Texts and
Monographs
in Physics

Bernd Thaller

The Dirac Equation

Springer-Verlag

Bernd Thaller

The Dirac Equation

Springer-Verlag
Berlin Heidelberg New York
London Paris Tokyo
Hong Kong Barcelona
Budapest

Dr. Bernd Thaller

Institut für Mathematik, Karl-Franzens-Universität Graz
Heinrichstr. 36, A-8010 Graz, Austria

Editors

Wolf Beiglböck

Institut für Angewandte Mathematik
Universität Heidelberg
Im Neuenheimer Feld 294
W-6900 Heidelberg 1, FRG

Walter Thirring

Institut für Theoretische Physik
der Universität Wien
Boltzmanngasse 5
A-1090 Wien, Austria

Elliott H. Lieb

Jadwin Hall
Princeton University
P. O. Box 708
Princeton, NJ 08544-0708, USA

ISBN 3-540-54883-1 Springer-Verlag Berlin Heidelberg New York
ISBN 0-387-54883-1 Springer-Verlag New York Berlin Heidelberg

Library of Congress Cataloging-in-Publication Data. Thaller, Bernd, 1956– The Dirac equation / Bernd Thaller. p. cm. – (Texts and monographs in physics)
Includes bibliographical references and index.
ISBN 3-540-54883-1 (Berlin : alk. paper). – ISBN 0-387-54883-1 (New York : alk. paper)
1. Dirac equation. 2. Relativistic quantum theory. 3. Quantum electrodynamics. I. Title. II. Series.
QC174.26.W28T43 1992 530.1'24–dc20 92-12288

Typesetting: Camera ready by author

55/3140-543210 - Printed on acid-free paper

Preface

Ever since its invention in 1929 the Dirac equation has played a fundamental role in various areas of modern physics and mathematics. Its applications are so widespread that a description of all aspects cannot be done with sufficient depth within a single volume. In this book the emphasis is on the role of the Dirac equation in the relativistic quantum mechanics of spin-1/2 particles. We cover the range from the description of a single free particle to the external field problem in quantum electrodynamics.

Relativistic quantum mechanics is the historical origin of the Dirac equation and has become a fixed part of the education of theoretical physicists. There are some famous textbooks covering this area. Since the appearance of these standard texts many books (both physical and mathematical) on the non-relativistic Schrödinger equation have been published, but only very few on the Dirac equation. I wrote this book because I felt that a modern, comprehensive presentation of Dirac's electron theory satisfying some basic requirements of mathematical rigor was still missing.

The rich mathematical structure of the Dirac equation has attracted a lot of interest in recent years. Many surprising results were obtained which deserve to be included in a systematic exposition of the Dirac theory. I hope that this text sheds a new light on some aspects of the Dirac theory which to my knowledge have not yet found their way into textbooks, for example, a rigorous treatment of the nonrelativistic limit, the supersymmetric solution of the Coulomb problem and the effect of an anomalous magnetic moment, the asymptotic analysis of relativistic observables on scattering states, some results on magnetic fields, or the supersymmetric derivation of solitons of the mKdV equation.

Perhaps one reason that there are comparatively few books on the Dirac equation is the lack of an unambiguous quantum mechanical interpretation. Dirac's electron theory seems to remain a theory with no clearly defined range of validity, with peculiarities at its limits which are not completely understood. Indeed, it is not clear whether one should interpret the Dirac equation as a quantum mechanical evolution equation, like the Schrödinger equation for a single particle. The main difficulty with a quantum mechanical one-particle interpretation is the occurrence of states with negative (kinetic) energy. Interaction may cause transitions to negative energy states, so that there is no hope for a stability of matter within that framework. In view of these difficulties R. Jost stated, "The unquantized Dirac field has therefore no useful physical interpretation" ([Jo 65], p. 39). Despite this verdict we are going to approach these questions in a pragmatic way. A tentative quantum mechanical interpre-

tation will serve as a guiding principle for the mathematical development of the theory. It will turn out that the negative energies anticipate the occurrence of antiparticles, but for the simultaneous description of particles and antiparticles one has to extend the formalism of quantum mechanics. Hence the Dirac theory may be considered a step on the way to understanding quantum field theory (see Chapter 10).

On the other hand, my feeling is that the relativistic quantum mechanics of electrons has a meaningful place among other theories of mathematical physics. Somewhat vaguely we characterize its range of validity as the range of quantum phenomena where velocities are so high that relativistic kinematical effects are measurable, but where the energies are sufficiently small that pair creation occurs with negligible probability. The successful description of the hydrogen atom is a clear indication that this range is not empty. The main advantages of using the Dirac equation in a description of electrons are the following: (1) The Dirac equation is compatible with the theory of relativity, (2) it describes the spin of the electron and its magnetic moment in a completely natural way. Therefore, I regard the Dirac equation as one step further towards the description of reality than a one-particle Schrödinger theory. Nevertheless, we have to be aware of the fact that a quantum mechanical interpretation leads to inconsistencies if pushed too far. Therefore I have included treatments of the paradoxes and difficulties indicating the limitations of the theory, in particular the localization problem and the Klein paradox. For these problems there is still no clear solution, even in quantum electrodynamics.

When writing the manuscript I had in mind a readership consisting of theoretical physicists and mathematicians, and I hope that both will find something interesting or amusing here. For the topics covered by this book a lot of mathematical tools and physical concepts have been developed during the past few decades. At this stage in the development of the theory a mathematical language is indispensable whenever one tries to think seriously about physical problems and phenomena. I hope that I am not too far from Dirac's point of view: "... a book on the new physics, if not purely descriptive of experimental work, must be essentially mathematical" ([Di 76], preface). Nevertheless, I have tried never to present mathematics for its own sake. I have only used the tools appropriate for a clear formulation and solution of the problem at hand, although sometimes there exist mathematically more general results in the literature. Occasionally the reader will even find a theorem stated without a proof, but with a reference to the literature.

For a clear understanding of the material presented in this book some familiarity with linear functional analysis – as far as it is needed for quantum mechanics – would be useful and sometimes necessary. The main theorems in this respect are the spectral theorem for self-adjoint operators and Stone's theorem on unitary evolution groups (which is a special case of the Hille-Yoshida theorem). The reader who is not familiar with these results should look up the cited theorems in a book on linear operators in Hilbert spaces. For the sections concerning the Lorentz and Poincaré groups some basic knowledge of Lie groups is required. Since a detailed exposition (even of the definitions

alone) would require too much space, the reader interested in the background mathematics is referred to the many excellent books on these subjects.

The selection of the material included in this book is essentially a matter of personal taste and abilities; many areas did not receive the detailed attention they deserved. For example, I regret not having had the time for a treatment of resonances, magnetic monopoles, a discussion of the meaning of indices and anomalies in QED, or the Dirac equation in a gravitational field. Among the mathematical topics omitted here is the geometry of manifolds with a spin structure, for which Dirac operators play a fundamental role. Nevertheless, I have included many comments and references in the notes, so that the interested reader will find his way through the literature.

Finally, I want to give a short introduction to the contents of this book. The first three chapters deal with various aspects of the relativistic quantum mechanics of free particles. The kinematics of free electrons is described by the free Dirac equation, a four-dimensional system of partial differential equations. In Chapter 1 we introduce the Dirac equation following the physically motivated approach of Dirac. The Hamiltonian of the system is the Dirac operator which as a matrix differential operator is not semibounded from below. The existence of a negative energy spectrum presents some conceptual problems which can only be overcome in a many particle formalism. In the second quantized theory, however, the negative energies lead to the prediction of antiparticles (positrons) which is regarded as one of the greatest successes of the Dirac equation (Chapter 10). In the first chapter we discuss the relativistic kinematics at a quantum mechanical level. Apart from the mathematical properties of the Dirac operator we investigate the behavior of observables such as position, velocity, momentum, describe the Zitterbewegung, and formulate the localization problem.

In the second chapter we formulate the requirement of relativistic invariance and show how the Poincaré group is implemented in the Hilbert space of the Dirac equation. In particular we emphasize the role of covering groups ("spinor representations") for the representation of symmetry transformations in quantum mechanics. It should become clear why the Dirac equation has four components and how the Dirac matrices arise in representation theory. In the third chapter we start with the Poincaré group and construct various unitary representations in suitable Hilbert spaces. Here the Dirac equation receives its group theoretical justification as a projection onto an irreducible subspace of the "covariant spin-1/2 representation".

In Chapter 4 external fields are introduced and classified according to their transformation properties. We discuss some necessary restrictions (Dirac operators are sensible to local singularities of the potential, Coulomb singularities are only admitted for nuclear charges $Z < 137$), describe some interesting results from spectral theory, and perform the partial wave decomposition for spherically symmetric problems. A very striking phenomenon is the inability of an electric harmonic oscillator potential to bind particles. This fact is related to the Klein paradox which is briefly discussed.

The Dirac operator in an external field – as well as the free Dirac operator – can be written in 2×2 block-matrix form. This feature is best described in the framework of supersymmetric quantum mechanics. In Chapter 5 we give an introduction to these mathematical concepts which are the basis of almost all further developments in this book. For example, we obtain an especially simple (and at the same time most general) description of the famous Foldy-Wouthuysen transformation which diagonalizes a supersymmetric Dirac operator. The diagonal form clearly exhibits a symmetry between the positive and negative parts of the spectrum of a "Dirac operator with supersymmetry". A possible breaking of this "spectral supersymmetry" can only occur at the thresholds $\pm mc^2$ and is studied with the help of the "index" of the Dirac operator which is an important topological invariant. We introduce several mathematical tools for calculating the index of Dirac operators and discuss the applications to concrete examples in relativistic quantum mechanics.

In Chapter 6 we calculate the nonrelativistic limit of the Dirac equation and the first order relativistic corrections. Again we make use of the supersymmetric structure in order to obtain a simple, rigorous and general procedure. This treatment might seem unconventional because it does not use the Foldy-Wouthuysen transformation – instead it is based on analytic perturbation theory for resolvents.

Chapter 7 is devoted to a study of some special systems for which additional insight can be obtained by supersymmetric methods. The first part deals with magnetic fields which give rise to very interesting phenomena and strange spectral properties of Dirac operators. In the second part we determine the eigenvalues and eigenfunctions for the Coulomb problem (relativistic hydrogen atom) in an almost algebraic fashion. We also consider the addition of an "anomalous magnetic moment" which is described by a very singular potential term but has in fact a regularizing influence such that the Coulomb-Dirac operator becomes well defined for all values of the nuclear charge.

Scattering theory is the subject of Chapter 8; we give a geometric, time-dependent proof of asymptotic completeness and describe the properties of wave and scattering operators in the case of electric, scalar and magnetic fields. For the purpose of scattering theory, magnetic fields are best described in the Poincaré gauge which makes them look short-range even if they are long-range (there is an unmodified scattering operator even if the classical motion has no asymptotes). The scattering theory of the Dirac equation in one-dimensional time dependent scalar fields has an interesting application to the theory of solitons. The Dirac equation is related to a nonlinear wave equation (the "modified Korteweg-de Vries equation") in quite the same way as the one-dimensional Schrödinger equation is related to the Korteweg-de Vries equation. Supersymmetry can be used as a tool for understanding (and "inverting") the Miura transformation which links the solutions of the KdV and mKdV equations. These connections are explained in Chapter 9.

Chapter 10 finally provides a consistent framework for dealing with the negative energies in a many-particle formalism. We describe the "second quantized" Dirac theory in an (unquantized) strong external field. The Hilbert space

of this system is the Fock space which contains states consisting of an arbitrary and variable number of particles and antiparticles. Nevertheless, the dynamics in the Fock space is essentially described by implementing the unitary time evolution according to the Dirac equation. We investigate the implementation of unitary and self-adjoint operators, the consequences for particle creation and annihilation and the connection with such topics as vacuum charge, index theory, and spontaneous pair creation.

For additional information on the topics presented here the reader should consult the literature cited in the notes at the end of the book. The notes describe the sources and contain some references to physical applications as well as to further mathematical developments.

This book grew out of several lectures I gave at the Freie Universität Berlin and at the Karl-Franzens Universität Graz in 1986–1988. Parts of the manuscript have been read carefully by several people and I have received many valuable comments. In particular I am indebted to W. Beiglböck, W. Bulla, V. Enss, F. Gesztesy, H. Grosse, B. Helffer, M. Klaus, E. Lieb, L. Pittner, S. N. M. Ruijsenaars, W. Schweiger, S. Thaller, K. Unterkofler, and R. Wüst, all of whom offered valuable suggestions and pointed out several mistakes in the manuscript.

I dedicate this book to my wife Sigrid and to my ten-year-old son Wolfgang, who helped me to write the computer program producing Fig. 7.1.

Graz, October 1991 *Bernd Thaller*

Contents

1 Free Particles

The free Dirac equation describes a relativistic electron or positron which moves freely as if there were no external fields or other particles. Nevertheless this equation is important for the asymptotic description of interacting particles because in the limit of large times interacting particles tend to behave like free ones, provided their mutual separation increases.

In Sect. 1.1 we "derive" the Dirac equation for a free particle following Dirac's original approach. In order to obtain a quantum mechanical interpretation we consider the Dirac equation as an evolution equation in a suitable Hilbert space whose vectors are related to the physical states via a statistical interpretation. We identify certain self-adjoint operators with physical observables in correspondence to nonrelativistic quantum mechanics (Sect. 1.3). Next we prove self-adjointness of the Dirac operator (energy observable) and determine its spectral properties in Sect. 1.4. The time evolution is described in Sect. 1.5. In particular we derive the evolution kernel (Feynman propagator) and show that it vanishes outside the light cone. This implies a causal propagation of wavefunctions. We also investigate the temporal behavior of position, velocity, spin and orbital angular momentum (Sect. 1.6).

By writing the Dirac equation as a quantum mechanical initial value problem we arrive at a one particle interpretation which, if pushed too far, leads to some inconsistencies — even at the level of free particles. The origin of all problems is the fact that the Dirac operator is not semibounded. Therefore a free electron can be in a state with negative energy. Via a charge conjugation these negative energy solutions can be identified as positive energy solutions of a positron Dirac equation. There remains, however, the problem that there are superpositions of electron and positron solutions in the original Hilbert space. The resulting interference effects lead to a paradoxical behavior of free wavepackets ("Zitterbewegung", see Sect. 1.6).

