{1}{\nu} \sum_{n=1}^{\nu} M(\omega_1)\cdots M(\omega_n)N(\omega_{n+1},\ldots,\omega_{n+l+r+1}) = |\psi_{\mathcal{S}}\rangle\langle\theta|\ \mathbb{E}[N],$$

where $\theta = P^*_{1,\mathbb{E}[M]}\psi_{\mathcal{S}}$.

As in the previous Section, a density argument based on the cyclicity and separability of the reference vector ψ_0 allows to obtain from Theorem 6.6 the asymptotic state for all normal initial states ϱ on $\mathfrak{M}$ given as Theorem 3.3

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THE MATHEMATICAL MODEL OF SCATTERING IN STEPWISE WAVEGUIDES

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We consider the mathematical model of the interface of two homogeneous waveguides. This model includes, as particular cases, most types of the acoustic, electrodynamic and quantum waveguide interfaces. We give an accurate mathematical construction of the most important object in the waveguide interface theory — the scattering operator — and discuss its most general properties.

Keywords: inhomogeneous waveguide, scattering in waveguide

1. Introduction

The problem of modes transformation in inhomogeneous waveguides has very long history, and a long list of publications in physics and mathematics was devoted to this problem during the last century. There exist now a lot of approximate methods to solve these problems analytically and numerically and, moreover, the commercial soft for such problems (see, e.g., Refs. 10,11). Nevertheless, the well-known and widely used term "scattering matrix" (see, e.g., Ref. 5) seems to be not yet mathematically well-defined in the waveguide problems, and, accordingly, the mathematical properties of the scattering operator of a waveguide (in any sense) are not well described. Such description is, however, necessary to understand the processes in the quantum, electrodynamic and acoustic waveguides, and, in particular, to develop good numerical algorithms for waveguide simulation.

Here we consider a mathematical model of the stepwise waveguide and demonstrate that the investigation of this model is, essentially, a problem of the theory of the self-adjoint extensions of the symmetric operators in the

Hilbert spaces. In such approach, the scattering operator appears naturally when the resolvent of the self-adjoint extension of some symmetric operator is calculated, and hence the scattering operator is, from the very beginning, the operator in an appropriate Hilbert space, namely, the deficiency space of the initial symmetric operator. This allows us to investigate the properties of the "scattering matrix" within the operator theory.

In addition to a construction of the scattering operator, we obtain in this way a description of some of its important properties. Some of them seem to be rather unexpected, as, for example, the fact that this operator may be, in general, unbounded in the Hilbert space of the sequences of mode amplitudes with the usual inner product. It is also interesting that, under some conditions, the scattering operator may be approximated (in some well-defined sense) by finite-dimensional operators which are scattering operators for appropriate "finite dimensional waveguides". This approximation preserves most of important properties of such operators, such as the flow conservation law, and can be used to numerical calculation of the scattering matrix for various types of waveguides.

Our work is mainly devoted to the simplest of problems mentioned above — the problem of mode transformation at the " interface" of two homogeneous waveguides. In this case, the field in each homogeneous part of waveguide may be represented as the superposition of the corresponding eigenwaves with coefficients depending on the longitudinal coordinate. From this point of view, the scattering operator in this case maps the vector of in-wave amplitudes to the vector of out-wave amplitudes. For such consideration, one must have a precise definition of what in- and out-waves are. If, as is the case in some problems of quantum mechanics, the number of eigenwaves in both waveguides is finite, it is not so difficult to explain what they are, and hence what the scattering operator is: It is simply a matrix of finite size. The situation becomes dramatically complicated in the infinite dimensional case which appears in most physical problems, such as acoustic or electrodynamic waveguides, quantum wires and so on. In such cases, the in- and out- waves belong to the infinite dimensional space which has not, as a rule, any natural structure of a Hilbert space. So, the scattering operator must be considered as the operator in the infinite dimensional space of quite complicated nature.

It is not that difficult to write the formal algebraic expression for the scattering operator in terms of the boundary conditions at the waveguide interface, and different kinds of such expressions appear in a number of books and papers, see, e.g., ref. 6. In the finite dimensional case, these ex-

pressions can be used for analytic, as well as numerical, investigation of mode transformation, although, if the dimension of the "transversal space" is large enough, this investigation may be not that simple. To do this formal expression valid in the infinite dimensional case, one must, however, investigate in some detail certain analytic properties of the operators entering in this expression, and we do this for our model.

2. A Mathematical Model of the Stepwise Waveguide

2.1. *An Abstract Homogeneous Waveguide*

For a mathematical model of a homogeneous waveguide, let us consider an infinite dimensional Hilbert space H and the self-adjoint negative operator $\hat{A}$ with compact resolvent in this space. We say that any essentially self-adjoint operator of the form

$$W = I_H \otimes \frac{d^2}{dz^2} \; + \; \hat{A} \otimes I_{L_2} \tag{2.1}$$

in the Hilbert space $H \otimes L_2(\mathbb{R})$ with the domain $D(\hat{A}) \otimes C_0^\infty(\mathbb{R})$ is a *waveguide*.

For any non-real point $\lambda \in \mathbb{C}$, the resolvent of the operator (2.1) is of the form

$$(R_W(\lambda)f)(z) = -\frac{1}{2}\int\limits_{\infty}^{\infty} d\zeta B(\lambda)^{-1} e^{-|z-\zeta|B(\lambda)} f(\zeta), \tag{2.2}$$

where $B(\lambda) = (\lambda - A)^{1/2}$ and for the branch of the square root we take $\mathrm{Re}\sqrt{\mu} > 0$ for any $\mu \in \mathbb{C}$ such that $\mathrm{Im}\mu \neq 0$. It is easy to see that (2.2) is a bounded operator in the space $H \otimes L_2(\mathbb{R})$. Further, for any real $-\omega^2 \notin \mathrm{spec}A$, there exist limit operators $R_W(-\omega^2 \pm i0)$ defined on a dense set; they map the domain $H \otimes C_0^\infty(\mathbb{R})$ into the space

$$\begin{gathered} (H \otimes L_2(\mathbb{R})) \oplus \\ \left(\bigoplus_{-\omega_k^2 \in \mathrm{spec}A,\ \omega_k^2 < \omega^2} V_k \otimes [e^{\pm i|z|\sqrt{\omega^2 - \omega_k^2}}] \right), \end{gathered} \tag{2.3}$$

where V_k is the eigenspace of the operator A corresponding to the eigenvalue $-\omega_k^2$, and in the last tensor product, $[e^{\pm i|z|\sqrt{\omega^2-\omega_k^2}}]$ is the one-dimensional space spanned by the function in square brackets. The last direct sum in (2.3) represents what is usually called the *in-* or *out-space*, depending on the sign.

This approach to the definition of the scattering states, instead of using the "radiation conditions",[3] rather complicated in the waveguide problems, is known as "limiting amplitude principle".[9] The passage to the limit of the resolvent of the stepwise waveguide and the corresponding scattering operator at the real values of spectral parameter does not contain any essential obstacles, so we will not consider this limit in what follows.

2.2. *The Abstract Stepwise Waveguide*

Let now consider two Hilbert spaces $H_\pm$ and two negative self-adjoint operators $A_\pm$ with compact resolvents in these spaces. Let further consider the Hilbert space and the dense domain in it:

$$\mathcal{L} = (H_+ \otimes L_2(\mathbb{R}_+)) \oplus (H_- \otimes L_2(\mathbb{R}_-)),$$
$$\mathcal{D}_0 = (H_+ \otimes C_0^\infty(\mathbb{R}_+)) \oplus (H_- \otimes C_0^\infty(\mathbb{R}_-)).$$

The operator

$$W_0 = \left(I_{H_+} \otimes \frac{d^2}{dz^2} + A_+ \otimes I_{L_2(\mathbb{R}_+)}\right) \oplus \left(I_{H_-} \otimes \frac{d^2}{dz^2} + A_- \otimes I_{L_2(\mathbb{R}_-)}\right) \tag{2.4}$$

is symmetric, but not self-adjoint on this domain. In what follows any self-adjoint extension of the operator (2.4) is said to be a *stepwise waveguide*. We will see that self-adjoint extensions of this operator are parameterized by the operator we refer to as a *scattering operator* in the stepwise waveguide.

3. The Scattering Operator

3.1. *The Self-adjoint Extensions of the Operator W_0*

To describe the self-adjoint extensions of the operator (2.4), we will follow the von Neumann approach.[1] We need first to describe the deficiency spaces, i.e., the kernels of the adjoint operators $W_0^* \pm i$. To do this, we need to find all solution in the space $\mathcal{L}$ of the equation

$$W_0^* u = \pm i u \ . \tag{3.1}$$

It is easy to see that these solutions are of the form

$$u^\pm(z) = \begin{cases} e^{-B_+(\pm i)z} v_+ & \text{if } z > 0, \\ e^{B_-(\pm i)z} v_- & \text{if } z < 0, \end{cases} \tag{3.2}$$

where $B_\pm(\lambda) = (\lambda - A_\pm)^{1/2}$ and $v_\pm$ are the right and left "limit values" of the function $u(z)$, respectively; for details, see subsection 2.1. For the

function $u(z)$ to belong to $\mathcal{L}$, these values must lie in the spaces $H_A^{\pm}$ which are the augmentations of the spaces $H_{\pm}$ with respect the norms

$$\|v\|_A^{\pm} = \|X_{\pm}^{-1} v\|_{H_{\pm}}. \tag{3.3}$$

The self-adjoint positive operators $X_{\pm}$ in (3.3) are defined as

$$X_{\pm} = (B_{\pm}(i) + B_{\pm}(-i))^{1/2},$$

and hence are the operators with compact resolvent. Hence, the deficiency spaces $\mathcal{N}_{\pm}$ are isomorphic to the space

$$H_A = H_A^+ \oplus H_A^- \ . \tag{3.4}$$

(Note that the extensions of the operators $e^{\mp B_{\pm}(\lambda)z} : \ H_{\pm} \longrightarrow H_{\pm} \otimes L_2(\mathbb{R})_{\pm}$ to the map $H_A^{\pm} \longrightarrow H_{\pm} \otimes L_2(\mathbb{R})_{\pm}$ are natural and these extensions give unitary isomorphisms desired. The inverse operators are given by the maps

$$u \mapsto \underset{z \longrightarrow \pm 0}{H_A \lim} u(z),$$

where hereafter $H_A \lim$ denotes a limit in H_A. The fact that the deficiency spaces do not coincide with the "transverse" space of the waveguide has a physical interpretation: It is well-known that the field may have singularities on the waveguide interface.

Any unitary operator V in the space H_A defines a unitary operator $\mathcal{N}_+ \longrightarrow \mathcal{N}_-$ given by

$$\left(e^{-B_+(i)z} \oplus e^{-B_-(i)z}\right) v \longmapsto \left(e^{-B_+(-i)z} \oplus e^{-B_-(-i)z}\right) Vv \ . \tag{3.5}$$

Hence, the set of the unitary operators in the space H_A parameterizes the set of self-adjoint extensions of the operator (2.4). We designate W_V the extension corresponding to a given unitary operator V. So, the interface of two homogeneous waveguides can be described by such an operator.

3.2. *The Self-adjoint Extensions and the Boundary Conditions*

Physicists like to describe the waveguide interface through "boundary conditions", i.e., some linear relations between the values of the function $u(z)$ and its first derivatives at the interface.[3] We now show how such conditions follow from the definition of the operator W_V. Note, however, that not *all* possible extensions can be obtained in such a way. Indeed, due to von Neumann's theory, the domain of this operator consists of elements of the form

$u_0 \oplus \tilde{u} \oplus V\tilde{u}$, where $u_0 \in \mathcal{D}_0$ and $\tilde{u} \in \mathcal{N}_+$. It follows from this relation that

$$\begin{aligned} H_A^{\pm} \lim_{z \to \pm 0} u(z) &= (I+V)\,\tilde{v}, \\ H_A^{\pm} \lim_{z \to \pm 0} u'(z) &= -\left(B(i) + B(-i)V\right) J\tilde{v}, \end{aligned} \tag{3.6}$$

where $\tilde{v} = \begin{pmatrix} v_+ \\ v_- \end{pmatrix} \in H_A = H_A^+ \oplus H_A^-$ is the vector of "limit values" of the function $\tilde{u}$ and where the operators $B(\pm i)$ in the space H_A are defined as $B(\pm i) = B_+(\pm i) \oplus B_-(\pm i)$. Hence, if both the operators in the right hand side of the equations (3.6) are invertible, we obtain the relation

$$Q_0 u(0) + Q_1 u'(0) = 0, \tag{3.7}$$

where the operators Q_0, Q_1 in the space H_A are defined in terms of the operator V as follows:

$$\begin{aligned} Q_0 &= (I+V)^{-1}, \\ Q_1 &= \left(B(i) + B(-i)\,V\right)^{-1} J, \end{aligned} \tag{3.8}$$

and operator J in the space $H_A = H_A^+ \oplus H_A^-$ is defined as $J = I_+ \oplus (-I_-)$. Note that these operators may be unbounded not only in H, but even in H_A.

As an example, let us consider the waveguide such that $H_+ = H_-$ and $A_+ = A_-$. Let further the boundary conditions be the continuity conditions of the function $u(z)$ and its z-derivative at $z = 0$. So, this waveguide is exactly an homogeneous waveguide. The corresponding unitary operator V is of the form

$$\begin{aligned} V_{++} = V_{--} &= -\tfrac{1}{2} B\,(-i)^{-1} X^2, \\ V_{-+} = V_{+-} &= -2iB\,(-i)^{-1} X^{-2}. \end{aligned}$$

3.3. *The Resolvent of the Operator W_V and the Scattering Operator*

We now calculate the resolvent of the waveguide operator and show how the scattering operator appears in a natural way. To do this, we need to find in $D(W_V)$ the solution for u of the equation

$$W_V u - \lambda u = f, \quad \text{where } f \in \mathcal{L} \text{ and } \mathrm{Im}\lambda \neq 0.$$

The general solution of this equation has the form

$$u\,(z) = -\frac{1}{2} B_{\pm}^{-1}\,(\lambda) \int_0^{\infty} e^{-||z|-\zeta|B_{\pm}(\lambda)} f\,(\pm\zeta)\,d\zeta + e^{-|z|B_{\pm}(\lambda)} u_{\pm},$$

where we take all + for $z > 0$ and all − for $z < 0$. The vectors $u_\pm \in H_A^\pm$ in these formulas are the constants of integration. To satisfy the conditions (3.6), we must choose these constants (i.e., the vector $u = u_+ \oplus u_-$) as follows. Let us consider the vectors

$$F_\pm = -\frac{1}{2} B_\pm^{-1}(\lambda) \int_0^\infty e^{\mp \zeta B_\pm(\lambda)} f(\pm\zeta)\, d\zeta \ . \tag{3.9}$$

One can see that these vectors, same as the vectors $B_\pm(\lambda)F_\pm$, belong to the spaces $H'_{A_\pm} = \{\varphi \in H_\pm \ \ \|X\varphi\| < \infty\}$. Let us now consider the system of equations (for a constant u and a vector $\tilde{v} \in H_A$) of the form

$$\begin{aligned} &F + u = (I + V)\,\tilde{v}, \\ &B(\lambda)\,(F - u) = -\,(B(i) + B(-i)V)\,\tilde{v}. \end{aligned} \tag{3.10}$$

This system is a direct consequence of the conditions (3.6). Formally, the solution (for u) of the system (3.10) can be expressed as

$$\begin{aligned} u &= 2\,(I + V)\,(B(\lambda) - B(i) + (B(\lambda) - B(-i))\,V)^{-1}\,B(\lambda)F - F \\ &\equiv S_V(\lambda)F \ . \end{aligned} \tag{3.11}$$

If the inverse operator in (3.11) exists, the operator $S_V(\lambda) : H'_A \mapsto H_A$, defined in this relation, is said to be a *scattering operator* for the stepwise waveguide W_V. In terms of the scattering operator the resolvent of the operator W_V is expressed as follows:

$$\begin{aligned} &u(z) \equiv (R_{W_V}(\lambda)f)(z) = \\ &-\tfrac{1}{2} B_\varepsilon^{-1}(\lambda) \int_0^\infty e^{-|\varepsilon z - \zeta| B_\varepsilon(\lambda)} f(\varepsilon\zeta)\, d\zeta + \\ &e^{-\varepsilon z B_\varepsilon(\lambda)} (S_V(\lambda)F)_\varepsilon, \quad \text{where } \varepsilon = \operatorname{sign}(z). \end{aligned} \tag{3.12}$$

We show now that the operator $S_V(\lambda) : H'_A \mapsto H_A$ exists and bounded. First, note that for $\operatorname{Im}\lambda > 0$, the operator $(B(\lambda) - B(-i))^{-1}$ is a bounded operator $H'_A \longrightarrow H_A$. This assertion is equivalent to the boundedness of the the operator $X^{-2}\,(B(\lambda) - B(-i))^{-1}$ in H, which follows from the obvious numerical inequality of the form

$$\sup_{q>0} \left| \frac{1}{(\sqrt{q+i} + \sqrt{q-i})(\sqrt{q+\lambda} - \sqrt{q-i})} \right| < \infty.$$

To prove the desired property of the scattering operator, it suffices now to prove that the operator $(B(\lambda) - B(-i))^{-1}\,(B(\lambda) - B(i)) + V$ has a bounded inverse in H_A. This fact follows form the inequality

$$\|\,(B(\lambda) - B(-i))^{-1}\,(B(\lambda) - B(i))\,\| = b(\lambda) < 1. \tag{3.13}$$

(Hereafter we consider all operators as operators in H_A and use the corresponding norms.) Indeed, if so, than for any $\varphi \in H_A$, one has

$$\begin{gathered} \left\| \left(\left(B(\lambda) - B(-i)\right)^{-1} \left(B(\lambda) - B(i)\right) + V \right) \varphi \right\| \geq \\ \|V\varphi\| - \| \left(B(\lambda) - B(-i)\right)^{-1} \left(B(\lambda) - B(i)\right) \varphi \| \geq \\ \|\varphi\| - b(\lambda)\|\varphi\| = (1 - b(\lambda)) \, \|\varphi\|, \end{gathered} \tag{3.14}$$

and hence the operator $\left(B(\lambda) - B(-i)\right)^{-1} \left(B(\lambda) - B(i)\right) + V$ has the bounded inverse. The inequality (3.13) follows from another numerical inequality of the form

$$\sup_{q>0} \left| \frac{\sqrt{q+\lambda} - \sqrt{q+i}}{\sqrt{q+\lambda} - \sqrt{q-i}} \right| = b(\lambda) < 1. \tag{3.15}$$

This is simple and we omit the proof. The case $\mathrm{Im}\lambda < 0$ can be considered by a similar way.

The boundedness of the scattering operator as the operator from H'_A to H_A seems to be a too weak assertion. But we show in what follows that it may be unbounded in H, and this fact seems to be rather unexpected from the physical point of view; we do not understand at the moment its physical consequences.

It is important to note that the constant $b(\lambda)$ in the estimate (3.13) does not depend on the operator V, but only on the spectra of the operators $A_\pm$. We use this fact in what follows to prove the existence of the finite dimensional approximations of the scattering operator.

4. The General Properties of the Scattering Operator

4.1. *On The Finite Dimensional Approximation of the Operators in the Hilbert Space*

In this section, we briefly discuss the main general notions concerned with the finite dimensional approximations of the operators in Hilbert spaces.[8]

Let H be an infinite dimensional Hilbert space and

$$\{H_n, \; T_n : H \longrightarrow H_n \mid n \in \mathbb{N}\}$$

a sequence of finite dimensional Hilbert spaces and linear surjections. We say that this sequence *approximates* the space H if the maps T_n are defined on some dense linear manifold $\mathcal{M} \subset H$ and, for each $x \in \mathcal{M}$, we have

$$\lim_{n\to\infty} \|T_n x\|_{H_n} = \|x\|_H \; .$$

Let further $A: H \to H$ be a linear operator such that $A\mathcal{M} \subset \mathcal{M}$ and $A_n: H_n \to H_n$ a sequence of linear maps. We say that this sequence *approximates* the operator A if, for each $x \in \mathcal{M}$, we have

$$\lim_{n\to\infty} \|T_n A x - A_n T_n x\|_{H_n} = 0 \ .$$

Such definitions of approximation of linear spaces and operators are widely used in Numerical Analysis.

The following properties of approximations used bellow are evident:

(i) If the operators A_n are uniformly bounded, then the operator A is bounded.

(ii) If the sequences A_n and B_n approximate the operators A and B and the sequence A_n is uniformly bounded, then the sequence $A_n B_n$ approximates the operator AB.

(iii) If the operator A^{-1} exists and is bounded, the sequence A_n approximates the operator A, and the operators A_n^{-1} exist and are uniformly bounded, then the sequence A_n^{-1} approximates the operator A^{-1}.

The example which we use below is as follows. Let A be a positive operator in H with compact resolvent, P_n the projection onto the linear span of the eigenvectors of A corresponding to the eigenvalues λ, where $\lambda < n$. Let $H_n = P_n H$, $T_n = P_n$,$A_n = A|_{H_n}$ and $\mathcal{M}$ be the set of vectors in H with finite spectral decompositions. Then the pairs (H_n, A_n) approximate (H, A).

4.2. *The Approximation of the Scattering Operator*

There exists a very limited number of physically interesting examples of the stepwise waveguides for which the scattering operator can be investigated analytically and most of these examples are finite dimensional. To calculate the scattering operator in the infinite dimensional case, a numerical procedure is usually needed. Such procedures are always based on some finite dimensional approximation of the original problem. The question of the convergence of such numerical procedures is the key question for the successful calculation and, as a rule, this question appears to be very complicated.

We show that, under certain conditions, a scattering operator for a given infinite dimensional step-wise waveguide can be approximated, in the above sense, by appropriate finite dimensional waveguides.

In Ref. 4 it was shown that such conditions are satisfied for certain physically interesting cases.

Suppose the approximating sequences of the operators $A_{\pm,n}$ are defined as in subsect. 4.1. Let further suppose there exists a sequence V_n of *unitary* operators approximating a given unitary operator V. The existence of such approximation is the main condition for the following constructions. Due to the fact that the operators P_n are projections on the eigenspaces of the operators $A_\pm$, the sequences $B_{(n,\pm)} = P_n B_\pm(\lambda) P_n$ approximate the operators $B_\pm$. It follows from the this fact and the relations (3.13), (3.15) that the sequence of operators

$$(B_n(\lambda) - B_n(-i))^{-1} (B_n(\lambda) - B_n(i)) + V_n$$

approximates the corresponding limiting operator and their inverses are uniformly bounded. Hence, the sequence

$$S_{V_n}(\lambda) = \\ 2 (I_n + V_n) (B_n(\lambda) - B_n(i) + (B_n(\lambda) - B_n(-i)) V_n)^{-1} B_n(\lambda) - I_n$$

approximates the operator $S_V(\lambda)$ and, moreover, is the sequence of scattering operators for the finite dimensional waveguides defined by the transversal operators $A_{\pm,n}$ and unitary operators V_n.

4.3. *Unboundedness of the Scattering Operator. An Example*

In this section, we show[4] that the scattering operator may indeed be unbounded in the space H. We emphasize that the example discussed is artificial and seems to have no physical meaning. But, first, it is mathematically natural, and, second, it shows that for the scattering operator in H to be bounded, some additional conditions are needed.

Let us consider a sequence of the finite dimensional waveguides of the form (where β_n is a constant)

$$H_{\pm,n} = \mathbb{C}^2,$$

$$A_{-,n} = \Lambda_n = \begin{pmatrix} -1 & 0 \\ 0 & -\beta_n^4 \end{pmatrix}, \; A_{+,n} = U_n A_{-,n} U_n^*,$$

where the unitary operators U_n are of form

$$U_n = U_n^* = U_n^{-1} = \frac{1}{1+\beta_n^2} \begin{pmatrix} 1-\beta_n^2 & 2\beta_n \\ 2\beta_n & \beta_n^2 - 1 \end{pmatrix}$$

and the boundary conditions are the continuity conditions of the function $u(z)$ and its first derivative. Let W_n be the corresponding waveguide. For a

given n, it is easy to calculate the scattering operator which is a 4×4-matrix of the form

$$S_n(\lambda) = \begin{pmatrix} R_n & T_n \\ U_nT_nU_n^* & U_nR_nU_n^* \end{pmatrix},$$

where the 2×2-matrices $T_n = T(\beta_n)$ and $R_n = E - T_n$ are matrix-valued functions of β. An explicit expressions for the T-matrix is quite complicated, but it can be shown that, for a given $\lambda \in \mathbb{C}$ and $\beta_n \to \infty$, the matrix element $T_{12}(\beta_n)$ is $O(\beta_n)$.

Now suppose $\beta_n \to \infty$ and consider a waveguide of the form

$$W = \bigoplus_{n=1}^{\infty} W_n \ .$$

The corresponding scattering operator is then

$$S(\lambda) = \bigoplus_{n=1}^{\infty} S_n(\lambda).$$

For any $\lambda \in \mathbb{C}$, the set of matrix elements of this operator is unbounded, and hence the operator can not be bounded.

5. The Multistep Waveguides and The Scattering Operator

To construct a mathematical model of the multistep waveguide, let us consider the set of real numbers $0 = a_0 < a_1 < ... < a_N < \infty$. Let

$$\mathcal{L} = \bigoplus_{j=0}^{N+1} H_j \otimes L_2(\Delta_j),$$

where $\Delta_0 = (-\infty, a_0)$ and $\Delta_j = (a_{j-1}, a_j)$ for $j = 1, ..., N$; let $\Delta_{N+1} = (a_N, \infty)$, and let

$$\mathcal{D}_0 = \bigoplus_{j=0}^{N+1} H_j \otimes C_0^{\infty}(\Delta_j).$$

Let the A_j, where $j = 0, ..., N + 1$, be negative operators in the respective Hilbert spaces H_j and let

$$W_0 = \bigoplus_{j=0}^{N+1} \left(\frac{d^2}{dz^2} \otimes I_{H_j} \oplus I_{L_2(\mathbb{R}_{\Delta_j})} \otimes A_j \right)$$

be the symmetric operator in $\mathcal{L}$ with the domain $\mathcal{D}_0$. This operator has many self-adjoint extensions; we will consider only local extensions, i.e.,

those defined by boundary conditions of the form (3.7) at each point a_j. Such extensions W we be referred to as *multistep waveguides*.

For each $j = 0, ..., N$, one can define the scattering operator $S_j(\lambda)$ for the pair $(A_j,\ A_{j+1})$ as in subsection 3.3. These operators completely define the waveguide, e.g., in terms of its resolvent. For a given scattering operator, the resolvent of the waveguide may be constructed as follows. Let

$$u = R_W(\lambda)f.$$

Let $P_j(t) = e^{-tB_j(\lambda)}$, where $t \in \Delta_j$. These operators are known in physics as *propagators*. Then, for $z \in \Delta_j$, we have

$$u\,(z) = -\tfrac{1}{2}B_j^{-1}(\lambda) \int\limits_{a_{j-1}}^{a_j} P_j(|\ z-\zeta\ |)f(\zeta)d\zeta + P_j(z-a_{j-1})u_j^+ + P_j(a_j-z)u_j^-,$$

where the vectors $u_j^{\pm} \in H_{A_j}$ are the constants of integration. Due to the boundary conditions at infinity, one has $u_0^+ = 0$ and $u_{N+1}^- = 0$. The definition of the scattering operator implies that

$$\begin{pmatrix} u_{j+1}^+ \\ u_j^- \end{pmatrix} = S_j(\lambda) \begin{pmatrix} P_{j+1}(|\Delta_{j+1}|)u_{j+1}^- + \psi_{j+1}^+ \\ P_j(|\Delta_j|)u_j^+ + \psi_j^- \end{pmatrix} \tag{5.1}$$

for $j = 0, ..., N$, where

$$\psi_j^- = -\tfrac{1}{2}B_j^{-1}(\lambda) \int\limits_0^{\Delta_j} P_j(\zeta)f(\zeta + a_{j-1})d\zeta,$$
$$\psi_j^+ = -\tfrac{1}{2}B_j^{-1}(\lambda) \int\limits_0^{\Delta_j} P_j(\zeta)f(a_j - \zeta)d\zeta.$$

The equations (5.1) define the vectors $u_j^{\pm}$, and hence the resolvent of the multistep waveguide is completely defined by the set of partial" scattering operators. Together with the finite dimensional approximation of the scattering operator described in subsect. 4.2, these equations give a way to numerical calculation of the different problems connected with multistep waveguides.[2,7]

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SCHRÖDINGER OPERATORS WITH RANDOM δ MAGNETIC FIELDS

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We consider the Schrödinger operators on $\mathbf{R}^2$ with the magnetic field given by a positive constant field plus random δ magnetic fields of the Poisson-Anderson type. We give sufficient conditions for the lower Landau levels to be infinitely degenerated eigenvalues, and for the lowest Landau level not to be an eigenvalue. The proof relies on the entire function theory by B. Ya. Levin.

Keywords: Quantum mechanics, Schrödinger operator, Random magnetic field, Aharonov-Bohm effect, Point interaction, Landau level, Entire function theory

1. Introduction

Define a differential operator $\mathcal{L}_\omega$ on $\mathbf{R}^2$ by

$$\mathcal{L}_\omega = \left(\frac{1}{i}\nabla + \mathbf{a}_\omega\right)^2,$$

where ω is an element of a probability space Ω, and $\mathbf{a}_\omega$ is the magnetic vector potential. The magnetic field corresponding to a vector potential $\mathbf{a} = (a_x, a_y)$ is defined by $\operatorname{rot}\mathbf{a} = \partial_x a_y - \partial_y a_x$ in the distribution sense. We assume the magnetic field $\operatorname{rot}\mathbf{a}_\omega$ is given by

$$\operatorname{rot}\mathbf{a}_\omega(z) = B + \sum_{\gamma\in\Gamma_\omega} 2\pi\alpha_\gamma(\omega)\delta(z-\gamma). \tag{1.1}$$

Here, B is a positive constant, δ is the Dirac measure concentrated on the origin. The random set Γ_ω is the Poisson configuration (the support of the Poisson point process) with intensity measure $\rho dxdy$, where ρ is a positive constant (for the definition of the Poisson point process, see e.g. Refs. 2,21). The random variables $\{\alpha_\gamma\}_{\gamma\in\Gamma_\omega}$ are i.i.d., $[0,1)$-valued random variables independent of Γ_ω [a], and their common distribution measure μ satisfies

$$\operatorname{supp}\mu \neq \{0\}.$$

We denote

$$\bar{\alpha} = \mathbf{E}[\alpha_\gamma], \quad p = \mathbf{P}\{\alpha_\gamma \neq 0\},$$

where $\mathbf{E}[X]$ denotes the expectation of a random variable X, and $\mathbf{P}\{E\}$ the probability of an event E. The values $\bar{\alpha}$ and p are independent of γ, since $\{\alpha_\gamma\}_{\gamma\in\Gamma}$ are i.i.d. We call the magnetic field satisfying these assumptions *the Poisson-Anderson type random δ magnetic fields* [b]. The assumption $\alpha_\gamma(\omega) \in [0,1)$ loses no generality, since the integral differences of $\alpha_\gamma(\omega)$'s can be gauged away.[15] These conditions are considered to be a mathematical model for the randomly distributed infinitesimally thin solenoids under the influence of a homogeneous magnetic field. A system of this type appears in the study of the Hall conductivity (see Desbois et. al.[8–10]).

A vector potential $\mathbf{a}_\omega$ satisfying (1.1) can be constructed as follows.[15] In the sequel, we identify a vector $z = (x,y) \in \mathbf{R}^2$ with a complex number $z = x + iy \in \mathbf{C}$. Put

$$\phi_\omega(z) = \frac{B\bar{z}}{2} + \frac{\alpha_0(\omega)}{z} + \sum_{\gamma\in\Gamma_\omega\setminus\{0\}} \alpha_\gamma(\omega)\left(\frac{1}{z-\gamma} + \frac{1}{\gamma} + \frac{z}{\gamma^2}\right), \tag{1.2}$$

where $\alpha_0(\omega) = 0$ if $0 \notin \Gamma_\omega$. Later we will prove that the right hand side of (1.2) converges locally uniformly in $\mathbf{C}\setminus\Gamma_\omega$, almost surely. Put

$$\mathbf{a}_\omega(z) = (\operatorname{Im}\phi_\omega(z), \operatorname{Re}\phi_\omega(z)).$$

[a] More precisely, we construct the random variables $\{\alpha_\gamma\}_{\gamma\in\Gamma_\omega}$ as follows. Let Ω_1 be the probability space on which the Poisson configuration Γ_ω is defined, and number the elements $\{\gamma_j\}_{j=1}^\infty$ of Γ_ω as $0 < |\gamma_1| < |\gamma_2| < \cdots$ (the probability that there exist two points of Γ_ω with the same absolute value is zero). Let Ω_2 be the probability space on which i.i.d. random variables $\{\alpha_j\}_{j=1}^\infty$ are defined. Put $\Omega = \Omega_1 \times \Omega_2$, and denote $\alpha_{\gamma_j}(\omega) = \alpha_j(\omega)$ $(j = 1,2,\ldots)$.