Since for free particles the sign of the energy is a conserved quantity one might think of restricting everything to the subspace of positive energies, and choosing observables which leave this subspace invariant. This procedure leads to the quantum analog of the classical relativistic relation between energy and velocity without Zitterbewegung (Sect. 1.7). But again there is an unexpected difficulty. This is the localization problem described in Sect. 1.8: Since the standard position operator (multiplication by x) mixes positive and negative energies one is forced to look for a new position operator (i.e., to reinterpret the wavefunction). But choosing any other position observable in the positive energy subspace leads inevitably to the possibility of an instantaneous spreading of initially localized states and therefore to an acausal behavior. On the other hand, we could keep $|\psi|^2$ as the usual expression for the position probability density. But then there are no localized states at all with positive energy, and hence there is no position observable in the usual sense. This problem indicates either that the usual quantum mechanical interpretation (which is basically a one-particle interpretation modelled on the nonrelativistic theory) is insufficient, or that "localization in a finite region" is not a property that one single relativistic particle can have.

In Sect. 1.9 we describe an approximate localization by the "method of (non-)stationary phase" (Sect. 1.9). In particular we estimate the probability of finding the particle at large times outside the "classically allowed" region. This is the region of space where a particle with a certain momentum distribution and initial localization is expected to be according to classical mechanics. We find that the tails of the wavefunction in the classically forbidden region decay rapidly in time. These results are needed for scattering theory in Chapter 8.

1.1 Dirac's Approach

In this section we follow closely Dirac's original arguments which led to the discovery of his famous equation describing the relativistic motion of a spin-1/2 particle in $\mathbb{R}^3$. A deeper understanding of the origin of the Dirac equation will be obtained on a group theoretical basis in Chapter 3.

Formally, the transition from classical to quantum mechanics can be accomplished by substituting appropriate operators for the classical quantities. Usually, these operators are differential or multiplication operators acting on suitable wavefunctions. In particular, for the energy E and the momentum $\boldsymbol{p}$ of a free particle the substitution

$$E \longrightarrow \mathrm{i}\hbar\frac{\partial}{\partial t}, \quad \boldsymbol{p} \longrightarrow -\mathrm{i}\hbar\nabla, \quad (\hbar = \text{Planck's constant}) \tag{1.1}$$

is familiar from the nonrelativistic theory. Moreover, (1.1) is formally Lorentz-invariant. If applied to the classical relativistic energy-momentum relation,

$$E = \sqrt{c^2p^2 + m^2c^4}, \tag{1.2}$$

(1.1) gives the square-root Klein-Gordon equation

$$\mathrm{i}\hbar\,\frac{\partial}{\partial t}\,\psi(t,\boldsymbol{x}) = \sqrt{-c^2\hbar^2\triangle + m^2c^4}\;\psi(t,\boldsymbol{x}), \quad t \in \mathbb{R}, \quad \boldsymbol{x} \in \mathbb{R}^3, \tag{1.3}$$

where $\triangle = \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2 + \partial^2/\partial x_3^2$ is the Laplace operator. The square-root of a differential operator can be defined with the help of Fourier-transformations, but due to the asymmetry of space and time derivatives Dirac found it impossible to include external electromagnetic fields in a relativistically invariant way. So he looked for another equation which can be modified in order to describe the action of electromagnetic forces. This new equation should also describe the internal structure of the electrons, the spin. The Klein-Gordon equation

$$-\hbar^2\frac{\partial^2}{\partial t^2}\,\psi(t,\boldsymbol{x}) = \left(-c^2\hbar^2\triangle + m^2c^4\right)\psi(t,\boldsymbol{x}) \tag{1.4}$$

with a scalar wavefunction ψ was not able to do so. Moreover, a quantum mechanical evolution equation should be of first order in the time derivative. So Dirac reconsidered the energy-momentum relation (1.2) and before translating it to quantum mechanics with the help of (1.1), he linearized it by writing

$$E = c\sum_{i=1}^{3}\alpha_i p_i + \beta mc^2 \equiv c\,\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2, \tag{1.5}$$

where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β have to be determined from (1.2). Indeed, (1.2) can be satisfied if one assumes that $\boldsymbol{\alpha}$ and β are anticommuting quantities which are most naturally represented by $n \times n$ matrices ("Dirac matrices").

Comparing E^2 according to Eqs. (1.2) and (1.5) we find that the following relations must hold

$$\begin{aligned} &\alpha_i\alpha_k + \alpha_k\alpha_i = 2\delta_{ik}\mathbf{1}, \quad i,k = 1,2,3, \\ &\alpha_i\beta + \beta\alpha_i = \mathbf{0}, \quad i = 1,2,3, \\ &\beta^2 = \mathbf{1}, \end{aligned} \tag{1.6}$$

where δ_{ik} denotes the Kronecker symbol ($\delta_{ik} = 1$ if $i = k$; $\delta_{ik} = 0$ if $i \neq k$), $\mathbf{1}$ and $\mathbf{0}$ are the n-dimensional unit and zero matrices. The $n \times n$-matrices $\boldsymbol{\alpha}$ and β should be Hermitian so that (1.5) can lead to a self-adjoint expression (which is necessary for a quantum mechanical interpretation, cf. the next section). The dimension n of the Dirac matrices can be determined as follows. From (1.6) we conclude

$$\operatorname{tr}\alpha_i = \operatorname{tr}\beta^2\alpha_i = -\operatorname{tr}\beta\alpha_i\beta = -\operatorname{tr}\alpha_i\beta\beta = -\operatorname{tr}\alpha_i = 0, \tag{1.7}$$

where tr denotes the trace of a matrix. On the other hand, in view of $\alpha_i^2 = 1$, the eigenvalues of α_i are either $+1$ or -1. This together with (1.7) shows that the dimension n of the matrices has to be an even number. For $n = 2$ there are at most three linearly independent anticommuting matrices: For example, the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{1.8}$$

together with the unit matrix $\mathbf{1}$ form a basis in the space of Hermitian 2×2 matrices. Hence there is no room for a "rest energy" matrix β in two dimensions. In four dimensions (1.6) can be satisfied, if we choose

$$\beta = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}, \quad \alpha_i = \begin{pmatrix} \mathbf{0} & \sigma_i \\ \sigma_i & \mathbf{0} \end{pmatrix}, \quad i = 1,2,3. \tag{1.9}$$

This "standard representation" was introduced by Dirac. Some other frequently used representations are listed in the appendix. If one now "translates" Eq. (1.5) to quantum mechanics one obtains the Dirac equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(t,\boldsymbol{x}) = H_0\,\psi(t,\boldsymbol{x}). \tag{1.10}$$

H_0 is given explicitly by the matrix-valued differential expression

$$H_0 = -\mathrm{i}\hbar c\,\boldsymbol{\alpha}\cdot\nabla + \beta mc^2 = \begin{pmatrix} mc^2\mathbf{1} & -\mathrm{i}\hbar c\,\boldsymbol{\sigma}\cdot\nabla \\ -\mathrm{i}\hbar c\,\boldsymbol{\sigma}\cdot\nabla & -mc^2\mathbf{1} \end{pmatrix}, \tag{1.11}$$

where $\boldsymbol{\alpha} = (\alpha_1,\alpha_2,\alpha_3)$, $\boldsymbol{\sigma} = (\sigma_1,\sigma_2,\sigma_3)$ are triplets of matrices. H_0 acts on vector-valued wavefunctions

$$\psi(t,\boldsymbol{x}) = \begin{pmatrix} \psi_1(t,\boldsymbol{x}) \\ \vdots \\ \psi_4(t,\boldsymbol{x}) \end{pmatrix} \in \mathbb{C}^4. \tag{1.12}$$

If $m = 0$ ("neutrinos"), then the mass term in (1.5) vanishes and only three anticommuting quantities α_i are needed. In this case it is sufficient to use 2×2 matrices. Indeed, $E = c\boldsymbol{\sigma} \cdot \boldsymbol{p}$ satisfies the condition $E^2 = c^2p^2$ with the Pauli matrices defined above. The corresponding two component equation

$$\mathrm{i}\hbar \frac{\partial}{\partial t} \psi(t) = c\boldsymbol{\sigma} \cdot \boldsymbol{p} \psi(t) \tag{1.13}$$

is called the Weyl equation. It is not invariant under space reflections and was therefore rejected until the discovery of parity violation in neutrino experiments.

If the space-dimension is one or two, then again we can use Pauli matrices instead of Dirac matrices. In this case the Dirac equation has the form (1.10) with

$$H_0 = -\mathrm{i}\hbar c \left(\sigma_1 \frac{\partial}{\partial x_1} + \sigma_2 \frac{\partial}{\partial x_2} \right) + \sigma_3 mc^2. \tag{1.14}$$

It is commonly accepted that the free Dirac operator, apart from some peculiarities, describes free relativistic electrons. Chapter 1 is devoted to a detailed description of (1.11) and the solutions to (1.10). In the following we shall always use units with $\hbar = 1$.

1.2 The Formalism of Quantum Mechanics

In this section we give an outline of the basic ideas which will guide us in our attempt to put the Dirac equation into a quantum mechanical framework.

1.2.1 Observables and States

According to the basic principles of quantum mechanics one defines a Hilbert space $\mathfrak{H}$ for each quantum mechanical system[1]. Every measurable quantity or "*observable*" (e.g., energy, momentum, etc.) has to be represented by a self-adjoint operator. The "*state*" of the system at time t_0 is given by a vector $\psi(t_0) \in \mathfrak{H}$. We assume that $\psi(t_0)$ is normalized, i.e., multiplied by a scalar constant such that

$$\|\psi(t_0)\|^2 \equiv (\psi(t_0), \psi(t_0)) = 1, \tag{1.15}$$

where "$(\cdot, \cdot)$" denotes the scalar product in $\mathfrak{H}$.

[1] For the basic principles of linear functional analysis in Hilbert spaces (the mathematical background of quantum mechanics), the reader is referred to the literature, e.g [Ka 80], [RS 72], or [We 80]. Here we assume some basic knowledge about linear operators, their domains and adjoints, self-adjointness, spectrum and so on.

1.2.2 Time Evolution

If the system at time t_0 is in the state $\psi(t_0)$, then at time t its state is given by

$$\psi(t) = e^{-\mathrm{i}Ht}\,\psi(t_0), \tag{1.16}$$

where the self-adjoint operator H ("*Hamiltonian*") represents the energy of the system. According to Stone's theorem (see [RS 72]) $\psi(t)$ is the unique strong solution of the Cauchy problem

$$\mathrm{i}\frac{d}{dt}\,\psi(t) = H\,\psi(t), \quad \psi(t_0) \in \mathfrak{D}(H) \subset \mathfrak{H}. \tag{1.17}$$

If $\mathfrak{H}$ is a function space, then ψ is often called "*wavefunction*". The unitary time evolution $\exp(-\mathrm{i}Ht)$ induces a transformation of the observables. Let A be self-adjoint on a domain of definition $\mathfrak{D}(A)$. Then

$$A(t) \equiv e^{\mathrm{i}Ht}\,A\,e^{-\mathrm{i}Ht} \tag{1.18}$$

is self-adjoint on $\mathfrak{D}(A(t)) = \exp(-\mathrm{i}Ht)\,\mathfrak{D}(A)$.

1.2.3 Interpretation

The usual interpretation linking these mathematical objects with the results of measurements is obtained as follows. For any self-adjoint operator A we can find, according to the spectral theorem, a "spectral measure" $\chi(A \in B)$ of a (Borel measurable) set B.

$$\chi(A \in B) = \int_{\mathbb{R}} \chi(\lambda \in B)\,dE_A(\lambda) = \int_B dE_A(\lambda), \tag{1.19}$$

where $E_A(\lambda)$ is the spectral family of A (see [RS 72]), and $\chi(\lambda \in B)$ is the characteristic function of B, i.e.,

$$\chi(\lambda \in B) = \begin{cases} 1 & \lambda \in B, \\ 0 & \lambda \notin B. \end{cases} \tag{1.20}$$

The operator $\chi(A \in B)$ is an orthogonal projection operator[2]. If $\|\psi\| = 1$, then $(\psi, \chi(A \in B)\,\psi)$ is a probability measure on $\mathbb{R}$.

Definition (Born's statistical interpretation). *If a quantum mechanical system is (at some time) in the state described by ψ, then*

$$(\psi, \chi(A \in B)\,\psi) = \int_B d(\psi, E_A(\lambda)\,\psi) \tag{1.21}$$

[2] An orthogonal projection P is a self-adjoint operator with $P^2 = P$, its range $\mathrm{Ran}\,P$ is a closed subspace of the Hilbert space, $\mathbf{1} - P$ projects onto the orthogonal complement of $\mathrm{Ran}\,P$

(where B is some Borel set in $\mathbb{R}$) is the probability for a measurement of the observable represented by A to give a result in B.

Thus the only possible results of measurements are the (real) numbers contained in the spectrum $\sigma(A)$. Eq. (1.21) predicts the probability zero for any value which is not in $\sigma(A)$, because $E_A(\lambda)$ is constant on any interval which contains no points of $\sigma(A)$. If the system is in a state ψ which is an eigenvector of A belonging to the eigenvalue λ_0, then the probability of finding the value λ_0 in a measurement of A is 1.

From (1.18) and the unitarity of the time evolution we find

$$(\psi, \chi(A(t) \in B)\,\psi) = (\psi(t), \chi(A \in B)\,\psi(t)), \quad \text{for all } t, \tag{1.22}$$

and if $\psi(t) = \exp(-\mathrm{i}Ht)\,\psi$ is in $\mathfrak{D}(A)$ for all t, then we can define the "*expectation value*"

$$(\psi, A(t)\,\psi) = (\psi(t), A\,\psi(t)). \tag{1.23}$$

According to our probabilistic interpretation this is the mean value of the results of many measurements which are all performed on systems identically prepared to be in the state ψ.