[b] Of course, we can consider the case Γ_ω is a non-random lattice Γ and $\{\alpha_\gamma\}$ are i.i.d. (Anderson type). The arguments below can be applied to this case with a little modification.

Then we can easily verify (1.1) holds.

We denote the Friedrichs extension of $\mathcal{L}_\omega|_{C_0^\infty(\mathbf{R}^2\setminus\Gamma_\omega)}$ by H_ω, then H_ω is a self-adjoint operator on the Hilbert space $L^2(\mathbf{R}^2)$. The domain of H_ω is given by

$$D(H_\omega) = \{u \in L^2(\mathbf{R}^2) \mid \mathcal{L}_\omega u \in L^2(\mathbf{R}^2), \limsup_{z\to\gamma} |u(z)| < \infty \text{ for any } \gamma \in \Gamma_\omega\}. \tag{1.3}$$

Remark that we can take another self-adjoint extensions of $\mathcal{L}_\omega|_{C_0^\infty(\mathbf{R}^2\setminus\Gamma_\omega)}$, since $\mathcal{L}_\omega|_{C_0^\infty(\mathbf{R}^2\setminus\Gamma_\omega)}$ is not essentially self-adjoint (see e.g. Refs. 1,7,17). When $\alpha_\gamma(\omega) \notin \mathbf{Z}$, the boundary condition $\limsup_{z\to\gamma} |u(z)| < \infty$ is equivalent to

$$\limsup_{z\to\gamma} |u(z)| = 0.$$

This boundary condition physically means that the solenoids are electrically shielded and the electron cannot penetrate inside the solenoids.

We denote the free operator (the operator corresponding to the constant magnetic field $\operatorname{rot} \mathbf{a} = B$) by H_0. The spectrum of H_0 is well-known:

$$\sigma(H_0) = \bigcup_{n=1}^{\infty} \{E_n\},$$

where $E_n = (2n-1)B$ is called the n-th Landau level. The Landau levels are infinitely degenerated eigenvalues of H_0.

In this paper, we shall investigate whether *the infinite degeneracy of the Landau levels changes under the perturbation of the δ-magnetic fields.* This problem is closely related to the infinite degeneracy of zero modes for the 2-dimensional Pauli operator.[14,15,22] The result is the following.

Theorem 1.1.

(1) If n is a positive integer satisfying $\dfrac{B}{2\pi\rho} + \bar{\alpha} > np$, then E_n is almost surely an infinitely degenerated eigenvalue of H_ω.

(2) If $\dfrac{B}{2\pi\rho} + \bar{\alpha} < p$, then E_1 is almost surely not an eigenvalue of H_ω.

The above theorem roughly means the lower Landau levels tend to be stable under the perturbation by δ magnetic fields, even if it is random. Similar results are obtained in the case of (scalar) point interactions[3–5,12,13,20] or in the case of δ magnetic fields.[14,15,17,18,22] It may be interesting to compare the above results with those in the case of regular potentials.[11,23] In that

case, it is widely believed that the Landau levels are broadened and there exist some extended states corresponding to the center of the Landau level.

It seems natural for the authors to conjecture E_n is not an infinitely degenerated eigenvalue when $B/(2\pi\rho) + \bar{\alpha} < np$. However, this conjecture could not be proved for some technical reasons (see the remark after the proof of Theorem 1.1 in section 4). The spectrum between Landau levels will be argued in our forthcoming paper.[19]

The rest of the paper is organized as follows. In section 2, we introduce a multi-valued holomorphic function on $\mathbf{C}$ called *the multi-valued canonical product*, and estimate its exponential growth order at infinity. In section 3, we give an explicit form of eigenfunctions corresponding to the Landau levels, using the multi-valued canonical products. This expression combined with the result of section 2 will lead us to the conclusion in section 4 (a similar argument is found in Ref. 6).

2. Multi-valued canonical product

There is a beautiful theory by B. Ja. Levin[16] about the relation between the exponential growth order of the canonical product and the distribution of its zeros. His theory also holds for the multi-valued function, with the modification as follows.

Let Γ be a discrete subset of $\mathbf{C}$ and $\alpha = (\alpha_\gamma)_{\gamma\in\Gamma}$ be a sequence of non-negative real numbers. For $r > 0$ and $\theta_1, \theta_2 \in \mathbf{R}$ with $0 \le \theta_2 - \theta_1 \le 2\pi$, put

$$n(r, \theta_1, \theta_2) = \sum_{0<|\gamma|\le r, \theta_1 \le \arg\gamma < \theta_2} \alpha_\gamma$$

(the sum is taken over $\gamma \in \Gamma$, as in the sequel). Put $n(r) = n(r, 0, 2\pi)$. We assume

$$n(r) = O(r^2) \quad \text{as } r \to \infty. \tag{2.1}$$

Define a sum $\zeta_{\Gamma,\alpha}$ and a product $\sigma_{\Gamma,\alpha}$ by

$$\zeta_{\Gamma,\alpha}(z) = \frac{\alpha_0}{z} + \sum_{\gamma\neq 0} \alpha_\gamma \left(\frac{1}{z-\gamma} + \frac{1}{\gamma} + \frac{z}{\gamma^2} \right), \tag{2.2}$$

$$\sigma_{\Gamma,\alpha}(z) = z^{\alpha_0} \prod_{\gamma\neq 0} \left(1 - \frac{z}{\gamma}\right)^{\alpha_\gamma} e^{\alpha_\gamma \left(\frac{z}{\gamma} + \frac{z^2}{2\gamma^2}\right)} \tag{2.3}$$

(we put $\alpha_0 = 0$ when $0 \notin \Gamma$). Particularly when Γ is a lattice of rank 2 and $\alpha_\gamma \equiv 1$, then $\zeta_{\Gamma,\alpha}$ is the Weierstrass ζ function, and $\sigma_{\Gamma,\alpha}$ is the Weierstrass σ function.

Let $\{C_j\}_{j=1}^{\infty}$ be a system of disks, where $C_j = \{|z - z_j| \le r_j\}$. We say $\mathcal{C} = \bigcup_{j=1}^{\infty} C_j$ is a C^0-set if

$$\limsup_{r\to\infty} \frac{1}{r} \sum_{|z_j|\le r} r_j = 0.$$

Proposition 2.1. *Assume (2.1) holds. Then the following holds:*

(1) The sum (2.2) converges uniformly in a compact subset of $\mathbf{C} \setminus \Gamma$. *If we take the branches of the functions* $\{(1 - \frac{z}{\gamma})^{\alpha_\gamma}\}_{\gamma\in\Gamma\setminus\{0\}}$ *appropriately, then the right hand side of (2.3) converges uniformly in a simply connected compact subset of* $\mathbf{C} \setminus \Gamma$. *For* $k = 0, 1, 2, \ldots$, *the function* $|\left(\frac{d}{dz}\right)^k \sigma_{\Gamma,\alpha}(z)|$ *is independent of the choice of the branches. Moreover, we have*

$$\frac{d}{dz}\sigma_{\Gamma,\alpha}(z) = \sigma_{\Gamma,\alpha}(z)\zeta_{\Gamma,\alpha}(z). \tag{2.4}$$

(2) Assume additionally that

(a) there exists $I_0 \subset [0, 2\pi)$ *such that* $[0, 2\pi) \setminus I_0$ *is countable and the limit*

$$\Delta(\theta_1, \theta_2) = \lim_{r\to\infty} \frac{n(r, \theta_1, \theta_2)}{r^2}$$

exists for any $\theta_1, \theta_2 \in I_0 + 2\pi\mathbf{Z}$ *with* $0 \le \theta_2 - \theta_1 \le 2\pi$, *and*

(b) the limit

$$\delta_{\Gamma,\alpha} = \frac{1}{2} \lim_{r\to\infty} \sum_{0<|\gamma|\le r} \frac{\alpha_\gamma}{\gamma^2} \tag{2.5}$$

exists and is finite.

Let $d\Delta$ *be the Lebesgue-Stieltjes measure given by the relation* $\int_{[\theta_1,\theta_2)} d\Delta(\psi) = \Delta(\theta_1, \theta_2)$. *Then, there exists a* C^0*-set* $\mathcal{C}$ *such that*

$$\lim_{r\to\infty, re^{i\theta}\notin\mathcal{C}} \frac{\log|\sigma_{\Gamma,\alpha}(re^{i\theta})|}{r^2} = H(\theta), \tag{2.6}$$

where the function $H(\theta)$ *is defined by the Stieltjes integral*

$$H(\theta) = -\int_{\theta-2\pi}^{\theta} (\psi - \theta)\sin 2(\psi - \theta)\ d\Delta(\psi) + \mathrm{Re}(e^{2i\theta}\delta_{\Gamma,\alpha}).$$

The convergence (2.6) is uniform with respect to $\theta \in [0, 2\pi)$.

Remark 2.1. The proof of the first assertion is easy. The second assertion is a generalization of Theorem 2 in Chap. II, Sec. 1 of Ref. 16, and its proof is also similar (there is a misprint in the first edition of Ref. 16; there must be the minus sign before the integral in (2.06) in Ref. 16). The outline of the proof will be given in Ref. 19.

Corollary 2.1. *In addition to the assumption of (ii) of Proposition 2.1, assume that*

$$\Delta(\theta_1, \theta_2) = c(\theta_2 - \theta_1)$$

for some positive constant c. Put

$$\widetilde{\sigma}_{\Gamma,\alpha}(z) = e^{-\delta_{\Gamma,\alpha} z^2} \sigma_{\Gamma,\alpha}(z).$$

Then, there exists some C^0-set $\mathcal{C}$ satisfying the following; for any $\epsilon > 0$, we have

$$|\widetilde{\sigma}_{\Gamma,\alpha}(z)| \leq e^{(c\pi+\epsilon)|z|^2} \tag{2.7}$$

for sufficiently large z, and

$$|\widetilde{\sigma}_{\Gamma,\alpha}(z)| \geq e^{(c\pi-\epsilon)|z|^2} \tag{2.8}$$

for sufficiently large z outside $\mathcal{C}$.

Proof. By Proposition 2.1 and the equality

$$-c \int_{\theta-2\pi}^{\theta} (\psi - \theta) \sin 2(\psi - \theta) d\psi = c\pi,$$

we see that there exists some C^0-set $\mathcal{C}$ such that both (2.7) and (2.8) hold for sufficiently large z outside $\mathcal{C}$. Since $\mathcal{C}$ is a C^0-set, the limitation $z \in \mathbf{C} \backslash \mathcal{C}$ on (2.7) can be eliminated by using the maximum modulus principle (see the argument after the proof of Lemma 5 in Chap. II, Sec. 3 of Ref. 16). □

For an entire function f, it is well-known that f and its derivatives $\frac{d^k f}{dz^k}$ have the same exponential growth order.[16] For a multi-valued holomorphic function f, we have the following.

Lemma 2.1. *Let f be a multi-valued holomorphic function on $\mathbf{C}$ and n_0 a nonnegative integer. Let Γ be the set of the branch points of f. Assume the following conditions hold:*

(1) In a neighborhood U_γ of each $\gamma \in \Gamma$, f is written as

$$f(z) = (z - \gamma)^{\alpha_\gamma} g_\gamma(z),$$

where $\alpha_\gamma > n_0$ and g_γ is a function holomorphic in U_γ.

(2) $\#\{\gamma \in \Gamma \mid |\gamma| \leq r\} = O(r^2)$ *as* $r \to \infty$.
(3) There exists a constant $a > 0$ *such that*

$$|f(z)| \leq e^{a|z|^2}$$

for sufficiently large z.

Then, for any $\epsilon > 0$, *we have for any* $k = 0, 1, \ldots, n_0$

$$\left|\frac{d^k f}{dz^k}(z)\right| \leq e^{(a+\epsilon)|z|^2} \tag{2.9}$$

for sufficiently large $z \in \mathbf{C} \setminus \Gamma$.

Remark 2.2. By (i), the function $|\frac{d^k f}{dz^k}(z)|$ is single-valued.

Proof. By (i), we have

$$\lim_{z \to \gamma} \left|\frac{d^k f}{dz^k}(z)\right| = 0$$

for $k = 0, \ldots, n_0$. Thus the function $M_k(r) = \max_{|z|=r} \left|\frac{d^k f}{dz^k}(z)\right|$ is monotone nondecreasing, by the maximum modulus principle. By (ii), we can take $A \in \mathbf{N}$ such that

$$\#\{\gamma \in \Gamma \mid |\gamma| \leq r\} \leq Ar^2 - 1.$$

Take $l \in \mathbf{N}$. Dividing the ring $\{l - 1 < |z| \leq l\}$ into Al^2 subrings, we find a subring $\{r_l - \frac{1}{2Al^2} < |z| \leq r_l + \frac{1}{2Al^2}\}$ which contains no point of Γ. Then, for $|z| = r_l$, we have by the Cauchy integral formula

$$\frac{d^k f}{dz^k}(z) = \frac{k!}{2\pi i} \int_{|w-z|=\frac{1}{3Al^2}} \frac{f(w)}{(w-z)^{k+1}} dw.$$

Using this formula, we have

$$M_k(l-1) \leq (3Al^2)^k k! M_0(l).$$

Therefore (2.9) follows from (iii). □

3. Eigenfunctions for Landau levels

Let us return to our model and construct the eigenfunctions for Landau levels. Similar solutions are found in Refs. 14,15,18,22.

Let ϕ_ω be the function given in (1.2). Define differential operators $\mathcal{A}_\omega$ and $\mathcal{A}_\omega^\dagger$ by

$$\mathcal{A}_\omega = 2\partial_z + \phi_\omega(z), \quad \mathcal{A}_\omega^\dagger = -2\partial_{\bar{z}} + \overline{\phi_\omega(z)},$$

where $\partial_z = (\partial_x - i\partial_y)/2$, $\partial_{\bar{z}} = (\partial_x + i\partial_y)/2$. These operators satisfy the canonical commutation relation

$$\mathcal{L}_\omega = \mathcal{A}_\omega^\dagger \mathcal{A}_\omega + B = \mathcal{A}_\omega \mathcal{A}_\omega^\dagger - B \tag{3.1}$$

as an operator on $\mathcal{D}'(\mathbf{C} \setminus \Gamma_\omega)$.

Put $\alpha(\omega) = (\alpha_\gamma(\omega))_{\gamma \in \Gamma_\omega}$, $\zeta_\omega = \zeta_{\Gamma_\omega, \alpha(\omega)}$ and $\sigma_\omega = \sigma_{\Gamma_\omega, \alpha(\omega)}$. Then, we have

$$\mathcal{A}_\omega = 2\partial_z + \frac{B\bar{z}}{2} + \zeta_\omega(z), \quad \mathcal{A}_\omega^\dagger = -2\partial_{\bar{z}} + \frac{Bz}{2} + \overline{\zeta_\omega(z)}. \tag{3.2}$$

Put

$$\widetilde{\alpha}_\gamma(\omega) = \begin{cases} 1 & (0 < \alpha_\gamma(\omega) < 1), \\ 0 & (\alpha_\gamma(\omega) = 0), \end{cases} \quad \widetilde{\sigma}_\omega = \sigma_{\Gamma_\omega, \widetilde{\alpha}(\omega)},$$

where $\widetilde{\alpha}(\omega) = (\widetilde{\alpha}_\gamma(\omega))_{\gamma \in \Gamma_\omega}$. Notice that $\widetilde{\sigma}_\omega$ is an entire function.

Lemma 3.1. *Let $n \in \mathbf{N}$. Then, the following holds:*

(1) Let f be an entire function. Put

$$u(z) = {\mathcal{A}_\omega^\dagger}^{n-1} \left(e^{-\frac{B}{4}|z|^2} |\sigma_\omega(z)|^{-1} \overline{\widetilde{\sigma}_\omega(z)^n f(z)} \right). \tag{3.3}$$

If $u \in L^2(\mathbf{C})$, then $u \in D(H_\omega)$ and $H_\omega u = E_n u$. Moreover, if $u \in D(H_\omega)$ satisfies $H_\omega u = Bu$, then there exists an entire function f such that (3.3) holds with $n = 1$.

(2) For almost all ω, the assumptions (a) and (b) in (ii) of Proposition 2.1 are satisfied with $\Gamma = \Gamma_\omega$, $\alpha = \beta(\omega) = (n\widetilde{\alpha}_\gamma(\omega) - \alpha_\gamma(\omega))_{\gamma \in \Gamma_\omega}$ and

$$\Delta(\theta_1, \theta_2) = \rho(\theta_2 - \theta_1)(np - \bar{\alpha})/2.$$

(3) Let $\omega \in \Omega$ satisfying the conclusion of (ii). Let $\delta_\omega = \delta_{\Gamma_\omega, \beta(\omega)}$ be the constant defined by (2.5) for $\Gamma = \Gamma_\omega$ and $\alpha = \beta(\omega)$. For a polynomial $g \not\equiv 0$, let $u_{n,g}$ be the function u defined by (3.3) with $f(z) = e^{-\delta_\omega z^2} g(z)$. Then, there exists a C^0-set $\mathcal{C}$ such that for any $\epsilon > 0$

$$|u_{n,g}(z)| \le \exp\left(\left(-\frac{B}{4} + \frac{\pi\rho(np - \bar{\alpha})}{2} + \epsilon \right) |z|^2 \right) \tag{3.4}$$

for sufficiently large z, and

$$|u_{1,g}(z)| \ge \exp\left(\left(-\frac{B}{4} + \frac{\pi\rho(p - \bar{\alpha})}{2} - \epsilon \right) |z|^2 \right) \tag{3.5}$$

for sufficiently large z outside $\mathcal{C}$.

Proof. In the sequel, we denote the inner product on $L^2(\mathbf{R}^2)$ by $(u,v) = \int_{\mathbf{R}^2} \overline{u}v dxdy$, the L^2-norm by $\|u\|^2 = (u,u)$.

(i) For simplicity of the notation, we omit the subscript ω for a while. Let u be the function given by (3.3). By (2.4) and (3.2), we have

$$\mathcal{A} = e^{-\frac{B}{4}|z|^2}|\sigma(z)|^{-1}(2\partial_z)e^{\frac{B}{4}|z|^2}|\sigma(z)|. \tag{3.6}$$

Put

$$v(z) = e^{-\frac{B}{4}|z|^2}|\sigma(z)|^{-1}\overline{\widetilde{\sigma}(z)^n f(z)}.$$

By (3.1) and (3.6), we have $(\mathcal{L} - B)v = \mathcal{A}^\dagger \mathcal{A} v = 0$. Then we can prove $\mathcal{L}\mathcal{A}^{\dagger j} v = E_{j+1}\mathcal{A}^{\dagger j} v$ for any nonnegative integer j, by an inductive argument using (3.1). Thus we have $\mathcal{L}u = E_n u$.

If $u \in L^2(\mathbf{R}^2)$, then we have $\mathcal{L}u = E_n u \in L^2(\mathbf{R}^2)$. Since $v(z) = O(|z-\gamma|^{n-\alpha_\gamma+l})$ as $z \to \gamma$ (l is the order of zero at γ for f), we have $u(z) = O(|z-\gamma|^{1-\alpha_\gamma+l})$ as $z \to \gamma$. Thus u satisfies the boundary conditions $\limsup_{z\to\gamma}|u(z)| < \infty$ for every $\gamma \in \Gamma$. By (1.3), we have $u \in D(H)$.

Next, suppose $u \in D(H)$ and $Hu = Bu$. Since H is the Friedrichs extension, (3.1) implies

$$((H-B)u, u) = (\mathcal{A}^\dagger \mathcal{A} u, u) = \|\mathcal{A}u\|^2.$$

Thus, we have

$$\mathcal{A}u = 0 \quad \text{in } \mathbf{R}^2 \setminus \Gamma. \tag{3.7}$$

By (3.6), any solution to (3.7) is written as

$$u(z) = e^{-\frac{B}{4}|z|^2}|\sigma(z)|^{-1}\overline{g(z)},$$

where $g(z)$ is a holomorphic function on $\mathbf{C}\setminus\Gamma$. Since u satisfies the boundary conditions $\limsup_{z\to\gamma}|u(z)| < \infty$ for every $\gamma \in \Gamma$, we see that the function g has to be factorized as $g(z) = \widetilde{\sigma}(z)f(z)$, where $f(z)$ is an entire function on $\mathbf{C}$. Thus the assertion holds.

(ii) First we prove the assumption (a) is satisfied. For $N = m + ni \in \mathbf{Z} \oplus \mathbf{Z}i$, define a square Q_N by

$$Q_N = \left\{ s + ti \mid m - \frac{1}{2} \le s < m + \frac{1}{2},\ n - \frac{1}{2} \le t < n + \frac{1}{2} \right\}$$

and put

$$X_N(\omega) = \sum_{\gamma \in \Gamma_\omega \cap Q_N} \beta_\gamma(\omega).$$

Then the random variables $\{X_N\}_{N\in\mathbf{Z}\oplus\mathbf{Z}i}$ are independent and

$$\mathbf{E}[X_N] = \mathbf{E}_{\Omega_1}[\#(\Gamma. \cap Q_N)]\mathbf{E}_{\Omega_2}[n\widetilde{\alpha}_\gamma - \alpha_\gamma] = \rho(np - \bar{\alpha}),$$

where we used $\mathbf{E}[\#(\Gamma_\cdot \cap U)] = \rho|U|$ (for the probability spaces Ω_1 and Ω_2, see the footnote about the definition of the Poisson-Anderson fields). For $r > 0$ and $\theta_1, \theta_2 \in \mathbf{R}$ with $0 \le \theta_2 - \theta_1 \le 2\pi$, put

$$\begin{aligned} S(r,\theta_1,\theta_2) &= \{se^{i\theta} \mid 0 < s \le r,\ \theta_1 \le \theta < \theta_2\}, \\ N(r,\theta_1,\theta_2) &= \{N \in \mathbf{Z} \oplus \mathbf{Z}i \mid Q_N \subset S(r,\theta_1,\theta_2)\}, \\ \widetilde{n}(r,\theta_1,\theta_2) &= \sum_{N \in N(r,\theta_1,\theta_2)} X_N. \end{aligned}$$

Then we have

$$\frac{\widetilde{n}(r,\theta_1,\theta_2)}{r^2} = \frac{\sum_{N \in N(r,\theta_1,\theta_2)} X_N}{\#N(r,\theta_1,\theta_2)} \frac{\#N(r,\theta_1,\theta_2)}{r^2} \to \frac{\rho(np-\bar{\alpha})(\theta_2-\theta_1)}{2}$$

almost surely, by the law of large numbers. Moreover, we readily have

$$\lim_{r\to\infty} \frac{\widetilde{n}(r,\theta_1,\theta_2) - n(r,\theta_1,\theta_2)}{r^2} = 0$$

almost surely. Thus we have

$$\lim_{r\to\infty} \frac{n(r,\theta_1,\theta_2)}{r^2} = \frac{\rho(np-\bar{\alpha})(\theta_2-\theta_1)}{2} \tag{3.8}$$

almost surely, for each $\theta_1, \theta_2 \in \mathbf{Q}$ with $0 \le \theta_2 - \theta_1 \le 2\pi$. By the monotonicity of the function $n(r,\theta_1,\theta_2)$ with respect to θ_1 or θ_2, we see that (3.8) holds for every $\theta_1, \theta_2 \in \mathbf{R}$, almost surely.

Next we show the assumption (b) holds. Put

$$\delta(r) = \sum_{1<|\gamma|\le r} \frac{\beta_\gamma}{\gamma^2}.$$

We shall prove $\delta(r)$ converges as $r \to \infty$, almost surely.

For $m = 1, 2, \ldots$ and $k = 0, \ldots, 4m-1$, put

$$U_{m,k} = \left\{ re^{i\theta} \;\middle|\; m^2 < r \le (m+1)^2, \frac{k\pi}{2m} \le \theta < \frac{(k+1)\pi}{2m} \right\},$$

$$c_{m,k} = m^2 e^{i\frac{k\pi}{2m}}, \quad \Gamma_{m,k} = \Gamma \cap U_{m,k}, \quad \delta_{m,k} = \sum_{\Gamma_{m,k}} \frac{\beta_\gamma}{\gamma^2}.$$

In the sequel, we denote the general constants independent of m, k, ω by C. For $\gamma \in U_{m,k}$, we have

$$\left| \frac{1}{\gamma^2} - \frac{1}{c_{m,k}^2} \right| = \left| \frac{(\gamma + c_{m,k})(\gamma - c_{m,k})}{\gamma^2 c_{m,k}^2} \right| \le Cm^{-5}. \tag{3.9}$$

Put $\bar{\beta} = \mathbf{E}[\beta_\gamma] = np - \bar{\alpha}$. Then we have

$$\begin{aligned}
&|\delta_{m,k} + \delta_{m,k+m}| \\
&\le m^{-4} \left| \sum_{\Gamma_{m,k}} \beta_\gamma - \sum_{\Gamma_{m,k+m}} \beta_\gamma \right| + Cm^{-5} \left(\#\Gamma_{m,k} + \#\Gamma_{m,k+m} \right) \\
&\le m^{-4} \left(\left| \sum_{\Gamma_{m,k}} (\beta_\gamma - \bar{\beta}) \right| + \left| \sum_{\Gamma_{m,k+m}} (\beta_\gamma - \bar{\beta}) \right| + |\#\Gamma_{m,k} - \#\Gamma_{m,k+m}| \bar{\beta} \right) \\
&\qquad + Cm^{-5} \left(\#\Gamma_{m,k} + \#\Gamma_{m,k+m} \right), \qquad (3.10)
\end{aligned}$$

where we used (3.9) and $c^2_{m,k+m} = -c^2_{m,k}$ in the first inequality. By the Schwarz inequality and the independence of $\{\beta_\gamma\}$, we have

$$\begin{aligned}
&\mathbf{E} \left[\left| \sum_{\Gamma_{m,k}} (\beta_\gamma - \bar{\beta}) \right| \right] = \mathbf{E}_{\Omega_1} \left[\mathbf{E}_{\Omega_2} \left[\left| \sum_{\Gamma_{m,k}} (\beta_\gamma - \bar{\beta}) \right| \right] \right] \\
&\le \mathbf{E}_{\Omega_1} \left[\left(\mathbf{V}_{\Omega_2} \left[\sum_{\Gamma_{m,k}} \beta_\gamma \right] \right)^{1/2} \right] = \mathbf{E}_{\Omega_1} \left[\left(\#\Gamma_{m,k} \mathbf{V}_{\Omega_2} [\beta_\gamma] \right)^{1/2} \right] \qquad (3.11) \\
&\le \left(\mathbf{E}_{\Omega_1} [\#\Gamma_{m,k}] \right)^{1/2} \left(\mathbf{V}_{\Omega_2} [\beta_\gamma] \right)^{1/2} \le Cm,
\end{aligned}$$

where $\mathbf{V}[X]$ denotes the variance of a random variable X. The expectation $\mathbf{E}\left[\left| \sum_{\Gamma_{m,k+m}} (\beta_\gamma - \bar{\beta}) \right| \right]$ is estimated in the same way. Moreover, we have

$$\begin{aligned}
\mathbf{E}[|\#\Gamma_{m,k} - \#\Gamma_{m,k+m}|] &\le 2\mathbf{E}[|\#\Gamma_{m,k} - \rho|U_{m,k}||] \\
&\le 2\mathbf{V}[\#\Gamma_{m,k}]^{1/2} \le Cm, \qquad (3.12) \\
\mathbf{E}[\#\Gamma_{m,k} + \#\Gamma_{m,k+m}] &= 2\rho|U_{m,k}| \le Cm^2, \qquad (3.13)
\end{aligned}$$

where we used $\mathbf{V}[\#\Gamma_{m,k}] = \rho|\Gamma_{m,k}| \le Cm^2$. By (3.10), (3.11), (3.12) and (3.13), we have

$$\mathbf{E}\left[|\delta_{m,k} + \delta_{m,k+m}| \right] \le Cm^{-3},$$

so

$$\sum_{m=1}^{\infty} \sum_{k=0}^{m-1} \mathbf{E}\left[|\delta_{m,k} + \delta_{m,k+m} + \delta_{m,k+2m} + \delta_{m,k+3m}| \right] < \infty.$$

Therefore we conclude the sequence $\{\delta(m^2)\}_{m=1}^{\infty}$ converges almost surely.

Now it is sufficient to show that

$$\sup_{m^2 < r < (m+1)^2} |\delta(r) - \delta(m^2)| \to 0 \quad \text{as } m \to \infty \qquad (3.14)$$

almost surely. As in the proof of (a), we can prove

$$\frac{\#\{\gamma \in \Gamma_\omega \mid m^2 < |\gamma| < (m+1)^2\}}{\pi(m+1)^4 - \pi m^4} \to \rho$$

almost surely. This implies

$$\#\{\gamma \in \Gamma_\omega \mid m^2 < |\gamma| < (m+1)^2\} \le Cm^3$$

almost surely. Thus we have

$$|\delta(r) - \delta(m^2)| \le \#\{\gamma \in \Gamma_\omega \mid m^2 < |\gamma| < (m+1)^2\} m^{-4} \le Cm^{-1}$$

for $m^2 < r < (m+1)^2$, which implies (3.14).

(iii) By (2.4) and (3.2), we have

$$\mathcal{A}_\omega^\dagger = \operatorname{sgn}\sigma_\omega(z)^{-1} \left(-2\partial_{\bar z} + \frac{Bz}{2}\right) \operatorname{sgn}\sigma_\omega(z),$$

where $\operatorname{sgn}(z) = \frac{z}{|z|} = \frac{|z|}{\bar z}$. Thus we have

$$\begin{aligned} &u_{n,g}(z) \\ &= e^{-\frac{B}{4}|z|^2} \operatorname{sgn}\sigma_\omega(z)^{-1} (-2\partial_{\bar z} + Bz)^{n-1} \overline{\sigma_\omega(z)^{-1} \widetilde{\sigma}_\omega(z)^n e^{-\delta_\omega z^2} g(z)} \\ &= e^{-\frac{B}{4}|z|^2} \operatorname{sgn}\sigma_\omega(z)^{-1} (-2\partial_{\bar z} + Bz)^{n-1} \overline{\widetilde{\sigma}_{\Gamma_\omega,\beta(\omega)}(z) g(z)}. \end{aligned}$$

Since

$$\frac{\#(\Gamma_\omega \cap B_r(0))}{r^2} \to \pi\rho$$

almost surely, we have

$$\#(\Gamma_\omega \cap B_r(0)) = O(r^2) \quad \text{as } r \to \infty$$

almost surely. So the conclusion follows from (ii) of this lemma, Corollary 2.1, Lemma 2.1 and the Leibniz rule. □

4. Proof of theorem 1.1

Proof. Suppose $B/(2\pi\rho) + \bar\alpha > np$. Then, there exists $\epsilon > 0$ such that $-B/4 + \pi\rho(np - \bar\alpha)/2 + \epsilon < 0$. For any polynomial g, the function $u_{n,g}$ is an eigenfunction of H_ω corresponding to the eigenvalue E_n, by (3.4). Thus we see that E_n is an infinitely degenerated eigenvalue of H_ω, almost surely.

Next, suppose $B/(2\pi\rho) + \bar\alpha < p$. Then, there exists $\epsilon > 0$ such that $-B/4 + \pi\rho(np - \bar\alpha)/2 - \epsilon > 0$. By (3.5), we have

$$|u_{1,1}(z)| \ge 1 \tag{4.1}$$

for sufficiently large z outside some C^0-set $\mathcal{C}$. Adding some disk centered at the origin to $\mathcal{C}$, we may assume (4.1) holds for every $z \in \mathbf{C} \setminus \mathcal{C}$. Let

$$S_0 = \{r > 0 \mid \{|z| = r\} \cap \mathcal{C} = \emptyset\}.$$

Suppose some $u \in D(H)$ satisfies $Hu = Eu$. By (i) of Lemma 3.1, u is written as $u = u_{1,1}\bar{f}$ for some entire function $f = \sum_{n=0}^{\infty} a_n z^n$. Then we have

$$\int_{\mathbf{C}} |u|^2 dxdy \geq 2\pi \sum_{n=0}^{\infty} \int_{S_0} |a_n|^2 r^{2n+1} dr. \tag{4.2}$$

Since $\mathcal{C}$ is a C^0-set, we have

$$\int_{(0,R)\cap S_0} r^{2n+1} dr \geq |(1,R) \cap S_0| \to \infty$$

as $R \to \infty$, where $|S|$ denotes the Lebesgue measure of S. Thus the right hand side of (4.2) diverges if some a_n is not zero. This implies $u = 0$, so we see that E_1 is not an eigenvalue of H_ω, almost surely. □

Remark 4.1. We could not prove the conjecture 'E_n is not an infinitely degenerated eigenvalue when $B/(2\pi\rho) + \bar{\alpha} < np$' for two reasons. First, we could not exclude the possibility of the existence of the exceptional solutions, which cannot be written as (3.3), when $n \geq 2$. Second, we could not establish the lower bound like (3.5) for the solution $u_{n,g}$, when $n \geq 2$.