The projection operator $E = \phi(\phi, \cdot)$ is the observable determining whether or not a system is in the state ϕ. The only possible results of single measurements of E are 0 ("system is not in ϕ") or 1 ("system is in the state ϕ"). If the system is prepared to be in the state ψ, then the expectation value of E (i.e., the probability of finding this system in the state ϕ is given by

$$(\psi, E\psi) = |(\phi, \psi)|^2, \tag{1.24}$$

and is called the "*transition probability*" from ψ to ϕ.

1.3 The Dirac Equation and Quantum Mechanics

Here we make some of the identifications which are necessary for a quantum mechanical interpretation of the Dirac equation. We need a Hilbert space and some operators representing basic observables.

1.3.1 A Hilbert Space for the Dirac Equation

If we compare (1.10) and (1.17) we see that it is most natural to interpret H_0 as the Hamiltonian for a free electron. H_0 is a 4×4-matrix differential operator which acts on $\mathbb{C}^4$-valued functions of $\boldsymbol{x} \in \mathbb{R}^3$. We choose the Hilbert space[3]

$$\mathfrak{H} = L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$$

[3] The various notations in Eq. (1.25) are explained, e.g., in [RS 72], Sects. II.1 and II.4

$$\equiv L^2(\mathbb{R}^3)^4 = L^2(\mathbb{R}^3, \mathbb{C}^4) = L^2(\mathbb{R}^3) \otimes \mathbb{C}^4. \tag{1.25}$$

It consists of 4-component column[4] vectors $\psi = (\psi_1, \psi_2, \psi_3, \psi_4)^\top$, where each component ψ_i is (a Lebesgue equivalence class of) a complex valued function of the space variable $\boldsymbol{x}$. The scalar product is given by

$$(\psi, \phi) \equiv \int_{\mathbb{R}^3} \sum_{i=1}^{4} \overline{\psi_i(\boldsymbol{x})}\, \phi_i(\boldsymbol{x})\, d^3x. \tag{1.26}$$

(The bar denotes complex conjugation).

In this Hilbert space we want to define the free Dirac operator

$$H_0\, \psi \equiv -\mathrm{i}c\, \boldsymbol{\alpha} \cdot \nabla \psi + \beta m c^2\, \psi, \quad \text{for all } \psi \in \mathfrak{D}(H_0), \tag{1.27}$$

on a suitable domain $\mathfrak{D}(H_0)$. We shall prove in Sect. 1.4.4 that H_0 is self-adjoint on

$$\mathfrak{D}(H_0) \equiv H^1(\mathbb{R}^3)^4 \subset \mathfrak{H}, \tag{1.28}$$

the first Sobolev space[5], which is a natural domain for first order differential operators. Now, by Stone's theorem, Eq. (1.10) becomes a well posed initial value problem in the Hilbert space $\mathfrak{H}$.

1.3.2 Position and Momentum

Having identified H_0 as the operator for the energy of a free electron, it remains to define self-adjoint operators for the other observables. Of course, this cannot be done without ambiguity and we know that any particular choice causes prejudices concerning the interpretation of the theory. This is indeed a subtle point of the Dirac theory, as we shall see in later sections. The following definitions are motivated mainly by the analogy to the nonrelativistic quantum mechanics of an electron.

The operator $\boldsymbol{x} = (x_1, x_2, x_3)$ of multiplication by $\boldsymbol{x}$ is called "*standard position operator*". In fact, $\boldsymbol{x}$ consists of the three self-adjoint operators x_i which are defined by

$$\mathfrak{D}(x_i) \equiv \left\{ \psi \in L^2(\mathbb{R}^3)^4 \;\middle|\; \int \sum_{k=1}^{4} |x_i \psi_k(\boldsymbol{x})|^2\, d^3x < \infty \right\}, \quad i = 1, 2, 3, \tag{1.29}$$

$$(x_i \psi)(\boldsymbol{x}) = \begin{pmatrix} x_i \psi_1(\boldsymbol{x}) \\ \vdots \\ x_i \psi_4(\boldsymbol{x}) \end{pmatrix} \quad \text{for } \psi \text{ in this domain, and } i = 1, 2, 3. \tag{1.30}$$

Remember that the spectral measure $\chi(x_i \in B_i)$ of x_i is just multiplication with the characteristic function of the Borel set $B_i \subset \mathbb{R}$. We define a projection operator valued measure on $\mathbb{R}^3$ by setting

[4] We write the column vector as a transposed row vector (superscript "$\top$").
[5] [RS 78], p. 253

$$E(B) \equiv \chi(x_1 \in B_1)\,\chi(x_2 \in B_2)\,\chi(x_3 \in B_3) = \chi(\boldsymbol{x} \in B), \tag{1.31}$$

for each $B = B_1 \times B_2 \times B_3$. Then the probability of finding the particle in the region $B \subset \mathbb{R}^3$ is

$$(\psi, E(B)\psi) \equiv \int_B |\psi(\boldsymbol{x})|^2\, d^3x, \qquad |\psi(\boldsymbol{x})|^2 \equiv \sum_{k=1}^{4} |\psi_k(\boldsymbol{x})|^2, \tag{1.32}$$

and $|\psi(\boldsymbol{x})|^2$ can be interpreted as a "position probability density". (There are other possible interpretations which we shall discuss in Sect. 1.7).

The differential operator $\boldsymbol{p} \equiv -\mathrm{i}\nabla = -\mathrm{i}(\partial/\partial x_1, \partial/\partial x_2, \partial/\partial x_3)$ (acting component-wise on the vector ψ is called "momentum operator". Mathematically, it can be defined as the Fourier transformation of the standard position operator. One obvious motivation for this choice is that $\boldsymbol{p}$ generates the space translations

$$\left(e^{-\mathrm{i}\boldsymbol{a}\cdot\boldsymbol{p}}\,\psi\right)(\boldsymbol{x}) = \psi(\boldsymbol{x} - \boldsymbol{a}). \tag{1.33}$$

1.3.3 Some Other Observables

Furthermore we define the "*angular momentum operators*"

$$\boldsymbol{S} \equiv -\tfrac{\mathrm{i}}{4}\,\boldsymbol{\alpha} \wedge \boldsymbol{\alpha} \quad (\textit{spin} \text{ angular momentum}), \tag{1.34}$$

$$\boldsymbol{L} \equiv \boldsymbol{x} \wedge \boldsymbol{p} \quad (\textit{orbital} \text{ angular momentum}), \tag{1.35}$$

$$\boldsymbol{J} \equiv \boldsymbol{L} + \boldsymbol{S} \quad (\textit{total} \text{ angular momentum}). \tag{1.36}$$

By $\boldsymbol{\alpha} \wedge \boldsymbol{\alpha}$ we denote the three matrices $\sum_{k,l} \epsilon_{jkl}\alpha_k\alpha_l$, $j = 1, 2, 3$, where ϵ is the totally antisymmetric tensor

$$\epsilon_{jkl} \equiv \begin{cases} 1, & \text{if } (jkl) \text{ is an even permutation of } (123), \\ -1, & \text{if } (jkl) \text{ is an odd permutation of } (123), \\ 0, & \text{if at least two indices are equal.} \end{cases} \tag{1.37}$$

The spin operator $\boldsymbol{S}$ is bounded, everywhere defined and self-adjoint. In the standard representation,

$$\boldsymbol{S} = \frac{1}{2}\begin{pmatrix} \boldsymbol{\sigma} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\sigma} \end{pmatrix}. \tag{1.38}$$

$\boldsymbol{\sigma}/2$ is just the spin operator of nonrelativistic quantum mechanics. Also the operator $\boldsymbol{L}$ is well known from nonrelativistic quantum mechanics, except that it acts now on 4-component wavefunctions. Finally, we define the "*center-of-energy operator*"

$$\boldsymbol{N} = \tfrac{1}{2}\,(H_0\boldsymbol{x} + \boldsymbol{x}H_0)\,, \tag{1.39}$$

which will play an important role as the generator of Lorentz boosts in Chapter 2. All the operators H_0, $\boldsymbol{p}$, $\boldsymbol{J}$, and $\boldsymbol{N}$ are essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)^4$ (see also Sect. 2.2.4).

1.4 The Free Dirac Operator

Next we describe the most important mathematical properties of the Dirac operator H_0. We prove its self-adjointness and analyze the spectrum which consists of all possible values resulting from an energy measurement. It will turn out that according to the Dirac equation a free particle can have negative energies.

1.4.1 The Free Dirac Operator in Fourier Space

The free Dirac operator H_0 is most easily analyzed in the Fourier space. The Fourier transformation

$$(\mathcal{F}\psi_k)(\boldsymbol{p}) \equiv \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{-i\boldsymbol{p}\cdot\boldsymbol{x}}\, \psi_k(\boldsymbol{x})\, d^3x, \quad k = 1,2,3,4, \tag{1.40}$$

defined for integrable functions extends to a uniquely defined unitary operator (which is again denoted by $\mathcal{F}$) in the Hilbert space $L^2(\mathbb{R}^3)^4$. Occasionally we shall write $\mathcal{F}L^2(\mathbb{R}^3, d^3x)^4 = L^2(\mathbb{R}^3, d^3p)^4$ to distinguish between the variables. The Hilbert space $L^2(\mathbb{R}^3, d^3p)^4$ is often called momentum space. Any matrix differential operator in $L^2(\mathbb{R}^3, d^3x)^4$ is transformed via $\mathcal{F}$ into a matrix multiplication operator in $L^2(\mathbb{R}^3, d^3p)^4$. For the Dirac operator one obtains

$$\big(\mathcal{F}H_0\mathcal{F}^{-1}\big)(\boldsymbol{p}) = \mathrm{h}(\boldsymbol{p}) \equiv \begin{pmatrix} mc^2\,\mathbf{1} & c\boldsymbol{\sigma}\cdot\boldsymbol{p} \\ c\boldsymbol{\sigma}\cdot\boldsymbol{p} & -mc^2\,\mathbf{1} \end{pmatrix}. \tag{1.41}$$

For each $\boldsymbol{p}$, this is a Hermitian 4×4-matrix which has the eigenvalues ($p \equiv |\boldsymbol{p}|$)

$$\lambda_1(p) = \lambda_2(p) = -\lambda_3(p) = -\lambda_4(p) = \sqrt{c^2p^2 + m^2c^4} \equiv \lambda(p). \tag{1.42}$$

The unitary transformation $\mathrm{u}(\boldsymbol{p})$ which brings $\mathrm{h}(\boldsymbol{p})$ to the diagonal form is given explicitly by

$$\mathrm{u}(\boldsymbol{p}) = \frac{\big(mc^2 + \lambda(p)\big)\mathbf{1} + \beta c\,\boldsymbol{\alpha}\cdot\boldsymbol{p}}{\sqrt{2\lambda(p)\big(mc^2 + \lambda(p)\big)}} = a_+(p)\,\mathbf{1} + a_-(p)\,\beta\,\frac{\boldsymbol{\alpha}\cdot\boldsymbol{p}}{p}, \tag{1.43}$$

where

$$a_\pm(p) \equiv \frac{1}{\sqrt{2}}\sqrt{1 \pm mc^2/\lambda(p)}\,. \tag{1.44}$$

It may be checked that

$$\mathrm{u}(\boldsymbol{p})\,\mathrm{h}(\boldsymbol{p})\,\mathrm{u}(\boldsymbol{p})^{-1} = \beta\,\lambda(p), \tag{1.45}$$

where

$$\mathrm{u}(\boldsymbol{p})^{-1} = a_+(p)\,\mathbf{1} - a_-(p)\,\beta\,\frac{\boldsymbol{\alpha}\cdot\boldsymbol{p}}{p}. \tag{1.46}$$

(In all these expressions $\boldsymbol{\alpha}$ and β denote the Dirac matrices in the standard representation (1.9), $\mathbf{1}$ is the 4×4 unit matrix).

From Eqs. (1.41) and (1.45) it is clear that the unitary transformation

$$\mathcal{W} = \mathrm{u}\,\mathcal{F} \tag{1.47}$$

converts the Dirac operator H_0 into an operator of multiplication by the diagonal matrix

$$\big(\mathcal{W} H_0 \mathcal{W}^{-1}\big)(p) = \beta\,\lambda(p). \tag{1.48}$$

in the Hilbert space $L^2(\mathbb{R}^3, d^3p)^4$. If $\phi = \mathcal{W}\psi$ is integrable, then we can write

$$\psi(\boldsymbol{x}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}}\, \mathrm{u}(\boldsymbol{p})^{-1}\, \phi(\boldsymbol{p})\, d^3p, \quad \phi \in L^1(\mathbb{R}^3)^4 \cap L^2(\mathbb{R}^3)^4. \tag{1.49}$$

Note that $\mathrm{u}(\boldsymbol{p})^{-1}\,\phi(\boldsymbol{p})$ is a linear combination of the four eigenvectors of the matrix $\mathrm{h}(\boldsymbol{p})$.

These eigenvectors can be chosen as simultaneous eigenvectors of the helicity $\boldsymbol{S}\cdot\boldsymbol{p}$, see Appendix 1.F.