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MEAN FIELD LIMIT FOR BOSONS AND SEMICLASSICAL TECHNIQUES

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We give a summary of results obtained with Z. Ammari in Ammari-Nier[2] after analyzing accurately the formal relationships between mean field and semiclassical asymptotics.

Keywords: Mean field limit; bosonic QFT; Wigner measures

1. Introduction

When the one particle states lie in a complex Hilbert space $\mathcal{Z}$, the many body problem is formulated in a Hilbert space $\mathcal{H} \subset \oplus_{n\in\mathbb{N}}\mathcal{Z}^{\otimes n}$, which contains the symmetry (resp. antisymmetry) constraint for bosons (resp. fermions). The mean field limit consists in studying states associated with a large number N of particles and their dynamics for some specific Hamiltonian. After introducing the small parameter $\varepsilon = \frac{1}{N}$, one can consider for example initial states $\Psi_0 = z_0^{\otimes N} = z_0^{\otimes \varepsilon^{-1}}$ and the evolved states $\Psi_t = e^{-i\frac{t}{\varepsilon}H_\varepsilon}\Psi_0$, when H_ε is the Wick quantized version of a polynomial expression $p(z,\overline{z})$ of $z \in \mathcal{Z}$ obtained after replacing the z_j (resp. $\overline{z_j}$) variable by a scaled annihilation (resp. creation) operator $\sqrt{\varepsilon}a_j$ (resp. $\sqrt{\varepsilon}a_j^*$) while fulfilling the Wick ordering rule (annihilation on the right-hand side). The mean field dynamics is given by $\Psi_t \simeq z_t^{\otimes \varepsilon^{-1}}$ where z_t evolves according to the Hamiltonian dynamics, $i\partial_t z_t = \partial_{\overline{z}} p(z_t, \overline{z_t})$, in the phase space $\mathcal{Z}$ endowed with the symplectic form Im $\langle\ ,\ \rangle$. The precise meaning of $\simeq$ is given after proving that with the normalization $|z_t| = 1$, the quantity

$$\langle \Psi_t\,,\, \varepsilon(A\otimes I\otimes\cdots\otimes I + I\otimes A\otimes I\otimes\cdots\otimes I\otimes +I\otimes\cdots\otimes I\otimes A)\Psi_t\rangle \tag{1.1}$$

is equivalent to $\langle z_t\,,\, Az_t\rangle$ in the limit $\varepsilon \to 0$ (i.e. $N \to \infty$). Within the bosonic framework, the observable involved in (1.1) is nothing but the Wick

quantized operator p_A^{Wick} for the polynomial $p_A(z,\overline{z}) = \langle z\,, Az\rangle$. Higher order correlations are also described after testing with Wick quantized higher order polynomials.

This summarizes the formal relationship between mean field limits and semiclassical analysis: they both involve the Hamiltonian dynamics on the phase space and ε-dependent quantizations of classical symbols. In spite of the strong development of semiclassical techniques for finite dimensional problems in the eighties, very little has been done in this spirit for mean field problems. One reason is the well-known difficulty to develop a pseudo-differential calculus in infinite dimension which is rich enough to catch the properties of realistic nonlinear dynamics. Another reason is that some other methods, based on the integral functional point of view or techniques of truncated Dyson expansions were more effective for other problems in quantum field theory.

This text provides a short presentation of a recent joint work with Z. Ammari, where the introduction of Wigner measures in infinite dimension allowed to analyze the links between various approaches to mean field problems and to prove new results. While doing so the differences between the inductive and projective approaches to the infinite dimensional case and the specificities of Weyl-, Wick- and anti-Wick quantizations have been completely clarified.

2. Review of the finite dimensional case

2.1. *Finite dimensional phase space and Schrödinger representation*

Consider $\mathcal{Z} = \mathbb{C}^d$ with its natural Hermite scalar product $\langle z_1\,, z_2\rangle = \sum_{j=1}^d \overline{z_{1,j}} z_{2,j}$, its real scalar product $S(z_1,z_2) = \mathrm{Re}\langle z_1\,, z_2\rangle$ and its symplectic form $\sigma(z_1,z_2) = \mathrm{Im}\langle z_1\,, z_2\rangle$. Set $\mathcal{H} = \bigoplus_{n=0}^\infty \bigvee^n \mathcal{Z} = \Gamma_s(\mathcal{Z})$ the bosonic Fock space, defined as a Hilbert direct sum. For any $n \in \mathbb{N}$, the orthogonal projection from $\bigotimes^n \mathcal{Z}$ onto the closed subspace $\bigvee^n \mathcal{Z}$ of symmetric tensors is denoted by $\mathcal{S}_n$. For any $(\xi_1, \xi_2, \ldots, \xi_n) \in \mathcal{Z}^n$, the vector $\xi_1 \vee \xi_2 \vee \cdots \vee \xi_n \in \bigvee^n \mathcal{Z}$ is

$$\xi_1 \vee \xi_2 \vee \cdots \vee \xi_n \mathcal{S}_n(\xi_1 \otimes \xi_2 \cdots \otimes \xi_n) = \frac{1}{n!} \sum_{\sigma\in\mathfrak{S}_n} \xi_{\sigma(1)} \otimes \xi_{\sigma(2)} \cdots \otimes \xi_{\sigma(n)}$$

After introducing a small parameter $\varepsilon > 0$, the ε-dependent annihilation and creation operators are defined by

$$a(z)_{|\bigvee^n \mathcal{Z}} = \sqrt{\varepsilon n}\ \ \langle z| \otimes I_{\bigvee^{n-1}\mathcal{Z}}$$

$$a^*(z)_{|\bigvee^n \mathcal{Z}} = \sqrt{\varepsilon(n+1)}\ \mathcal{S}_{n+1} \circ (\ z \otimes I_{\bigvee^n \mathcal{Z}}) = \sqrt{\varepsilon(n+1)}\ z \bigvee I_{\bigvee^n \mathcal{Z}}\,,$$

when $z \in \mathcal{Z}$ is identified with the operator $\mathbb{C} \ni \lambda \mapsto \lambda z \in \mathcal{Z}$. The quantized real variables

$$\Phi(z) = \frac{1}{\sqrt{2}}(a^*(z) + a(z)) \quad \text{and} \quad \Pi(z) = \Phi(iz) = \frac{1}{i\sqrt{2}}(a(z) - a^*(z))\,.$$

They are self-adjoint operators on $\mathcal{H}$ and satisfy the identities:

$$[\Phi(z_1), \Phi(z_2)] = i\varepsilon\sigma(z_1, z_2)I, \qquad [\Phi(z_1), \Pi(z_2)] = i\varepsilon S(z_1, z_2)I.$$

The representation of the Weyl commutation relations in the Fock space

$$\begin{aligned} W(z_1)W(z_2) &= e^{-\frac{i\varepsilon}{2}\sigma(z_1,z_2)}W(z_1+z_2) \\ &= e^{-i\varepsilon\sigma(z_1,z_2)}W(z_2)W(z_1), \end{aligned} \tag{2.1}$$

is obtained by setting $W(z) = e^{i\Phi(z)}$. After introducing the vacuum vector $(1, 0, \dots) \in \mathcal{H}$, the coherent state vectors are given by

$$E(z) = W\left(\frac{\sqrt{2}z}{i\varepsilon}\right)\Omega = e^{\frac{1}{\varepsilon}[a^*(z)-a(z)]}\Omega\,,$$

for any $z \in \mathcal{Z}$, with the explicit form

$$E(z)e^{-\frac{|z|^2}{2\varepsilon}} \sum_{n=0}^{\infty} \frac{1}{\varepsilon^n}\frac{a^*(z)^n}{n!}\Omega = e^{-\frac{|z|^2}{2\varepsilon}} \sum_{n=0}^{\infty} \varepsilon^{-n/2}\frac{z^{\otimes n}}{\sqrt{n!}}\,. \tag{2.2}$$

They should not be confused with Hermite or product states of the form

$$H_n(z) = z^{\otimes n}\,. \tag{2.3}$$

The number operator is also scaled with the small parameter $\varepsilon > 0$ according to

$$N_{|\bigvee^n \mathcal{Z}} = \varepsilon n I_{|\bigvee^n \mathcal{Z}} = \sum_{j=1}^{d} a^*(e_j)a(e_j)$$

where the last identity holds for any orthonormal basis $(e_1, \dots, e_d) \in \mathcal{Z}^d$.

The relationship with the Schrödinger representation which can be formulated with a Bargmann transform in the finite dimensional case (see Folland,[9] Martinez,[22] Aftalion-Blanc-Nier[1]) can be explicitly given after setting $z = x + i\xi$, with $(x, \xi) \in T^*\mathbb{R}^d$. The symplectic form $[\![\ ,\ ]\!]$ and the scalar product $(\ ,\ )$ on $T^*\mathbb{R}^d$ are usually defined according to

$$\begin{aligned}]\ &= \xi.y - x.\eta = -\mathrm{Im}\,\langle x + i\xi\,,\, y + i\eta\rangle = -\sigma(x + i\xi, y + i\eta) \\ ((x,\xi),(y,\eta)) &= x.y + \xi.\eta = \mathrm{Re}\,\langle x + i\xi\,,\, y + i\eta\rangle = S(x + i\xi, y + i\eta)\,. \end{aligned}$$

In order to recover easily the correspondence with the standard pseudodifferential calculus of operators $a(\sqrt{h}x, \sqrt{h}D_x)$, it is convenient to set

$$\varepsilon = 2h\,.$$

While specifying the relationship between the usual presentations of the bosonic Fock space and the semiclassical analysis of finite dimensional problems, fixing the normalizations in a coherent way for both approaches is probably the hardest task. Here is a summary of these correspondences:

$\mathcal{Z} = \mathbb{C}^d$	$T^*\mathbb{R}^d$
$\Gamma_s(\mathbb{C}^d)\,,$	$L^2(\mathbb{R}^d)$
$S(z_1, z_2) = \mathrm{Re}\langle z_1, z_2\rangle$	$((x_1,\xi_1)\,,\,(x_2,\xi_2)) = \xi_1.\xi_2 + x_1.x_2 = S(z_1, z_2)$
$\sigma(z_1, z_2) = \mathrm{Im}\langle z_1, z_2\rangle$	$[\![(x_1,\xi_1),(x_2,\xi_2)]\!] = \xi_1.x_2 - x_1.\xi_2 = -\sigma(z_1, z_2)$
$a(z) = a(\sum_{j=1}^d \alpha_j e_j)$	$a(z) = \sum_{j=1}^d \overline{\alpha_j}(\sqrt{h}\partial_{x_j} + \sqrt{h}x_j)$
$a^*(z) = a^*(\sum_{j=1}^d \alpha_j e_j)$	$a^*(z) = \sum_{j=1}^d \alpha_j(-\sqrt{h}\partial_{x_j} + \sqrt{h}x_j)$
$[a(z_1), a^*(z_2)] = \varepsilon\,\langle z_1\,,\,z_2\rangle$	$[a(z_1), a^*(z_2)] = 2h\,\langle z_1\,,\,z_2\rangle$
$\Phi(z_0) = \frac{1}{\sqrt{2}}(a(z_0) + a^*(z_0))$	$\sqrt{2h}(x_0.x + \xi_0.D_x)$
$W(z_0) = e^{i\Phi(z_0)}$	$\tau_{(-\sqrt{2h}\xi_0, \sqrt{2h}x_0)} = e^{i(\sqrt{2h}x_0.x + \xi_0.\sqrt{2h}D_x)}$
$E(z_0) = W(\frac{\sqrt{2}}{i\varepsilon}z_0)\Omega$	$\tau_{(\frac{x_0}{\sqrt{h}}, \frac{\xi_0}{\sqrt{h}})}(\pi^{-d/4}e^{-\frac{x^2}{2}})$
$z_0^{\otimes n}, \lvert z_0\rvert = 1$	Hermite function $(n!)^{-1/2}[z_0.(-\partial_x + x)]^n(\pi^{-d/4}e^{-\frac{x^2}{2}})$
$N = \sum_{j=1}^d a^*(e_j)a(e_j)$	$h(-\Delta + x^2 - d)$

2.2. *Quantizations*

The Wick quantization is defined for any polynomial symbol while following the Wick ordering rule with creation operators on the left-hand side and annihilation operators on the right-hand side. After choosing an orthonormal basis $(e_1, \ldots, e_d)$ in $\mathcal{Z}$, $a^*(e_j)$ is associated with the antilinear form $\overline{z_j} = \langle z\,,\,e_j\rangle$, the annihilation operator $a(e_j)$ with the linear $z_j = \langle e_j\,,\,z\rangle$, and with the polynomial $b(\overline{z}, z) = \sum_{|\alpha|+|\beta|\le m} c_{\alpha,\beta}\overline{z}^\alpha z^\beta$ is associated the operator $b^{Wick} = \sum_{|\alpha|+|\beta|\le m} c_{\alpha,\beta}(a^*)^\alpha a^\beta$. A more intrinsic way can be done by considering for a (p, q)-homogeneous polynomial, the associated sesquilinear form. In *finite dimension*, this amounts to

$$b(\overline{z}, z) = \left\langle z^{\otimes q}\,,\,\tilde{b}z^{\otimes p}\right\rangle\,,\quad \tilde{b} = \frac{1}{p!}\frac{1}{q!}\partial_z^p\partial_{\overline{z}}^q b(\overline{z}, z) \in \mathcal{L}(\bigvee^p \mathcal{Z}, \bigvee^q \mathcal{Z}) \qquad (2.4)$$

The general definition of the unbounded operator b^{Wick} (see for example Derezinski-Gérard[6]), is given by its action on any n-particles sector

$$b^{Wick}_{|\bigvee^n \mathcal{Z}} = 1_{[p,+\infty)}(n) \frac{\sqrt{n!(n+q-p)!}}{(n-p)!} \, \varepsilon^{\frac{p+q}{2}} \, \left(\tilde{b} \bigvee I_{\bigvee^{n-p} \mathcal{Z}} \right) \\ b^{Wick}_{|\bigvee^n \mathcal{Z}} \in \mathcal{L}(\bigvee^n \mathcal{Z}, \bigvee^{n+q-p} \mathcal{Z}) \, . \tag{2.5}$$

The Weyl quantization is defined after considering the Fourier transform of the symbol b,

$$\mathcal{F}[b](z) = \int_{\mathcal{Z}} b(\xi) \; e^{-2\pi i \, S(z,\xi)} \; L(d\xi) \, , \quad b(z) = \int_{\mathcal{Z}} \mathcal{F}[b](z) \; e^{2\pi i \, S(z,\xi)} \; L(dz) \, ,$$

when $L(dz)$ denotes the Lebesgue measure on $\mathcal{Z} = \mathbb{C}^d$. The Weyl quantization (corresponding to the standard definition of $a^{Weyl}(\sqrt{h}x, \sqrt{h}D_x)$, $\varepsilon = 2h$) is then given by

$$b^{Weyl} = \int_{\mathcal{Z}} \mathcal{F}[b](z) \quad W(\sqrt{2}\pi z) \; L(dz) \, . \tag{2.6}$$

After taking good Weyl-Hörmander symbol classes, this makes an algebra with the Moyal product with full asymptotic expansions w.r.t. $\varepsilon > 0$ (see Hörmander,[19] Bony-Chemin,[3] Bony-Lerner,[4] Helffer,[16] Nataf-Nier,[23] Robert[24]). A good choice which contains polynomial symbols is $\cup_{s \in \mathbb{R}} S(\langle z \rangle^s \, , g)$ with $g = dz^2 = dx^2 + d\xi^2$ or $g = \frac{dz^2}{\langle z \rangle^2}$. Moreover for any polynomial symbol, the relationship between the Wick and Weyl quantization is explicit according to

$$b^{Weyl} \left(b * \frac{e^{-\frac{|z|^2}{\varepsilon/2}}}{(\pi\varepsilon/2)^d} \right)^{Wick} \, . \tag{2.7}$$

The Anti-Wick quantization can be defined in different ways. Either by associating with any polynomial symbol $b(\overline{z}, z) = \sum_{|\alpha|+|\beta| \leq m} c_{\alpha,\beta} \overline{z}^{\alpha} z^{\beta}$ the operator $b^{A-Wick} = \sum_{|\alpha|+|\beta| \leq m} c_{\alpha,\beta} a^{\beta} (a^*)^{\alpha}$. Equivalent definitions which make its properties more obvious are given by:

$$b^{A-Wick} = \int_{\mathcal{Z}} b(\xi) \;\; |E(\xi)\rangle\langle E(\xi)| \;\; \frac{L_p(d\xi)}{(\pi\varepsilon)^d} \tag{2.8}$$

$$b^{A-Wick} = \left(b * \frac{e^{-\frac{|z|^2}{\varepsilon/2}}}{(\pi\varepsilon/2)^d} \right)^{Weyl} \tag{2.9}$$

$$= \int_{\mathcal{Z}} \mathcal{F}[b](\xi) \;\; W(\sqrt{2}\pi\xi) \;\; e^{-\frac{\varepsilon\pi^2}{2}|\xi|^2} \; L(d\xi) \, . \tag{2.10}$$

For example, the Anti-Wick quantization appears directly as a non negative quantization in (2.8) while the comparison with the Weyl quantization can be derived from (2.9) or (2.10). In *finite dimension*, all these quantization are asymptotically equivalent in the sense that they are asymptotically equal up to a well controlled $O(\varepsilon)$ term when one deals with good classes of symbols.

2.3. *Mean field or semiclassical asymptotics*

The semiclassical asymptotic can be written

$$\begin{cases} ih\partial_t\psi = p^{Weyl}(\sqrt{h}x, \sqrt{h}D_x)\psi \\ \psi(t=0) = \psi_0^h\,, \end{cases}$$

and there are several ways to handle the limit $h \to 0$:

1a) Use the WKB-ansatz, $\psi(t) = e^{i\frac{S(x,t)}{h}} \sum_{k=0}^{\infty} h^k a_k(x,t)$, when the initial data equals $\psi_0^h = e^{i\frac{S_0(x)}{h}} \sum_{k=0}^{\infty} h^k a_k(x,0)$;

1b) Express more generally $e^{-\frac{it}{h}p(\sqrt{h}x,\sqrt{h}D_x)}$ as a Fourier integral operator;

1c) Express $e^{\frac{it}{h}p(\sqrt{h}x,\sqrt{h}D_x)}b^{Weyl}(\sqrt{h}x,\sqrt{h}D_x)e^{-\frac{it}{h}p(\sqrt{h}x,\sqrt{h}D_x)}$ as an h-pseudodifferential operator with principal part solving $\partial_t b = \{p, b\}$ according the classical Hamiltonian dynamics associated with p;

2) Analyze the propagation of squeezed coherent states when $\psi_0^h = E(z_0)$ also known as the Hepp method;

3) Use Wigner measures which solve $\partial_t\mu + \{p, \mu\} = 0\,.$

We refer the reader for example to Grigis-Sjöstrand,[15] Martinez,[22] Robert[24] for the first approach and to Combescure-Ralston-Robert[5] for the second one in finite dimension and Gérard,[12] Gérard-Markowich-Mauser-Poupaud,[13] Helffer-Martinez-Robert,[17] Lions-Paul[20] for the introduction of Wigner measures.

The bosonic mean field limit writes with $\varepsilon \to 0$ when $\varepsilon = \frac{1}{n}$ and n is the characteristic number of bosons. It is usually written

$$\begin{cases} i\varepsilon\partial_t\psi = p^{Wick}\psi \\ \psi(t=0) = \psi_{z_0} \quad \text{with } \psi_{z_0} = E(z_0) \text{ or } \psi_{z_0} = z_0^{\otimes n}, \quad n = \frac{1}{\varepsilon}\,. \end{cases}$$

The problem is to show

$$\langle \psi(t)\,, A\psi(t)\rangle \overset{\varepsilon\to 0}{\sim} \langle \psi_{z_t}\,, A\psi_{z_t}\rangle$$

where A is any Wick-quantized polynomial $A = b^{Wick}$ and z_t is the solution to the associated classical equation

$$i\partial_t z_t = \partial_{\overline{z}} p(\overline{z_t}, z_t), \qquad z_{t=0} = z_0\,.$$

In the framework of mean field limits, this has been considered first with the Hepp method. This method was actually first developed for the infinite dimensional case by Hepp[18] and Ginibre-Velo.[14] Another approach widely studied consists, when $\psi_{z_0} = z_0^{\otimes n}$, in computing explicitly the evolution of Wick observables tested on such states via a Dyson expansion (see Fröhlich-Graffi-Schwarz,[11] Fröhlich-Knowles-Pizzo,[10] Erdös-Schlein-Yau[7,8]). Both methods work essentially for some specific initial data contrarily to the methods 1b), 1c) and 3) used in the finite dimensional semiclassical framework.

3. Infinite dimensional case

Considering the infinite dimensional case which is the relevant one within the mean field theory presents some well known difficulties. First of all building a good pseudodifferential calculus is not so trivial and the different approaches carry different pieces of information. Even when a good pseudodifferential algebra is built, it has to be preserved by nonlinear deformations according to the mean field dynamics. In the infinite dimensional case, this essentially never happens.

There are essentially two ways to consider the extension of the pseudodifferential calculus in infinite dimension: one is inductive and occurs within the problems of thermodynamical limits, the other one is projective and fits better with a stochastic processes point of view. The first one consists in having a good control of phase-space integrals like (2.6), (2.8), (2.10), with respect to the dimension or by replacing the Lebesgue measure with Gaussian measures. The quasi-equivalence of two Gaussian measures is ensured by some Hilbert-Schmidt condition which occurs in the presentation by Lascar[21] of some infinite dimensional pseudodifferential calculus and is reminiscent of Shale's theorem. Such Hilbert-Schmidt conditions do not ensure that all the infinite dimensional phase space is well explored and brings difficulties after applying a nonlinear Hamiltonian dynamics.

The second one relies on the tensor decomposition

$$\Gamma_s(\mathcal{Z}) \sim \Gamma_s(p\mathcal{Z}) \otimes \Gamma_s(p^\perp \mathcal{Z}) \tag{3.1}$$

with

$$W(\xi + \xi') = W(\xi)W(\xi') = W_p(\xi) \otimes W_{p^\perp}(\xi') \quad \text{when } \xi \in p\mathcal{Z}\,,\ \xi' \in p^\perp \mathcal{Z}\,, \tag{3.2}$$

where p is any finite rank orthogonal projection and $p^\perp = 1 - p$ (the tensor product is the Hilbert tensor product). Hence it is possible to define cylindrical Weyl (resp. Anti-Wick) observable by restricting the integral (2.6)

(resp. (2.10)), and testing with such an observable corresponds to tracing out (or integrating) with respect to all the directions but $p\mathcal{Z}$.

This distinction can be considered within the Wick quantization of polynomial symbols. Actually it is contained in the discussion of what is the right continuity assumption for polynomials $b(\overline{z}, z) = \left\langle z^{\otimes q}, \tilde{b} z^{\otimes p} \right\rangle$ which amounts to the right notion of completed tensor product. The Hilbert-Schmidt condition would say that $\tilde{b} \in \mathcal{L}^2(\bigvee^p \mathcal{Z}, \bigvee^q \mathcal{Z})$ is a Hilbert-Schmidt operator ($\mathcal{L}^p(E, F)$ denotes the p-Schatten class and $\mathcal{L}^\infty(E, F)$ the set of compact operators). The condition (2.4) actually provides the right algebra property and it is a mixture of Hilbert-Schmidt (the symmetric tensor products $\bigvee^p \mathcal{Z}$ and $\bigvee^p \mathcal{Z}$ are Hilbert tensor products) and projective topology ($\tilde{b}$ is a general bounded operator). Here again the difficulty comes from the fact that a nonlinear Hamiltonian dynamics does not preserve the class of polynomial symbols.

Although the possible pseudodifferential calculi do not lead in infinite dimension to good notions of Fourier integral operators and yet do not allow nonlinear deformations, some results about the mean field dynamics are available via the Hepp method (see Hepp,[18] Ginibre-Velo[14]) or via the truncated Dyson expansion approach (see Erdös-Schlein-Yau,[7,8] Fröhlich-Graffi-Schwarz,[11] Fröhlich-Knowles-Pizzo[10]). The most flexible way to approach the semiclassical limit, that is Wigner measures, allows to clarify the situation in infinite dimension.

Wigner measures are easily defined with the Weyl and Anti-Wick quantization within the projective approach according to (2.6), (2.10), (3.2). When the trace class operator $\varrho \geq 0$ on $\mathcal{H}$ with $\mathrm{Tr}[\varrho] = 1$, the family of probability measures defined by duality according to

$$\mathrm{Tr}\left[\varrho(b^{A-Wick} \otimes \mathrm{Id}_{\Gamma_s(p^\perp \mathcal{Z})})\right] \int_{p\mathcal{Z}} b(z) d\mu(z)$$

on any finite dimensional subspace $p\mathcal{Z}$, is a projective family of probability measures also called a weak distribution. When the phase space $\mathcal{Z}$ is separable and under the additional assumption that $\mathrm{Tr}\left[(1+N)^{\delta/2} \varrho^\varepsilon (1+N)^{\delta/2}\right]$ is uniformly bounded w.r.t $\varepsilon \in (0, \bar{\varepsilon})$ for some $\delta > 0$, it is possible to carry out the diagonal extraction process which leads to the definition of the Wigner measure. Moreover such an asymptotic weak distribution is actually a Radon measure on the infinite dimensional phase space $\mathcal{Z}$ (see Skohorod,[26] Schwartz[25]).

Theorem 3.1. *Assume that $\mathcal{Z}$ is a separable Hilbert space. Let $(\varrho^\varepsilon)_{\varepsilon \in (0, \bar{\varepsilon})}$ be a family of normal states on $\mathcal{L}(\mathcal{H})$ parametrized by ε. Assume*

$\mathrm{Tr}[N^{\delta/2}\rho^\varepsilon N^{\delta/2}] \leq C_\delta$ *uniformly w.r.t.* $\varepsilon \in (0,\overline{\varepsilon})$ *for some fixed* $\delta > 0$ *and* $C_\delta \in (0,+\infty)$. *Then for every sequence* $(\varepsilon_n)_{n\in\mathbb{N}}$ *with* $\lim_{n\to\infty}\varepsilon_n = 0$ *there exists a subsequence* $(\varepsilon_{n_k})_{k\in\mathbb{N}}$ *and a Borel probability measure* μ *on* $\mathcal{Z}$ *such that*

$$\lim_{k\to\infty} Tr[\rho^{\varepsilon_{n_k}} b^{Weyl}] \lim_{k\to\infty} Tr[\rho^{\varepsilon_{n_k}} b^{A-Wick}] \int_{\mathcal{Z}} b(z)\, d\mu(z)\,,$$

for all cylindrical functions $b \in \cup_{p\in\mathbb{P}} \mathcal{F}^{-1}\left(\mathcal{M}_b(p\mathcal{Z})\right)$ *of which the Fourier transform is a bounded measure (*$\mathbb{P}$ *is the set of orthogonal projections with a finite rank).*

Moreover this probability measure μ *satisfies* $\displaystyle\int_{\mathcal{Z}} |z|^{2\delta}\, d\mu(z) < \infty$.

Definition 3.1. For a family $(\varrho^\varepsilon)_{\varepsilon\in(0,\overline{\varepsilon})}$ which satisfy the assumptions of Theorem 3.1, $\mathcal{M}(\varrho^\varepsilon)$ denotes the set of all its Wigner measures defined after extracting a subsequence $\varepsilon_{n_k} \to 0$.

Once these asymptotic objects are defined it is possible to handle them and to compare the action of different quantizations (the comparison of Weyl and Anti-Wick quantized cylindrical observables is contained in the theorem), of different kinds of results (Hepp method, truncated Dyson expansion) and of different points of view (inductive or projective). For every questions several limits have to be considered: the limit $\varepsilon \to 0$, the limit with respect to the dimension going to or being infinite and possibly the limit due to an approximation process which allows to switch from one kind of observables to another (cylindrical, polynomial). The order of taking the limits is often crucial and makes the analysis non trivial. For example, the asymptotic equivalence of quantizations is only partially true.

Proposition 3.1. *Assume the uniform estimate*

$$\left|(1+N)^{\delta/2}\varrho^\varepsilon(1+N)^{\delta/2}\right|_{\mathcal{L}^1(\mathcal{H})} \leq C_\delta \text{ for all } \delta > 0$$

and further that the family $(\varrho^\varepsilon)_{\varepsilon\in(0,\overline{\varepsilon})}$ *has a unique Wigner measure* μ *as* $\varepsilon \to 0$. *Then the limit*

$$\lim_{\varepsilon\to 0} Tr\left[\beta^{Wick}\varrho^\varepsilon\right] = \int_{\mathcal{Z}} \beta(z)\, d\mu(z)$$

holds for any polynomial $\beta(\overline{z},z) = \left\langle z^{\otimes q}\,,\, \tilde{\beta} z^{\otimes p}\right\rangle$, *with a* compact *kernel* $\tilde{\beta} \in \mathcal{L}^\infty(\bigvee^p \mathcal{Z}, \bigvee^q \mathcal{Z})$.

Dimensional defect of compactness: The restriction

$$\beta \in \mathcal{L}^\infty(\bigvee^p \mathcal{Z}, \bigvee^q \mathcal{Z})$$

is not an artefact of our approach. It accounts for what we called the dimensional defect of compactness. Here is the basic example: Take an orthonormal basis $(e_j)_{j\in\mathbb{N}}$ of $\mathcal{Z}$ and consider for ϱ^ε the projector

$$\varrho^\varepsilon = |E(e_{[1/\varepsilon]})\rangle\langle E(e_{[1/\varepsilon]})|$$

when $[1/\varepsilon]$ denotes the integer part of $1/\varepsilon$. This family admits the unique Wigner measure δ_0 as $\varepsilon \to 0$. For any Wick quantized polynomial with a compact kernel

$$\lim_{\varepsilon\to 0} \left\langle E(e_{[1/\varepsilon]}) \, , b^{Wick} E(e_{[1/\varepsilon]}) \right\rangle = 0 \, .$$

But taking $b^{Wick} = N$, that is $b(z) = |z|^2$ gives

$$\left\langle E(e_{[1/\varepsilon]}) \, , b^{Wick} E(e_{[1/\varepsilon]}) \right\rangle = \langle E(e_j) \, , NE(e_j) \rangle = 1 \, .$$

4. Applications

Three applications have been given with details in Ammari-Nier.[2]

(1) Reconsidering the thermodynamic limit of the ideal Bose gas as a small parameter limit allows to reconsider the Bose-Einstein condensation phenomenon. It provides an interesting illustration of the dimensional defect of compactness.

(2) It is possible to specify the relationship between various approaches and various results about mean field limits. For example a slightly weaker version of the propagation of chaos, that is for products states $|z^{\otimes n}\rangle\langle z^{\otimes n}|$ tested on Wick observables, can be derived from the result given by the Hepp method for coherent states.

Theorem 4.1. *Let U_ε be a unitary operator on $\mathcal{H}$ possibly depending on $\varepsilon \in (0, \bar{\varepsilon})$ which commutes with the number operator $[N, U_\varepsilon] = 0$. Assume that for a given $z \in \mathcal{Z}$ such that $|z| = 1$, there exists $z_U \in \mathcal{Z}$ such that*

$$\mathcal{M}\left(|U_\varepsilon E(z)\rangle\langle U_\varepsilon E(z)|\right) = \{\delta_{z_U}\} \, .$$

Then for any non negative function $\varphi \in L^1(\mathbb{R}, ds)$ such that $\int_{\mathbb{R}} \varphi(s)(1+|s|)^\delta \, ds < \infty$ for some $\delta > 0$ and $\int_{\mathbb{R}} \varphi(s) \, ds = 1$, the family

$$\varrho^\varepsilon_\varphi = \sum_{n=0}^{\infty} \varepsilon^{1/2} \varphi(\varepsilon^{1/2}(n - \varepsilon^{-1}))|U_\varepsilon z^{\otimes n}\rangle\langle U_\varepsilon z^{\otimes n}|$$

admits a unique Wigner measure

$$\mathcal{M}\left(\varrho^\varepsilon_\varphi\right)\frac{1}{2\pi}\int_0^{2\pi}\delta_{e^{i\theta}z_U}\;d\theta\,.$$

(3) Non trivial superpositions: It is possible to derive from the results obtained for the mean field dynamics of coherent states or product states, the mean field dynamics of non trivial superposition of states. For example the Wigner measure allows to use some orthogonality of measures arguments.

Proposition 4.1. *Assume that the family of vectors* $(u^\varepsilon)_{\varepsilon\in(0,\overline{\varepsilon})}$ *and* $(v^\varepsilon)_{\varepsilon\in(0,\overline{\varepsilon})}$ *satisfy the uniform estimates*

$$\left|(1+N)^{\delta/2}u^\varepsilon\right|_{\mathcal{H}}+\left|(1+N)^{\delta/2}v^\varepsilon\right|_{\mathcal{H}}\leq C\quad,\quad |u^\varepsilon|_{\mathcal{H}}=|v^\varepsilon|_{\mathcal{H}}=1$$

for some fixed $\delta>0$ *and* $C>0$. *Set*

$$\varrho^\varepsilon_{uv}=|u^\varepsilon\rangle\langle v^\varepsilon|\,.$$

Assume further that any $\mu\in\mathcal{M}(\varrho^\varepsilon_{uu})$ *and any* $\nu\in\mathcal{M}(\varrho^\varepsilon_{vv})$ *are mutually orthogonal. Then the family* $(\varrho^\varepsilon_{uv})_{\varepsilon\in(0,\overline{\varepsilon})}$ *is pure with*

$$\mathcal{M}(\varrho^\varepsilon_{uv},\varepsilon\in(0,\overline{\varepsilon}))=\{0\}$$
$$\textit{i.e.}\lim_{\varepsilon\to0}\left\langle u^\varepsilon\,,\,b^{Weyl}v^\varepsilon\right\rangle\lim_{\varepsilon\to0}\left\langle u^\varepsilon\,,\,b^{A-Wick}v^\varepsilon\right\rangle=0$$

for any $b\in\mathcal{F}^{-1}(\mathcal{M}_b(p\mathcal{Z}))$ *and any* $p\in\mathbb{P}$.

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VARIATIONAL PRINCIPLE FOR HAMILTONIANS WITH DEGENERATE BOTTOM

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Perturbations of Hamiltonians whose Fourier symbol attains its minimum along a hypersurface are considered. Such operators arise in several domains, like spintronics, theory of superconductivity, or theory of superfluidity. Variational estimates for the number of eigenvalues below the essential spectrum in terms of the perturbation potential are provided.

Keywords: Schrödinger operator, variational principle, Fourier symbol

1. Introduction

We are studying quantum Hamiltonians $H = H_0 + V$ acting on $L^2(\mathbb{R}^n)$, $n \geq 2$, where V is a potential and H_0 is a self-adjoint (pseudodifferential) operator whose Fourier symbol $H_0(p)$ attains its minimal value on a certain $(n-1)$-dimensional submanifold of $\mathbb{R}^n$ (surface of extrema). A possible example for H_0 is the Hamiltonian

$$H_0(p) = \Delta + \frac{\big(|p| - p_0\big)^2}{2\mu}, \quad \Delta, \mu, p_0 > 0, \quad p \in \mathbb{R}^3, \tag{1.1}$$

arising in the study of the roton spectrum in liquid helium II[1] and introduced by Landau.[2] Another example can be the three-dimensional Hamiltonian

$$H_0(p) = (p^2 - \mu)\frac{e^{\beta(p^2-\mu)} + 1}{e^{\beta(p^2-\mu)} - 1}, \quad \mu, \beta > 0, \tag{1.2}$$

which has appeared very recently in the theory of superconductivity;[3,4] we refer to the papers cited for the physical meaning of all the constants.

Similar situations appear in the study of matrix Hamiltonians related to the spintronics (see below) and in the elasticity theory.[5] We will be interested in situations when V is has a short range (in a suitable sense) and does not change the bottom of the essential spectrum, hence one arrives at a couple of questions concerning the eigenvalues lying below the threshold. A rather detailed analysis of the eigenvalues can be carried out using the constructions of Laptev-Safronov-Weidl, see Ref. 6.

Our aim here is more methodological. It is a classical result that the existence of a negative eigenvalue for the Schrödinger operator $-\Delta + V$ in dimensions one and two is guaranteed by the condition $\int V(x)dx < 0$. We are going to find some analogs of these conditions for the above Hamiltonians, in particular, estimates for the number of discrete eigenvalues below the threshold. While estimates of this kind along with a more detailed spectral information could, in principle, be achieved using more sophisticated methods of Ref. 6, they can be useful for an a priori analysis; moreover, this provides an intuitive illustration of the role of one-dimensional dynamics in the direction transversal to the surface of extrema and shows the origin of an infinite discrete spectrum appearing under negative perturbations.

It seems that the presence of an infinite discrete spectrum in the physics literature in such a setting has been observed first rather recently in Ref. 7 on example of rotationally invariant perturbations of the Rashba Hamiltonian. In Refs. 8,9 we gave a rigorous justification for a class of spin-orbit Hamiltonians and rather general potentials, including distributional interactions and interactions supported by null sets, using variational arguments and specific test functions for two-dimensional systems. Here we develop this idea in a different direction and use the one-dimensional character of the dynamics in the direction transversal to the surface of extrema to construct another type of test functions using exact eigenfunctions of a certain integral operator.

2. Assumptions and basic construction

Let us list our assumptions. Below we consider a self-adjoint operator $H_0 = H_0(-i\nabla)$, where $\mathbb{R}^n \ni p \mapsto H_0(p) \in \mathbb{R}$ is a semibounded below continuous function attaining its minimum value $\min H_0 = m$. Denote $\Gamma = \{p \in \mathbb{R}^n : H_0(p) = m\}$; we will assume that for some domain $\Omega \subset \mathbb{R}^n$ the intersection $S = \Omega \cap \Gamma$ is a smooth $(n-1)$-dimensional submanifold of $\mathbb{R}^n$ (in general, with boundary); by ω we denote the induced volume form on S. Without loss of generality we assume that $\overline{S}$ is compact and orientable (otherwise one can take a smaller Ω). We also suppose that H_0 is twice continuously

differentiable near S.

For both the Hamiltonians (1.1) and (1.2) one takes $\Omega = \mathbb{R}^3$. For the example of Eq. (1.1), one has $m = 0$ and S is the sphere of radius p_0 centered at the origin. In Eq. (1.1) one has $m = 2\beta^{-1}$ and S is the sphere of radius $\sqrt{\mu}$ centered at the origin.

Consider a real-valued potential $V \in L^1(\mathbb{R}^n)$. We will assume that the operator $H = H_0 + V$ defined as a form sum is self-adjoint with

$$\inf \operatorname{spec}_{\mathrm{ess}}(H_0 + V) = \inf \operatorname{spec}_{\mathrm{ess}} H_0 = m. \tag{2.1}$$

For both the Hamiltonians (1.1) and (1.2) the assumption (2.1) holds for $V \in L^{3/2}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$; indeed, such V is relatively compact with respect to the Laplacian. As the difference ($H_0 -$ Laplacian) is infinitely small with respect to the Laplacian, V is a relatively compact perturbation of H_0 as well.

In what follows we will work in the p-representation. The operator H is then associated with the bilinear form

$$\langle f, Hf\rangle = \int_{\mathbb{R}^n} H_0(p)|f(p)|^2 dp + \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} \hat{V}(p-p')\overline{f(p)}f(p')dp\,dp',$$

where $\hat{V}$ is the Fourier transform of V; in our case $\hat{V}$ is a bounded continuous function due to $V \in L^1(\mathbb{R}^n)$. By $\mathcal{V}$ we denote the operator on $L^2(S,\omega)$ acting by the rule

$$\mathcal{V}f(s) = \int_S \hat{V}(s-s')f(s')\omega(ds').$$

Theorem 2.1. *The number of eigenvalues of H below m is not less than the number of negative eigenvalues for $\mathcal{V}$ counting multiplicities.*

Proof. Let $n(s)$ be a unit normal vector to S at a point $s \in S$ and depend on s continuously. For $r > 0$ consider the map $\sigma : S \times (-r,r) \to \mathbb{R}^n$, $(s,t) \mapsto s + tn(s)$; we choose r sufficiently small in order that L becomes a diffeomorphism between $S \times (-r,r)$ and $\sigma\big(S \times (-r,r)\big)$. Note that due to $H_0 \in C^2$ one has $H_0\big(\sigma(s,t)\big) - m \le Ct^2$ for $t \to 0$ with some $C > 0$ independent of s and that $\sigma(s,0) = s$ for any $s \in S$.

Consider two arbitrary function $\Psi_1, \Psi_2 \in L^2(S,\omega)$. Take $\varphi \in C_0^\infty(\mathbb{R})$ with $\int \varphi = 1$ and $\varepsilon > 0$. Consider functions $f_j^\varepsilon \in L^2(\mathbb{R}^n)$ given by

$$f_j^\varepsilon(p) = \begin{cases} \varepsilon^{-1}\,\varphi(\varepsilon^{-1}t)\Psi_j(s), & p = \sigma(s,t), \quad (s,t) \in S \times (-r,r), \\ 0, & \text{otherwise.} \end{cases} \tag{2.2}$$

Clearly,

$$\langle f_1^\varepsilon, (H-m) f_2^\varepsilon\rangle = \int_{\mathbb{R}^n} \overline{f_1^\varepsilon(p)}\big(H_0(p)-m\big) f_2^\varepsilon(p)dp + \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} \hat V(p-p')\overline{f_1^\varepsilon(p)} f_2^\varepsilon(p')\,dp\,dp'.$$

One has $dp = \rho(s,t)\omega(ds)dt$ with $\rho(s,t) = 1 + O(t)$ for $t \to 0$ uniformly in $s \in S$, hence

$$\begin{aligned}
&\left| \int_{\mathbb{R}^n} \big(H_0(p)-m\big)\overline{f_1^\varepsilon(p)} f_1^\varepsilon(p)dp \right| \\
&= \left| \varepsilon^{-2}\int_{-r}^{r}\int_S \Big(H_0\big(\sigma(s,t)\big)-m\Big)\big|\varphi(\varepsilon^{-1}t)\big|^2\overline{\Psi_1(s)}\Psi_2(s)\rho(s,t)\omega(ds)dt \right| \\
&\le C\left| \int_{-r}^{r}\int_S \varepsilon^{-2}t^2\big|\varphi(\varepsilon^{-1}t)\big|^2\overline{\Psi_1(s)}\Psi_2(s)\rho(s,t)\omega(ds)dt \right| \\
&\le C\varepsilon\left| \int_{-r/\varepsilon}^{r/\varepsilon}\int_S t^2\big|\varphi(t)\big|^2\overline{\Psi_1(s)}\Psi_2(s)\rho(s,\varepsilon t)\omega(ds)\,dt \right| = O(\varepsilon).
\end{aligned}$$

On the other hand, for any bounded continuous function $v : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ one has

$$\begin{aligned}
&\int_{\mathbb{R}^n}\int_{\mathbb{R}^n} v(p,p')\overline{f_1^\varepsilon(p)} f_2^\varepsilon(p')\,dp\,dp' \\
&= \varepsilon^{-2}\int_{-r}^{r}\int_{-r}^{r}\int_S\int_S v\big(\sigma(s,t),\sigma(s',t')\big)\overline{\varphi(\varepsilon^{-1}t)}\varphi(\varepsilon^{-1}t') \\
&\quad\times\overline{\Psi_1(s)}\Psi_2(s')\rho(s,t)\rho(s',t')\,\omega(ds)\omega(ds')dt\,dt' \\
&= \int_{-r/\varepsilon}^{r/\varepsilon}\int_{-r/\varepsilon}^{r/\varepsilon}\int_S\int_S v\big(\sigma(s,\varepsilon t),\sigma(s',\varepsilon t')\big)\overline{\varphi(t)}\varphi(t') \\
&\quad\times\overline{\Psi_1(s)}\Psi_2(s')\rho(s,\varepsilon t)\rho(s',\varepsilon t')\,\omega(ds)\omega(ds')dt\,dt' =: I(\varepsilon).
\end{aligned} \tag{2.3}$$

Due to the obvious estimate

$$\begin{aligned}
&\left| \int_S\int_S v\big(\sigma(s,\varepsilon t),\sigma(s',\varepsilon t')\big)\overline{\Psi_1(s)}\Psi_2(s')\rho(s,\varepsilon t)\rho(s',\varepsilon t')\,\omega(ds)\omega(ds')\right| \\
&\qquad\le \tilde C\int_S \big|\Psi_1(s)\big|\omega(ds)\int_S|\Psi_2(s)|\omega(ds)
\end{aligned}$$

with $\tilde C = \sup_{p,p'\in\mathbb{R}^n}|v(p,p')|\sup_{(s,t)\in S\times(-r,r)}|\rho(s,t)|$, one has, by the Lebesgue dominated convergence,

$$\begin{aligned}
\lim_{\varepsilon\to0} I(\varepsilon) &= \int_S\int_S v\big(\sigma(s,0),\sigma(s',0)\big)\overline{\Psi_1(s)}\Psi_2(s')\omega(ds)\omega(ds') \\
&= \int_S\int_S v(s,s')\overline{\Psi_1(s)}\Psi_2(s')\omega(ds)\omega(ds').
\end{aligned} \tag{2.4}$$

Taking $v(p,p') = \hat{V}(p-p')$, we have shown that for any $\Psi_1, \Psi_2 \in L^2(S,\omega)$ and the functions f_1^ε, f_2^ε given by Eq. (2.2) one has

$$\lim_{\varepsilon\to 0}\langle f_1^\varepsilon, (H-m) f_2^\varepsilon\rangle = \langle \Psi_1, \mathcal{V}\Psi_2\rangle. \tag{2.5}$$

Assume now that $\mathcal{V}$ has N negative eigenvalues $E_1,\dots,E_N$ and let $\Psi_1,\dots,\Psi_N$ be the corresponding normalized eigenfunctions orthogonal to each other. Consider the functions f_j^ε, $j=1,\dots,N$, given by the expressions (2.2). Then, by Eq. (2.5), the matrix $h(\varepsilon) = \big(\langle f_j^\varepsilon, (H-m) f_k^\varepsilon\rangle\big)$ converges to $\mathrm{diag}(E_1,\dots,E_N)$. In particular, $h(\varepsilon)$ is negative definite for sufficiently small ε, which means, by the variational principle, that H has at least N eigenvalues below m. □

3. Estimates for the number of eigenvalues

Due to the obvious estimate

$$\int_S\int_S |\hat{V}(s-s')|^2 \omega(ds)\,\omega(ds') < \infty$$

$\mathcal{V}$ is a Hilbert-Schmidt operator and hence compact, which implies $\mathrm{spec}_{\mathrm{ess}}\,\mathcal{V} = \{0\}$.

Theorem 3.1. *If $V \le 0$ and $V \not\equiv 0$, then the discrete spectrum of $\mathcal{V}$ consists of an infinite sequence of negative eigenvalues converging to* 0*, and* 0 *is not an eigenvalue.*

Proof. Let $f \in L^2(S,\omega)$. One has

$$\begin{aligned}\langle f, \mathcal{V} f\rangle &= \int_S\int_S \hat{V}(s-s')\overline{f(s)} f(s')\omega(ds)\omega(ds') \\ &= \frac{1}{(2\pi)^{n/2}}\int_S\int_S\int_{\mathbb{R}^n} V(x) e^{i\langle s'-s,x\rangle}\overline{f(s)} f(s') dx\,\omega(ds)\,\omega(ds') \\ &= \frac{1}{(2\pi)^{n/2}}\int_{\mathbb{R}^n} V(x)\big|g(x)\big|^2\,dx \le 0\end{aligned}$$

with

$$g(x) := \int_S f(s) e^{-i\langle s,x\rangle}\omega(ds). \tag{3.1}$$

Therefore, $\mathrm{spec}\,\mathcal{V} \subset (-\infty, 0]$.

Assume that $\langle f, \mathcal{V} f\rangle = 0$ for some f. The function g in Eq. (3.1) is analytic as the Fourier transform of the compactly supported (and hence tempered) distribution $(2\pi)^{n/2} f(s)\delta_S(s)$, where δ_S is the Dirac measure

concentrated on S. To have $\langle f, \mathcal{V}f\rangle = 0$ the function g must vanish on a set of non-zero Lebesgue measure (the support of V) and hence, due to the analyticity, must vanish everywhere. As the Fourier transform is a bijection on the set of the tempered distributions, this means $f = 0$. Therefore, 0 cannot be an eigenvalue of $\mathcal{V}$, and it remains to recall that $\mathcal{V}$ is a compact operator in a Hilbert space of infinite dimension. □

Combining Theorems 2.1 and 3.1 one arrives at

Corollary 3.1. *If $V \leq 0$ and $V \not\equiv 0$, then H has infinitely many eigenvalues below the essential spectrum.*

If the condition $V \leq 0$ does not hold, one still can try to estimate the number of negative eigenvalues for $\mathcal{V}$ using the values of the Fourier transform at some points. Due to $\operatorname{spec}_{\mathrm{ess}} \mathcal{V} = \{0\}$ the number of negative eigenvalues for $\mathcal{V}$ can be estimated using the variational principle as well.

Theorem 3.2. *Let $N \in \mathbb{N}$. Assume that there exist points $s_j \in S$, $j = 1, \dots, N$, such that the matrix $\big(\hat{V}(s_j - s_k)\big)$ is negative definite, then V has at least N negative eigenvalues and hence H has at least N eigenvalues below m.*

Proof. Fix some neighborhoods $S_j \subset S$ of s_j such that there exist diffeomorphisms $J_j : B \to S_j$, where B is the unit ball centered at the origin in $\mathbb{R}^{n-1}$. Without loss of generality we assume $J_j(0) = s_j$. Let us take functions $\varphi_j \in C_0^\infty(\mathbb{R}^{n-1})$ with $D_j(0) \int \varphi_j = 1$, where D_j is the Jacobian for J_j, $j = 1, \dots, N$. Denote $\Psi_j^\varepsilon(s) = \varepsilon^{1-n} \varphi_j(\varepsilon^{-1} J_j^{-1}(s)) \chi_B(J_j^{-1}(s))$ where χ_B stands for the characteristic function of B. Clearly, $\Psi_j^\varepsilon \in L^2(S, \omega)$. One has

$$\begin{aligned}
\langle \Psi_j^\varepsilon, \mathcal{V}\Psi_k^\varepsilon\rangle &= \int_S \int_S \overline{\Psi_j^\varepsilon(s)} \hat{V}(s - s') \Psi_k^\varepsilon(s') \omega(ds)\, \omega(ds') \\
&= \varepsilon^{2-2n} \int_B \int_B \overline{\varphi_j(\varepsilon^{-1}u)} \hat{V}\big(J_j(u) - J_k(u')\big) \varphi_k(\varepsilon^{-1}u) D_j(u) D_k(u') du\, du' \\
&= \int_{B/\varepsilon} \int_{B/\varepsilon} \overline{\varphi_j(u)}\, \hat{V}\big(J_j(\varepsilon u) - J_k(\varepsilon u')\big) \varphi_k(u') D_j(\varepsilon u) D_k(\varepsilon u') du\, du' \\
&\overset{\varepsilon \to 0}{\longrightarrow} \hat{V}(s_j - s_k).
\end{aligned}$$

Therefore, the matrix $\big(\langle \Psi_j^\varepsilon, \mathcal{V}\Psi_k^\varepsilon\rangle\big)$ is negative definite for small ε. The rest follows from the variational principle and Theorem 2.1. □

Taking $N = 1$ in Theorem 3.2 we obtain a simple condition resembling that for perturbations of the Laplacian in one and two dimensions.

Corollary 3.2. *If*

$$\int_{\mathbb{R}^n} V(x)dx < 0,$$

then H has at least one eigenvalue below m.

We note that Corollary 3.1 can be also obtained from Theorem 3.2 because for $V \le 0$ and $V \not\equiv 0$ the matrix $\big(\hat{V}(s_j - s_k)\big)$ is negative definite for any choice and any number of mutually distinct points $s_j \in \mathbb{R}^n$ by the Bochner theorem.

4. Matrix Hamiltonians

The above constructions can be also applied to a class of matrix Hamiltonians. Namely, consider an operator H_0 acting in $L^2(\mathbb{R}^n) \otimes \mathbb{C}^d$ whose Fourier symbol in the multiplication by a $d \times d$ Hermitian matrix $H_0(p)$. Then there exist unitary matrices $U(p)$, $p \in \mathbb{R}^n$, and real-valued continuous functions $p \mapsto \lambda_1(p)$, $\dots$, $p \mapsto \lambda_d(p)$ with $\lambda_1(p) \le \lambda_2(p) \le \dots \le \lambda_d(p)$ such that

$$H_0(p) = U(p) \operatorname{diag}\big(\lambda_1(p), \dots, \lambda_d(p)\big) U^*(p). \tag{4.1}$$

We assume that $\lambda_1(p)$ satisfies the same conditions as the symbol $H_0(p)$ in the scalar case. We will use the same notation; in particular, $\min \lambda_1(p) = \inf \operatorname{spec} H_0 = m$.

A class of such matrix operators is delivered by spin-orbit Hamiltonians[10] acting in $L^2(\mathbb{R}^2) \otimes \mathbb{C}^2$ and given by the matrices

$$H_0(p) = \begin{pmatrix} p^2 & a(p) \\ \overline{a(p)} & p^2 \end{pmatrix} \tag{4.2}$$

with some linear functions a. In particular, the case $a(p) = \alpha(p_2 + ip_1)$ corresponds to the Rashba Hamiltonian,[11] and $a(p) = -\alpha(p_1 + ip_2)$ gives the Dresselhaus Hamiltonian;[12] in both cases α is a non-zero constant. Here one has $\lambda_1(p) = p^2 - \big|a(p)\big|$, and the minimum $-\alpha^2/4$ is attained at the circle $|p| = |\alpha|/2$.

Again consider a *scalar* real-valued potential $V \in L^1(\mathbb{R}^n)$. Assume that the operator $H_0 + V$ defined through the form sum is self-adjoint and that $\inf \operatorname{spec}_{\mathrm{ess}}(H_0 + V) = \inf \operatorname{spec}_{\mathrm{ess}} H_0 = m$. The preservation of the essential spectrum for the above Rashba and Dresselhaus Hamiltonians is guaranteed, e.g. for $V \in L^1(\mathbb{R}^2) \cap L^2(\mathbb{R}^2)$, which is achieved by comparison with the two-dimensional Laplacian.

Also in this case we can prove an analogue of Corollary 3.1.

Theorem 4.1. *Let $V \le 0$ and $V \not\equiv 0$, then the matrix Hamiltonian H has infinitely many eigenvalues below m.*

Proof. The proof follows the construction in the proof of Theorem 2.1. Consider the vector $h = (1, 0, \dots, 0)^T \in \mathbb{C}^d$, and for $\varepsilon > 0$ denote $F_j^\varepsilon(p) = U(p) f_j^\varepsilon(p) h$ with the functions f_j^ε from Eq. (2.2). Then by Eq. (4.1) one has

$$\langle F_j^\varepsilon, (H-m) F_k^\varepsilon \rangle = \int_{\mathbb{R}^n} \lambda_1(p)\, \overline{f_j^\varepsilon(p)} f_k^\varepsilon(p) dp + \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} \hat V(p-p') \langle U(p)h, U(p')h\rangle \overline{f_j^\varepsilon(p)} f_k^\varepsilon(p')\, dp\, dp'.$$

By Eqs. (2.3) and (2.4), there holds

$$\lim_{\varepsilon\to 0} \langle F_j^\varepsilon, (H-m) F_k^\varepsilon\rangle = \int_S\int_S \hat V(s-s') \big\langle U(s)h, U(s')h\big\rangle \overline{\Psi_1(s)} \Psi_2(s')\, \omega(ds)\, \omega(ds').$$

By the same arguments as in the proof of Theorem 2.1, the number of eigenvalues of H below m is not less than the number of negative eigenvalues of the operator $\mathcal{U}$ acting on $L^2(S,\omega)$ and given by

$$\mathcal{U} f(s) = \int_S \hat V(s-s') \big\langle U(s)h, U(s')h\big\rangle f(s) ds'.$$

Again, $\mathcal{U}$ is a compact operator by

$$\int_S\int_S \Big|\hat V(s-s') \big\langle U(s)h, U(s')h\big\rangle\Big|^2 \omega(ds)\, \omega(ds') \le \int_S\int_S \big|\hat V(s-s')\big|^2 \omega(ds)\, \omega(ds') < \infty.$$

Let us show that all eigenvalues of $\mathcal{U}$ are negative (this, like in Theorem 3.1, will mean that $\mathcal{U}$ has an infinite number of negative eigenvalues). For $f \in L^2(S,\omega)$ one has

$$\begin{aligned} \langle f, \mathcal{U} f\rangle &= \int_S\int_S \hat V(s-s') \big\langle U(s)h, U(s')h\big\rangle \overline{f(s)} f(s') \omega(ds)\omega(ds') \\ &= \int_S\int_S\int_{\mathbb{R}^n} \frac{V(x) e^{i\langle s'-s, x\rangle}}{(2\pi)^{n/2}} \big\langle U(s)h, U(s')h\big\rangle \overline{f(s)} f(s') dx\, \omega(ds)\, \omega(ds') \quad (4.3) \\ &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} V(x) \big|g(x)\big|^2 dx \le 0 \end{aligned}$$

with

$$g(x) := \int_S U(s) f(s) h e^{-i\langle s, x\rangle} \omega(ds).$$

It remains to show that 0 is not an eigenvalue of $\mathcal{U}$. Assuming $\mathcal{U}f = 0$ we obtain from Eq. (4.3) that g vanishes on the support of V having non-zero Lebesgue measure. As g is again the Fourier transform of a compactly supported distribution and hence analytic, it must vanish everywhere, which means that the vector function $s \mapsto U(s)f(s)h$ is zero a.e. As the matrix $U(s)$ is unitary for any s, this means $f = 0$. □

We note that Corollary 3.1 and Theorem 3.2 for the Rashba and Dresselhaus Hamiltonians were shown in Ref. 8 using special test functions for two-dimensional operators.[13] The above analysis can be extended to the case when the perturbation V is not a potential, but a measure with some regularity conditions. For the Hamiltonians (4.2) one can still prove the infiniteness of the discrete spectrum for perturbations by negative measures supported by curves.[9]

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VORTICES AND SPONTANEOUS SYMMETRY BREAKING IN ROTATING BOSE GASES *

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We present a rigorous proof of the appearance of quantized vortices in dilute trapped Bose gases with repulsive two-body interactions subject to rotation, which was obtained recently in joint work with Elliott Lieb.[14] Starting from the many-body Schrödinger equation, we show that the ground state of such gases is, in a suitable limit, well described by the nonlinear Gross-Pitaevskii equation. In the case of axially symmetric traps, our results show that the appearance of quantized vortices causes spontaneous symmetry breaking in the ground state.

1. Introduction

In recent remarkable experiments,[1,12,21,22] the appearance of quantized vortices in the ground state (and low temperature equilibrium states) of rotating dilute Bose gases was beautifully demonstrated. These quantized vortices are a consequence of the superfluid nature of the system under investigation. In particular, since the system is almost completely Bose condensed, it behaves like a single quantum particle.

The state of ultracold dilute Bose gases is usually described by means of the Gross-Pitaevskii (GP) equation.[2,4,5,9,10] This non-linear Schrödinger equation originates as the variational equation from the corresponding *GP energy functional*, given by

$$\mathcal{E}^{\mathrm{GP}}[\phi] = \langle\phi|H_0|\phi\rangle + 4\pi g \int_{\mathbb{R}^3} |\phi(x)|^4 d^3x \ . \tag{1.1}$$

Here, $\phi \in L^2(\mathbb{R}^3)$, and H_0 denotes the one-particle Hamiltonian, describing the kinetic, potential and rotational energy of the particles. In fact, if Ω

denotes the angular velocity vector and $V(x)$ the trap potential, H_0 is, in appropriate units, given by

$$H_0 = -\Delta + V(x) - \Omega \cdot L\,, \tag{1.2}$$

where $L = -ix \wedge \nabla$ denotes the angular momentum operator. The parameter g in (1.1) is nonnegative and measures the interaction strength among the particles. The trap potential $V(x)$ is assumed to be locally bounded and to increase fast enough at infinity in order to have the particles confined to the trap (and, in particular, to ensure that H_0 is bounded from below). More precisely, we assume that

$$\lim_{|x|\to\infty} \left(V(x) - \frac{1}{4}|\Omega \wedge x|^2 \right) = +\infty\,. \tag{1.3}$$

Since $-\Delta - \Omega \cdot L = (-i\nabla + \Omega \wedge x/2)^2 - |\Omega \wedge x|^2/4$, this implies the desired property.

The GP energy is the minimal value of $\mathcal{E}^{\mathrm{GP}}[\phi]$ among all (appropriate normalized) functions ϕ, i.e.,

$$E^{\mathrm{GP}}(g,\Omega) = \inf_{\|\phi\|_2=1} \mathcal{E}^{\mathrm{GP}}[\phi]\,.$$

Using (1.3) and the fact that $g \geq 0$, it is in fact not difficult to show that the infimum is actually a minimum (see Ref. 20). That is, there exists a minimizer of the GP functional (1.1). Note that, in general, there may be many different minimizers. In any case, any minimizer satisfies the *GP equation*

$$\boxed{-\Delta\phi(x) + V(x)\phi(x) - \Omega \cdot L\,\phi(x) + 8\pi g|\phi(x)|^2\phi(x) = \mu\phi(x)}$$

where $\mu = E^{\mathrm{GP}}(g,\Omega) + 4\pi g \int_{\mathbb{R}^3} |\phi(x)|^4 d^3x$ is the corresponding chemical potential.

For axially symmetric $V(x)$, i.e., in case $V(x)$ commutes with $\Omega \cdot L$, the GP functional is invariant under rotation about the Ω axis. It turns out that for any $\Omega \neq 0$, this rotational symmetry is broken in the GP minimizer for large enough interaction strength g.[23,24] This symmetry breaking is the result of the appearance of quantized vortices since, in case of more than one vortex, they cannot be arrange in a symmetric way. Note that, in particular, this implies that there will be many GP minimizers (for g large enough).

We remark that the phenomenon just described is a special feature of rotating systems and cannot be observed in a non-rotating system. In fact, for $\Omega = 0$ there is always a unique minimizer of the GP functional.[20]

It turns out that the appearance of quantized vortices, and the resulting symmetry breaking, which we have just described, are not merely a property of the GP theory, but can actually be derived out of the underlying (many-particle) Schrödinger equation. This was proved in Ref. 14. In the following sections, we will give a summary of these results, and we will explain the key ideas leading to their proof.

2. The Schrödinger Equation for Many Particles

Consider a quantum-mechanical system of a large number, N, of bosons, with one-particle energies described by H_0 (given in (1.2) above). We assume that the particles interact via a repulsive pair interaction potential $v_a(x)$. The Hamiltonian for this system is given by

$$H_N = \sum_{i=1}^{N} H_0^{(i)} + \sum_{1\leq i<j\leq N} v_a(x_i - x_j)\,, \tag{2.1}$$

where the superscript (i) refers to the fact that H_0 acts on the i'th variable. Since the particles under consideration are bosons, the Hamiltonian H_N acts on the subspace of totally symmetric functions in $\bigotimes^N L^2(\mathbb{R}^3)$, which we denote by $\mathcal{H}_N$.

The interaction potential $v_a(x)$ is assumed to be nonnegative and of short range. More precisely, it is assumed to have finite *scattering length*,[17,20] denoted by a, which means that it has to be integrable at infinity (i.e., it has to decay faster than $|x|^{-3}$). A typical example would be a hard sphere interaction, which formally means that $v_a(x) = \infty$ for $|x| \leq a$ and $v_a(x) = 0$ otherwise. We shall, in fact, choose some fixed (nonnegative) interaction potential $w(x)$ with scattering length 1 and obtain $v_a(x)$ by scaling as

$$v_a(x) = a^{-2} w(x/a)\,.$$

It is then easy to see that $v_a(x)$ has scattering length a. Moreover, a now appears as a parameter in the Hamiltonian H_N, which can be freely varied. In particular, we can (and will) let a depend on N. We note that this scaling of $v_a(x)$ is, of course, mathematically and physically equivalent to scaling the trap potential $V(x)$ (and the angular velocity Ω) in an appropriate way, while keeping the interaction potential fixed.