1.4.2 Spectral Subspaces of H_0

In the Hilbert space $\mathcal{W}\,L^2(\mathbb{R}^3)^4$ where the Dirac operator is diagonal, see Eq. (1.48), the upper two components of wavefunctions belong to positive energies, while the lower components correspond to negative energies. Hence we define the *subspace of positive energies* $\mathfrak{H}_{\mathrm{pos}} \subset L^2(\mathbb{R}^3)^4$ as the subspace spanned by vectors of the type

$$\psi_{\mathrm{pos}} \equiv \mathcal{W}^{-1}\,\tfrac{1}{2}(\mathbf{1} + \beta)\,\mathcal{W}\psi, \qquad \psi \in L^2(\mathbb{R}^3, d^3x). \tag{1.50}$$

Similarly, the vectors

$$\psi_{\mathrm{neg}} \equiv \mathcal{W}^{-1}\,\tfrac{1}{2}(\mathbf{1} - \beta)\,\mathcal{W}\psi, \qquad \psi \in L^2(\mathbb{R}^3, d^3x), \tag{1.51}$$

span the *negative energy subspace* $\mathfrak{H}_{\mathrm{neg}}$. Since $\mathfrak{H}_{\mathrm{pos}}$ is orthogonal to $\mathfrak{H}_{\mathrm{neg}}$, we can write

$$\mathfrak{H} = \mathfrak{H}_{\mathrm{pos}} \oplus \mathfrak{H}_{\mathrm{neg}} \quad \text{(orthogonal direct sum)}. \tag{1.52}$$

Every state ψ can be uniquely written as a sum of ψ_{pos} and ψ_{neg}. Obviously, H_0 acts as a positive operator on $\mathfrak{H}_{\mathrm{pos}}$ because with $\phi_\pm = \frac{1}{2}(1 \pm \beta)\mathcal{W}\psi$ we have

$$(\psi_{\mathrm{pos}},\, H_0\,\psi_{\mathrm{pos}}) = (\mathcal{W}^{-1}\phi_+\,, \mathcal{W}^{-1}\,\lambda(\cdot)\,\phi_+) = (\phi_+, \lambda(\cdot)\,\phi_+) \;>\; 0. \tag{1.53}$$

Similarly, H_0 is negative on $\mathfrak{H}_{\mathrm{neg}}$. The orthogonal projection operators onto the positive/negative energy subspaces are given by

$$P^{\mathrm{pos}}_{\mathrm{neg}} = \mathcal{W}^{-1}\,\tfrac{1}{2}(\mathbf{1} \pm \beta)\,\mathcal{W} = \frac{1}{2}\Big(\mathbf{1} \pm \frac{H_0}{|H_0|}\Big). \tag{1.54}$$

Here the operator $|H_0|$ is given as

$$|H_0| \equiv \sqrt{H_0^2} = \sqrt{-c^2\triangle + m^2c^4}\,\mathbf{1}\,. \tag{1.55}$$

The square root operator may be defined as the inverse Fourier transformation of the multiplication operator $\sqrt{c^2p^2 + m^2c^4}$ in $L^2(\mathbb{R}^3, d^3p)$. Obviously we have

$$H_0\psi^{\text{pos}}_{\text{neg}} = \pm|H_0|\psi^{\text{pos}}_{\text{neg}}\,. \tag{1.56}$$

With $\operatorname{sgn} H_0 \equiv H_0/|H_0|$ we have $H_0 = |H_0|\operatorname{sgn} H_0$ (polar decomposition of H_0, see also Sect. 5.2.3 below).

1.4.3 The Foldy-Wouthuysen Transformation

The transformation

$$U_{\text{FW}} = \mathcal{F}^{-1}\mathcal{W} \tag{1.57}$$

is usually called the *Foldy-Wouthuysen transformation*. Obviously it transforms the free Dirac operator into the 2×2-block form

$$U_{\text{FW}} H_0 U_{\text{FW}}^{-1} = \begin{pmatrix} \sqrt{-c^2\triangle + m^2c^4} & 0 \\ 0 & -\sqrt{-c^2\triangle + m^2c^4} \end{pmatrix} = \beta|H_0|. \tag{1.58}$$

This should be compared to (1.3). We see that the free Dirac equation is unitarily equivalent to a pair of (two component) square-root Klein-Gordon equations.

1.4.4 Self-Adjointness and Spectrum of H_0

An operator is called essentially self-adjoint, if it has a unique extension to a larger domain, where it is self-adjoint (see [RS 72], Sect. VIII.2).

Theorem 1.1. The free Dirac operator is essentially self-adjoint on the dense domain $\mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{0\})^4$ and self-adjoint on the Sobolev space

$$\mathfrak{D}(H_0) = H^1(\mathbb{R}^3)^4. \tag{1.59}$$

Its spectrum is purely absolutely continuous and given by

$$\sigma(H_0) = (-\infty, -mc^2] \cup [mc^2, \infty). \tag{1.60}$$

Proof. From (1.53) we see that H_0 is unitarily equivalent to the operator $\beta\lambda(\cdot)$ of multiplication by a diagonal matrix-valued function of $\boldsymbol{p}$, and hence is self-adjoint on

$$\mathfrak{D}(H_0) = \mathcal{W}^{-1}\mathfrak{D}\big(\beta\lambda(\cdot)\big) = \mathcal{F}^{-1}\mathrm{u}^{-1}\mathfrak{D}\big(\lambda(\cdot)\big) = \mathcal{F}^{-1}\mathfrak{D}\big(\lambda(\cdot)\big). \tag{1.61}$$

We have used that $\mathrm{u}(\boldsymbol{p})^{-1}$ is multiplication by a unitary matrix and does not change the domain of any multiplication operator. The Sobolev space $H^1(\mathbb{R}^3)^4$ is defined as the inverse Fourier transform of the set

$$\{ f \in L^2(\mathbb{R}^3, d^3p)^4 \mid (1+|\boldsymbol{p}|^2)^{1/2} f \in L^2(\mathbb{R}^3, d^3p)^4 \}. \tag{1.62}$$

By the definition of λ, Eq. (1.42), this set equals $\mathfrak{D}(\lambda(\cdot))$ (for $m \neq 0$). The spectrum of H_0 equals the spectrum of the multiplication operator $\beta\lambda$ which is simply given by the range of the functions $\lambda_i(p)$, $i = 1, \ldots, 4$.

In order to prove the essential self-adjointness we first consider the free Dirac operator on the set $\mathcal{S}(\mathbb{R}^3)^4$ of (4-component) functions of rapid decrease[6]. The Dirac operator with this domain will be denoted by $\tilde{H}_0$, i.e.,

$$\mathfrak{D}(\tilde{H}_0) = \mathcal{S}(\mathbb{R}^3)^4, \quad \tilde{H}_0 \psi \equiv -\mathrm{i}c\,\boldsymbol{\alpha} \cdot \nabla \psi + \beta mc^2 \psi, \quad \psi \in \mathcal{S}(\mathbb{R}^3)^4. \tag{1.63}$$

The set $\mathcal{S}(\mathbb{R}^3)^4$ is invariant with respect to Fourier transformations,

$$\mathcal{F}\mathcal{S}(\mathbb{R}^3)^4 = \mathcal{S}(\mathbb{R}^3)^4. \tag{1.64}$$

Therefore, $\tilde{H}_0$ is unitarily equivalent to the restriction of $\mathrm{h}(\boldsymbol{p})$ to $\mathcal{S}(\mathbb{R}^3)^4$. Since the restricted multiplication operator is essentially self-adjoint (its closure is the self-adjoint multiplication operator $\mathrm{h}(\boldsymbol{p})$), the same is true for $\tilde{H}_0$, and its closure is H_0, the self-adjoint Dirac operator. The Dirac operator on the domain $\mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{\mathrm{O}\})^4$ will be denoted by $\dot{H}_0$. We want to show that the closure[7] of $\dot{H}_0$ equals H_0. Since we have $\mathfrak{D}(\dot{H}_0) \subset \mathfrak{D}(\tilde{H}_0)$, and the same relation holds for the closures of the operators, it is sufficient to prove

$$\mathfrak{D}(\tilde{H}_0) \subset \mathfrak{D}(\text{closure of } \dot{H}_0). \tag{1.65}$$

For every $\psi \in \mathcal{S}(\mathbb{R}^3)^4$, we have to find a sequence $\psi_n \in \mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{\mathrm{O}\})^4$ with

$$\lim_{n\to\infty} \psi_n = \psi, \qquad \lim_{n\to\infty} \dot{H}_0 \psi_n = \tilde{H}_0 \psi. \tag{1.66}$$

Choose $f \in \mathcal{C}^\infty(\mathbb{R}^3)$ with $f(\boldsymbol{x}) = 1$ for $|\boldsymbol{x}| \leq 1$, $f(\boldsymbol{x}) = 0$ for $|\boldsymbol{x}| \geq 2$, and let $0 \leq f(\boldsymbol{x}) \leq 1$ for all $\boldsymbol{x}$. For $\psi \in \mathcal{S}(\mathbb{R}^3)^4$ define

$$\psi_n(\boldsymbol{x}) = f(n^{-1}\boldsymbol{x}) \big(1 - f(n\boldsymbol{x})\big)\, \psi(\boldsymbol{x}). \tag{1.67}$$

Clearly, $\psi_n \in \mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{\mathrm{O}\})^4$, and $\psi_n \to \psi$. Next we calculate

$$\dot{H}_0 \psi_n(\boldsymbol{x}) - \tilde{H}_0 \psi(\boldsymbol{x}) = -\mathrm{i}c\,\psi(\boldsymbol{x}) \big(1 - f(n\boldsymbol{x})\big)\, n^{-1} \big(\boldsymbol{\alpha} \cdot \nabla f\big)(n^{-1}\boldsymbol{x}) \tag{1.68}$$

$$+ \mathrm{i}c\,\psi(\boldsymbol{x})\, f(n^{-1}\boldsymbol{x})\, n \big(\boldsymbol{\alpha} \cdot \nabla f\big)(n\boldsymbol{x}) \tag{1.69}$$

$$+ \big[f(n^{-1}\boldsymbol{x}) \big(1 - f(n\boldsymbol{x})\big) - 1\big] \tilde{H}_0 \psi(\boldsymbol{x}). \tag{1.70}$$

The norm of the first summand can be estimated by $\mathrm{const.} n^{-1} \|\psi\|$, the second summand (1.69) is bounded in norm by $\mathrm{const.} n^{-1/2} \sup |\psi(\boldsymbol{x})|$ because

$$\int |\psi(\boldsymbol{x})|^2\, n^2\, |\big(\nabla f\big)(n\boldsymbol{x})|^2\, d^3x \leq \sup_{\boldsymbol{x}} |\psi(\boldsymbol{x})|^2 \frac{1}{n} \int |(\nabla f)(\boldsymbol{x})|^2\, d^3x. \tag{1.71}$$

(1.70) vanishes in norm, as $n \to \infty$ by our assumptions on f. This proves Eq. (1.66) and hence Eq. (1.65). □

[6] [RS 72], Sect. V.3, p.133.

[7] The closure of an operator is explained, e.g., in [RS 72], Sect. VIII.1.

1.4.5 The Spectral Transformation

The spectral transform $U_{\rm sp}$ of H_0 is defined as the unitary transformation to a Hilbert space $\mathfrak{K}$ where $U_{\rm sp}H_0U_{\rm sp}^{-1}$ acts as a multiplication operator. This Hilbert space $\mathfrak{K}$ is given by

$$\mathfrak{K} = L^2\big(\sigma(H_0), L^2(S^2)^2\big)^2. \tag{1.72}$$

It consists of two-component functions $(g_1(E), g_2(E))$ of one single real variable E which can only take values in $\sigma(H_0)$. For any E, the values $g_i(E)$ lie in the Hilbert space $L^2(S^2)^2$. This means that (for each i and E) $g_i(E)$ is a (two-component) square integrable function on the unit sphere S^2. The scalar product in $L^2(S^2)^2$ is

$$(\phi, \psi)_s = \int_{S^2} d\omega \sum_{a=1}^{2} \overline{\phi_a(\omega)}\psi_a(\omega), \quad \text{all } \phi,\ \psi \in L^2(S^2)^2, \tag{1.73}$$

where $\omega = (\vartheta, \varphi) \in S^2$, and $d\omega = \sin\vartheta\, d\vartheta d\varphi$. For elements g and h in $\mathfrak{K}$ the scalar product is defined as

$$(g, h)_{\mathfrak{K}} = \int_{\sigma(H_0)} dE \sum_{i=1}^{2} \big(g_i(E), h_i(E)\big)_s\,. \tag{1.74}$$

Next we introduce a unitary transformation

$$\mathcal{K}\colon L^2(\mathbb{R}^3, d^3p)^4 \to \mathfrak{K}. \tag{1.75}$$

For $\phi \in L^2(\mathbb{R}^3, d^3p)^4$ we use polar coordinates and write

$$\phi(\boldsymbol{p}) = \boldsymbol{f}(p, \omega), \quad p \equiv |\boldsymbol{p}|. \tag{1.76}$$

Then the vector $\mathcal{K}\phi \in \mathfrak{K}$ is defined by its values $[\mathcal{K}\phi](E)$ as follows (remember that $[\mathcal{K}\phi](E)$ is a two-component function of $\omega \in S^2$).

$$\begin{aligned}
&[\mathcal{K}\phi](E, \omega) \\
&\quad = \tfrac{1}{c^{3/2}}\left\{E^2(E^2 - m^2c^4)\right\}^{1/4} \tfrac{1}{2}(1 + \operatorname{sgn}(E)\beta)\, \boldsymbol{f}\big(\tfrac{1}{c}(E^2 - m^2c^4)^{1/2}, \omega\big) \\
&\quad = \tfrac{1}{c^{3/2}}\left\{E^2(E^2 - m^2c^4)\right\}^{1/4} \begin{cases} \begin{pmatrix} f_1(\dots) \\ f_2(\dots) \end{pmatrix}, & E > 0, \\ \begin{pmatrix} f_3(\dots) \\ f_4(\dots) \end{pmatrix}, & E < 0. \end{cases}
\end{aligned} \tag{1.77}$$

(For the last expression we have chosen the standard representation of Dirac matrices). The operator $\mathcal{K}$ is essentially a variable substitution composed with a projection onto upper/lower components of $\boldsymbol{f}$. It is easy to check that $\mathcal{K}$ is unitary, thanks to the complicated factor in (1.77). Now we can define the "*spectral transform*" of H_0 by

$$U_{\rm sp} = \mathcal{K}\mathcal{W}\colon L^2(\mathbb{R}^3, d^3x)^4 \to \mathfrak{K}, \tag{1.78}$$

and verify that $U_{\rm sp}H_0U_{\rm sp}^{-1}$ = multiplication by E, i.e.,

$$\big[U_{\rm sp}H_0\psi\big](E) = E\big[U_{\rm sp}\psi\big](E). \tag{1.79}$$

1.4.6 Interpretation of Negative Energies

According to Sect. 1.3.1 the free Dirac operator represents the energy of the system described by the Dirac equation. Since the spectrum of the Dirac operator has a negative part, this system can be in a state with negative energy. Originally our intention was to describe a single free electron, for which the occurrence of negative energies is a most peculiar fact. Moreover, the unboundedness of the Dirac operator provides us with an infinite energy reservoir. In spite of various attempts there is still no commonly accepted solution for some of the interpretational problems with negative energies.