2.1. *Ground State Energy*

For fixed $w(x)$ and $V(x)$, we shall denote the ground state energy of H_N as $E_0(N, a, \Omega)$, i.e.,

$$E_0(N, a, \Omega) = \inf_{\Psi \in \mathcal{H}_N} \frac{\langle \psi | H_N | \Psi \rangle}{\langle \Psi | \Psi \rangle} .$$

Since the ground state energy per unit volume of a homogeneous Bose gas with interaction $v_a(x)$ at density ρ is given by $4\pi a \rho^2$ for low density,[18] it is reasonable to expect that $E_0(N, a, \Omega) \approx N E^{\mathrm{GP}}(Na, \Omega)$ for dilute gases. Here, dilute means that $a^3 \bar{\rho} \ll 1$, where $\bar{\rho}$ denotes the average density. This condition is, in particular, satisfied if $N \gg 1$ and $Na = O(1)$. We call this the *GP limit*. In this limit, we have the following result.[14]

Theorem 2.1. *For any $g \geq 0$ and $\Omega \in \mathbb{R}^3$,*

$$\boxed{\lim_{N \to \infty} \frac{E_0(N, g/N, \Omega)}{N} = E^{\mathrm{GP}}(g, \Omega)} \tag{2.2}$$

That is, for large N and $a = O(1/N)$, the ground state energy per particle is given by the GP energy with coupling parameter $g = Na$. Theorem 2.1 holds for all angular velocities Ω (satisfying the stability criterion (1.3)). It extends previous results in the nonrotating case $\Omega = 0$.[20]

Note that the right side of (2.2) is independent of the choice of the unscaled interaction potential $w(x)$. In the dilute limit considered here, only the scattering length a matters, and not the details of the interaction potential. Note also that the result cannot be obtained by simple perturbation theory; in fact, the $\int |\phi|^4$ term in the GP functional is partly kinetic energy, and not the average value of $v_a(x)$ (which might even be zero, as in the case of the hard-sphere interaction).

As will be pointed out in Subsect. 2.3 below, it is essential to restrict to symmetric wave functions (bosons) in Theorem 2.1. For the absolute ground state energy (defined as the infimum of H_N over all wavefunctions, not necessarily symmetric ones), the result is wrong, in general. For the absolute ground state, the right side has to be replaced by minimizing a density-matrix functional instead.[23]

2.2. *Bose-Einstein Condensation*

The GP energy functional (1.1) and its minimizers contain information not only about the ground state energy of the many-body Hamiltonian (2.1), but also about the ground state or, more precisely, its reduced density

matrices. Recall that for any wavefunction $\Psi \in \mathcal{H}_N$, its *reduced one-particle density matrix* $\gamma_N^{(1)}$ is given by the kernel

$$\gamma_N^{(1)}(x,x') = N \int_{\mathbb{R}^{3(N-1)}} \Psi(x,x_2,\ldots,x_N)\Psi^*(x',x_2,\ldots,x_N)d^3x_2\cdots d^3x_N\,.$$

Note that this defines a positive trace class operator on the one-particle space $L^2(\mathbb{R}^3)$.

The one-particle density matrix of a state Ψ contains all the information about the system concerning expectation values of one-particle operators. It particular, the concept of *Bose-Einstein condensation* (BEC) is defined in terms of $\gamma_N^{(1)}$.

Note that if Ψ is normalized, i.e., $\|\Psi\|_2 = 1$, then the trace of $\gamma_N^{(1)}$ is N. BEC means that $\gamma_N^{(1)}$ has an eigenvalue of order N. The corresponding eigenfunction is called the *condensate wave function*. For dilute systems, as we consider here, one expects in fact *complete BEC*, meaning that $\gamma_N^{(1)}$ is approximately a rank one projection, or $\gamma_N^{(1)}(x,x') \approx N\phi(x)\phi(x')$ for some normalized $\phi \in L^2(\mathbb{R}^3)$.

In the non-rotating case $\Omega = 0$, complete BEC in the ground state of H_N was proved in Ref. 15. Moreover, it was shown that the condensate wave function equals the GP minimizer. Recall that in the case $\Omega = 0$ there is a unique minimizer of the GP functional (1.1) (up to constant phase factor, of course), which we denote by ϕ^{GP}. That is, if $\gamma_N^{(1)}$ denotes the one-particle density matrix of the ground state Ψ of H_N for $\Omega = 0$, then

$$\boxed{\lim_{N\to\infty} \frac{1}{N}\gamma_N^{(1)}(x,x') = \phi^{\mathrm{GP}}(x)\phi^{\mathrm{GP}}(x')} \tag{2.3}$$

in the GP limit $N \to \infty$, $Na \to g$. To be precise, the limit (2.3) holds in trace norm sense. Note that although a is scaled to zero in the limit considered, the right side of (2.3) depends on $g = Na$ via ϕ^{GP}.

The corresponding result for $\Omega \neq 0$ is necessarily more complicated because of non-uniqueness of the GP minimizer ϕ^{GP}. It is actually more natural to not just look at a ground state of H_N (which may not be unique in the rotating case either), but on the set of all *approximate ground states*. These are defined as sequences of (bosonic) N-particle density matrices γ_N (that is, positive operators on $\mathcal{H}_N$ with trace one) with $\mathrm{Tr}\, H_N\gamma_N \approx NE^{\mathrm{GP}}$. One can then expect that the reduced one-particle density matrix $\gamma_N^{(1)}$ of any such approximate ground state is a convex combination of GP minimizers, i.e.,

$$\gamma_N^{(1)}(x,x') \approx \sum_i \lambda_i \phi_i^{\mathrm{GP}}(x)\phi_i^{\mathrm{GP}}(x')^*$$

where each $\phi_i^{\rm GP}$ is a GP minimizer, and $\sum_i \lambda_i = N$.

Theorem 2.2 below states that this is indeed the case. The mathematically precise formulation is slightly complicated by the fact that the set of GP minimizers is, in general, not countable.

Let Γ be the set of all limit points of one-particle density matrices of approximate ground states:

$$\Gamma = \Bigg\{ \gamma \,:\, \exists \text{ sequence } \gamma_N, \lim_{N\to\infty,\, Na\to g} \frac{1}{N} \mathrm{Tr}\, H_N \gamma_N = E^{\rm GP}(g,\Omega), \\ \lim_{N\to\infty} \frac{1}{N} \gamma_N^{(1)} = \gamma \Bigg\} \,. \tag{2.4}$$

Since H_0 has a compact resolvent by our assumption (1.3), one easily sees that $\mathrm{Tr}\,\gamma = 1$ for all $\gamma \in \Gamma$. Moreover, because of the linearity of the conditions in (2.4), Γ is clearly convex.

Theorem 2.2. *For given value of $g \geq 0$ and Ω, let Γ denote the set of all limit points of one-particle density matrices of approximate ground states of H_N, defined in (2.4).*

(i) *Γ is a compact and convex subset of the set of all trace class operators.*

(ii) *Let $\Gamma_{\rm ext} \subset \Gamma$ denote the set of extreme points in Γ. We have $\Gamma_{\rm ext} = \{|\phi\rangle\langle\phi| \,:\, \mathcal{E}^{\rm GP}[\phi] = E^{\rm GP}(g,\Omega)\}$, i.e., the extreme points in Γ are given by the rank-one projections onto GP minimizers.*

(iii) *For each $\gamma \in \Gamma$, there is a positive (regular Borel) measure $d\mu_\gamma$, supported in $\Gamma_{\rm ext}$, with $\int_{\Gamma_{\rm ext}} d\mu_\gamma(\phi) = 1$, such that*

$$\boxed{\gamma = \int_{\Gamma_{\rm ext}} d\mu_\gamma(\phi)\, |\phi\rangle\langle\phi|}$$

where the integral is understood in the weak sense. That is, every $\gamma \in \Gamma$ is a convex combination of rank-one projections onto GP minimizers.

We remark that item (iii) of Theorem 2.2 follows from item (ii) by Choquet's Theorem.[6]

As explained above, Theorem 2.2 is the natural analogue of (2.3) in the rotating case. It can also be interpreted as a rigorous proof of superfluidity. As typical for superfluids, angular momentum in rotating systems is acquired in terms of quantized vortices. These can be seen by solving the GP equation.

Theorem 2.2 also shows the occurrence of spontaneous symmetry breaking. As remarked earlier, axial symmetry of the trap $V(x)$ leads to non-uniqueness of the GP minimizer for g large enough.[23,24] Uniqueness can

be restored by perturbing H_0 to break the symmetry and favor one of the minimizers. This then leads to complete BEC in the usual sense, since Γ contains contains only one element in case the GP functional (1.1) has a unique minimizer.

As in the case of the ground state energy discussed in the previous subsection, the situation is very different for the absolute ground state. The set Γ consists of only one element in this case (namely the minimizer of the density matrix functional discussed below, which is unique for any value of Ω and g). In particular, there is no spontaneous symmetry breaking in the absolute ground state. This will be discussed in the next subsection.

2.3. *The Absolute Ground State*

Let $E_{\rm abs}(N, a, \Omega)$ denote the absolute ground state energy of H_N in (2.1), irrespective of symmetry constraints, i.e.,

$$E_{\rm abs}(N, a, \Omega) = \inf_{\Psi \in L^2(\mathbb{R}^{3N})} \frac{\langle \psi | H_N | \Psi \rangle}{\langle \Psi | \Psi \rangle} \,.$$

Note that necessarily $E_{\rm abs}(N, a, \Omega) \leq E_0(N, a, \Omega)$. As is well known, for $\Omega = 0$ the two energies are equal. This turns out not to be the case for $\Omega \neq 0$, in general.

In the GP limit, the absolute ground state energy, and the corresponding one-particle reduced density matrices of approximate ground states, turn out to be described by a *GP density matrix functional*, introduced in Ref. 24,

$$\mathcal{E}^{\rm DM}[\gamma] = {\rm Tr}\,[H_0 \gamma] + 4\pi g \int_{\mathbb{R}^3} \rho_\gamma(x)^2 d^3x \,.$$

Here, γ is a positive trace class operator on $L^2(\mathbb{R}^3)$, and ρ_γ denotes the density of γ, i.e., $\rho_\gamma(x) = \gamma(x, x)$. The functional $\mathcal{E}^{\rm DM}$ can be shown[24] to have a unique minimizer (under the normalization condition ${\rm Tr}\,\gamma = 1$), which we denote by $\gamma^{\rm DM}$. We denote the corresponding energy by $E^{\rm DM}(g, \Omega) = \mathcal{E}^{\rm DM}[\gamma^{\rm DM}]$.

The following Theorem concerning the absolute ground state of H_N was proved in Ref. 23.

Theorem 2.3. *For any fixed $g \geq 0$ and $\Omega \in \mathbb{R}^3$,*

$$\boxed{\lim_{N\to\infty} \frac{E_{\rm abs}(N, g/N, \Omega)}{N} = E^{\rm DM}(g, \Omega) \quad \text{and} \quad \lim_{N\to\infty} \frac{1}{N} \gamma^{(1)}_{\rm abs} = \gamma^{\rm DM}}$$

Here, $\gamma^{(1)}_{\rm abs}$ denotes the one-particle density matrix of any approximate (absolute) ground state sequence of H_N. In other words, the set Γ defined as in (2.4), but for the absolute ground state, contains only one element, namely the unique minimizer of $\mathcal{E}^{\rm DM}$.

Note that $\mathcal{E}^{\rm GP}$ is the restriction of $\mathcal{E}^{\rm DM}$ to rank one projections. In the case of symmetry breaking (i.e., for g large enough), $\operatorname{rank}\gamma^{\rm DM} \geq 2$, and hence $E^{\rm DM} < E^{\rm GP}$. In particular, in view of Theorems 2.1–2.3, the absolute and bosonic ground state differ significantly, in general, both in terms of their energy and their reduced one-particle density matrix.

We remark that the results explained in this subsection become physically relevant if one considers bosons with internal degrees of freedom. Internal degrees of freedom effectively increase the number of allowed symmetry classes (see, e.g., Ref. 8). In particular, if the number of states of the internal degrees of freedom of the bosons is greater or equal to the rank of $\gamma^{\rm DM}$, $E^{\rm DM}(g,\Omega)$ equals the (bosonic) ground state energy per particle in the GP limit. More generally, one can show that in the GP limit the functional $\mathcal{E}^{\rm DM}$, when restricted to density matrices of rank at most n, correctly describes the ground state energy (and corresponding one-particle density matrix) of bosons with n internal states.

3. Sketch of the Proof of Theorem 2.1

In the following, we shall give a brief outline of the main ideas in the proof of Theorem 2.1. For details we refer to the original work in Ref. 14. We shall restrict our attention to the appropriate lower bound on the ground state energy $E_0(N,a,\Omega)$. The corresponding upper bound can be obtained via a variational argument, as explained in Ref. 23.

A convenient way to keep track of the bosonic symmetry requirement is to work in Fock space. Recall that the bosonic Fock space $\mathcal{F}$ is given by $\mathcal{F} = \bigoplus_{N\geq 0} \mathcal{H}_N$. In terms of creation and annihilation operators $a_j^\dagger$ and a_j on $\mathcal{F}$, the Hamiltonian can be written as

$$H = \sum_{j\geq 1} e_j a_j^\dagger a_j + \tfrac{1}{2} \sum_{ijkl} a_i^\dagger a_j^\dagger a_k a_l \, W_{ijkl} \,. \tag{3.1}$$

Here, we choose the basis in the one-particle space $L^2(\mathbb{R}^3)$ as to diagonalize H_0, i.e., $H_0 = \sum_j e_j |\varphi_j\rangle\langle\varphi_j|$, and $a_j^\dagger$ creates a particle with wavefunction φ_j, whereas a_j annihilates it. The coefficients W_{ijkl} are given in terms of expectation values of $v_a(x)$, namely $W_{ijkl} = \langle \varphi_i \otimes \varphi_j | v_a | \varphi_k \otimes \varphi_l \rangle$.

Note that H in (3.1) commutes with total particle number operator $\sum_{j\geq 1} a_j^\dagger a_j$. Hence it splits into a direct sum of operators on $\mathcal{H}_N$ for $N =$

$0, 1, \ldots$. In fact, our H_N in (2.1) is just the restriction of H to $\mathcal{H}_N$.

The analysis employed for obtaining a lower bound on the ground state energy of H in the sector of N particles consists of two main steps:

1. Eq. (3.1) is not necessarily well defined. E.g., if $v_a(x)$ is the hard-core interaction potential (or, more generally, is not integrable), then $W_{ijkl} = \infty$ for any set of indices. In order to overcome this problem, we shall first show that, for a lower bound, one can replace $v_a(x)$ by a "soft" and longer ranged potential $U(x)$ (with the same scattering length), at the expense of the high-momentum part of the kinetic energy. We note that this step is necessary even in the case when $v_a(x)$ is integrable (and hence (3.1) is well defined) in order to proceed with the second step.
2. After having replaced $v_a(x)$ by the softer potential $U(x)$, one then shows that it is possible to replace the operators $a_j^\dagger$ and a_j by complex numbers z_j without changing the ground state energy too much.[19] Note that if all the $a_j^\dagger$ and a_j in (3.1) are treated as numbers, the expression (3.1) looks very similar to the GP energy functional (1.1); in fact, it is given by

$$\langle \phi_{\mathbf{z}} | H_0 | \phi_{\mathbf{z}} \rangle + \tfrac{1}{2} \int_{\mathbb{R}^6} v_a(x-y) |\phi_{\mathbf{z}}(x)|^2 |\phi_{\mathbf{z}}(y)|^2 \, d^3x \, d^3y \,,$$

with $\phi_{\mathbf{z}}(x) = \sum_j z_j \varphi_j(x)$.

In the following, we shall explain these two main steps in more detail.

3.1. *Step 1: Generalized Dyson Lemma*

The following Lemma can be viewed as a generalization of an idea of Dyson.[7] The purpose of the lemma is give a lower bound on the interaction potential $v_a(x)$ in terms of a softer and longer ranged potential $U(x)$, at the expense of some kinetic energy (see also Ref. 18). For our purpose, we can only spare the high momentum part of the kinetic energy, however; the low momentum part is needed for the H_0 term in the GP functional.

We thus have to separate the high momentum from the low momentum part of the kinetic energy. This can be done in the following way. The proof of Lemma 3.1 is given in Ref. 16.

Lemma 3.1. *Let $v_a(x)$ have scattering length a and range R_0. Let θ_R be the characteristic function of the ball $\{x : |x| < R\}$. Let $0 \leq \chi(p) \leq 1$, such*

that $h(x) \equiv \widehat{1-\chi}(x)$ *is bounded and integrable,*

$$f_R(x) = \sup_{|y|\leq R} |h(x-y) - h(x)|\,,$$

and

$$w_R(x) = \frac{2}{\pi^2} f_R(x) \int_{\mathbb{R}^3} f_R(y) d^3y\,.$$

Then for any $\varepsilon > 0$ *and any positive radial function* $U(x)$ *supported in* $R_0 \leq |x| \leq R$ *with* $\int U = 4\pi$ *we have the operator inequality*

$$-\nabla\chi(p)\theta_R(x)\chi(p)\nabla + \tfrac{1}{2}v_a(x) \geq (1-\varepsilon)aU(x) - \frac{a}{\varepsilon}w_R(x)\,. \tag{3.2}$$

Here, $\chi(p)$ denotes a multiplication operator in momentum space. Note that the operator $-\nabla\chi(p)\theta_R(x)\chi(p)\nabla$ can be interpreted as a Laplacian that has been localized to the ball of radius R and cut off in momentum space. Because of the cut-off, this is not a local operator, however. The parameter R is chosen such that $a \ll R \ll N^{-1/3}$. Note that to leading order in a/R, the scattering length of $2aU(x)$ is given in terms of its first order Born approximation as $(8\pi)^{-1}2a\int_{\mathbb{R}^3} U(x)d^3x = a$.

Because of the appearance of the characteristic function $\theta_R(x)$ in (3.2), Lemma 3.1 has the following immediate consequence. If $y_1, \ldots, y_n$ are n points in $\mathbb{R}^3$ whose mutual distance is at least $2R$, then

$$-\nabla\chi(p)^2\nabla + \tfrac{1}{2}\sum_{i=1}^n v_a(x-y_i) \geq \sum_{i=1}^n \left[(1-\varepsilon)aU(x-y_i) - \frac{a}{\varepsilon}w_R(x-y_i)\right]\,.$$

This bound accomplishes the replacement of the hard interaction potential $v_a(x)$ by a soft one, at the expense of the high momentum part of the kinetic energy. For given configuration of $N-1$ particles, this estimate is applied to the remaining particle. Of course one still has to estimate the contribution from configurations where 2 (or more) of the $N-1$ fixed particles are closer together than $2R$. This can be achieved by a Feynman-Kac integral representation[25] of the ground state. We refer to Ref. 14 for details.

3.2. *Step 2: Coherent States*

The Fock space $\mathcal{F}$ can be viewed as an infinite tensor product of the form $\mathcal{F} = \bigotimes_{j\geq 1}\mathcal{F}_j$, with $\mathcal{F}_j$ spanned by the vectors $(a_j^\dagger)^n|0\rangle$ for $n = 0, 1, \ldots$. Here, $|0\rangle$ denotes the Fock space vacuum.

Consider first the case of a single mode, $\mathcal{F}_1$, say. For $z \in \mathbb{C}$, a *coherent state*[13] in $\mathcal{F}_1$ is defined by

$$|z\rangle = e^{-|z|^2/2 + za_1^\dagger}|0\rangle\,.$$

These states span in the whole space $\mathcal{F}_1$. In fact, they satisfy the completeness relation

$$\int_{\mathbb{C}} dz|z\rangle\langle z| = \mathbb{I}\,, \tag{3.3}$$

where dz stands for $\pi^{-1}dxdy$, and $z = x + iy$, $x, y \in \mathbb{R}$.

In terms of coherent states, *upper and lower symbols* of operators can be defined. Lower symbols are simply the expectation values of operators in coherent states, e.g., $\langle z|a_1|z\rangle = z$ and $\langle z|a_1^\dagger a_1|z\rangle = |z|^2$. Upper symbols, on the other hand, represent functions of z which, when integrated against $|z\rangle\langle z|dz$ over $\mathbb{C}$, yield given operators. For instance, it is not difficult to see that $a_1 = \int dz\, z|z\rangle\langle z|$, while $a_1^\dagger a_1 = \int dz\,(|z|^2 - 1)|z\rangle\langle z|$. Hence, upper and lower symbols of a_1 are given by z, whereas the lower symbol of $a_1^\dagger a_1$ is $|z|^2$ and the upper symbol is $|z|^2 - 1$.

Note that lower symbols yield upper bounds on ground state energies, by the variational principle, while upper symbols are useful for lower bounds. The difference in the symbols thus quantifies the error one makes in replacing the operators $a_1^\dagger$ and a_1 by numbers. In particular, for every quadratic term $a_1^\dagger a_1$ a factor -1 has to be taken into account. For this reason, one cannot introduce coherent states of all the modes j, but only for a finite number of them.

In fact, we shall introduce coherent states of all the modes $1 \leq j \leq J$ for some $J \gg 1$. That is, we first write $\mathcal{F} = \mathcal{F}_< \otimes \mathcal{F}_>$, where $\mathcal{F}_<$ is spanned by the vectors of the form $(a_1^\dagger)^{n_1} \cdots (a_J^\dagger)^{n_J}|0\rangle$, with $n_j \in \mathbb{N}$ for $1 \leq j \leq J$. For $\mathbf{z} = (z_1, \ldots, z_J) \in \mathbb{C}^J$, we introduce the projection operator $\Pi(\mathbf{z})$ on $\mathcal{F}_<$, given by

$$\Pi(\mathbf{z}) = |z_1 \otimes \cdots \otimes z_J\rangle\langle z_1 \otimes \cdots \otimes z_J|\,.$$

Using upper symbols, we can then write the Hamiltonian H in (3.1) as

$$H = \int_{\mathbb{C}^J} d\mathbf{z}\, \Pi(\mathbf{z}) \otimes h(\mathbf{z})\,.$$

Here, $h(\mathbf{z})$ represents the upper symbol of H. Since only the modes $1 \leq j \leq J$ have been replaced by numbers, $h(\mathbf{z})$ is an *operator* on $\mathcal{F}_>$. Using the completeness property of the coherent states, Eq. (3.3), it is then easy to see that

$$\inf \operatorname{spec} H \geq \inf_{\mathbf{z}} \inf \operatorname{spec} h(\mathbf{z})\,.$$

One then proceeds to show that $h(\mathbf{z}) \approx \mathcal{E}^{\mathrm{GP}}[\phi_{\mathbf{z}}]$ modulo controllable error terms. These error terms are, in fact, operators on $\mathcal{F}_>$ which describe

both the interactions among particles in high modes as well as the interaction between particles in modes $j \leq J$ and $j > J$. Precise bounds on these terms can be found in Ref. 14.

4. Sketch of the Proof of Theorem 2.2

In order to obtain information on (approximate) ground states from bounds on the energy, one proceeds as follows. One first perturbs the Hamiltonian H_N in (2.1) by some one-particle perturbation S, and applies the same perturbation to the GP functional (1.1). One then shows that the result of Theorem 2.1 still holds for the perturbed system. In fact, the proof of Theorem 2.1 outlined in the previous section is sufficiently robust in order to easily incorporate such a modification.

Griffiths' argument[11] then implies that, for any $\gamma \in \Gamma$, and any bounded hermitian operator S,

$$\operatorname{Tr} S\gamma \geq \min_{\phi=\phi^{\mathrm{GP}}} \langle \phi | S | \phi \rangle \,, \tag{4.1}$$

where the minimum on the right side is taken over all GP minimizers. Inequality (4.1) is the key to the proof of Theorem 2.2. The rest follows from convexity theory,[26] as we shall explain now.

Recall that an exposed point of a convex set $\mathcal{C}$ is an extreme point p with the additional property that there is a tangent plane to $\mathcal{C}$ containing p but no other point of $\mathcal{C}$. Hence, for $\widetilde{\gamma} \in \Gamma$ an exposed point, there exists an S such that

$$\operatorname{Tr} S\widetilde{\gamma} \leq \operatorname{Tr} S\gamma \quad \text{for all } \gamma \in \Gamma \,. \tag{4.2}$$

with equality *if and only if* $\gamma = \widetilde{\gamma}$.

It is not very difficult to show that $|\phi^{\mathrm{GP}}\rangle\langle\phi^{\mathrm{GP}}| \in \Gamma$ for any GP minimizer ϕ^{GP}. Hence, if we choose γ in (4.2) to be equal to $|\phi^{\mathrm{GP}}\rangle\langle\phi^{\mathrm{GP}}|$ for the ϕ^{GP} that minimizes the right side of (4.1) for this particular S, the inequalities (4.1) and (4.2) imply that

$$\min_{\phi=\phi^{\mathrm{GP}}} \langle \phi | S | \phi \rangle = \langle \phi^{\mathrm{GP}} | S | \phi^{\mathrm{GP}} \rangle \leq \operatorname{Tr} S\widetilde{\gamma} \leq \operatorname{Tr} S\gamma = \langle \phi^{\mathrm{GP}} | S | \phi^{\mathrm{GP}} \rangle$$

and hence there is actually equality in (4.2). This, in turn, implies that $\widetilde{\gamma} = |\phi^{\mathrm{GP}}\rangle\langle\phi^{\mathrm{GP}}|$. We have thus shown that all exposed points of Γ are of this form!

In order to extend this result to all extreme points, now merely exposed points, we employ Straszewicz's Theorem,[26] which states that the exposed points are a dense subset of the extreme points. Strictly speaking, this

theorem only holds in finite dimensions and not, *a priori*, in the infinite dimensional case under consideration here. However, because of compactness, the set Γ is "almost" finite dimensional, and hence the theorem can be applied via an approximation argument. We refer again to Ref. 14 for details.

5. Conclusions

We have presented a rigorous justification of the Gross-Pitaevskii approximation for sufficiently dilute rotating Bose gases. For large particle number N and both Na and Ω of order 1, the ground state of a rotating Bose gas is well approximated by the solution to the GP equation. This is true both for the energy and the reduced density matrices. In particular, our analysis proves the appearance of quantized vortices and the occurrence of spontaneous symmetry breaking in the parameter regime where these phenomena can be observed in the GP equation, e.g., for $\Omega \neq 0$ and g large enough.

We point out that one of the major open problems in this field is the validity of the GP equation for *rapidly* rotating gases, where either $|\Omega| \to \infty$ as $N \to \infty$ (in case the trap potential grows faster than quadratic at infinity), or Ω approaches the trap frequency (for traps that are asymptotically quadratic). There is evidence that the GP descriptions breaks down once the number of vortices in the system is of the same order as the number of particles. Despite recent progress in this direction,[3] a proof of this assertion is still lacking.

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THE MODEL OF INTERLACING SPATIAL PERMUTATIONS AND ITS RELATION TO THE BOSE GAS

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The model of spatial permutations is related to the Feynman-Kac representation of the Bose gas. The transition to infinite cycles corresponds to Bose-Einstein condensation. We review the general setting and some results, and we derive a multi-body interaction between permutation jumps, that is due to the original interactions between quantum particles.

Keywords: spatial random permutations, infinite cycles, interacting Bose gas, Bose-Einstein condensation

1. Introduction

One purpose of this article is to review the setting for the model of *spatial permutations* and its relation with the quantum Bose gas, and to summarize some of the material presented in a recent collaboration with Volker Betz.[2] Another purpose is to compute the effective interaction between permutation jumps. It involves the original interaction potential between quantum particles. While several mathematical questions remain unanswered, it is argued that the model of interacting spatial permutations describes the quantum interacting Bose gas *exactly*, and in a simpler way. The main phenomenon in bosonic systems is the *Bose-Einstein condensation*. We discuss the links between this phase transition and the occurrence of *infinite cycles* in random permutations.

Given points $x_1, \dots, x_N$ in $\mathbb{R}^d$, one considers random permutations π of

N elements with weight

$$\prod_{i=1}^{N} \exp\{-\tfrac{1}{4\beta}|x_i - x_{\pi(i)}|^2\}.$$

Permutation jumps are essentially finite, but permutation cycles can be large. This model is illustrated in Fig. 1. It is motivated in large part by the Feynman-Kac representation of the Bose gas. We actually discuss a more general setting where permutation jumps interact.

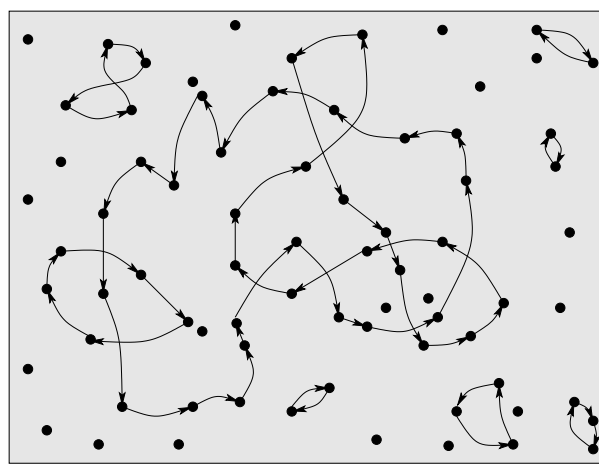

Fig. 1. Illustration for a random set of points $\boldsymbol{x} = (x_1, \dots, x_N)$, and for a permutation $\pi \in \mathcal{S}_N$. Isolated points are sent onto themselves. Permutation jumps are small, but long cycles can occur nonetheless.

The precise setting is introduced in Section 2. We recall the Feynman-Kac representation of the Bose gas in Section 3; it makes the relation between the ideal Bose gas and non-interacting spatial permutations clear. The two-body interaction between permutation jumps, that is expected to give the exact behaviour to lowest order in the strength of the particle interactions, is computed in Section 4. Finally, we describe a simple model of interacting permutations in Section 5. It is exactly solvable, and it provides some understanding about the effects of interactions on the Bose-Einstein condensation.

2. The model of spatial permutations

Let $\Lambda \subset \mathbb{R}^d$ be a cube of size L and volume $V = L^d$, and let $N \in \mathbb{N}$. The state space of the model of spatial permutations is

$$\Omega_{\Lambda,N} = \Lambda^N \times \mathcal{S}_N,$$

with $\mathcal{S}_N$ the symmetric group of permutations of N elements. We are interested in the properties of permutations, and all our random variables are functions $\theta : \mathcal{S}_N \to \mathbb{R}$. Their probability distributions depend on spatial variables in an indirect but essential way. Let $\ell_i(\pi)$ denote the length of the cycle that contains i, i.e., the smallest integer $n \geq 1$ such that $\pi^n(i) = i$. The most important random variable is the density of points in cycles of certain lengths. For $n, n' \in \mathbb{N}$, let

$$\boldsymbol{\varrho}_{n,n'}(\pi) = \frac{1}{V} \#\big\{i = 1, \dots, N : n \leq \ell_i(\pi) \leq n'\big\}. \tag{2.1}$$

The expectation of the random variable θ is defined by

$$E_{\Lambda,N}(\theta) = \frac{1}{Z(\Lambda,N)N!} \int_{\Lambda^N} \mathrm{d}\boldsymbol{x} \sum_{\pi \in \mathcal{S}_N} \theta(\pi)\, \mathrm{e}^{-H(\boldsymbol{x},\pi)}\,. \tag{2.2}$$

Here, the normalization factor $Z(\Lambda, N)$ is chosen so that $E_{\Lambda,N}(1) = 1$. The term $N!$ is present in order that $Z(\Lambda, N)$ scales like the exponential of the volume of Λ — thus behaving like a partition function in statistical mechanics. The integral is over N points in Λ, denoted $\boldsymbol{x} = (x_1, \dots, x_N)$.

We consider Hamiltonians of the form

$$H(\boldsymbol{x}, \pi) = \sum_{i=1}^{N} \xi(x_i - x_{\pi(i)}) + \sum_{1 \leq i < j \leq N} V(x_i, x_{\pi(i)}, x_j, x_{\pi(j)}), \tag{2.3}$$

with ξ a spherically symmetric function $\mathbb{R}^d \to [0, \infty]$, and V a translation invariant function $\mathbb{R}^{4d} \to \mathbb{R}$. We also suppose that ξ is increasing and that $\xi(0) = 0$. One should think of typical permutations as involving finite jumps, i.e., $|x_i - x_{\pi(i)}|$ stays bounded as $\Lambda, N \to \infty$.

The major question concerns the occurrence of infinite cycles. It turns out that the distribution of cycles can be well characterized in the absence of interactions, with the potential $V \equiv 0$. We need a few hypotheses on ξ. Let $C = \int \mathrm{e}^{-\xi}$. We suppose that $\mathrm{e}^{-\xi}$ has positive Fourier transform, which we denote $C\,\mathrm{e}^{-\varepsilon(k)}$. Precisely, we have

$$C\,\mathrm{e}^{-\varepsilon(k)} = \int_{\mathbb{R}^d} \mathrm{e}^{-2\pi \mathrm{i} k x}\, \mathrm{e}^{-\xi(x)}\, \mathrm{d}x.$$

The case of physical relevance is $\xi(x) = \frac{1}{4\beta}|x|^2$ with β the inverse temperature, in which case $\varepsilon(k) = 4\pi^2\beta|k|^2$. But it may be of mathematical

interest to consider other functions, including some where $\mathrm{e}^{-\xi}$ has bounded support. Criteria that guarantee positivity of the Fourier transform are discussed e.g. in Ref. 6.