A better understanding of the negative energy solutions can perhaps be obtained if we consider for a moment the Dirac equation in an external field, and the operation of charge conjugation. The Dirac operator for a charge e in an external electromagnetic field $(\phi_{\mathrm{el}}, \boldsymbol{A})$ is given by

$$H(e) = c\boldsymbol{\alpha} \cdot \left(\boldsymbol{p} - \tfrac{e}{c}\boldsymbol{A}(t, \boldsymbol{x})\right) + \beta mc^2 + e\phi_{\mathrm{el}}(t, \boldsymbol{x}). \tag{1.80}$$

Now consider the antiunitary transformation

$$C\psi = U_C\,\overline{\psi}. \tag{1.81}$$

where U_C is a unitary 4×4 matrix with $\beta U_C = -U_C\overline{\beta}$, and $\alpha_k U_C = U_C\overline{\alpha_k}$, for $k = 1, 2, 3$. In the standard representation we take $U_C = \mathrm{i}\beta\alpha_2$ (in the Majorana representation, cf. Appendix 1A, one simply has $U_C = \mathbf{1}$). A short calculation shows that if $\psi(t)$ is a solution of the Dirac equation with Hamiltonian $H(e)$, then $C\psi(t)$ is a solution of the Dirac equation with Hamiltonian $H(-e)$. This motivates the name *charge conjugation* for the operator C. Moreover,

$$C\,H(e)\,C^{-1} = -H(-e). \tag{1.82}$$

Thus, the negative energy subspace of $H(e)$ is connected via a symmetry transformation with the positive energy subspace of the Dirac operator $H(-e)$ for a particle with opposite charge (antiparticle, positron). For $C\psi$ in the positive energy subspace of $H(-e)$ we can interpret $|C\psi(\boldsymbol{x})|^2$ as a position probability density. Then the equation

$$|C\psi(\boldsymbol{x})|^2 = |\psi(\boldsymbol{x})|^2 \tag{1.83}$$

shows that the motion of a negative energy electron state ψ is indeed indistinguishable from that of a positive energy positron. This suggests the following interpretation: *A state $\psi \in \mathfrak{H}_{\mathrm{neg}}$ describes an antiparticle with positive energy.*

The problem now is that the Hilbert space $\mathfrak{H} = L^2(\mathbb{R}^3)^4$ contains states which are superpositions of positive and negative energy states. But a single particle state can hardly be imagined as a superposition of electrons and positrons. So one might try to modify the theory by restricting everything to the Hilbert space $\mathfrak{H}_{\mathrm{pos}}$ with the help of the projection operator P_{pos} defined in (1.54). This projection operator commutes with H_0 and hence with $\exp(-\mathrm{i}H_0 t)$ so that an initial state with positive energy has positive energies for all times, i.e.,

$$\psi(t) \equiv e^{-iH_0 t}\psi = P_{\text{pos}}\psi(t) \quad \text{if and only if} \quad \psi = P_{\text{pos}}\psi. \tag{1.84}$$

For free particles this point of view has indeed some attractive features. The main problem with it is that some observables do not leave $\mathfrak{H}_{\text{pos}}$ invariant. One might even think of interactions which, say in a scattering experiment, turn an initial state with positive energy into a final state which has negative energy admixtures.

1.5 The Free Time Evolution

The time evolution operator $\exp(-iH_0 t)$ is an integral operator in the Hilbert space $L^2(\mathbb{R}^3, d^3x)^4$. In this section we determine the integral kernel.

If at time $t = 0$ the system described by the free Dirac equation is in the state $\psi = \mathcal{W}^{-1}\phi$, then its time evolution is given by

$$\psi(t) = \mathcal{W}^{-1}\big(e^{-i\lambda(\cdot)t}\phi_+ + e^{+i\lambda(\cdot)t}\phi_-\big) \tag{1.85}$$

(see Sect. 1.4.1 for notation). Writing the inverse Fourier transform as an integral and expressing $\phi_\pm$ with the help of (1.47) again in terms of ψ we obtain the time evolution in form of an integral operator. As in Sect. 1.4.4, $\mathcal{S}(\mathbb{R}^3)^4$ denotes the space of 4-component functions of rapid decrease, the test-functions for tempered distributions.

Theorem 1.2. Assume $\psi \in \mathcal{S}(\mathbb{R}^3)^4$. Then for $t \neq 0$

$$\psi(t, \boldsymbol{x}) = \int_{\mathbb{R}^3} S(t, \boldsymbol{x} - \boldsymbol{y})\, \psi(\boldsymbol{y})\, d^3y, \tag{1.86}$$

where

$$S(t, \boldsymbol{x}) = i\big(i\frac{\partial}{\partial t} - ic\,\boldsymbol{\alpha}\cdot\nabla + \beta mc^2\big)\triangle(t, \boldsymbol{x}). \tag{1.87}$$

$\triangle(t, \cdot)$ is a distribution of the form

$$\triangle(t, \boldsymbol{x}) = \frac{\operatorname{sgn}(t)}{2\pi c}\big\{-\delta(c^2t^2 - |\boldsymbol{x}|^2) + \frac{m^2c^2}{4}\theta(c^2t^2 - |\boldsymbol{x}|^2) + \ldots\big\}, \tag{1.88}$$

where the remainder is continuous (δ denotes the Dirac delta function, and θ the Heaviside step function). For $|\boldsymbol{x}| \neq c|t|$ we have

$$\triangle(t, \boldsymbol{x}) = \frac{m^2c}{4\pi}\operatorname{sgn}(t)\begin{cases} \dfrac{J_1\left(mc\sqrt{c^2t^2 - |\boldsymbol{x}|^2}\right)}{mc\sqrt{c^2t^2 - |\boldsymbol{x}|^2}} & \text{if } c|t| > |\boldsymbol{x}|, \\ 0 & \text{if } c|t| < |\boldsymbol{x}|. \end{cases} \tag{1.89}$$

(J_1 is the first Bessel function[8]).

[8] For the definition of the Bessel functions J_ν, modified Bessel functions K_ν and Hankel functions $H_\nu^{(1,2)}$ see the book of Gradshteyn and Ryzhik [GR 80]

Proof. We consider separately the action of $\exp(-\mathrm{i}H_0 t)$ on the positive and negative energy parts of the wavefunction. Define $t_\pm = t \mp \mathrm{i}\epsilon$. We have

$$\lim_{\epsilon \to 0} e^{-\mathrm{i}H_0 t_\pm} \psi = e^{-\mathrm{i}H_0 t} \psi, \quad \text{for all } \psi \in \mathfrak{H}^{\text{pos}}_{\text{neg}}. \tag{1.90}$$

Next consider

$$\begin{aligned}
\big(e^{-\mathrm{i}H_0 t_\pm} P^{\text{pos}}_{\text{neg}} \psi\big)(\boldsymbol{x}) &= \Big(\mathcal{F}^{-1}\, e^{\mp \mathrm{i}\lambda t_\pm}\, \frac{1}{2}\big(1 \pm \frac{\mathrm{h}}{\lambda}\big)\, \mathcal{F}\psi\Big)(\boldsymbol{x}) \\
&= \frac{1}{(2\pi)^{3/2}} \int \Big\{ \frac{\pm 1}{(2\pi)^{3/2}} \int e^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})} \big(\pm\lambda(p) + \mathrm{h}(\boldsymbol{p})\big)\, \frac{e^{\mp \mathrm{i}\lambda(p) t_\pm}}{2\lambda(p)}\, d^3p \Big\}\, \psi(\boldsymbol{y})\, d^3y \\
&\equiv \int S_\pm(t_\pm, \boldsymbol{x} - \boldsymbol{y})\, \psi(\boldsymbol{y})\, d^3y.
\end{aligned} \tag{1.91}$$

The imaginary part of $t_\pm$ has been chosen such that the integral in curly parenthesis exists, as long as $\epsilon > 0$. Hence

$$S_\pm(t_\pm, \boldsymbol{x}) = \mathrm{i}\big(\mathrm{i}\frac{\partial}{\partial t} - \mathrm{i}c\,\boldsymbol{\alpha}\cdot\nabla + \beta mc^2\big) \triangle_\pm(t_\pm, \boldsymbol{x}), \tag{1.92}$$

with

$$\triangle_+(t_+, \boldsymbol{x}) = \overline{\triangle_-(t_-, \boldsymbol{x})} = \frac{-\mathrm{i}}{(2\pi)^3} \int e^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}}\, \frac{e^{-\mathrm{i}\lambda(p)t_+}}{2\lambda(p)}\, d^3p. \tag{1.93}$$

Introducing polar coordinates and writing $r \equiv |\boldsymbol{x}|$, $p \equiv |\boldsymbol{p}|$, we obtain

$$\triangle_\pm(t_\pm, \boldsymbol{x}) = \frac{\mp \mathrm{i}}{4\pi^2 r} \int_0^\infty p \sin(pr)\, \frac{e^{\mp \mathrm{i}\lambda(p)t_\pm}}{\lambda(p)}\, dp. \tag{1.94}$$

Inserting the definition (1.42) of λ we can write this as[9]

$$\triangle_+(t_+, r) = \frac{-\mathrm{i}m^2 c}{4\pi^2}\, \frac{K_1\big(mc(r^2 - c^2t_+^2)^{1/2}\big)}{mc(r^2 - c^2t_+^2)^{1/2}}. \tag{1.95}$$

Next we apply the formulas

$$K_1(e^{-\mathrm{i}\frac{\pi}{2}} z) = -\frac{\pi}{2} H_1^{(1)}(z), \quad -\pi < \arg z < \frac{\pi}{2}, \tag{1.96}$$

$$K_1(e^{\mathrm{i}\frac{\pi}{2}} z) = -\frac{\pi}{2} H_1^{(2)}(z), \quad -\frac{\pi}{2} < \arg z < \pi, \tag{1.97}$$

and note that

$$e^{\mathrm{i}\frac{\pi}{2}}(r^2 - c^2t_+^2)^{1/2} \overset{\epsilon \to 0}{\longrightarrow} \sqrt{c^2t^2 - r^2} \quad \text{if } ct < -r, \tag{1.98}$$

$$e^{-\mathrm{i}\frac{\pi}{2}}(r^2 - c^2t_+^2)^{1/2} \overset{\epsilon \to 0}{\longrightarrow} \sqrt{c^2t^2 - r^2} \quad \text{if } ct > r, \tag{1.99}$$

(where "$\sqrt{\ }$" denotes the positive square root of a positive real number). From this we obtain for $c|t| \neq r$ in the limit $\epsilon \to 0$ the following expression,

[9] [GR 80], Eq. 3.961.1

$$\triangle_+(t,\boldsymbol{x}) = \frac{m^2 c}{8\pi} \begin{cases} -\dfrac{H_1^{(1)}\left(mc\sqrt{c^2t^2-r^2}\right)}{mc\sqrt{c^2t^2-r^2}} & \text{if } ct < -r, \\ -\dfrac{2\mathrm{i}}{\pi}\dfrac{K_1\left(mc\sqrt{r^2-c^2t^2}\right)}{mc\sqrt{r^2-c^2t^2}} & \text{if } c|t| < r, \\ +\dfrac{H_1^{(2)}\left(mc\sqrt{c^2t^2-r^2}\right)}{mc\sqrt{c^2t^2-r^2}} & \text{if } ct > r. \end{cases} \tag{1.100}$$

Using

$$\triangle(t,\boldsymbol{x}) = \triangle_+(t,\boldsymbol{x}) + \triangle_-(t,\boldsymbol{x}) = \triangle_+(t,\boldsymbol{x}) + \overline{\triangle_+(t,\boldsymbol{x})}, \tag{1.101}$$

we finally arrive at Eq. (1.89).

Next we calculate the behavior of the kernel $S(t,\boldsymbol{x})$ at the light cone $c|t| = |\boldsymbol{x}|$. From (1.94) we obtain

$$\begin{aligned} &\triangle_+(t_+,\boldsymbol{x}) + \triangle_-(t_-,\boldsymbol{x}) \\ &\quad = \frac{-1}{2\pi^2 c^2 r}\,\mathrm{sgn}(t) \int_{mc^2}^{\infty} \sin\big(p(\lambda)r\big)\,\sin\big(\lambda|t|\big)\,e^{-\lambda\epsilon}\,d\lambda, \end{aligned} \tag{1.102}$$

where $p(\lambda) = \frac{1}{c}\sqrt{\lambda^2 - m^2c^4}$. Next we expand

$$\sin\big(p(\lambda)r\big) = \sin\Big(\frac{\lambda r}{c}\Big) - \frac{m^2c^3 r}{2\lambda}\,\cos\Big(\frac{\lambda r}{c}\Big) + O\Big(\frac{1}{\lambda^2}\Big) \tag{1.103}$$

and insert this in (1.102). The last summand is of order $1/\lambda^2$ and hence integrable, therefore we can perform the limit $\epsilon \to 0$ to obtain a function which is continuous in r and t. The remaining expressions can be evaluated explicitly if we replace the lower bound of the integral in (1.102) by 0. This replacement again produces a continuous error term in the limit $\epsilon \to 0$. The first summand gives[10]

$$\begin{aligned} &\frac{-1}{2\pi^2 c^2 r}\,\mathrm{sgn}(t) \int_0^{\infty} \sin\Big(\frac{\lambda r}{c}\Big)\,\sin\big(\lambda|t|\big)e^{-\lambda\epsilon}\,d\lambda = \\ &\frac{-\mathrm{i}}{4\pi^2 c}\,\mathrm{sgn}(t)\Big(\frac{1}{c^2t^2 - r^2 - c^2\epsilon^2 + 2\mathrm{i}c^2|t|\epsilon} - \frac{1}{c^2t^2 - r^2 - c^2\epsilon^2 - 2\mathrm{i}c^2|t|\epsilon}\Big). \end{aligned} \tag{1.104}$$

In the limit $\epsilon \to 0$ this expression becomes

$$\begin{aligned} &\frac{-\mathrm{i}}{4\pi^2 c}\,\mathrm{sgn}(t)\Big(\frac{1}{c^2t^2 - r^2 + \mathrm{i}0} - \frac{1}{c^2t^2 - r^2 - \mathrm{i}0}\Big) \\ &\quad = -\frac{\mathrm{sgn}(t)}{2\pi c}\,\delta(c^2t^2 - r^2). \end{aligned} \tag{1.105}$$

From the second term in the expansion (1.103) we obtain[11]

[10] [GR 80], Eq. 3.895.12
[11] [GR 80], Eq. 3.947.3

$$\frac{m^2c}{4\pi^2}\,\mathrm{sgn}(t)\int_0^\infty \cos\Big(\frac{\lambda r}{c}\Big)\,\sin\big(\lambda|t|\big)\,e^{-\lambda\epsilon}\,\frac{d\lambda}{\lambda}$$

$$= \frac{m^2c}{4\pi^2}\,\mathrm{sgn}(t)\Big(\frac{1}{2}\arctan\frac{2\epsilon|t|}{\epsilon^2-t^2+r^2/c^2}+\frac{\pi}{2}\theta(c^2t^2-r^2-\epsilon^2)\Big). \tag{1.106}$$

From

$$\lim_{\epsilon\to 0}\arctan\frac{2\epsilon|t|}{\epsilon^2-t^2+r^2/c^2} = \begin{cases}\pi/2 & \text{if } c^2t^2-r^2=0\\ 0 & \text{if } c^2t^2-r^2\neq 0\end{cases} \tag{1.107}$$

we conclude that the limit $\epsilon\to 0$ of the distribution (1.106) is simply given by

$$\frac{1}{2\pi c}\,\mathrm{sgn}(t)\,\frac{m^2c^2}{4}\,\theta(c^2t^2-r^2). \tag{1.108}$$

This finally proves (1.88). □

Remark. The theorem states that $S(t,\boldsymbol{x})$ vanishes for $c|t|<|\boldsymbol{x}|$. This shows that *wavefunctions* propagate at most with the speed of light: If a spinor ψ at time $t=0$ has compact support in a sphere with radius r, then $\psi(t)$ still vanishes outside a sphere of radius $r+ct$.

In the Foldy-Wouthuysen representation the time evolution of positive energy states is given by

$$\exp\big(-\mathrm{i}t\sqrt{-c^2\triangle+m^2c^4}\,\big). \tag{1.109}$$

The integral kernel $K(t,\boldsymbol{x}-\boldsymbol{y})$ of this operator does not vanish outside the light cone:

$$K(t,\boldsymbol{x}) = \frac{m^2c^3t}{4\pi(c^2t^2-|\boldsymbol{x}|^2)}\begin{cases}-H_2^{(1)}\big(mc\sqrt{c^2t^2-|\boldsymbol{x}|^2}\big) & \text{if } ct<-|\boldsymbol{x}|,\\ -\dfrac{2\mathrm{i}}{\pi}K_2\big(mc\sqrt{|\boldsymbol{x}|^2-c^2t^2}\big) & \text{if } c|t|<|\boldsymbol{x}|,\\ +H_2^{(2)}\big(mc\sqrt{c^2t^2-|\boldsymbol{x}|^2}\big) & \text{if } ct>|\boldsymbol{x}|.\end{cases} \tag{1.110}$$

This implies an acausal behavior for the wavefunctions $(U_{\mathrm{FW}}\psi)(t)$. We shall discuss these problems further in Sect. 1.8.

1.6 Zitterbewegung

It is only for very special initial states that the time evolution can be determined explicitly with the methods of the previous section (i.e., by evaluating Eq. (1.86)). In order to get a qualitative description of the behavior of relativistic particles, it is useful to investigate the temporal behavior (cf. Eq (1.18)) of some selected observables.

1.6.1 The Velocity Operator

For free particles the velocity operator is usually defined as the time derivative of the position operator $\boldsymbol{x}(t) \equiv \exp(\mathrm{i}H_0 t)\,\boldsymbol{x}\,\exp(-\mathrm{i}H_0 t)$. If $\boldsymbol{x}$ is chosen as the standard position operator (1.30), we obtain the *standard velocity operator*

$$\frac{d}{dt}\boldsymbol{x}(t) = \mathrm{i}\,[H_0, \boldsymbol{x}(t)] = e^{\mathrm{i}H_0 t}\,\mathrm{i}\,[H_0, \boldsymbol{x}]\,e^{-\mathrm{i}H_0 t}$$

$$= e^{\mathrm{i}H_0 t}\,c\boldsymbol{\alpha}\,e^{-\mathrm{i}H_0 t} \equiv c\boldsymbol{\alpha}(t). \tag{1.111}$$

(A domain for the commutators in Eq. (1.111) is given below, see the remark in Sect. 1.6.2). The matrix $c\boldsymbol{\alpha}$ has the eigenvalues $+c$, $-c$, i.e., a purely discrete spectrum. The operator $c\boldsymbol{\alpha}(t)$ is unitarily equivalent to $c\boldsymbol{\alpha}$, therefore also $\sigma(c\boldsymbol{\alpha}(t)) = \{+c, -c\}$ for all t. We arrive at the somewhat paradoxical conclusion that a velocity measurement at any time yields c or $-c$ as the only possible values.

In *classical* relativistic kinematics one is accustomed to the relation $\boldsymbol{v} = c^2\boldsymbol{p}/E$, and by the correspondence principle one would have expected the operator $c^2\boldsymbol{p}H_0^{-1}$ to be the correct velocity operator. This operator is bounded, commutes with H_0 (which means that it is a constant of motion for free particles) and has purely continuous spectrum in the interval $[-c, c]$. (Note that H_0^{-1} is a bounded operator since 0 is not in the spectrum of H_0). We call $c^2\boldsymbol{p}H_0^{-1}$ the *classical velocity operator.*

The time derivative of the standard velocity operator is

$$\frac{d}{dt}\,c\boldsymbol{\alpha}(t) = e^{\mathrm{i}H_0 t}\,\mathrm{i}[H_0, c\boldsymbol{\alpha}]\,e^{-\mathrm{i}H_0 t} = 2\mathrm{i}H_0\,\boldsymbol{F}(t), \tag{1.112}$$

which shows that $\boldsymbol{\alpha}(t)$ is not a constant of motion. The operator $\boldsymbol{F}$, defined as the difference between $c\boldsymbol{\alpha}$ and the classical velocity operator,

$$\boldsymbol{F} \equiv c\boldsymbol{\alpha} - c^2\boldsymbol{p}H_0^{-1}, \tag{1.113}$$

is bounded. Since (each component of) $\boldsymbol{F}$ anticommutes with H_0,

$$\boldsymbol{F}H_0 = -H_0\boldsymbol{F} \quad \text{on } \mathfrak{D}(H_0), \tag{1.114}$$

we easily obtain

$$\boldsymbol{F}(t) = e^{2\mathrm{i}H_0 t}\boldsymbol{F}, \qquad \int_0^t \boldsymbol{F}(t)\,dt = \frac{1}{2\mathrm{i}H_0}\,e^{2\mathrm{i}H_0 t}\,\boldsymbol{F}. \tag{1.115}$$

Integrating (1.112) and using $c\boldsymbol{\alpha}(0) = c\boldsymbol{\alpha}$ we arrive at

$$c\boldsymbol{\alpha}(t) = c^2\boldsymbol{p}H_0^{-1} + \boldsymbol{F}(t). \tag{1.116}$$

Thus the velocity oscillates without damping around the conserved mean value $c^2\boldsymbol{p}H_0^{-1}$ which is just the classical velocity operator. This phenomenon is usually called "*Zitterbewegung*".

1.6.2 Time Evolution of the Standard Position Operator

The formal time derivative of $\boldsymbol{x}(t)$ in Eq. (1.111) implies

$$\boldsymbol{x}(t) = \boldsymbol{x} + \int_0^t c\,\boldsymbol{\alpha}(t)\,dt. \tag{1.117}$$

Here the second summand is bounded for all finite t and thus $\mathfrak{D}\big(\boldsymbol{x}(t)\big) = \mathfrak{D}(\boldsymbol{x})$ by a standard perturbation theoretic argument. This heuristic argument is made precise in the following theorem. We mention that in nonrelativistic quantum mechanics the domain of $\boldsymbol{x}$ is *not* invariant under the free time evolution.

Theorem 1.3. The domain $\mathfrak{D}(\boldsymbol{x})$ of the multiplication operator $\boldsymbol{x}$ is left invariant by the free time evolution,

$$\mathfrak{D}\big(\boldsymbol{x}(t)\big) = e^{-\mathrm{i}H_0 t}\,\mathfrak{D}(\boldsymbol{x}) = \mathfrak{D}(\boldsymbol{x}). \tag{1.118}$$

On this domain we have

$$\boldsymbol{x}(t) = \boldsymbol{x} + c^2 \boldsymbol{p} H_0^{-1} t + \frac{1}{2\mathrm{i}H_0}\left(e^{2\mathrm{i}H_0 t} - 1\right)\boldsymbol{F}. \tag{1.119}$$

Proof. Formally, (1.119) is easily verified by differentiating it with respect to t, which gives (1.116) in accordance with (1.111). The integration constant comes from the condition $\boldsymbol{x}(0) = \boldsymbol{x}$.

In order to prove the invariance of the domain we consider the regularization

$$\boldsymbol{x}_\lambda \equiv \frac{\boldsymbol{x}}{1 + \lambda|\boldsymbol{x}|}, \quad \lambda > 0. \tag{1.120}$$

For $\lambda > 0$, $\boldsymbol{x}_\lambda$ is a bounded multiplication operator which is defined everywhere in the Hilbert space. A vector ψ is in the domain of $\boldsymbol{x}$ if and only if $\|\boldsymbol{x}_\lambda \psi\|$ remains bounded uniformly in λ, as $\lambda \to 0$.

Since also the derivative of $\boldsymbol{x}_\lambda$ is bounded, we have $\boldsymbol{x}_\lambda \psi \in \mathfrak{D}(H_0)$, whenever $\psi \in \mathfrak{D}(H_0)$. On these states we can evaluate the time derivative of $\boldsymbol{x}_\lambda(t)$,

$$\frac{d}{dt}\,\boldsymbol{x}_\lambda(t)\,\psi = e^{+\mathrm{i}H_0 t}\,\mathrm{i}[H_0, \boldsymbol{x}_\lambda]\,e^{-\mathrm{i}H_0 t}\,\psi, \quad \text{for } \psi \in \mathfrak{D}(H_0). \tag{1.121}$$

But the commutator extends to a bounded operator on all of $\mathfrak{H}$. Integrating from 0 to t and taking the norm gives for all $\psi \in \mathfrak{H}$ and $\lambda > 0$,

$$\begin{aligned} \|\,\boldsymbol{x}_\lambda(t)\,\psi\,\| &= \|\,\boldsymbol{x}_\lambda\,e^{-\mathrm{i}H_0 t}\,\psi\,\| \\ &\le \|\,\boldsymbol{x}_\lambda\,\psi\,\| + \int_0^t \left\| \frac{\boldsymbol{\alpha} - \lambda(\boldsymbol{\alpha}\cdot\boldsymbol{x}/|\boldsymbol{x}|)\,\boldsymbol{x}_\lambda}{1+\lambda|\boldsymbol{x}|}\,e^{-\mathrm{i}H_0 t}\,\psi \right\| ds. \end{aligned} \tag{1.122}$$

If, in addition, ψ is in the domain of $\boldsymbol{x}$, then the right hand side remains bounded uniformly, as $\lambda \to 0$. Hence also $\exp(-\mathrm{i}H_0 t)\psi$ is in the domain of $\boldsymbol{x}$. From this the equality of $\mathfrak{D}(\boldsymbol{x})$ with $\exp(-\mathrm{i}H_0 t)\mathfrak{D}(\boldsymbol{x})$ follows immediately. □

Remark. Eq. (1.111) makes sense if applied to vectors in the domain of the commutator $[H_0, \boldsymbol{x}(t)]$. We show that the set

$$\mathfrak{D} \equiv H_0^{-1}\mathfrak{D}(\boldsymbol{x}) \subset \mathfrak{D}(\boldsymbol{x}) \cap \mathfrak{D}(H_0) \tag{1.123}$$

is dense, invariant under the free time evolution, and $[H_0, \boldsymbol{x}(t)]$ is well defined on $\mathfrak{D}$. If $\mathfrak{D}$ were not dense, then there would exist a nonzero vector $f \in \mathfrak{H}$ for which

$$0 = (f, H_0^{-1}\psi) = (H_0^{-1}f, \psi), \quad \text{all } \psi \in \mathfrak{D}(\boldsymbol{x}). \tag{1.124}$$

Since $\mathfrak{D}(\boldsymbol{x})$ is dense, (1.124) implies $H_0^{-1}f = 0$ and hence $f = H_0 H_0^{-1} f = 0$. This is a contradiction, therefore $\mathfrak{D}$ is dense in $\mathfrak{H}$. The inclusion $\mathfrak{D} \subset \mathfrak{D}(\boldsymbol{x})$ is most easily seen in momentum space. Let $\psi \in \mathfrak{D}(\boldsymbol{x})$, i.e., $\mathcal{F}\psi \in \mathfrak{D}(\nabla_{\boldsymbol{p}})$. From

$$\mathcal{F}\boldsymbol{x}H_0^{-1}\psi = \mathrm{i}\nabla_{\boldsymbol{p}}\,\mathrm{h}(\boldsymbol{p})^{-1}\,\mathcal{F}\psi \tag{1.125}$$

we find $H_0^{-1}\psi \in \mathfrak{D}(\boldsymbol{x})$, because the derivative with respect to $\boldsymbol{p}$ of

$$\mathrm{h}(\boldsymbol{p})^{-1} = \frac{c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2}{c^2p^2 + m^2c^4} \tag{1.126}$$

is bounded. This implies $\mathfrak{D} \subset \mathfrak{D}(\boldsymbol{x})$ and hence $\mathfrak{D} \subset \mathfrak{D}(\boldsymbol{x}) \cap \mathfrak{D}(H_0)$, because the inclusion $\mathfrak{D} \subset \mathfrak{D}(H_0)$ is trivial. Finally, it is easily seen that the commutator $[H_0, \boldsymbol{x}(t)]$ is well defined on $e^{-\mathrm{i}H_0 t}H_0^{-1}\mathfrak{D}(\boldsymbol{x}) = \mathfrak{D}$. On this domain the commutator can be evaluated to give $c\boldsymbol{\alpha}(t)$. Since the result is bounded, it can be extended uniquely to all of $\mathfrak{H}$.