We define the *critical density* by

$$\rho_{\mathrm{c}} = \int_{\mathbb{R}^d} \frac{\mathrm{d}k}{\mathrm{e}^{\varepsilon(k)} - 1}. \tag{2.4}$$

The critical density is finite for $d \geq 3$, but it can be infinite for $d = 1, 2$. The experienced physicist will have recognized the formula for the critical density of Bose-Einstein condensation. The relation with the Bose gas will be discussed in the next section. In the following theorem we fix the density ρ and we let $N = \rho V$ in the expectation (2.2).

Theorem 2.1. *Let ξ satisfy the assumptions above. Then for any $0 < a < b < 1$, and any $s \geq 0$,*

$$\text{(a)} \quad \lim_{V\to\infty} E_{\Lambda,\rho V}(\boldsymbol{\varrho}_{1,V^a}) = \begin{cases} \rho & \text{if } \rho \leq \rho_{\mathrm{c}}; \\ \rho_{\mathrm{c}} & \text{if } \rho \geq \rho_{\mathrm{c}}; \end{cases}$$

$$\text{(b)} \quad \lim_{V\to\infty} E_{\Lambda,\rho V}(\boldsymbol{\varrho}_{V^a,V^b}) = 0;$$

$$\text{(c)} \quad \lim_{V\to\infty} E_{\Lambda,\rho V}(\boldsymbol{\varrho}_{V^b,sV}) = \begin{cases} 0 & \text{if } \rho \leq \rho_{\mathrm{c}}; \\ s & \text{if } 0 \leq s \leq \rho - \rho_{\mathrm{c}}; \\ \rho - \rho_{\mathrm{c}} & \text{if } 0 \leq \rho - \rho_{\mathrm{c}} \leq s. \end{cases}$$

In order to understand the meaning of these claims, one should think of a as barely bigger than 0, and b barely smaller than 1. In part (a), $\boldsymbol{\varrho}_{1,V^a}$ is the density of points in finite cycles. All points belong to finite cycles if $\rho \leq \rho_{\mathrm{c}}$. However, if $\rho > \rho_{\mathrm{c}}$, a fraction $\rho - \rho_{\mathrm{c}}$ of points belong to infinite cycles. It is natural to ask oneselves about the size of "infinite cycles" in a finite domain of volume $L^d = V$. One could expect the typical length to be of order L^2, since the continuum limit of random walks has Hausdorff dimension 2, and cycles are somewhat like closed random walks. However, part (b) shows that cycles of length V^b, with $0 < b < 1$, have vanishing density. Thus infinite cycles are *macroscopic*, i.e., each cycle involves a strictly positive fraction of points. The statistics of macroscopic cycles is characterized in part (c).

The proof of Theorem 2.1 can be found in Ref. 2. Actually, the correct statement involves periodic boundary conditions; the interested reader is invited to look in Ref. 2 for the precise statement. Theorem 2.1 extends an earlier result of Sütő for the ideal Bose gas.[13]

A different model is investigated in Ref. 4, where the positions $x_1, \ldots, x_N$ form a cubic lattice. The density is always equal to 1, but the function $\xi(x)$ depends on a parameter that represents the temperature of the system. It is found numerically that the critical temperature for the occurrence of infinite cycles is close but different from that of the ideal Bose gas. Many properties are similar, however; infinite cycles are also macroscopic. A surprising fact is that the expectation of the length of the longest cycle seems to be identical to that in the ideal Bose gas; this suggests that the distribution of macroscopic cycles may be the same.

3. Feynman-Kac representation of the Bose gas

The Feynman-Kac formula relates the kernel of $\mathrm{e}^{-\beta H}$, with H a Schrödinger operator, to the Brownian motion, whose mathematical expression is the Wiener measure. It seems to have first appeared in Ref. 3, precisely in the context of bosonic systems and in the discussion of cycles. Ginibre wrote an excellent mathematical introduction to the Wiener measure, the Feynman-Kac formula, and its application to bosonic systems.[5] We review these notions here without introducing the full mathematical setting, but all equations below can be justified with a bit of analysis. In particular, we do not discuss the details arising from the boundary conditions; as usual in statistical mechanics, they are irrelevant for large systems.

Let $\Lambda \subset \mathbb{R}^d$ be a cube of size L, and let g_β denote the normalized Gaussian function

$$g_\beta(x) = \frac{1}{(2\pi\beta)^{d/2}} \, \mathrm{e}^{-|x|^2/2\beta} .$$

It is not hard to check that

$$\int_\Lambda g_s(x-a) g_t(x-b) \mathrm{d}x = g_{s+t}(a-b),$$

and that, after iteration,

$$\int_{\Lambda^{n-1}} \mathrm{d}x_2 \ldots \mathrm{d}x_n \prod_{i=1}^{n} g_t(x_{i+1} - x_i - a_i) = g_{nt}\big(x_{n+1} - x_1 - \Sigma_{i=1}^n a_i\big). \quad (3.1)$$

Let $H = -\Delta + U$ be a Schrödinger operator in $L^2(\Lambda)$, with Δ the Laplacian and U a smooth real function. This operator is unbounded and we need to specify its domain. We can choose the space of C^2 functions on Λ with Dirichlet boundary conditions. Then H is symmetric and we consider its self-adjoint extension. Of relevance to statistical mechanics is the operator $\mathrm{e}^{-\beta H}$. It is a nice operator, bounded and compact, but these

properties are not important here. The Feynman-Kac formula states that (with $x_{n+1} \equiv x_1$)

$$\begin{aligned} \mathrm{Tr}\ \mathrm{e}^{-\beta H} &= \lim_{n\to\infty} \int_{\Lambda^n} \mathrm{d}x_1 \dots \mathrm{d}x_n \Big[\prod_{i=1}^n g_{2\beta/n}(x_{i+1} - x_i) \Big] \exp\Big\{ -\frac{\beta}{n} \sum_{i=1}^n U(x_i) \Big\} \\ &\equiv \int_\Lambda \mathrm{d}x \, \exp\Big\{ -\tfrac{1}{2} \int_0^{2\beta} U\big(\omega(s)\big) \mathrm{d}s \Big\} \mathrm{d}W_{xx}^{2\beta}(\omega). \end{aligned}$$

Here, ω is a Brownian bridge starting and ending at x and traveling in time 2β, and $W_{xx}^{2\beta}$ is the Wiener measure. In the second line we should restrict the paths to stay inside Λ, because of Dirichlet boundary conditions; we neglect these technicalities, however.

Let us turn to the description of bosonic systems. The state space for N quantum bosons in a domain $\Lambda \subset \mathbb{R}^d$ is the subspace $L^2_{\mathrm{sym}}(\Lambda^N)$ of symmetric complex functions of N variables. The Hamiltonian is given by the Schrödinger operator

$$H = -\sum_{i=1}^N \Delta_i + \sum_{1\le i,j\le N} U(x_i - x_j).$$

Here, Δ_i denotes the d-dimensional Laplacian for the i-th variable, and $U(x_i - x_j)$ is a multiplication operator that represents the interaction between particles i and j. We always suppose that $U(x) \ge 0$. We can choose the self-adjoint extension of H that corresponds to Dirichlet boundary conditions. Of course, the sum of N Laplacians in Λ^d can be viewed as a Laplacian in Λ^{dN}, so we can apply the Feynman-Kac formula.

The canonical partition function is equal to

$$\mathrm{Tr}_{L^2_{\mathrm{sym}}(\Lambda^N)}\ \mathrm{e}^{-\beta H} = \mathrm{Tr}_{L^2(\Lambda^N)}\, P_+\, \mathrm{e}^{-\beta H}$$

where P_+ is the projector onto symmetric functions,

$$P_+ \varphi(x_1, \dots, x_N) = \frac{1}{N!} \sum_{\pi\in\mathcal{S}_N} \varphi(x_{\pi(1)}, \dots, x_{\pi(N)}).$$

Using this projection and the Feynman-Kac formula, the partition function of the Bose gas can be written as

$$\mathrm{Tr}\ \mathrm{e}^{-\beta H} = \frac{1}{N!} \int_{\Lambda^N} \mathrm{d}\boldsymbol{x} \sum_{\pi\in\mathcal{S}_N} \mathrm{e}^{-H'(\boldsymbol{x},\pi)},$$

with the Gibbs factor given by

$$\begin{aligned} \mathrm{e}^{-H'(\boldsymbol{x},\pi)} &= \Big[\prod_{i=1}^{N} \int \mathrm{d}W^{2\beta}_{x_i x_{\pi(i)}}(\omega_i)\Big] \times \\ &\times \exp\Big(-\tfrac{1}{2} \sum_{1\le i<j\le N} \int_0^{2\beta} U\big(\omega_i(s)-\omega_j(s)\big)\mathrm{d}s\Big). \end{aligned} \tag{3.2}$$

This formula is illustrated in Fig. 2. It involves spatial positions and permutations of these positions.

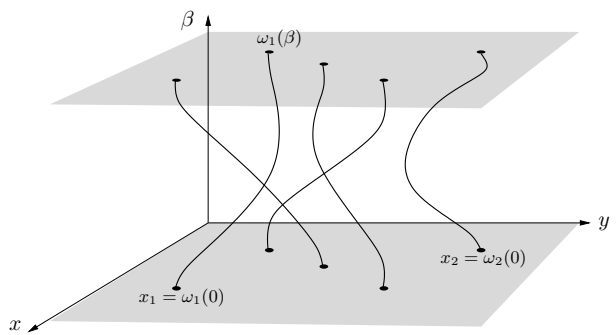

Fig. 2. Feynman-Kac representation of a gas of N bosons. The horizontal plane represents the d spatial dimensions, and the vertical axis is the imaginary time dimension. The picture shows five particles and two cycles, of respective length 4 and 1.

In the case of the ideal gas, $U \equiv 0$, the paths no longer interact and the Wiener integrals in (3.2) can be computed. We find that

$$\mathrm{e}^{-H'(\boldsymbol{x},\pi)} = (4\pi\beta)^{-dN/2}\, \mathrm{e}^{-H^{(0)}(\boldsymbol{x},\pi)} \tag{3.3}$$

with

$$H^{(0)}(\boldsymbol{x},\pi) = \frac{1}{4\beta} \sum_{i=1}^{N} \big|x_i - x_{\pi(i)}\big|^2. \tag{3.4}$$

The prefactor in (3.3) plays no rôle in expectations of random variables and it can be ignored. Thus the ideal Bose gas is equivalent to the "ideal" model of spatial permutations with Gaussian weights. Random variables of permutations have same distribution in both models, and the transition to infinite cycles takes place at the same critical density.

The equivalence between the occurrence of infinite cycles and Bose-Einstein condensation is an open problem. It is known to be true in the

ideal gas, see Refs. 12,13,15, but it does not seem to be true in strongly interacting systems in a solid phase. Pollock and Ceperley have argued that superfluidity is related to *spatially winding* cycles.[11] Such cycles are clearly infinite in the thermodynamic limit. On the other hand, we know from Theorem 2.1 that infinite cycles are macroscopic (i.e., they have strictly positive density), so they certainly have non-zero winding number. Infinite and winding cycles should therefore be equivalent. Superfluidity is by no means equivalent to Bose-Einstein condensation. These facts bring some level of confusion and we can only hope that they will be clarified in the future.

However, it is expected that, in dimension $d \geq 3$, weakly interacting bosonic systems have the *same critical density* for Bose-Einstein condensation, superfluidity, infinite cycles, and winding cycles. Hereafter, we study the occurrence of infinite cycles in the weakly interacting regime, and we implicitly assume that they reveal a Bose-Einstein condensation.

4. Exact two-body interaction for permutation jumps

4.1. *Expansion of path interactions*

The two-body interactions between quantum particles translate into many-body interactions for permutations. But we can perform an expansion and see that, to lowest order, we obtain a two-body interaction between permutation jumps.

Let $\widehat{W}^t_{x,y} = g_t^{-1}(x-y)W^t_{x,y}$ be a Wiener measure normalized such that $\int \mathrm{d}\widehat{W}^t_{x,y}(\omega) = 1$. From (3.2), we have

$$\mathrm{e}^{-H'(\boldsymbol{x},\pi)} = (4\pi\beta)^{-dN/2}\, \mathrm{e}^{-H^{(0)}(\boldsymbol{x},\pi)}\, \mathrm{e}^{-H^{(1)}(\boldsymbol{x},\pi)}$$

with $H^{(0)}$ given by (3.4), and

$$\begin{aligned} \mathrm{e}^{-H^{(1)}(\boldsymbol{x},\pi)} &= \Big[\prod_{i=1}^N \int \mathrm{d}\widehat{W}^{2\beta}_{x_i x_{\pi(i)}}(\omega_i)\Big] \prod_{1\leq i<j\leq N} \mathrm{e}^{-\frac{1}{2}\int_0^{2\beta} U\left(\omega_i(s)-\omega_j(s)\right)\mathrm{d}s} \\ &= \Big[\prod_{i=1}^N \int \mathrm{d}\widehat{W}^{2\beta}_{x_i x_{\pi(i)}}(\omega_i)\Big] \prod_b \big(1-\Upsilon(\omega_b)\big). \end{aligned} \tag{4.1}$$

The last product is over bonds $b = \{i,j\}$ with $i \neq j$. For $i < j$, we defined $\omega_b = \omega_i - \omega_j$, and

$$\Upsilon(\omega_b) = 1 - \mathrm{e}^{-\frac{1}{2}\int_0^{2\beta} U(\omega_b(s))\mathrm{d}s}. \tag{4.2}$$

Expanding the product in (4.1), we have

$$\mathrm{e}^{-H^{(1)}(\boldsymbol{x},\pi)} = \Big[\prod_{i=1}^{N}\int \mathrm{d}\widehat{W}^{2\beta}_{x_i x_{\pi(i)}}(\omega_i)\Big] \sum_{k=0}^{\frac{1}{2}N(N-1)} (-1)^k \sum_{\{b_1,\dots,b_k\}} \prod_{m=1}^{k} \Upsilon(\omega_{b_m}). \tag{4.3}$$

In the regime of weak interactions, the typical k in the above sum is a small fraction of the volume, and the typical $b_1, \dots, b_k$ are mostly disjoint.

We first perform the expansion in a somewhat cavalier fashion. We will be more precise in Section 4.2, where we will check that we have identified the leading order. Let $b_m = \{i_m, j_m\}$. Let us assume that $b_\ell \cap b_m = \emptyset$ for all $\ell \neq m$; then

$$\Big[\prod_{i=1}^{N}\int \mathrm{d}\widehat{W}^{2\beta}_{x_i x_{\pi(i)}}(\omega_i)\Big] \prod_{m=1}^{k} \Upsilon(\omega_{b_m}) = \prod_{m=1}^{k} V(x_{i_m}, x_{\pi(i_m)}, x_{j_m}, x_{\pi(j_m)}) \tag{4.4}$$

where the potential V has been defined by

$$V(x,y,x',y') = \int \mathrm{d}\widehat{W}^{2\beta}_{xy}(\omega) \int \mathrm{d}\widehat{W}^{2\beta}_{x'y'}(\omega')\Upsilon(\omega-\omega'). \tag{4.5}$$

This is the two-body interaction between jumps $x \mapsto y$ and $x' \mapsto y'$. The expression (4.5) can be simplified, see Eq. (4.16) below. We use the identity (4.4) for all $b_1, \dots, b_k$ that appear in (4.3), not only disjoint ones. This is an approximation; it assumes that either the terms with intersecting b_m's are not important, or that their contribution is close to (4.4). We obtain

$$\mathrm{e}^{-H^{(1)}(\boldsymbol{x},\pi)} \approx \sum_{k\geq 0}(-1)^k \sum_{\{b_1,\dots,b_k\}} \prod_{m=1}^{k} V(x_{i_m}, x_{\pi(i_m)}, x_{j_m}, x_{\pi(j_m)}).$$

Ignoring the possibility that a same bond may occur several times, we get

$$\begin{aligned} \mathrm{e}^{-H^{(1)}(\boldsymbol{x},\pi)} &\approx \sum_{k\geq 0} \frac{(-1)^k}{k!} \sum_{b_1,\dots,b_k} \prod_{m=1}^{k} V(x_{i_m}, x_{\pi(i_m)}, x_{j_m}, x_{\pi(j_m)}) \\ &= \exp\Big\{- \sum_{1\leq i<j\leq N} V(x_i, x_{\pi(i)}, x_j, x_{\pi(j)})\Big\}. \end{aligned} \tag{4.6}$$

These approximations suggest that, to lowest order in the strength of the interaction, the multi-body interaction arising from the Feynman-Kac representation can be approximated by the two-body interaction defined in (4.5).

4.2. *Cluster expansion*

It is not clear that the approximations above have produced the correct terms, that are exact to lowest order. In this section we perform a cluster expansion. It cannot be entirely justified from a mathematical point of view, but it nevertheless clarifies the approximations.

Consider the graph with vertices $\{1,\dots,k\}$, and with an edge between ℓ and m whenever $b_\ell \cap b_m \neq \emptyset$. We say that a set of bonds $B = \{b_1,\dots,b_k\}$ is *connected* if this graph is connected. Let $\operatorname{supp} B = \cup_{b\in B} b$. We say that B and B' are *compatible* if their supports are disjoint, $\operatorname{supp} B \cap \operatorname{supp} B' = \emptyset$. Then the sum over sets of bonds in (4.3) can be written as a sum over connected and mutually compatible B's, namely

$$\sum_{k\geq 0} (-1)^k \sum_{\{b_1,\dots,b_k\}} \prod_{m=1}^{k} \Upsilon(\omega_{b_m}) = \sum_{\ell\geq 0} \frac{1}{\ell!} \sum_{\substack{B_1,\dots,B_\ell \\ \text{compatible}}} \prod_{m=1}^{\ell} \Big[(-1)^{|B_m|} \prod_{b\in B_m} \Upsilon(\omega_b) \Big]. \tag{4.7}$$

The contribution of compatible B's factorizes. For a connected B, let us introduce

$$\Phi_B(\boldsymbol{x},\pi) = (-1)^{|B|} \Big[\prod_{i\in \operatorname{supp} B} \int \mathrm{d}\widehat{W}^{2\beta}_{x_i x_{\pi(i)}}(\omega_i) \Big] \prod_{b\in B} \Upsilon(\omega_b).$$

Notice that $\Phi_B(\boldsymbol{x},\pi)$ depends only on positions x_i and $x_{\pi(i)}$ for $i \in \operatorname{supp} B$. Then we have

$$\mathrm{e}^{-H^{(1)}(\boldsymbol{x},\pi)} = \sum_{\ell\geq 0} \frac{1}{\ell!} \sum_{\substack{B_1,\dots,B_\ell \\ \text{compatible}}} \prod_{m=1}^{\ell} \Phi_{B_m}(\boldsymbol{x},\pi). \tag{4.8}$$

We now apply the cluster expansion method, see e.g. Ref. 9,14 for references. Given $B_1,\dots,B_\ell$, let $\varphi(B_1,\dots,B_\ell)$ be the following combinatorial function:

$$\varphi(B_1,\dots,B_\ell) = \begin{cases} 1 & \text{if } \ell = 1; \\ \dfrac{1}{\ell!} \displaystyle\sum_{G\subset \mathcal{G}(B_1,\dots,B_\ell)} (-1)^{|G|} & \text{if } \ell \geq 2. \end{cases}$$

Here, $\mathcal{G}(B_1,\dots,B_\ell)$ denotes the graph with ℓ vertices, and with an edge between i and j whenever B_i and B_j are *not* compatible. The sum is over all *connected* subgraphs of ℓ vertices, and $|G|$ is the number of edges of G. Notice that $\varphi(B_1,\dots,B_\ell)$ is zero unless $B_1,\dots,B_\ell$ form a cluster, i.e., unless $\mathcal{G}(B_1,\dots,B_\ell)$ is connected.

The cluster expansion yields a convergent series for the logarithm of (4.8), hence for $H^{(1)}$. Precisely,

$$H^{(1)}(\boldsymbol{x},\pi) = -\sum_{\ell\geq 1}\sum_{B_1,\dots,B_\ell} \varphi(B_1,\dots,B_\ell)\prod_{m=1}^{\ell}\Phi_{B_m}(\boldsymbol{x},\pi). \tag{4.9}$$

Let $i_1,\dots,i_k$ be distinct indices. The previous equation suggests to define the k-body interaction by

$$\begin{aligned} &V^{(k)}\big((x_{i_\ell},x_{\pi(i_\ell)})_{\ell=1}^{k}\big) \\ &= -\sum_{m\geq 1}\sum_{\substack{B_1,\dots,B_m \\ \cup_\ell \operatorname{supp} B_\ell=\{i_1,\dots,i_k\}}} \varphi(B_1,\dots,B_m)\prod_{\ell=1}^{m}\Phi_{B_\ell}(\boldsymbol{x},\pi). \end{aligned} \tag{4.10}$$

Then $H^{(1)}$ is given by

$$H^{(1)}(\boldsymbol{x},\pi) = \sum_{k\geq 2}\sum_{1\leq i_1<\cdots<i_k\leq N} V^{(k)}\big((x_{i_\ell},x_{\pi(i_\ell)})_{\ell=1}^{k}\big). \tag{4.11}$$

Everything here is exact, and it is rigorous provided we can prove the absolute convergence of the series of cluster terms in (4.9). A sufficient criterion is that, for any i,

$$\sum_{B,\operatorname{supp} B\ni i} |\Phi_B(\boldsymbol{x},\pi)|\,\mathrm{e}^{a|B|} \leq a \tag{4.12}$$

for some constant $a>0$. See e.g. Ref. 9,14 for concise statements about cluster expansions. The sum above involves bonds whose positions are far away. In order to get such an estimate, one needs to control spatial decay. It depends on permutations, and there are combinatorial difficulties.

We conclude this subsection by discussing various estimates for the terms above. Using $1-\mathrm{e}^{-x}\leq x$, we have that

$$\|\Upsilon\|_\infty = \sup_\omega \Upsilon(\omega) \leq \beta\|U\|_\infty.$$

The interesting regime of parameters is $\beta\sim 1/T_{\mathrm{c}}^{(0)}$ and $U\to 0$, so Υ is arbitrarily small. If the potential U is a hard-core with small radius, then $\|\Upsilon\|_\infty = 1$, but $\|\Upsilon\|_p$ is small for $p<\infty$. We also have that, for any B, $\boldsymbol{x}$, and π,

$$|\Phi_B(\boldsymbol{x},\pi)| \leq \|\Upsilon\|_\infty^{|B|}.$$

Consider the series (4.10) for the potential at order k. The sets $B_1,\dots,B_m$ that contribute to lowest order are such that $\sum_\ell |B_\ell| = k-1$. It follows that $V^{(k)}$ is of order $\|\Upsilon\|_\infty^{k-1}$.

We can extract the lowest order term. The expression for $V^{(2)}(x_i, x_{\pi(i)}, x_j, x_{\pi(j)})$ involves terms of arbitrary orders. But we only need to consider $-\Phi_B$ with B containing the single bond $b = \{i, j\}$. We then obtain the potential V defined in (4.5).

4.3. *A simpler expression for the interaction*

We now seek to simplify the formula (4.5). Namely, we can replace the two integrals over Brownian bridges by a single integral, which will lead to the nicer formula (4.16). We have

$$\int \mathrm{d}W^{2\beta}_{xy}(\omega) \int \mathrm{d}W^{2\beta}_{x'y'}(\omega')\Upsilon(\omega-\omega')$$

$$= \lim_{n\to\infty} \int_{\Lambda^{2(n-1)}} \mathrm{d}x_2 \dots \mathrm{d}x_n \, \mathrm{d}x'_2 \dots \mathrm{d}x'_n \Big[\prod_{i=1}^{n} g_{2\beta/n}(x_{i+1}-x_i) g_{2\beta/n}(x'_{i+1}-x'_i)\Big] \times$$

$$\times \Big[1 - \exp\Big\{-\frac{\beta}{n}\sum_{i=1}^{n} U(x_i - x'_i)\Big\}\Big] \tag{4.13}$$

with $x_1 = x$, $x_{n+1} = y$, $x'_1 = x'$, $x'_{n+1} = y'$. Let us introduce $z_i = x_i - x'_i$. It is not hard to check that

$$\begin{aligned} &g_{2\beta/n}(x_{i+1}-x_i)\, g_{2\beta/n}(x'_{i+1}-x'_i) \\ &= g_{\beta/n}(x_{i+1} - x_i - \tfrac{1}{2}z_{i+1} + \tfrac{1}{2}z_i)\, g_{4\beta/n}(z_{i+1}-z_i). \end{aligned} \tag{4.14}$$

Substituting into (4.13), we get

$$\lim_{n\to\infty} \int_{\Lambda^{n-1}} \mathrm{d}z_2 \dots \mathrm{d}z_n \Big[\prod_{i=1}^{n} g_{4\beta/n}(z_{i+1}-z_i)\Big] \Big[1 - \exp\Big\{-\frac{\beta}{n}\sum_{i=1}^{n} U(z_i)\Big\}\Big]$$

$$\int_{\Lambda^{n-1}} \mathrm{d}x_2 \dots \mathrm{d}x_n \prod_{i=1}^{n} g_{\beta/n}(x_{i+1} - x_i - \tfrac{1}{2}z_{i+1} + \tfrac{1}{2}z_i). \tag{4.15}$$

Using Eq. (3.1), the last line is equal to

$$g_\beta\big(y - x - \tfrac{1}{2}(y - y' - x + x')\big) = g_\beta\big(\tfrac{1}{2}(y + y' - x - x')\big).$$

The first line of (4.15) yields an integral over Brownian paths. Then (4.15) is equal to

$$g_\beta\big(\tfrac{1}{2}(y + y' - x - x')\big) \int \big[1 - \mathrm{e}^{-\frac{1}{4}\int_0^{4\beta} U(\omega(s))\mathrm{d}s}\big] \mathrm{d}W^{4\beta}_{x-x',y-y'}(\omega).$$

Finally, we have the following identity, similar to (4.14)

$$g_{2\beta}(y-x) g_{2\beta}(y'-x') = g_\beta\big(\tfrac{1}{2}(y + y' - x - x')\big) g_{4\beta}(y - y' - x + x').$$

Recall that the two-body interaction defined in (4.5) involves normalized Wiener measures. Putting normalizations back, we get the following elegant formula for the interaction between jumps $x \mapsto y$ and $x' \mapsto y'$,

$$\boxed{V(x,y,x',y') = \int \left[1 - \mathrm{e}^{-\frac{1}{4}\int_0^{4\beta} U(\omega(s))\mathrm{d}s}\right] \mathrm{d}\widehat{W}^{4\beta}_{x-x',y-y'}(\omega).} \tag{4.16}$$

It would be useful to obtain a closed form expression in terms of special functions, if it is possible. When U consists of a hard-core potential of radius a, $V(x,y,x',y')$ is equal to the probability that a Brownian bridge, starting at $x-x'$ and ending at $y-y'$, intersects the ball of radius a centered at 0.

4.4. *Effect of interactions on the critical temperature*

The model of spatial permutations should help to clarify the effects of interactions on the critical temperature of Bose-Einstein condensation.

Let $T_{\mathrm{c}}^{(a)}$ be the critical temperature for Bose-Einstein condensation as a function of the scattering length a of the interaction potential U between quantum particles. It is believed that $T_{\mathrm{c}}^{(a)}$ behaves in three dimensions as

$$\frac{T_{\mathrm{c}}^{(a)} - T_{\mathrm{c}}^{(0)}}{T_{\mathrm{c}}^{(0)}} = c\rho^{1/3}a + o(\rho^{1/3}a), \tag{4.17}$$

with c a *universal* constant that does not depend on the mass of particles or on the interactions. The value and even the sign of c has been contested in the physics literature, although a consensus has recently emerged that $c \approx 1.3$. See Refs. 1,7,8,10 and references therein.

The model of spatial permutations is clearly simpler than the Feynman-Kac representation of the Bose gas, and is therefore better suited to Monte-Carlo simulations. More importantly, we expect that this model, with the interaction (4.16), is *exactly* related to the original quantum boson model, to lowest order in a. Numerical simulations should allow to determine the constant c in the model of permutations with high precision, and with high confidence. It should be identical to the universal constant of (4.17) for the interacting Bose gas.

5. A simple model of interacting spatial permutations

In this final section, we discuss a simple model of interacting spatial permutations that was introduced in Ref. 2. We consider only interactions between permutation jumps of 2-cycles, arguably the most important. The resulting model is exactly solvable, and it provides a heuristic description for the shift in the critical temperature of the Bose-Einstein condensation.