1.6.3 Evolution of the Expectation Value

Due to the third summand in (1.119) the expectation value of $\boldsymbol{x}(t)$ contains an oscillating part $z_\psi(t)$. We can show that this oscillation tends to zero, as $t \to \infty$. Writing $(U_{\mathrm{sp}}\psi)(\lambda) = g(\lambda)$ we obtain

$$\begin{aligned} z_\psi(t) &\equiv \Big(\psi\,, \frac{1}{2\mathrm{i}H_0}\,e^{2\mathrm{i}H_0 t}\,\boldsymbol{F}\psi\Big) = \Big(U_{\mathrm{sp}}\psi\,, \frac{1}{2\mathrm{i}\lambda}\,e^{2\mathrm{i}\lambda t}\,U_{\mathrm{sp}}\boldsymbol{F}\,\psi\Big) \\ &= \int_{\sigma(H_0)} \frac{1}{2\mathrm{i}\lambda}\,e^{2\mathrm{i}\lambda t} \sum_{i=1,2} \big(g_i(\lambda)\,, \{U_{\mathrm{sp}}\boldsymbol{F}U_{\mathrm{sp}}^{-1}g\}_i(\lambda)\big)_s\,d\lambda, \end{aligned} \tag{1.127}$$

which is the (inverse) Fourier transform of an integrable function of λ. The Riemann Lebesgue-Lemma implies that $z_\psi(t)$ is a continuous function of t, vanishing as $t \to \infty$.

The Zitterbewegung is a consequence of the negative energies. Since $\boldsymbol{F}$ anticommutes with H_0 we obtain

$$\boldsymbol{F}\,P_{\substack{\mathrm{pos}\\\mathrm{neg}}} = P_{\substack{\mathrm{neg}\\\mathrm{pos}}}\,\boldsymbol{F}. \tag{1.128}$$

Therefore the bounded operator $\boldsymbol{F}$ maps the positive energy subspace into the subspace of negative energy and vice versa, in particular, $P_{\mathrm{pos}}\boldsymbol{F}P_{\mathrm{pos}} = 0$. For

any state $\psi_{\text{pos}} \in \mathfrak{H}_{\text{pos}}$, which is also in the domain of $\boldsymbol{x}$, we can form the expectation value

$$\big(\psi_{\text{pos}}(t), \boldsymbol{x}\,\psi_{\text{pos}}(t)\big) = \big(\psi_{\text{pos}}, P_{\text{pos}}\boldsymbol{x}(t)P_{\text{pos}}\,\psi_{\text{pos}}\big), \tag{1.129}$$

and see, that it performs no Zitterbewegung at all. A similar conclusion holds for the negative energy states. We summarize our results in the following theorem.

Theorem 1.4. The expectation value of $\boldsymbol{x}$ in the state $\psi(t) = e^{-\mathrm{i}H_0 t}\psi$, where $\psi \in \mathfrak{D}(\boldsymbol{x})$, is of the form

$$(\psi(t), \boldsymbol{x}\,\psi(t)) = (\psi, \{\boldsymbol{x} + \frac{1}{2\mathrm{i}H_0}\boldsymbol{F}\}\,\psi) + (\psi, c^2\boldsymbol{p}H_0^{-1}\,\psi)\,t + z_\psi(t), \tag{1.130}$$

where $z_\psi(t)$, given by (1.127), is continuous in t and vanishes at infinity. If ψ is an initial state with positive (negative) energy, then the expectation value of $\boldsymbol{x}$ in the state $\psi(t)$ performs no Zitterbewegung at all. In this case we have

$$(\psi(t), \boldsymbol{x}\,\psi(t)) = (\psi, \boldsymbol{x}\,\psi) + (\psi, c^2\boldsymbol{p}H_0^{-1}\,\psi)\,t, \quad \psi \in \mathfrak{H}_{\text{pos}} \text{ or } \mathfrak{H}_{\text{neg}}. \tag{1.131}$$

The velocity of a negative energy particle is always *antiparallel* to its momentum because $c^2\boldsymbol{p}H_0^{-1}\psi_{\text{neg}} = -c^2\boldsymbol{p}\,|H_0|^{-1}\psi_{\text{neg}}$.

1.6.4 Evolution of Angular Momenta

We want to stress that not only $\boldsymbol{x}(t)$ shows the phenomenon of Zitterbewegung. It is present also for example in the angular momentum operators $\boldsymbol{L}$ and $\boldsymbol{S}$. A little calculation shows that

$$\boldsymbol{L}(t) = \boldsymbol{x}(t) \wedge \boldsymbol{p} = \boldsymbol{L} + \frac{1}{2\mathrm{i}H_0}(e^{2\mathrm{i}H_0 t} - 1)\boldsymbol{F} \wedge \boldsymbol{p}, \tag{1.132}$$

$$\boldsymbol{S}(t) = -\frac{\mathrm{i}}{4}\boldsymbol{\alpha}(t) \wedge \boldsymbol{\alpha}(t) = \boldsymbol{S} - \frac{1}{2\mathrm{i}H_0}(e^{2\mathrm{i}H_0 t} - 1)\boldsymbol{F} \wedge \boldsymbol{p}. \tag{1.133}$$

Thus we see that orbital and spin angular momentum are not conserved because of Zitterbewegung. In the sum $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$, however, the time-dependent terms cancel, and we obtain the important result

$$\boldsymbol{J}(t) = \boldsymbol{J}, \tag{1.134}$$

which can be also verified directly from

$$[\boldsymbol{J}, H_0] = 0. \tag{1.135}$$

1.6.5 The Operators F and G

Eq. (1.116) gives the connection of the α-matrices with the classical velocity. We now give a similar relation for the Dirac matrix β in order to shed some light on its physical meaning. We first calculate

$$\mathrm{i}[H_0, \beta] = 2\mathrm{i} H_0 G, \tag{1.136}$$

where

$$G = \beta - \frac{mc^2}{H_0}. \tag{1.137}$$

G is a bounded operator which again anticommutes with H_0, i.e.,

$$GH_0 + H_0 G = 0 \quad \text{on } \mathfrak{D}(H_0). \tag{1.138}$$

G maps $\mathfrak{H}_{\mathrm{pos}}$ onto $\mathfrak{H}_{\mathrm{neg}}$ and vice versa. We see that

$$G(t) = e^{2\mathrm{i}H_0 t} G, \qquad \int_0^t G(t)\, dt = \frac{1}{2\mathrm{i}H_0}\, e^{2\mathrm{i}H_0 t}\, G. \tag{1.139}$$

Therefore, also β performs a Zitterbewegung,

$$\beta(t) = \frac{mc^2}{H_0} + G(t). \tag{1.140}$$

The operator G describes the difference between the Dirac matrix β and the operator corresponding to the classical expression

$$\frac{mc^2}{E} = \sqrt{1 - \frac{v^2}{c^2}}. \tag{1.141}$$

The operators $\boldsymbol{F}$ and G are closely related. From $H_0^2 = c^2 p^2 + m^2 c^4$ we obtain the relation

$$\boldsymbol{F} \cdot \boldsymbol{p} + mc^2 G = 0 \tag{1.142}$$

(i.e., the free Dirac operator is not changed if we replace $c\boldsymbol{\alpha}$ by $c^2 \boldsymbol{p} H_0^{-1}$ and β by $mc^2 H_0^{-1}$). We finally note the relations

$$\frac{1}{c}\, \boldsymbol{\alpha} \cdot \boldsymbol{F} + \beta G = 3, \tag{1.143}$$

$$G^2 = 1 - \frac{m^2 c^4}{H_0^2} = \frac{c^2 p^2}{H_0^2} = 3 - \frac{\boldsymbol{F}^2}{c^2}. \tag{1.144}$$

1.7 Relativistic Observables

The results of the previous section present some interpretational difficulties which we try to overcome by choosing different sets of operators for the observables of the theory.

1.7.1 Restriction to Positive Energies

The Zitterbewegung is mathematically well understood but presents some difficulties for the interpretation of the theory. Why should a free relativistic particle violate Newton's second law? The origin of this difficulty might well be that the choice of relativistic observables in Sect. 1.3 has been incorrect. We have chosen the standard position operator $\boldsymbol{x}$ because of its simplicity. But now we have learned that $\boldsymbol{x}$ mixes up positive and negative energy states in a very complex manner. This effect is the origin of the Zitterbewegung. It would be absent if there were only positive (or only negative) energies. Also the electron-positron interpretation in Sect. 1.4.6 suggests to consider the positive and negative energy subspaces separately, $\mathfrak{H}_{\text{pos}}$ for electrons, and $\mathfrak{H}_{\text{neg}}$ (or better $C\mathfrak{H}_{\text{neg}}$, see Eq. (1.82)) for positrons. Therefore it seems to be more natural to represent observables by operators which do not mix positive and negative energies. So we try to replace $\boldsymbol{x}$ by the part $\tilde{\boldsymbol{x}}$ which leaves $\mathfrak{H}_{\text{pos}}$ and $\mathfrak{H}_{\text{neg}}$ separately invariant. A little calculation shows that

$$\tilde{\boldsymbol{x}} \equiv P_{\text{pos}}\boldsymbol{x}P_{\text{pos}} + P_{\text{neg}}\boldsymbol{x}P_{\text{neg}} = \boldsymbol{x} - \frac{1}{2\mathrm{i}H_0}\boldsymbol{F}. \tag{1.145}$$

$\tilde{\boldsymbol{x}}$ is obtained from $\boldsymbol{x}$ by subtracting

$$P_{\text{pos}}\boldsymbol{x}P_{\text{neg}} + P_{\text{neg}}\boldsymbol{x}P_{\text{pos}} = \frac{1}{2\mathrm{i}H_0}\boldsymbol{F}. \tag{1.146}$$

This is a bounded operator and hence $\tilde{\boldsymbol{x}}$ is self-adjoint on $\mathfrak{D}(\tilde{\boldsymbol{x}}) = \mathfrak{D}(\boldsymbol{x})$. From (1.111), (1.115) and (1.116) it is clear that on this domain (cf. Theorem 1.3 in Sect. 1.6.2)

$$\tilde{\boldsymbol{x}}(t) = \tilde{\boldsymbol{x}} + c^2\boldsymbol{p}H_0^{-1}t. \tag{1.147}$$

Hence the corresponding velocity is just the operator expected from classical relativistic mechanics. From (1.145) it is also clear that $\tilde{\boldsymbol{x}}$ satisfies the canonical commutation relations with $\boldsymbol{p}$, since $\boldsymbol{p}$ commutes with $(2\mathrm{i}H_0)^{-1}\boldsymbol{F}$.

In the same way one could restrict also the other operators which mix the spectral subspaces:

$$c\,\tilde{\boldsymbol{\alpha}} = c^2\boldsymbol{p}H_0^{-1}, \tag{1.148}$$

$$\tilde{\beta} = mc^2H_0^{-1}, \tag{1.149}$$

$$\tilde{\boldsymbol{L}} = \boldsymbol{L} - \frac{1}{2\mathrm{i}H_0}\boldsymbol{F} \wedge \boldsymbol{p}, \tag{1.150}$$

$$\tilde{\boldsymbol{S}} = \boldsymbol{S} + \frac{1}{2\mathrm{i}H_0}\boldsymbol{F}\wedge\boldsymbol{p} = -\frac{\mathrm{i}}{4}c^2\boldsymbol{F}\wedge\boldsymbol{F}. \tag{1.151}$$

In (1.151) we have used the relation

$$\boldsymbol{S} = -\frac{\mathrm{i}}{4}\boldsymbol{\alpha}\wedge\boldsymbol{\alpha} = -\frac{\mathrm{i}}{4c^2}\boldsymbol{F}\wedge\boldsymbol{F} + \frac{1}{2\mathrm{i}H_0}\boldsymbol{F}\wedge\boldsymbol{p}. \tag{1.152}$$

Of course the operators H_0 and $\boldsymbol{p}$ commute with the projectors P_{pos} and P_{neg}, hence $\tilde{\boldsymbol{p}} = \boldsymbol{p}$, and

$$\tilde{H}_0 = H_0 = \sqrt{c^2p^2 + m^2c^4}\,P_{\mathrm{pos}} - \sqrt{c^2p^2 + m^2c^4}\,P_{\mathrm{neg}}. \tag{1.153}$$

From (1.150) and (1.151) we see that also $\tilde{\boldsymbol{J}} = \boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$, as expected.