The approximation consists in replacing the Hamiltonian (2.3) by

$$\tilde{H}(\boldsymbol{x},\pi) = \frac{1}{4\beta}\sum_{i=1}^{N} |x_i - x_{\pi(i)}|^2 + \sum_{\substack{1\le i<j\le N \\ \pi(i)=j,\pi(j)=i}} V(x_i,x_j,x_j,x_i).$$

The interaction term $V(\cdot)$ is given by (4.16) as before. From now on, all computations will be exact, at least to lowest order in the scattering length of the original potential U. We consider the three-dimensional case, obviously the most interesting. A computation shows that

$$V(x,y,y,x) = \frac{2a}{|x-y|} + O(a^2). \tag{5.1}$$

The lowest order term in the right side does not depend on β, surprisingly. The expectation of a random variable of permutations is given by (2.2),

$$E_{\Lambda,N}(\theta) = \frac{1}{Z(\Lambda,N)N!} \sum_{\pi\in\mathcal{S}_N} \theta(\pi) \int_{\Lambda^N} \mathrm{d}\boldsymbol{x}\, \mathrm{e}^{-\tilde{H}(\boldsymbol{x},\pi)}.$$

We now substitute $\tilde{H}$ with the following simpler Hamiltonian $H^{(\alpha)}$:

$$H^{(\alpha)}(\boldsymbol{x},\pi) = \frac{1}{4\beta}\sum_{i=1}^{N} |x_i - x_{\pi(i)}|^2 + \alpha N_2(\pi), \tag{5.2}$$

with $N_2(\pi)$ denoting the number of 2-cycles in the permutation π. The substitution is exact provided that, for any given permutation π,

$$\int_{\Lambda^N} \mathrm{d}\boldsymbol{x}\, \mathrm{e}^{-H(\boldsymbol{x},\pi)} = \int_{\Lambda^N} \mathrm{d}\boldsymbol{x}\, \mathrm{e}^{-H^{(\alpha)}(\boldsymbol{x},\pi)}.$$

Isolating the contribution of 2-cycles, this equation reduces to

$$\int_{\Lambda^2} \mathrm{d}x_1\mathrm{d}x_2\, \mathrm{e}^{-\frac{1}{2\beta}|x_1-x_2|^2 - V(x_1,x_2,x_2,x_1)} = \int_{\Lambda^2} \mathrm{d}x_1\mathrm{d}x_2\, \mathrm{e}^{-\frac{1}{2\beta}|x_1-x_2|^2-\alpha}.$$

With $V(\cdot)$ in (5.1), we find that

$$\alpha = \Big(\frac{8}{\pi\beta}\Big)^{1/2} a + O(a^2). \tag{5.3}$$

We now compute the pressure of the model with Hamiltonian $H^{(\alpha)}$. The grand-canonical partition function is given by

$$Z'(\beta,\Lambda,\mu) = \sum_{N\ge 0} \frac{\mathrm{e}^{\beta\mu N}}{N!} \sum_{\pi\in\mathcal{S}_N} \int_{\Lambda^N} \mathrm{d}\boldsymbol{x}\, \mathrm{e}^{-H^{(\alpha)}(\boldsymbol{x},\pi)}.$$

It is convenient to work in the Fourier space. Let us introduce a new partition function,

$$Z(\beta,\Lambda,\mu)=\sum_{N\geq 0}\frac{\mathrm{e}^{\beta\mu N}}{N!}\sum_{k_1,\dots,k_N\in\Lambda^*}\sum_{\pi\in\mathcal{S}_N}\mathrm{e}^{-\alpha N_2(\pi)}\prod_{i=1}^{N}\mathrm{e}^{-\beta|2\pi k_i|^2}\,\delta_{k_i,k_{\pi(i)}}. \tag{5.4}$$

Here, $\Lambda^*=\frac{1}{L}\mathbb{Z}^3$ is the dual lattice. The thermodynamic pressure is defined by

$$p^{(\alpha)}(\beta,\mu)=\lim_{V\to\infty}\frac{1}{\beta V}\log Z(\beta,\Lambda,\mu) \tag{5.5}$$

One can verify that the partition functions Z and Z' differ in two respects only. First, a normalization is missing, which results in a shift of the chemical potential. Second, Z has been defined with periodic boundary conditions, unlike Z' (where boundary conditions are neither periodic, nor Dirichlet). But both partition functions yield the same thermodynamics; precisely,

$$\lim_{V\to\infty}\frac{1}{\beta V}\log Z'(\beta,\Lambda,\mu)=p^{(\alpha)}\big(\beta,\mu+\tfrac{3}{2\beta}\log(4\pi\beta)\big).$$

We now compute $p^{(\alpha)}$. Introducing occupation numbers, (5.4) becomes

$$Z(\beta,\Lambda,\mu)=\sum_{(n_k)_{k\in\Lambda^*}}\prod_{k\in\Lambda^*}\left[\mathrm{e}^{-\beta(|2\pi k|^2-\mu)n_k}\sum_{\pi_k\in\mathcal{S}_{n_k}}\frac{1}{n_k!}\,\mathrm{e}^{-\alpha N_2(\pi_k)}\right].$$

We decomposed the permutation π into permutations (π_k) for each Fourier mode, and we also used

$$N_2(\pi)=\sum_{k\in\Lambda^*}N_2(\pi_k).$$

Notice that the chemical potential needs to be strictly negative, as in the ideal gas. We get

$$p^{(\alpha)}(\beta,\mu)=\lim_{V\to\infty}\frac{1}{\beta V}\sum_{k\in\Lambda^*}\log\left[\sum_{n\geq 0}\mathrm{e}^{-\beta(|2\pi k|^2-\mu)n}\sum_{\pi\in\mathcal{S}_n}\frac{1}{n!}\,\mathrm{e}^{-\alpha N_2(\pi)}\right]. \tag{5.6}$$

Let us compute the bracket above. For given $\pi\in\mathcal{S}_n$, let r_j denote the number of cycles of length j. Then $\sum_j jr_j=n$, and the number of permutations for given (r_j) is equal to

$$n!\Big/\prod_{j\geq 1}j^{r_j}r_j!.$$

The bracket in (5.6) is equal to

$$\sum_{n\geq 0} \frac{1}{n!} \sum_{\substack{r_1,r_2,\cdots\geq 0 \\ \sum_j j r_j = n}} \frac{n!}{\prod_{j\geq 1} j^{r_j} r_j!} \, \mathrm{e}^{-\beta(|2\pi k|^2-\mu)\sum_j j r_j} \, \mathrm{e}^{-\alpha r_2}$$

$$= \sum_{r_1,r_3,r_4,\cdots\geq 0} \prod_{j=1,3,4,\ldots} \frac{1}{r_j!} \big[\tfrac{1}{j} \, \mathrm{e}^{-j\beta(|2\pi k|^2-\mu)}\big]^{r_j} \sum_{r_2\geq 0} \frac{1}{r_2!} \big[\tfrac{1}{2} \, \mathrm{e}^{-2\beta(|2\pi k|^2-\mu)-\alpha}\big]^{r_2}$$

$$= \exp\Big\{ \sum_{j=1,3,4,\ldots} \tfrac{1}{j} \, \mathrm{e}^{-j\beta(|2\pi k|^2-\mu)} + \tfrac{1}{2} \, \mathrm{e}^{-2\beta(|2\pi k|^2-\mu)-\alpha} \Big\}$$

$$= \exp\Big\{ -\log(1 - \mathrm{e}^{-\beta(|2\pi k|^2-\mu)}) - \tfrac{1}{2} \, \mathrm{e}^{-2\beta(|2\pi k|^2-\mu)} \, (1 - \mathrm{e}^{-\alpha}) \Big\}.$$

This can be inserted into (5.6). In the limit $V \to \infty$ the expression converges to a Riemann integral. If $\alpha = 0$, we get the pressure of the ideal gas

$$p^{(0)}(\beta,\mu) = -\frac{1}{\beta} \int_{\mathbb{R}^3} \log\big(1 - \mathrm{e}^{-\beta(|2\pi k|^2-\mu)}\big) \mathrm{d}k, \tag{5.7}$$

as expected. And if $\alpha \neq 0$, we get

$$p^{(\alpha)}(\beta,\mu) = p^{(0)}(\beta,\mu) - \frac{\mathrm{e}^{2\beta\mu}}{2^{11/2}\pi^{3/2}\beta^{5/2}} (1 - \mathrm{e}^{-\alpha}).$$

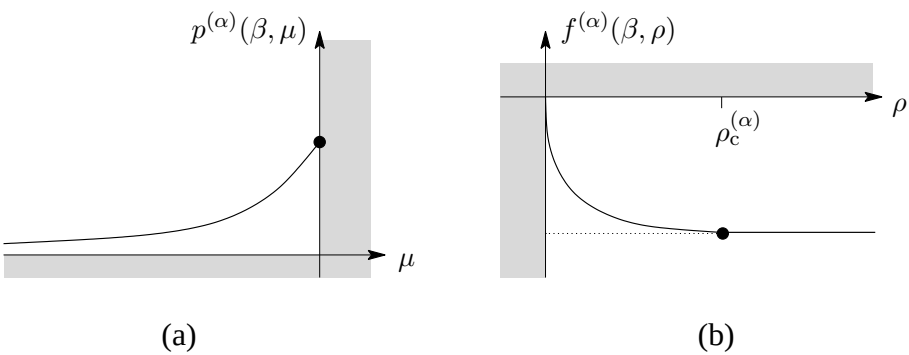

Fig. 3. The pressure and the free energy of the simple interacting model in three dimensions.

The pressure $p^{(\alpha)}$ is plotted in Fig. 3 (a) as a function of μ. One can consider other thermodynamic potentials as well. Recall that the free energy $f^{(\alpha)}$ is function of the (inverse) temperature and of the density, and it is related to the pressure by a Legendre transform:

$$f^{(\alpha)}(\beta,\rho) = \sup_{\mu} \big[\rho\mu - p^{(\alpha)}(\beta,\mu)\big].$$

One then obtains the graph depicted in Fig. 3 (b). It is strictly decreasing up to the *critical density* $\rho_{\rm c}^{(\alpha)} = \rho_{\rm c}^{(\alpha)}(\beta)$, and it is constant afterwards. The critical density is equal to the derivative of $p^{(\alpha)}$ with respect to μ at $0-$. We have

$$\rho_{\rm c}^{(\alpha)} = \rho_{\rm c}^{(0)} - \frac{1}{2^{9/2}\pi^{3/2}\beta^{3/2}}(1 - {\rm e}^{-\alpha}). \tag{5.8}$$

The first term of the right side, $\rho_{\rm c}^{(0)}$, is equal to the critical density of the ideal gas, Eq. (2.4). The second term is the correction due to our simple interaction.

We see that $\rho_{\rm c}^{(\alpha)}$ is smaller than $\rho_{\rm c}^{(0)}$ — interactions favour Bose-Einstein condensation. This observation is in line with physicists' expectations. The heuristics is particularly simple in this model: 2-cycles are penalized and this favours all other cycles, including infinite cycles. The latter occur therefore at a lower density. While elementary, this heuristics may well be correct.

Let us now estimate the change in the critical temperature. Using (5.3) with $\beta = 1/T_{\rm c}^{(0)}$, we find that, to lowest order,

$$\frac{T_{\rm c}^{(a)} - T_{\rm c}^{(0)}}{T_{\rm c}^{(0)}} = \tfrac{1}{3\sqrt{2}}\zeta(\tfrac{3}{2})^{-1}\alpha = \tilde{c}\,\rho^{1/3}a$$

with $\tilde{c} = 0.37$. This formula can be compared to (4.17). If we believe the value $c = 1.3$ found numerically, then 2-cycle interactions account only for a fraction of the effect of all interactions. One could also take into account the interactions within 3-cycles and longer cycles; the constant $\tilde{c}$ would increase a bit.

One would expect infinite cycles to occur for all densities larger than the critical density (5.8). More precisely, Theorem 2.1 should remain valid for $\alpha > 0$, replacing $\rho_{\rm c}$ by $\rho_{\rm c}^{(\alpha)}$. But only a weaker claim has been proved so far.

Theorem 5.1. *For any $b < 1$,*

$$\lim_{V\to\infty} E_{\Lambda,\rho V}(\boldsymbol{\varrho}_{V^b,\rho V}) \geq \rho - \frac{4}{(1 + {\rm e}^{-\alpha})^2}\rho_{\rm c}^{(0)}.$$

Theorem 5.1 guarantees the existence of macroscopic cycles for large enough densities. The proof can be found in ref. 2.

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BOSON GAS WITH BCS INTERACTIONS *

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This talk contains a review of some results about homogeneous boson models, which are a special case of the general variational problem of statistical mechanics that can be solved in terms of quasi-free states. We apply these results to the model of the Mean-Field Boson Gas with Bardeen-Cooper-Schrieffer (BCS) interaction.

Keywords: Solvable boson models, Bose-Einstein condensation, canonical commutation relations, equilibrium states, quasi-free states, gauge breaking, entropy densities, variational principles, pairing boson model

1. Introduction

1.1. *Motivation*

Shortly after the discovery of superfluidity F. London made a connection between this phenomenon and the almost forgotten Bose-Einstein condensation (BEC) in the free Bose gas.[28] His arguments were essentially based on fact that Helium-4 atoms are bosons, and their superfluidity can be understood in terms of the Bose statistics that they obey. Almost ten years later N.N Bogoliubov[8] proposed a microscopic theory of the superfluidity of Helium-4 showing that it can be regarded as a consequence of combination of *two factors*: the Bose-Einstein *condensation* and *interaction* between bosons. The Bogoliubov theory had a serious impact, since just a few years before L.D. Landau had developed a spectral criterion for superfluidity and according to this criterion the *free* Bose gas is not superfluid even in the presence of BEC.[23]

But more than eighty years after the prediction of Bose-Einstein con-

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densation the problem of whether this phenomenon is stable with respect to realistic pair-interaction is still unsolved and seems beyond the reach of the present methods. Either one must use special pair-potentials and limits[27] or one must truncate the Hamiltonian. The second course was followed by many authors. One such approach is to use a Hamiltonian which is a function of the occupation of the free-gas single particle states.[42] Since all the operators in these models commute, they can be investigated by probabilistic techniques using Laplace's method (*Large Deviations*).[6,7] However these models (which include mean-field or imperfect Bose gas) produce a spectrum identical to that of the free Bose gas and therefore does not satisfy the superfluidity criterion.

A more plausible model is the so-called Bogoliubov model, also called the weakly imperfect Bose-gas, see Refs.8,45. This model takes into account more interaction terms without losing its exact solvability. The basic ingredients of this model in terms of states on the (Canonical Commutation Relations) CCR-algebra of the boson observables, including the problem of the Bogoliubov-Landau spectral behaviour, has been analyzed in Refs. 1,2. Later the boson *Pairing Model* was introduced as a further refinement of the Bogoliubov model by including of BCS boson interaction.[46] Theoretical work on this model resulted into some intriguing properties like the occurrence of two types of condensation, a boson BCS-type *pair condensation* and the standard *one-particle* condensation, as well the presence of a spectral gap in the elementary excitations spectrum.[18,20,21,29,35]

The methods that have been used so far for the study of these solvable models have been the Bogoliubov approximating Hamiltonian method[45] and some form of Laplace's method,[67] One should also mention the noncommutative large deviation method developed in Ref. 32 for lattice systems and later refined in Ref. 39. This method has not been rigorously extended to Bose systems mainly due to technical problems with unbounded operators. However on a formal level it gives the right variational formulas (see for example Ref. 35.) Here we develop a new method based on the *quasi-free* states on the algebra of observables given by the algebra of the canonical commutation relations.[9,30]

1.2. *Solvable Models*

All the solvable models referred to above share the property that their equilibrium states and/or ground states, which are states on the algebra of the Canonical Commutation Relations (CCR) are completely determined by the one- and two-point correlation functions. Such states are called quasi-

free states. This class of states has been intensively studied in the sixties and seventies. Although quasi-free states are frequently used as the ideal laboratory for performing tests of all kinds, this mathematical analysis turned out to be much too technical to be very practical for its utility in the study of Bose systems in physics, see e.g. Refs. 12,40.

Recently we found in Ref. 36 a presentation of the quasi-free states suitable for the study of space homogeneous systems and in particular the explicit form of the variational principle of statistical mechanics for all solvable boson models. Then for these models the set of states over which one minimizes the free-energy density (or grand-canonical pressure) is reducible to the set of homogeneous quasi-free states. The main technical step in this is the explicit formula for the entropy density of a general quasi-free state including the non-gauge symmetric ones.

Though the variational principle when solved fully, in principle contains all the information about the model, in practice it is often difficult to solve. A very useful additional tool is the use of *condensate equations* introduced in Refs. 43,44. They form an essential part of the study of the variational principle and can be derived without any explicit knowledge of the entropy of the system, Section 2. Moreover, they are always valid as opposed to the Euler-Lagrange equations which are not always satisfied because either the stationary point is a maximum or the minimum does not correspond to any stationary point.

In Section 3 we apply our method to the Pairing Boson Model with Mean-Field and Bardeen-Cooper-Schrieffer (BCS) interactions to obtain the variational principle conjectured in Ref. 35 (and proved in Ref. 38), supplemented by the *condensate equations*. This model with BCS *attraction* is a very good example of a situation, when the condensate equations can give some conclusions more directly. For instance, from the condensate equations (3.11), (3.12), one immediately concludes that there is neither pairing nor zero-mode condensation for negative chemical potentials and also that zero-mode condensation implies a non-trivial boson pairing. An unusual property of this model is that for the BCS *repulsion* it is not completely equivalent to the mean-field case: the repulsion does not change the density of corresponding thermodynamic potentials but produces a generalized (*type* III) condensation à la van den Berg-Lewis-Pulé.

2. Quasi-Free Boson Systems

2.1. *Mathematical Heuristics*

Traditional approach to boson systems in mathematical physics is to start with symmetric Fock Hilbert space $\mathfrak{F}$ of vector states. Let $L^2(\mathbb{R}^n)$ be the space of square integrable functions on $\mathbb{R}^n$, here n stands for dimensionality. One considers the creation and annihilation operators: for any $f, g \in L^2(\mathbb{R}^n)$. The creation operator is given by $a^*(f) = \int dx f(x) a^*(x)$ acting in some domain $\mathrm{dom}(a^*(f)) \subset \mathfrak{F}$, the annihilation operator is its adjoint operator $a(f)$, and satisfying the usual canonical commutation relations

$$[a(x), a^*(y)] = \delta(x-y)\,, [a(x), a(y)] = 0,$$

leading to the relations

$$[a(f), a^*(g)] = (f, g)\,,\ [a(f), a(g)] = 0.$$

It is assumed that there exists a particular normalized vector Ω in $\mathfrak{F}$ such that it is annihilated by all $a(x)$ and hence that for all f:

$$a(f)\Omega = 0. \tag{2.1}$$

The symmetric Fock space $\mathfrak{F}$ is then the Hilbert space is the linear span generated by all vectors of the set: $\{a^*(f_1)a^*(f_2)...a^*(f_n)\Omega\}_n$ for all f_i and for all $n \in \mathbb{N}$.

A vector-state ω_Ψ of a boson system is an expectation value of the type $\omega(A) = (\Psi, A\Psi)$, where Ψ is a normalized vector of the Fock space and where A is any observable of the boson system. Remark that each observable is a function of the boson creation and annihilation operators. In particular, the physical model is defined through the energy observable, called Hamiltonian. For a two-body interaction v the general model takes the following form in a finite volume $V = |\Lambda|$:

$$\begin{aligned} H_\Lambda = \int_\Lambda dx \frac{1}{2m} \nabla a^*(x) \cdot \nabla a(x) \\ + \frac{1}{2V} \int_\Lambda dx \int_\Lambda dy\, a^*(x) a^*(y) v(x-y) a(x) a(y)\ . \end{aligned} \tag{2.2}$$

Stability of the model requires that the Hamiltonian operator acting in the Fock space is bounded from below.

In this paper we adopt the following definition: we shall say that a system is *solvable* if the corresponding density of thermodynamic potential can be expressed explicitly via a finite number of correlation functions.

We shall make this definition more exact later. In general the model (2.2) described above is not solvable. The natural way of defining solvability is in terms of the correlation functions.

The state ω is known if one can find all its correlation functions

$$\omega(a^*(f_1)...a^*(f_n)a(g_1)...a(g_m)) \tag{2.3}$$

for all functions f_i, g_j. One should realize that in order to know the state one has to know an infinity of correlation functions, for all $n, m \in \mathbb{N}$. This makes the many-body problem unsolvable in most cases.

In the literature one can find many approximation procedures, where the original state ω is replaced by a state $\widetilde{\omega}$ constructed via various *decoupling* procedures such that all higher order correlation functions can be expressed in terms of those of order less than some $n+m$. It must remarked that on the basis of the Marcinkiewicz theorem,[33,41] many of them are erroneous. Indeed, this theorem tells us that if the decoupling holds for all correlation functions from some $n+m$ on, then the decoupling holds for all correlation of order $n+m>2$. This means that the only decoupling, not contradicting the positivity of the state $\widetilde{\omega}$, is the one in terms of the one-point function, $\widetilde{\omega}(a(f))$ and two-point functions, $\widetilde{\omega}(a^*(f)a(g))$, $\widetilde{\omega}(a(f)a(g))$, for all f and g. Any state satisfying the decoupling procedure described above is called a "quasi-free state" (qf-state).

In the rest of this section we recall the main features of the boson Gibbs states, in particular the class of space homogeneous quasi-free states which are necessary for the formulation of the variational principle of statistical mechanics for solvable models.

Our main original contribution in this section is a proof of the existence of a canonical automorphism mapping a gauge breaking state in a gauge invariant one. This result will be essential for the explicit computation of the entropy density of the state, which makes possible the explicit formulation the variational principle for our class of solvable boson models.

2.2. *Canonical Commutation Relations and Quasi-Free States*

In order to define the total set of all *quasi-free* states it is convenient to work with the boson field which is defined on $\mathfrak{S}$ a suitable subspace of $L^2(\mathbb{R}^n)$, called a space of *test functions*. This field is defined by the map $b : f \in \mathfrak{S} \mapsto b(f)$, where the linear operator $b(f)$ on Fock space is given by

$$b(f) = a(f) + a^*(f).$$

The *Canonical Commutation Relations* (CCR) for these fields are now

$$[b(f), b(g)] = 2i\sigma(f, g) \ , \tag{2.4}$$

with $\sigma(f, g) = \mathrm{Im}\, \mathrm{m}(f, g)$. Note that the fields are real-linear in their argument: $b(\lambda f) = \lambda b(f)$, for $\mathrm{Im}\, \mathrm{m}\lambda = 0$, but $b(if) = i(-a(f) + a^*(f))$ and $a(f) = \frac{1}{2}((b(f) + ib(if))$.

It is equivalent to use the field operators as the generators of all observables instead of creation and annihilation operators. To avoid using unbounded operators we use the *Weyl operators* as the generators of the algebra of observables $\mathfrak{A}$ of the system. These are given by

$$W(f) \ = \exp\{ib(f)\}, \tag{2.5}$$

for any $f \in \mathfrak{S}$. The CCR are then equivalent to the relations

$$W(f)W(g) = e^{-i\sigma(f,g)}W(f + g). \tag{2.6}$$

We shall denote the set of states on $\mathfrak{A}$ by $\mathfrak{S}$. We recall that a state $\omega \in \mathfrak{S}$, is any *normalized linear positive* form on $\mathfrak{A}$.

Very often it is convenient to define states though their *truncated functions* $\omega(b(f_1)b(f_2)\dots b(f_n))_t$ for $f_1, f_2, \dots f_n \in \mathfrak{S}$. These functions are defined recursively through the formula

$$\omega(b(f))_t = \omega(b(f)), \quad \omega(b(f_1)\dots b(f_n)) = \sum \omega(b(f_k)\dots)_t \dots \omega(\cdots(f_l))_t,$$

where the sum is over all possible partitions of $\{1, \dots, n\}$, and where the order within each of the clusters is carried over from the left to the right.

Let ω be an arbitrary state on the Weyl algebra $\mathfrak{A}$, then for all $f \in \mathfrak{S}$, the expectation values $\omega(W(f))$ are known and can be expressed in terms of the truncated functions (see e.g., Ref. 9),

$$\begin{aligned} \omega(W(f)) = \omega(e^{i\lambda b(f)}) &= \sum_{n=0}^{\infty} \frac{i^n\lambda^n}{n!}\omega(b(f)^n) \\ &= \exp\left\{\sum_{n=1}^{\infty} \frac{i^n\lambda^n}{n!}\omega(b(f)^n)_t\right\}. \end{aligned} \tag{2.7}$$

For the models that we study in this paper we shall see that only the one- and two-point functions play a role. The one-point function is determined by the linear functional ϕ on $\mathfrak{S}$ and the two-point functions by two (unbounded) operators R and S on $\mathfrak{S}$. These are defined by

$$\phi(f) = \omega(a^*(f)) \tag{2.8}$$

and the truncated two-point functions

$$\begin{aligned}\langle f, Rg\rangle &= \omega(a(f)a^*(g)) - \omega(a(f))\omega(a^*(g)),\\ \langle f, Sg\rangle &= \omega(a(f)a(\overline{g})) - \omega(a(f))\omega(a(\overline{g})),\end{aligned} \tag{2.9}$$

where $\overline{g}$ stands for the complex conjugate of g. Clearly $\omega(b(f)b(f))$ can be expressed in terms of these two operators and ϕ. Note that the operator R is self-adjoint. We shall denote by $\mathfrak{S}_{\phi,R,S}$ the elements of $\mathfrak{S}$ determined by the triplet ϕ, R and S.

Since $*$-automorphisms (canonical transformations) leave the CCR invariant, many properties of a state are conserved under these transformations. We shall say that states are *canonically equivalent* if they can be transformed into each other in such a way.

It is easy to see that in general there is a canonical transformation which transforms a state ω into a state ω_0 with $\phi = 0$. For any real linear functional χ on $\mathfrak{S}$, the transformation τ_χ on the boson algebra defined by

$$\tau_\chi(W(f)) \;=\; e^{i\chi(f)}W(f) \tag{2.10}$$

together with linearity and conservation of products, is a canonical transformation. Clearly this transformation translates the boson field, $\tau_\chi b(f) = b(f) + \chi(f)$. Now the composition of a state ω with the transformation τ_χ, $\omega_0 = \omega \circ \tau_\chi$ is again a state and $\omega_0(b(f)) = \omega(b(f)) + \chi(f)$. Therefore if we choose $\chi(f) = -\omega(b(f)) = -2\Re e\,\phi(f)$, which is real linear, then the one-point function of ω_0 vanishes. Moreover the reduced two-point functions are left invariant so that operators R and S are unchanged.

It is clear that the positivity of the state ω implies that

$$\omega((a(f) + a^*(\overline{g}))(a(f) + a^*(\overline{g}))^*) \geq 0 \tag{2.11}$$

for all $f, g \in \mathfrak{S}$. Assuming $\phi = 0$ the inequality (2.11) is equivalent to

$$\langle f, Rf\rangle + \langle f, Sg\rangle + \langle g, S^*f\rangle + \langle g, (R-1)g\rangle \geq 0$$

for all $f, g \in \mathfrak{S}$. Putting $f = 0$ we see that $R \geq 1$, and putting $g = -R^{1/2}h$ and $f = R^{-1/2}Sh$ gives

$$R(R-1) + S^*S - R^{-1/2}S^*SR^{1/2} - R^{1/2}S^*SR^{-1/2} \geq 0.$$

Notice that if operators R and S *commute*, then the latter simplifies to

$$T^2 \equiv R(R-1) - S^*S \geq 0. \tag{2.12}$$

We now introduce the one-parameter group of gauge transformations. This group of canonical transformations or CCR-automorphisms, $\{\tau_\lambda |\, \lambda \in \mathbb{R}\}$, is defined by

$$\tau_\lambda(a^*(f)) = e^{i\lambda}a^*(f),\ \tau_\lambda(a(f)) = e^{-i\lambda}a(f). \tag{2.13}$$

A state ω is called *gauge invariant* if the relation $\omega \circ \tau_\lambda = \omega$ holds for all $\lambda \in \mathbb{R}$. In particular for a state $\omega \in \mathfrak{S}_{\phi,R,S}$ the one- and two-point functions transform under such a gauge transformation as follows

$$\begin{aligned}(\omega \circ \tau_\lambda)(a^*(f)) &= e^{i\lambda}\omega(a^*(f)),\\ (\omega \circ \tau_\lambda)(a(f)a^*(g)) &= \omega(a(f)a^*(g)),\\ (\omega \circ \tau_\lambda)(a(f)a(g)) &= e^{-i2\lambda}(\omega)(a(f)a(g)),\end{aligned}$$

or equivalently (ϕ, R, S) is transformed into $(e^{i\lambda}\phi, R, e^{-i2\lambda}S)$. Therefore a necessary condition for gauge invariance is that $\phi = 0$ and $S = 0$.

We now prove that any $\omega \in \mathfrak{S}_{\phi,R,S}$ is canonically equivalent to a state $\widetilde{\omega} \in \mathfrak{S}_{\widetilde{R}} \equiv \mathfrak{S}_{0,\widetilde{R},0}$ if R and S commute and $\overline{Rf} = R\overline{f}$ for all $f \in \mathfrak{S}$. We shall see later that these conditions are satisfied for translation invariant states. We determine explicitly the operator $\widetilde{R}$ as a function of R and S. This result is similar to the more restricted result stated in Ref. 30, where only the existence of such a map between pure quasi-free states (see definition later) is proved. Here we prove not only the existence of this map but we give its explicit construction.

Theorem 2.1. *Let $\omega \in \mathfrak{S}_{\phi,R,S}$ with R and S commuting and $\overline{Rf} = R\overline{f}$ for all $f \in \mathfrak{S}$. Then there exists a canonical transformation τ mapping ω into $\widetilde{\omega} \in \mathfrak{S}_{\widetilde{R}}$ where the operator $\widetilde{R}$ is given, in terms of the operators $R \geq 1$ and $T \geq 0$, by*

$$\widetilde{R} = \frac{1}{2} + \left(T^2 + \frac{1}{4}\right)^{\frac{1}{2}}. \tag{2.14}$$

Proof. Clearly we can assume that $\phi = 0$. By applying a canonical transformation similar to the gauge transformation in (2.13) we can transform operator S into $|S|$. Then we consider another canonical transformation γ (also called Bogoliubov transformation)

$$\widetilde{a}(f) = \gamma(a(f)) = a(Uf) - a^*(\overline{Vf}),$$

where U and V are commuting self-adjoint operators commuting with R and S and satisfying $\overline{Uf} = U\overline{f}$, $\overline{Vf} = V\overline{f}$ and $U^2 - V^2 = I$. We consider the two equations

$$\begin{aligned}\langle f, \widetilde{R}g\rangle &= \widetilde{\omega}(a(f)a^*(g)) = \omega(\gamma(a(f)a^*(g))),\\ 0 = \langle f, \widetilde{S}g\rangle &= \widetilde{\omega}(a(f)a(\overline{g})) = \omega(\gamma(a(f)a(\overline{g}))),\end{aligned}$$

in order to express $\widetilde{R}$ as a function of R and S or preferably T. One computes explicitly the following equations from the former ones, using the symmetry

of R and S, as follows

$$\widetilde{R} = U^2 R + V^2(R-1) - 2UVS, \tag{2.15}$$

$$0 = U^2 S - UV(2R-1) + V^2 S. \tag{2.16}$$

From the second relation (2.16) one gets a quadratic equation for the operator $X := UV^{-1}$, which is semi-bounded from below by I. Then solution of this equation has the form

$$X = \left(R - 1/2 + \left((R-1/2)^2 - S^2 \right)^{1/2} \right) S^{-1}.$$

Using the relation (2.12) between the operators S and T, one gets

$$X = \left(R - 1/2 + \left(T^2 + 1/4 \right)^{1/2} \right) \left(R(R-1) - T^2 \right)^{-1/2}.$$

This gives for U and V,

$$U = X(X^2-1)^{-1/2}, \quad V = (X^2-1)^{-1/2},$$

which we insert into the first equation (2.15) to obtain $\widetilde{R}$ as a function (2.14) of R and T.

The canonical transformation τ of the theorem is of course given by the composition of the gauge transformation with the Bogoliubov transformation. □

The states we shall be considering will be translation invariant. Space translations are again realized by a group of canonical transformations $\{\tau_x | \, x \in \mathbb{R}^n\}$ of the algebra of observables $\mathfrak{A}$ given by $\tau_x(a(f)) = a(T_x f)$ where $(T_x f)(y) = f(y-x)$. The translation invariance of a state ω, given by $\omega \circ \tau_x = \omega$ for all $x \in \mathbb{R}^n$, is immediately translated to the operators R, S by the property that they both commute with the operators T_x for $x \in \mathbb{R}^n$.

Translation invariance implies that $\phi(f) = c\widehat{f}(0)$ where $\widehat{f}$ denotes the Fourier transform of f and $c = \omega(a^*(0))$. On the other hand it is well known[19] that if A is such a translation invariant operator, then there exists a function ξ on $\mathbb{R}^n$ whose Fourier transform is a tempered distribution such that for all functions f, $(\widehat{Af})(k) = \xi(k)\widehat{f}(k)$. This is due to the kernel theorem for operator-valued distributions and the convolution theorem for Fourier transforms. In particular, our operators R and S are simple multiplication operators with functions denoted by $r(k)$ and $s(k)$. It is easily checked that for $k \neq 0$, $r(k) = \omega(\widehat{a}(k)\widehat{a}^*(k))$ and $s(k) = \omega(\widehat{a}(k)\widehat{a}(-k)) = s(-k)$ where $\widehat{a}(k)$ is the operator-valued distribution given by the Fourier transform of $a(x)$. For our purposes (see later) we

can assume in addition that $r(-k) = r(k)$. This last property is equivalent to $\overline{Rf} = R\overline{f}$. As R and S are multiplication operators they commute so that (2.12) holds and can be written in terms of r and s:

$$r(k)(r(k) - 1) - |s(k)|^2 \geq 0.$$

It is convenient to introduce a non-negative function $t(k)$, corresponding to the operator T, defined by

$$t(k)^2 = r(k)(r(k) - 1) - |s(k)|^2. \tag{2.17}$$

The class of translation invariant states $\mathfrak{S}_{\phi,R,S}$ can now be parameterized by the complex number c and the functions $r \geq 1$, $t \geq 0$ and $\alpha(k) = \arg s(k)$.

Now we turn to the *quasi-free* states.

Definition 2.1. A state ω is called a *quasi-free* state (qf-state) if all truncated functions of order $n > 2$ vanish. This means that a qf-state is completely determined by its one- and two-point functions:

$$\omega(W(f)) = \exp\{i\omega(b(f)) - \frac{1}{2}\omega(b(f)b(f))_t\} \tag{2.18}$$

The set of qf-states will be denoted by $\mathfrak{Q}$.

Note that a qf-state is completely determined by ϕ, R and S. We denote the qf-state corresponding to ϕ, R and S by $\omega_{\phi,R,S}$. Of course, translation invariant qf-states can be parameterized uniquely by the complex number c and the functions $r \geq 1$, $t \geq 0$ and $\alpha(k) = \arg s(k)$. Note also that a qf-state is gauge invariant if and only if $\phi = 0$ and $S = 0$. The above arguments show that $\omega_{\phi,R,S}$ is canonically equivalent to $\omega_{\widetilde{R}} \equiv \omega_{0,\widetilde{R},0}$.

We end this section by calculating the entropy for qf-states. For any normal (density matrix) state ω with density matrix ρ the von Neumann entropy is defined by the formula $S(\omega) = -\mathrm{Tr}\,\rho \ln \rho$. The entropy is left invariant under any canonical transformation τ (see e.g., Ref. 34, Chapters 1 and 9), that is, $S(\omega \circ \tau) = S(\omega)$. Let ω be a translation invariant, locally normal state on the algebra $\mathfrak{A}$ (i.e., its restriction to every bounded region of $\mathbb{R}^n$ is normal). Let $\Lambda \subset \mathbb{R}^n$ be a family of bounded regions increasing to $\mathbb{R}^n$. Then the entropy density of ω is defined by

$$\mathcal{S}(\omega) = \lim_{\Lambda} \frac{S(\omega_\Lambda)}{V}, \tag{2.19}$$

where $V = |\Lambda|$ denotes the volume of Λ, ω_Λ is the restriction of ω to Λ and $\lim_\Lambda := \lim_{\Lambda \uparrow \mathbb{R}^n}$. For translation invariant qf-states of the type ω_R, $\mathcal{S}$ has

been calculated in Ref. 15 and is given by

$$\mathcal{S}(\omega_R) = \int \nu(\mathrm{d}k)\ \{r(k)\ln r(k) - (r(k)-1)\ln(r(k)-1)\} \tag{2.20}$$

where $\nu(\mathrm{d}k) = \mathrm{d}^n k/(2\pi)^n$. It is clear from the above argument that the entropy density of $\omega_{\phi,R,S}$ is the same as that for $\omega_{\widetilde{R}}$. We state this result in the following proposition.

Proposition 2.1. *The entropy density of qf-state with two-point functions defined by R and S is given by*

$$\begin{aligned}\mathcal{S}(\omega_{\phi,R,S}) &= \mathcal{S}(\omega_{\widetilde{R}}) \\ &= \int \nu(\mathrm{d}k)\ \{\widetilde{r}(k)\ln\widetilde{r}(k) - (\widetilde{r}(k)-1)\ln(\widetilde{r}(k)-1)\}\end{aligned} \tag{2.21}$$

where $\widetilde{r}$ *is given by* (2.14),

$$\widetilde{r}(k) = \frac{1}{2} + \left(t^2(k) + \frac{1}{4}\right)^{\frac{1}{2}}. \tag{2.22}$$

In particular, the entropy density is independent of the one-point function ϕ.

2.3. *Equilibrium States*

An equilibrium state at inverse temperature β of a homogeneous boson system will be defined by the variational principle of statistical mechanics, that is, an equilibrium state is one that minimizes the free energy density.

The free-energy density (or more precisely the grand-canonical pressure) functional is defined on the state space by

$$f(\omega) := \beta\,\mathcal{E}(\omega) - \mathcal{S}(\omega)\ , \tag{2.23}$$

where $\mathcal{S}(\omega)$ is defined in the previous section and $\mathcal{E}(\omega)$ is the energy density. The energy density is determined by the local Hamiltonians of the system under consideration, H_Λ, defined for each bounded region of volume V

$$\mathcal{E}(\omega) = \lim_V \frac{1}{V}\omega(H_\Lambda - \mu N_\Lambda)\ ,$$

where μ is the chemical potential and N_Λ is the particle number operator.

The variational principle of statistical mechanics states that each translation invariant (or periodic) equilibrium state ω_β is the minimizer of the free energy density functional, that is, for any state ω,

$$f(\omega_\beta) = \inf_\omega f(\omega). \tag{2.24}$$

In the definition of $\mathcal{E}$ and $\mathcal{S}$ it has been presupposed that the states are locally normal in the sense that ω_Λ is a normal state. This is a reasonable assumption since we are basically interested in equilibrium states which are thermodynamic limits of local Gibbs states given locally by their (grand) canonical density matrices $\rho_\Lambda = e^{-\beta(H_\Lambda - \mu N_\Lambda)}/\mathrm{Tr}\, e^{-\beta(H_\Lambda - \mu N_\Lambda)}$.

Let ω be a normal state with density matrix ρ on Fock space $\mathfrak{F}$, with zero one-point function and with two-point functions given by the operators R and $S = 0$. Let $\{f_j\}$ be an orthonormal basis of eigenvectors of R with eigenvalues r_j. Consider the operator (trial diagonal Hamiltonian) $H = \sum_j \epsilon_j a_j^* a_j$ with $a_j = a(f_j)$ and $\epsilon_j = \ln(r_j/(r_j - 1))$. Let σ be the density matrix given by $\sigma = e^{-H}/\mathrm{Tr}\, e^{-H}$. It is clear that the state defined by σ is a qf-state which has two point function

$$\mathrm{Tr}\, \sigma\, a(f)a^*(g) = \langle f, Rg\rangle = \mathrm{Tr}\, \rho\, a(f)a^*(g).$$

Thus σ is the density matrix for the qf-state ω_R.

We use this construction to prove the entropy inequality

$$S(\omega) \leq S(\omega_R). \tag{2.25}$$

Using the Bogoliubov-Klein convexity inequality [9, Lemma 6.2.21], one gets

$$S(\omega_{(R,0)}) - S(\omega) = \mathrm{Tr}\, \rho \ln \rho - \mathrm{Tr}\, \sigma \ln \sigma \geq \mathrm{Tr}\, (\rho - \sigma) \ln \sigma$$

where $\ln \sigma = -\sum_j \epsilon_j a_j^* a_j - \ln\, \mathrm{Tr}\, (\exp -H)$ and hence

$$S(\omega_\sigma) - S(\omega) \geq -\sum_j \epsilon_j (\mathrm{Tr}\, \rho\, a_j^* a_j - \mathrm{Tr}\, \sigma\, a_j^* a_j) \,=\, 0,$$

since the states ρ and σ have the same two-point functions. This proves the inequality (2.25), which is a mathematical expression with the following physical interpretation: The state ω is a state with more non-trivial correlations than its associated qf-state ω_R and therefore it is understandable that the entropy of the state is smaller than or equal than the entropy of its associated qf-state.

Clearly this inequality carries over to the entropy density of locally normal states and using canonical equivalence to locally normal states with non-vanishing ϕ and S. Thus for locally normal states in $\mathfrak{S}_{\phi,R,S}$ we have

$$\mathcal{S}(\omega) \leq \mathcal{S}(\omega_{\phi,R,S}) = \mathcal{S}(\omega_{\widetilde{R}}). \tag{2.26}$$

From now on we shall study *solvable models*, i.e., models with a Hamiltonian whose energy density $\lim_\Lambda \omega(H_\Lambda)/V$ for any translation invariant state ω depends only on the one- and two-point correlation functions of the

state. This will be made more precise in Definition 2.3. But we first impose one last restriction on the states.

Definition 2.2. A translation invariant state ω is called *space-ergodic*, if for any three A, B, C *local* observables the following holds

$$\lim_{\Lambda} \omega(AB_\Lambda C) = \omega(AC)\omega(B),$$

where B_Λ the space-average

$$B_\Lambda = \frac{1}{V}\int_\Lambda dx\, \tau_x(B).$$

Note that for translation invariant states one has that $\omega(B) = \lim_\Lambda \omega(B_\Lambda)$, and therefore the above definition can be written in the form

$$\omega(A(\lim_{\Lambda} B_\Lambda - \omega(B)I)C) = 0.$$

In other words, for a space-ergodic state ω, the *limiting space-average* operator $\overline{B} := \omega - \lim_\Lambda B_\Lambda$ is proportional to identity I. In the same way one gets $\omega - \lim_\Lambda [B_\Lambda, A] = 0$ for any local observables A and B. For these reasons the limiting operator $\overline{B}$ is called an *observable at infinity*.[9] Note that $\overline{B}$ is a normal operator since $[\overline{B}, \overline{B^*}] = 0$

As a first application of the ergodicity of states we have

$$\lim_{\Lambda} \omega\left(\frac{a_0^* a_0}{V}\right) = |c|^2 := \rho_0, \tag{2.27}$$

where ρ_0 is the zero-mode condensate density for boson systems.

Definition 2.3. We say that a model is *solvable* if for every ergodic state ω, the energy density $\mathcal{E}(\omega)$ depends only on the *one-point* and *two-point* correlation functions of ω.

Note that if a model is solvable then the energy density $\mathcal{E}(\omega)$ is the same for all $\omega \in \mathfrak{S}_{\phi,R,S}$. We shall denote this common value by $\mathcal{E}(r, t, \alpha, c)$. On the other hand we have shown that for $\omega \in \mathfrak{S}_{\phi,R,S}$, $S(\omega)$ attains its maximum at the qf-state $\omega = \omega_{\phi,R,S}$. Thus we have

$$\begin{aligned} &\inf_{\omega \in \mathfrak{S}_{\phi,R,S}} f(\omega) = f(\omega_{\phi,R,S}) \\ &= \beta\mathcal{E}(r,t,\alpha,c) - \int \nu(\mathrm{d}k)\, \left\{\widetilde{r}(k)\ln\widetilde{r}(k) - (\widetilde{r}(k)-1)\ln(\widetilde{r}(k)-1)\right\}. \end{aligned} \tag{2.28}$$

Taking the infimum in (2.28) over ϕ, R and S we obtain our main result.

Theorem 2.2. *For a solvable boson system the equilibrium state ω_β is a qf-state and it is defined by*

$$f(\omega_\beta) = \inf_{\omega\in\mathfrak{Q}} f(\omega)$$

$$= \inf_{r,\,t,\,\alpha,\,c}\left\{\beta\mathcal{E}(r,t,\alpha,c) - \int\nu(\mathrm{d}k)\ \{\widetilde{r}(k)\ln\widetilde{r}(k) - (\widetilde{r}(k)-1)\ln(\widetilde{r}(k)-1)\}\right\}\ ,$$

where $\widetilde{r}(k)$ is given by (2.22) *as a function of r and t.*

2.4. *Condensate Equations*

Now we are in position to introduce the notion of *condensate equations* for equilibrium states of general boson system. They constitute essential tools for the study of the equilibrium as well as ground states of boson models. For a full discussion of this topic we refer the reader to Refs. 43,44. These equations are derived directly from the variational principle of statistical mechanics formulated above. However they have certain advantages over the Euler-Lagrange equations. First of all that they can be derived without any explicit knowledge of the entropy of the system. Secondly, while the Euler-Lagrange equations are not always satisfied because either the stationary point is a maximum or the minimum occurs on the boundary, the condensate equations are always valid.

To this end, consider the following completely-positive semigroups of transformations on the locally normal states in $\mathfrak{S}$. Let A be any local (quasi-local) observable (with space-average A_Λ over region Λ) and let

$$\Gamma_\Lambda = \int\limits_\Lambda dx\{[\tau_x(A_\Lambda^*),.]\tau_x(A_\Lambda) + \tau_x(A_\Lambda^*)[.,\tau_x(A_\Lambda)]\}.$$

Then for each finite region Λ one can define a semigroup of completely-positive maps on $\mathfrak{S}$[13] given by

$$\{\gamma_{\lambda,V} = \exp\lambda\Gamma_\Lambda\,|\,\lambda\geq 0\}.$$

Let ω_β be any locally normal state satisfying the variational principle with density matrix ρ_Λ. Then using the notation of Definition 2.2, one gets

$$0 \leq \lim_{\lambda\to 0}\frac{1}{\lambda}(f(\lim_\Lambda \omega\circ e^{\lambda\Gamma_\Lambda}) - f(\omega))$$
$$\leq \lim_\Lambda\left\{\beta\,\mathrm{Tr}\,\rho_\Lambda A_\Lambda^*[H_\Lambda(\mu),A_\Lambda] - \mathrm{Tr}\,\rho_\Lambda A_\Lambda^*\,A_\Lambda\ln\frac{\mathrm{Tr}\,\rho_\Lambda A_\Lambda^*\,A_\Lambda}{\mathrm{Tr}\,\rho_\Lambda A_\Lambda\,A_\Lambda^*}\right\}$$

The second inequality is a consequence of the bi-convexity of the function $x,y\to x\ln(x/y)$. Since the limiting space-average operator $\overline{A}$ is normal,

the second term of the right-hand side of the inequality vanishes and one gets

$$\lim_{\Lambda} \beta\omega_\beta(A_\Lambda^*[H_\Lambda(\mu), A_\Lambda]) \geq 0, \tag{2.29}$$

along with the same inequality with A_Λ replaced by A_Λ^*.

Using the same argument as above, but now working with the group of unitary operators $\{U_t = \exp(\mathrm{i}tH_\Lambda(\mu))|\, t \in \mathbb{R}\}$, one gets immediately $\lim_\Lambda \omega_\beta([H_\Lambda(\mu), X]) = 0$ for any observable X. Therefore

$$\begin{aligned} 0 &= \lim_{\Lambda} \omega_\beta([H_\Lambda(\mu), A_\Lambda^*\, A_\Lambda]) \\ &= \lim_{\Lambda} \{\omega_\beta([H_\Lambda(\mu), A_\Lambda^*]A_\Lambda) + \omega_\beta(A_\Lambda^*[H_\Lambda(\mu), A_\Lambda])\}. \end{aligned} \tag{2.30}$$

Using (2.29) and the property that the space-averages commute with all local observables, one gets the general condensate equation.

Theorem 2.3. *Let ω_β be any limit Gibbs state, satisfying the variational principle for equilibrium states at inverse temperature β, including $\beta = \infty$ which means that ω_∞ is a ground state, and let A be any local (or quasi-local) observable, then the condensate equation with respect to A is given by*

$$\lim_{\Lambda} \omega_\beta(A_\Lambda^*\,[H_\Lambda(\mu), A_\Lambda]) = 0. \tag{2.31}$$

3. Pairing Boson Model with BCS and Mean-Field Interactions

The model was invented in Ref. 46 as an attempt to improve the Bogoliubov theory of the weakly imperfect boson gas, see a detailed discussion in Refs 25,45. Using the notation of the previous section the Hamiltonian of the *Pairing Boson Model* (PBH) is then given as in Refs. 35,38 by

$$H_\Lambda = T_\Lambda - \frac{u}{2V} Q_\Lambda^* Q_\Lambda + \frac{v}{2V} N_\Lambda^2, \tag{3.1}$$

where

$$T_\Lambda = \sum_{k\in\Lambda^*} \epsilon(k)\, a_k^* a_k, \quad Q_\Lambda = \sum_{k\in\Lambda^*} \lambda(k) a_k a_{-k}, \quad N_\Lambda = \sum_{k\in\Lambda^*} a_k^* a_k.$$

The coupling λ is for simplicity a real L^2-function on $\mathbb{R}^n$ satisfying $\lambda(-k) = \lambda(k)$, $1 = \lambda(0) \geq |\lambda(k)|$. The coupling constant v is positive and satisfies $v - u > 0$, implying that the Hamiltonian defines a *superstable* system.[38] For a discussion of the origin of this model, see Ref. 38 and the references therein.

Again since the operators N_Λ/V and Q_Λ/V are both space averages, by the arguments of Section 2.3, this model is solvable in the sense of Definition 2.3 and the energy density is given by

$$\mathcal{E}(r,t,\alpha,c) = \int \nu(\mathrm{d}k)\,(\epsilon(k)-\mu)(r(k)-1) - \mu|c|^2$$
$$+\frac{v}{2}\left(\int \nu(\mathrm{d}k)\,(r(k)-1)+|c|^2\right)^2 - \frac{u}{2}\left|\lambda(0)c^2 + \int \nu(\mathrm{d}k)\,\lambda(k)s(k)\right|^2.$$

We have used the relations

$$\omega(a_k^* a_k) = \langle \phi_k, (R-1)\phi_k\rangle + |c|^2 V\delta_{k0},$$
$$\omega(a_k a_{-k}) = \langle \phi_k, S\phi_k\rangle + c^2 V\delta_{k0}.$$

With

$$\rho(k) = r(k)-1, \quad c = \sqrt{\rho_0}e^{i\alpha},$$
$$\overline{\rho} = \int \nu(\mathrm{d}k)\,\rho(k) + \rho_0, \quad \sigma = \int \nu(\mathrm{d}k)\,\lambda(k)s(k),$$

the energy density $\mathcal{E}(r,t,\alpha,c)$ becomes

$$\mathcal{E}(r,t,\alpha,c) = \int \nu(\mathrm{d}k)\,\epsilon(k)\rho(k) - \mu\overline{\rho} + \frac{v}{2}\overline{\rho}^2 - \frac{u}{2}\left|\rho_0 e^{2i\alpha} + \sigma\right|^2. \tag{3.2}$$

Since the cases $u > 0$ and $u \le 0$ are very different, we shall consider them separately.

3.1. *BCS attraction $u > 0$: Coexistence of BEC and BCS-boson pairing*

First we consider $u > 0$. Clearly, in this case the minimum in (3.2) is attained when $2\alpha = \arg\sigma$. Therefore, instead of (3.2) one can take for further analysis the function $\widetilde{\mathcal{E}}(r,t,c) := \mathcal{E}(r,t,\alpha = (\arg\sigma)/2, c)$, which has the form

$$\widetilde{\mathcal{E}}(r,t,c) = \int \nu(\mathrm{d}k)\,\epsilon(k)\rho(k) - \mu\overline{\rho} + \frac{v}{2}\overline{\rho}^2 - \frac{u}{2}\left(\rho_0 + |\sigma|\right)^2. \tag{3.3}$$

The corresponding entropy density $\mathcal{S}(\omega)$ is given in (2.21). It is independent of ρ_0 and depends only on $\rho(k)$ and $|s(k)|$. Then for real $\lambda(k)$, after optimizing with respect to the argument of $s(k)$, for $2\alpha = \arg\sigma$ the Euler-Lagrange equations in the parameters r, t and c, take the form

$$2\rho(k) + 1 = \frac{f(k)}{E(k)}\coth(\beta E(k)/2), \tag{3.4}$$

$$s(k) = \frac{u(\rho_0 + |\sigma|)\lambda(k)}{2E(k)}\coth(\beta E(k)/2), \tag{3.5}$$

$$0 = -\mu + v\overline{\rho} - u(\rho_0 + |\sigma|) \ , \tag{3.6}$$

where

$$f(k) = \epsilon(k) - \mu + v\overline{\rho}, \tag{3.7}$$

and

$$E(k) = \left\{ f^2(k) - u^2\lambda(k)^2(\rho_0 + |\sigma|)^2 \right\}^{1/2} . \tag{3.8}$$

As usual these equations are useful only if they have solutions within the admissible domain of r, t and c, which corresponds to the positivity of the state. These three equations coincide respectively with equations (2.8), (2.9) and (2.10) in Ref. 35. The integrated form of the first two equations also coincide with equations (5.1) and (5.2) in Ref. 38:

$$\overline{\rho} = \frac{1}{2}\int_{\mathsf{R}^n} \nu(\mathrm{d}k) \left\{ \frac{f(k)}{E(k)} \ \coth\frac{1}{2}\beta E(k) - 1 \right\} + \rho_0 \ , \tag{3.9}$$

$$(|\sigma| + \rho_0) = \frac{u\,(|\sigma| + \rho_0)}{2} \int_{\mathsf{R}^n} \nu(\mathrm{d}k) \frac{\lambda(k)^2}{E(k)} \ \coth\frac{1}{2}\beta E(k) \ + \rho_0 \ . \tag{3.10}$$

On the other hand, we find that the *condensate equation* (2.31) with respect to $a_0/V^{1/2}$ is

$$\rho_0(-\mu + v\overline{\rho} - u(\rho_0 + |\sigma|)) = 0, \tag{3.11}$$

cf. (3.6), and that with respect to Q_Λ/V it takes the form

$$\begin{aligned} (\overline{c}^2 + \overline{\sigma})\Bigg\{ & \int \nu(\mathrm{d}k)\, \lambda(k)(\epsilon(k) - \mu + v\overline{\rho}\,)\, s(k) + (-\mu + v\overline{\rho}\,)\ c^2 \\ & -u\left[\int \nu(\mathrm{d}k)\, \lambda(k)^2(\rho(k) + 1/2) + \rho_0\right] (c^2 + \sigma)\Bigg\} = 0. \end{aligned} \tag{3.12}$$

Taking into account that $|c|^2 = \rho_0$, one can check that these condensate equations are consistent with the Euler-Lagrange equations (3.4)-(3.6) and/or (3.9)-(3.10).

Remark 3.1. Notice that there is a relation between the condensate equation (3.11) and the Euler-Lagrange equation (3.6). Indeed, by (3.3) the ρ_0-dependent part of the variational functional has the form

$$\widetilde{\mathcal{E}}_0(\rho_0) := \frac{1}{2}(v - u)\rho_0^2 - (\mu - v\rho + u|\sigma|)\rho_0 \ ,$$

where $\rho := \overline{\rho} - \rho_0$. Since $v > u$, $\widetilde{\mathcal{E}}_0$ is strictly convex and has a unique minimum at $\rho_0^{\min}$. For $\mu \leq v\rho - u|\sigma|$ one gets $\rho_0^{\min} = 0$, which is not a

stationary point, whereas for $\mu > v\rho - u|\sigma|$ the minimum occurs at the unique *stationary point* $\rho_0^{\min} = (\mu - v\rho + u|\sigma|)/(v-u) > 0$. These of course correspond to the solutions of the Euler-Lagrange equation (3.6), or the condensate equation (3.11).

Remark 3.2. We have assumed above that $E(k) \geq 0$. It is clear that $E(k)$ corresponds to the spectrum of the quasi-particles of the model (3.1) and that it should be real and non-negative for all k. We can see this by applying the general and well-known inequality (see e.g. Refs. 9,17 or Ref. 43)

$$\lim_V \omega([X^*, [H_V - \mu N_V, X]]) > 0$$

holding for each equilibrium state and for each observable X. Let $X = \widetilde{a}_k$, where $\widetilde{a}_k = u_k a_k - v_k a^*_{-k}$, with

$$u_k^2 = \frac{1}{2}\left(\frac{f(k)}{E(k)} + 1\right), \quad v_k^2 = \frac{1}{2}\left(\frac{f(k)}{E(k)} - 1\right). \tag{3.13}$$

Then one obtains $\lim_V \omega([\widetilde{a}_k^*, [H_V - \mu N_V, \widetilde{a}_k]]) = E(k) \geq 0$, as should be by the stability of the original system.

There are two order parameters in the model (3.1), namely ρ_0 (Bose condensate density) and the function $s(k)$, or the density of condensed BCS-type bosons pairs σ with opposite momenta. By virtue of equations (3.9), (3.10) and (3.6) it is clear that there exists always a trivial solution given by $\rho_0 = s(k) = 0$, i.e., no boson condensation and no boson pairing. The interesting question is about the existence of non-trivial solutions.

The variational problem for the Boson pairing model for constant λ has been studied in detail in Ref. 35. It was shown there that the phase diagram is quite complicated and it was only possible to solve the problem for some values of u and v, see Fig. 2 in Ref. 35.

The first Euler-Lagrange equation (3.9) implies that for $u > 0$ (*attraction* in the BCS part of the PBH (3.1)) the existence of Bose-Einstein condensation, $\rho_0 > 0$ for large chemical potentials μ, or the total particle density $\overline{\rho}$. Moreover, it causes (in ergodic states) a *boson pairing*, $\sigma \neq 0$. This clearly follows from the condensate equations (3.11), (3.12) or the second Euler-Lagrange equation (3.10), since (3.10) is impossible for $\rho_0 > 0$ and $\sigma = 0$. However from the same equation it can be seen that the boson pairing $\sigma \neq 0$ can survive without Bose-Einstein condensation i.e. for $\rho_0 = |c|^2 = 0$. This is proved in the next remark.

Remark 3.3. In this remark we prove that it is possible to have a solution of the condensate equations (3.11), (3.12) with $\rho_0 = 0$ and $\sigma \neq 0$. The proof

is based on the analysis in Ref. 35. For simplicity let us take $n = 3$ and $\lambda(k) = 1$. For $x \geq 0$ we let

$$E(k,x) := \left\{ (\epsilon(k) + x)^2 - x^2 \right\}^{1/2}. \tag{3.14}$$

and for fixed $v > 0$

$$I_2(x) = \frac{v}{2} \int_{\mathsf{R}^3} \nu(\mathrm{d}k) \left\{ \frac{\epsilon(k) + x}{E(k,x)} \coth \frac{1}{2}\beta E(k,x) - 1 \right\}. \tag{3.15}$$

Let ρ_c be the critical density of the Perfect Bose Gas at inverse temperature β,

$$\rho_c := \int_{\mathbb{R}^3} \nu(\mathrm{d}k) \frac{1}{e^{\beta\epsilon(k)} - 1}. \tag{3.16}$$

Let $\mu_1 = \sup_{x \geq 0}(I_2(x) - x)$. From (3.15) one can check that $I_2(0) = v\rho_c$ and $I_2'(0) = +\infty$, and therefore $\mu_1 > v\rho_c$. Choose $v\rho_c < \mu < \mu_1$ and let $\hat{x}$ be one of the solutions of $\mu = I_2(x) - x$.

Now for $x \geq 0$, let

$$\begin{aligned} I_1(x) &= \frac{v}{2} \int_{\mathsf{R}^3} \nu(\mathrm{d}k) \frac{1}{E(k,x)} \coth \frac{1}{2}\beta E(k,x), \\ A(x) &= xI_1(x) - I_2(x). \end{aligned} \tag{3.17}$$

One can check that A is a strictly concave increasing function of x with $A(0) = -v\rho_c$. Let

$$\alpha := (A(\hat{x}) + \mu)/\hat{x} + 1 = I_1(\hat{x}). \tag{3.18}$$

Note that $A(\hat{x}) + \mu > A(0) + \mu > \mu - v\rho_c > 0$ and therefore $\alpha > 1$. Let the BCS coupling constant $u = v/\alpha$.

We now propose the following solution:

$$\rho_0 = 0, \tag{3.19}$$

$$\rho(k) = \frac{\epsilon(k) + \hat{x}}{2E(k,\hat{x})} \coth \frac{1}{2}\beta E(k,\hat{x}) - \frac{1}{2}, \tag{3.20}$$

$$s(k) = \frac{\hat{x}}{2E(k,\hat{x})} \coth \frac{1}{2}\beta E(k,\hat{x}). \tag{3.21}$$

From the definitions above it can be verified that $(s(k))^2 \leq \rho(k)(\rho(k) + 1)$. Then using the identities

$$\begin{aligned} v\overline{\rho} &= v \int_{\mathsf{R}^3} \nu(\mathrm{d}k)\rho(k) = I_2(\hat{x}) = \mu + \hat{x}, \\ u\sigma &= \frac{v}{\alpha}\,\sigma = \frac{1}{\alpha}\, I_1(\hat{x})\hat{x} = \hat{x}, \end{aligned}$$

we can check that the condensate equations (3.11), (3.12)) are satisfied. Note that (3.19)-(3.21) is also a solution of the Euler-Lagrange (3.4)-(3.6). In fact, in Ref. 35 we have proved that there is a whole region in the μ-α phase space for which this happens.

Suppose now that $(\tilde{\rho}_0 \neq 0, \tilde{\rho}(k), \tilde{s}(k))$ is another solution of (3.4)-(3.6) for the same values of μ, v and u. Then from (3.6) we can let

$$y := v \int_{\mathsf{R}^3} \nu(\mathrm{d}k)\tilde{\rho}(k) - \mu = u(\tilde{\rho}_0 + |\tilde{\sigma}|) > 0 \tag{3.22}$$

and so from (3.4)) and (3.5)) we obtain

$$\tilde{\rho}(k) = \frac{\epsilon(k) + y}{2E(k,y)} \coth \frac{1}{2}\beta E(k,y) - \frac{1}{2},$$
$$\tilde{s}(k) = \frac{y}{2E(k,y)} \coth \frac{1}{2}\beta E(k,y).$$

Integrating these identities we get

$$y + \mu - v\tilde{\rho}_0 = I_2(y),$$
$$\alpha y - v\tilde{\rho}_0 = yI_1(y)$$

and subtracting gives $A(y) = (\alpha - 1)y - \mu$. But from the properties of the function A mentioned above the last equation has only one solution for $\mu > v\rho_c$ and therefore $y = \hat{x}$. Thus the solution coincides with (3.19)-(3.21).

3.2. *BCS repulsion $u < 0$: suppression of BCS pearing and generalized (type III) Bose condensation*

The "two-stage" phase transitions with one-particle $\rho_0 = |c|^2 \neq 0$ and pair $\sigma \neq 0$ condensations described in Section is possible only for *attractive* BCS interaction $u > 0$. This behaviour was predicted in the physics literature (see for example Refs.20,46) and then was proved in Refs. 35,38.

The case of *repulsion* ($u < 0$) in the BCS part of the PBH (3.1) is very *different* than attraction. Despite general belief,[18,20,21,29] repulsion $u < 0$ is *not* identical to the case $u = 0$, i.e., to the Mean-Field Bose gas. The latter model has been studied in great details by different methods and it shows a simple *type I* BEC in the ground state, see Refs. 5,14,16,22,26,37.

Remark 3.4. Formally one deduces that (3.10) for $u < 0$ implies only trivial solutions $\rho_0 = 0$, $\sigma = 0$, but since the equation gives stationary points of the variational problem, this observation can not be conclusive. On the other hand the condensate equations (3.11), (3.12) give immediate but only partial information that for $\mu < 0$ the Bose condensation ρ_0 and

boson pairing σ must be zero. The inequalities of Remark 3.2 do not give more information about those parameters. The pressure for $u \leq 0$ was obtained rigorously in Ref. 35, in fact for a wider class of interactions then we consider here. The nature of the phase transition was studied in Ref. 38, where a method of external sources was used to prove the variational principle. Below we give another argument that solves the problem for the BCS repulsion in the PBH model (3.1).

Let us therefore take $u < 0$. Then clearly

$$\mathcal{E}(r,t,\alpha,c) \geq \int \nu(\mathrm{d}k)\, \epsilon(k)\rho(k) - \mu\overline{\rho} + \frac{v}{2}\overline{\rho}^2.$$

Therefore, since $r \mapsto r\ln r - (r-1)\ln(r-1)$ is increasing and $\widetilde{r}(k) \leq r(k)$, we have

$$\mathcal{S}(\omega_{\phi,R,S}) \leq \mathcal{S}(\omega_{\widetilde{R}}) \leq \mathcal{S}(\omega_R),$$

where $\mathcal{S}(\omega_R) = \mathcal{S}(\omega_{\phi,R,S=0}) = \mathcal{S}(\omega_{\phi=0,R,S=0})$ as in (2.20), the free-energy density $f(\omega_\beta)$ is bounded below by the free-energy density $f^{MF}(\beta,\mu)$ of the MF boson model. On the other hand

$$\begin{aligned} f(\omega_\beta) &= \inf_{\rho_0,\,\alpha,\,r,\,s} \{\beta\mathcal{E}(r,t,\alpha,c) - \mathcal{S}(\omega_{\phi,R,S})\} \\ &\leq \inf_{\rho_0=0,\,s=0} \{\beta\mathcal{E}(r,t,\alpha,c) - \mathcal{S}(\omega_{\phi,R,S})\} \\ &= \inf_{\rho} \left\{ \beta \left(\int \nu(\mathrm{d}k)\, \epsilon(k)\rho(k) - \mu\rho + \frac{v}{2}\rho^2 \right) - \mathcal{S}(\omega_R) \right\}, \end{aligned} \tag{3.23}$$

where $\rho = \int \nu(\mathrm{d}k)\rho(k)$. It is well known that the last infimum gives the free-energy density of the MF model (though this infimum is not attained with $\rho_0 = 0$ for $\mu > v\rho_c(\beta)$) and therefore $f(\omega_\beta)$ coincides with the free-energy density $f^{MF}(\beta,\mu)$. Here $\rho_c(\beta)$ is the critical density for the Perfect Bose Gas (3.16). Thus we have the following: *In the case of BCS repulsion* $u < 0$ *the free energy for the PBH is the same as for the mean-field case*

$$f(\omega_\beta) = f^{MF}(\beta,\mu)\ . \tag{3.24}$$

Returning to the variational principle this means that the infimum of the free-energy functional in the repulsive case is not attained for $\mu > v\rho_c(\beta)$. Since the critical density $\rho_c(\beta)$ is bounded (for $n > 2$), we must have BEC in this domain. But now it cannot be a simple accumulation of bosons in the mode $k = 0$, i.e. $\rho_0 \neq 0$, since it would imply that $c \neq 0$, and by consequence a positive BCS energy in $\mathcal{E}(r,t,\alpha,c)$, see PBH (3.1).

The situation which one finds strongly suggests a relation to what is known as *generalized condensation*. The possibility of such condensation

was predicted by Casimir[11] and studied extensively by van den Berg, Lewis and Pulé.[4] One form of generalized condensation is called *type III*; here the condensate is spread over an infinite number of single particle states with energy near the bottom of the spectrum, without any of the states being macroscopically occupied. To make the connection with the large deviation and variational techniques developed by van den Berg, Lewis and Pulé, see e.g., Refs. 6,7, note that though the infimum in the right-hand side of (3.23) cannot be reached within the space of *regular* measures $\rho(k)$ with $\rho_0 = 0$, there is a sequence of regular measures $\{\rho^{(l)}(k)\}_l$ such that $\rho^{(l)}(k) = 0 \cdot \delta(k) + \rho^{(l)}(k) \to \widetilde{\rho}_0\delta(k) + \widetilde{\rho}(k),\ l \to \infty$. Here $\widetilde{\rho}_0 > 0$ when $\mu > v\rho_c(\beta)$.

If $\mathcal{F}$ denotes the free-energy density functional in terms of $(\rho_0, \rho(k), s(k))$, then we get

$$\lim_{l\to\infty} \mathcal{F}(0, \rho^{(l)}(k), s^{(l)}(k) = 0) = \mathcal{F}(\widetilde{\rho}_0, \widetilde{\rho}(k), \widetilde{s}(k)). \tag{3.25}$$

Mathematically this is due to the fact that the functional $\mathcal{F}$ is not *lower* semi-continuous on the set of *regular measures*. The physical explanation was given in Ref. 38: In the case $u < 0$ this model corresponds to the *mean-field* model but with *type III* Bose condensation, i.e. with approximative regular measures that have no atom at $k = 0$. The fact that repulsive interaction is able to "spread out" the one-mode (*type I*) condensation into the *type III* was also discovered in other models.[10,31]

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