1.7.2 Operators in the Foldy-Wouthuysen Representation

The operator $\tilde{\boldsymbol{x}}$ has the interesting property that its components do not commute,

$$[\tilde{x}_i, \tilde{x}_k] = -\mathrm{i}\frac{c^2}{H_0^2}\tilde{S}_l, \tag{1.154}$$

where (i,k,l) is a cyclic permutation of $(1,2,3)$. Eq. (1.154) is very unfamiliar for position operators. It implies that localization in a finite region is not a meaningful concept any longer (see Sect. 1.7.3). There is, however, another position operator leaving $\mathfrak{H}_{\mathrm{pos}}$ and $\mathfrak{H}_{\mathrm{neg}}$ invariant, which has commuting components and time derivative $c^2\boldsymbol{p}H_0^{-1}$. This is the so called "*Newton Wigner position operator*" $\boldsymbol{x}_{\mathrm{NW}}$. It can be obtained most easily in the Foldy-Wouthuysen (FW) representation (cf. Sect. 1.4.3). Let $\boldsymbol{x}$ denote, as usual, the operator of multiplication by $\boldsymbol{x}$ (acting now in the Hilbert space of the FW-representation). We define the Newton-Wigner position operator to be the inverse FW-transformation of $\boldsymbol{x}$

$$\boldsymbol{x}_{\mathrm{NW}} = U_{\mathrm{FW}}^{-1}\,\boldsymbol{x}\,U_{\mathrm{FW}}. \tag{1.155}$$

We see immediately that the components $(x_{\mathrm{NW}})_i$ commute with each other and that the positive/negative energy subspaces are left invariant by $\boldsymbol{x}_{\mathrm{NW}}$, since

$$[\boldsymbol{x}_{\mathrm{NW}}, P_{\substack{\mathrm{pos}\\\mathrm{neg}}}] = U_{\mathrm{FW}}^{-1}\,[\boldsymbol{x}, \tfrac{1}{2}(1\pm\beta)]\,U_{\mathrm{FW}} = 0. \tag{1.156}$$

Similarly, we obtain for the time dependence

$$\boldsymbol{x}_{\mathrm{NW}}(t) = \boldsymbol{x}_{\mathrm{NW}} + \mathrm{c}^2\boldsymbol{p}H_0^{-1}t. \tag{1.157}$$

A less agreeable feature of the Newton-Wigner operator is its explicit form in the standard representation, which is obtained from (1.155) and (1.57) after some calculation.

$$\boldsymbol{x}_{\mathrm{NW}} = \boldsymbol{x} - \frac{\beta}{2\mathrm{i}\lambda}\left(c\,\boldsymbol{\alpha} - \frac{\mathrm{c}^2}{\lambda(\lambda+mc^2)}c(\boldsymbol{\alpha}\cdot\boldsymbol{p})\boldsymbol{p}\right) - \frac{\mathrm{c}^2}{\lambda(\lambda+mc^2)}\boldsymbol{S}\wedge\boldsymbol{p}, \tag{1.158}$$

where $\lambda = (c^2p^2 + m^2c^4)^{1/2}$. Of course we can also define other observables first in the FW-representation and then transform them to the standard representation.

The following list gives the FW-representation of some important operators. For any observable A we denote $A_{\mathrm{FW}} = U_{\mathrm{FW}} A U_{\mathrm{FW}}^{-1}$.

$$\boldsymbol{p}_{\mathrm{FW}} = \boldsymbol{p}, \tag{1.159}$$

$$(H_0)_{\mathrm{FW}} = \beta\sqrt{c^2p^2 + m^2c^4}, \tag{1.160}$$

$$(P^{\mathrm{pos}}_{\mathrm{neg}})_{\mathrm{FW}} = \tfrac{1}{2}(1 \pm \beta), \tag{1.161}$$

$$G_{\mathrm{FW}} = -\frac{c}{\lambda}\boldsymbol{\alpha}\cdot\boldsymbol{p}, \tag{1.162}$$

$$\boldsymbol{F}_{\mathrm{FW}} = c\,\boldsymbol{\alpha} + \frac{c^2\boldsymbol{p}}{\lambda + mc^2}G_{\mathrm{FW}}, \tag{1.163}$$

$$\boldsymbol{x}_{\mathrm{FW}} = \boldsymbol{x} + \frac{1}{2iH_{\mathrm{FW}}}\boldsymbol{F}_{\mathrm{FW}} - \frac{c^2}{\lambda(\lambda + mc^2)}\boldsymbol{S}\wedge\boldsymbol{p}, \tag{1.164}$$

$$\boldsymbol{S}_{\mathrm{FW}} = \boldsymbol{S} - (\boldsymbol{x}_{\mathrm{FW}} - \boldsymbol{x})\wedge\boldsymbol{p}, \tag{1.165}$$

$$\boldsymbol{L}_{\mathrm{FW}} = \boldsymbol{x}_{\mathrm{FW}}\wedge\boldsymbol{p}, \tag{1.166}$$

$$\boldsymbol{J}_{\mathrm{FW}} = \boldsymbol{J}, \tag{1.167}$$

$$(\boldsymbol{x}_{\mathrm{NW}})_{\mathrm{FW}} = \boldsymbol{x}. \tag{1.168}$$

1.7.3 Notions of Localization

There are several possible choices for position operators, each having attractive features but also disadvantages. So it seems worthwhile to describe some requirements which are often regarded as fundamental for any position observable. We consider a single particle and assume (at least for the moment) that it can have the property of being localized in some subset B of $\mathbb{R}^3$. If this property is indeed observable, then for each region B there must be a self-adjoint operator $E(B)$ in the Hilbert space of that particle which describes the two possibilities of being localized either within B or outside B. Thus $E(B)$ should only have the eigenvalues 1 ("within B") and 0 ("outside B"). An operator $E(B)$ with these properties must be a projection operator. Indeed, any observable which describes whether or not a physical system has a certain property, is a projection operator.

Our requirements are the following:

1. For every (Borel-measurable) set $B \subset \mathbb{R}^3$ there is a projection operator $E(B)$ such that $(\psi, E(B)\psi)$ is the probability of finding the particle in B, if it is currently in the state ψ, $\|\psi\| = 1$. The particle must be somewhere, hence

$$E(\mathbb{R}^3) = \mathbf{1}. \tag{1.169}$$

2. If the system is at the same time localized in B_1 and in B_2 then it is localized in $B_1 \cap B_2$,

$$E(B_1 \cap B_2) = E(B_1)\,E(B_2) \quad \text{for all } B_1 \text{ and } B_2. \tag{1.170}$$

3. The range of $E(B_1 \cup B_2)$ is the subspace of states which are localized in $B_1 \cup B_2$. This subspace should be spanned by the vectors in $E(B_1)$ and those in $E(B_2)$. Hence

$$E(B_1 \cup B_2) = E(B_1) + E(B_2) - E(B_1 \cap B_2) \quad \text{for all } B_1 \text{ and } B_2. \tag{1.171}$$

If $B_1, B_2, \ldots$ are disjoint then

$$E(B_1 \cup B_2 \cup \ldots) = \sum_{i=1}^{\infty} E(B_i). \tag{1.172}$$

4. Let $U(\boldsymbol{a}, \mathbf{R})$, $\boldsymbol{a} \in \mathbb{R}^3$, $\mathbf{R} \in SO(3)$, be a unitary representation (Sect. 2.2.4) of the (covering group of the) Euclidean group in the Hilbert space of the particle. For any Borel set B in $\mathbb{R}^3$ the set denoted by $\mathbf{R}B + \boldsymbol{a}$ is obtained from B by a rotation $\mathbf{R}$ and a translation with the vector $\boldsymbol{a}$. Then

$$E(\mathbf{R}B + \boldsymbol{a}) = U(\boldsymbol{a}, \mathbf{R})E(B)U(\boldsymbol{a}, \mathbf{R})^*. \tag{1.173}$$

If $E(B)$ satisfies the requirements 1-4 above, then it is the spectral measure of a unique "position" operator $\boldsymbol{q} = (q_1, q_2, q_3)$. We can define spectral families $E_{q_i}(\lambda) \equiv E\big(\{\boldsymbol{x} \in \mathbb{R}^3 \mid x_i \leq \lambda\}\big)$ and the operators

$$q_i = \int_{-\infty}^{+\infty} \lambda \, dE_{q_i}(\lambda), \quad i = 1, 2, 3. \tag{1.174}$$

From (1.170) it is clear that

$$E_{q_i}(\lambda)\,E_{q_k}(\lambda) = E_{q_k}(\lambda)\,E_{q_i}(\lambda), \quad i, k = 1, 2, 3, \tag{1.175}$$

i.e., the components of $\boldsymbol{q}$ commute. Conversely, for any position operator with commuting components we can define $E(B) = \chi(\boldsymbol{q} \in B)$ via the spectral theorem. Here χ denotes the characteristic function of B.

A spectral measure on $\mathbb{R}^3$ cannot be associated with the operator $\tilde{\boldsymbol{x}}$ of (1.145) because its components do not commute. According to this operator the notion of "localization in a region B" has no clear meaning.

For the standard position operator $E(B) = \chi(\boldsymbol{x} \in B)$ is simply the operator of multiplication by the characteristic function of the set B and hence the requirements 1-4 are trivial (cf. Sect. 1.3.2).

$$(\psi, E(B)\psi) = \int_B |\psi(\boldsymbol{x})|^2 \, d^3x \tag{1.176}$$

is the probability for finding the particle in B. According to this notion of localization a particle is localized in B if and only if its wavefunction ψ vanishes almost everywhere outside B.

For the Newton Wigner operator $\boldsymbol{x}_{\rm NW}$, the spectral measure

$$E(B) = \chi(\boldsymbol{x}_{\rm NW} \in B) = U_{\rm FW}^{-1}\, \chi(\boldsymbol{x} \in B)\, U_{\rm FW} \tag{1.177}$$

satisfies 1–4 because these statements are not affected by the unitary transformation $U_{\rm FW}^{-1}$. If $(\psi, E(B)\psi) = 1$, then the *particle* is localized in B, but this does not mean that the *wavefunction* ψ has to be localized in B. There is a remarkable theorem of Newton, Wigner and Wightman, which we state here in the form needed for the Dirac theory.

Theorem 1.5. Let $\boldsymbol{q} = (q_1, q_2, q_3)$ be a set of self-adjoint operators in $\mathfrak{H} = L^2(\mathbb{R}^3)^4$ such that $E(B) = \chi(\boldsymbol{q} \in B)$ fulfils requirements 1-4 and in addition

5. $E_{\boldsymbol{q}}(B)$ leaves $\mathfrak{H}_{\rm pos}$ and $\mathfrak{H}_{\rm neg}$ invariant, i.e.,

$$E_{\boldsymbol{q}}(B)\mathfrak{H}_{\substack{\rm pos\\ \rm neg}} \subset \mathfrak{H}_{\substack{\rm pos\\ \rm neg}}. \tag{1.178}$$

Then $\boldsymbol{q}$ is the Newton Wigner operator.

Therefore, if "localization in a region B" is a meaningful concept, then the theorem above is a strong argument in favor of the Newton Wigner operator. There are, however, some a priori arguments against the possibility of a strict localization in a region for particles with a definite sign of energy. These are considered in the next section.

1.8 Localization and Acausality

The restriction to operators leaving the positive/negative energy subspaces invariant solves the problem of Zitterbewegung. But there is another, more subtle difficulty. This is the localization problem.

1.8.1 Superluminal Propagation

The Einstein causality requires a finite propagation speed for all physical particles. Indeed, any solution of the Dirac equation (1.10), whether it has positive energy or not, cannot propagate faster than with the velocity of light (cf. Sect. 1.5). On the other hand, in the Foldy-Wouthuysen representation, we expect a possible superluminal spreading of the wavepackets in the corresponding Hilbert space $U_{\rm FW}\mathfrak{H}$. Thus, if we take the Newton Wigner operator (which is just multiplication by $\boldsymbol{x}$ in the FW-representation) as a position observable, then we have to live with an acausal propagation of initially localized particles. This problem, which we already mentioned in Sect. 1.5, comes with all position operators commuting with the sign of energy. This is the content of the next theorem.

Theorem 1.6. Let $\mathfrak{H}$ be a Hilbert space. For every Borel set $B \subset \mathbb{R}^3$ let $F(B)$ be a bounded, self-adjoint operator in $\mathfrak{H}$ such that for all $\psi \in \mathfrak{H}$ with $\|\psi\| = 1$, $(\psi, F(B)\psi)$ is a probability measure with the following properties:

i) $(\psi, F(B)\psi) = 1$ and $(\phi, F(B)\phi) = 0$ implies $(\phi, \psi) = 0$.

ii) There is a self-adjoint operator $\boldsymbol{p}$ (the generator of space translations) such that for all $\boldsymbol{a} \in \mathbb{R}^3$

$$(e^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{a}}\,\psi, F(B+\boldsymbol{a})\,e^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{a}}\,\psi) = (\psi, F(B)\psi). \tag{1.179}$$

Furthermore, define $H \equiv \lambda(\boldsymbol{p})$, where λ is a continuous function, positive, and not identically constant. Let $\psi \in \mathfrak{H}$ with $\|\psi\| = 1$.

Then for all nonempty open sets $B \subset \mathbb{R}^3$ and for all $\epsilon > 0$ there is a time $t \in (0, \epsilon)$ such that

$$(e^{-\mathrm{i}Ht}\psi, F(B)e^{-\mathrm{i}Ht}\psi) \neq 0. \tag{1.180}$$

Proof. We give an indirect proof. Assume that

$$(e^{-\mathrm{i}Ht}\,\psi\,, F(B)\,e^{-\mathrm{i}Ht}\,\psi) \equiv \|\,F(B)^{1/2}\,e^{-\mathrm{i}Ht}\,\psi\,\|^2 = 0 \tag{1.181}$$

for all $t \in (0, \epsilon)$. From (1.181) we see that $F(B)\,e^{-\mathrm{i}Ht}\,\psi = 0$. Next define for arbitrary $\phi \in \mathfrak{H}$ the complex function

$$g(z) = (\phi\,, F(B)e^{-\mathrm{i}Hz}\,\psi) = (\phi_{\boldsymbol{B}}\,, e^{-\mathrm{i}Hz}\,\psi), \tag{1.182}$$

where $\phi_{\boldsymbol{B}} = F(B)\phi$. Since

$$\frac{d}{dz}\,g(z) = -\mathrm{i}\int_0^\infty \lambda\,e^{-\mathrm{i}\lambda z}\,d(\phi_{\boldsymbol{B}}\,, E_H(\lambda)\,\psi) \tag{1.183}$$

exists for $\mathrm{Im}(z) < 0$, g is analytic in the lower half plane. Since moreover g is continuous by the strong continuity of $\exp(-\mathrm{i}Hz)$, we can apply the Schwarz reflection principle. g can thus be analytically continued to a holomorphic function on $\mathbb{C}$. Since it is zero on the interval $(0, \epsilon)$ of the real axis, it must vanish everywhere,

$$g(z) = 0 \quad \text{for all } z \in \mathbb{C}. \tag{1.184}$$

Now for all ψ satisfying (1.181) and all $\phi \in \mathfrak{H}$ we have

$$(\phi_{\boldsymbol{B}}, \chi(a \leq H < b)\psi) = \frac{1}{\sqrt{2\pi}}\int dt\,g(t)\,\tilde{\chi}(t) = 0, \tag{1.185}$$

where $\tilde{\chi}(t)$ is the Fourier transform of the characteristic function of the interval (a, b). Thus $F(B)\chi(a \leq H < b)\psi = 0$. Now let B' be an open subset of B such that the distance d of the boundaries of B and B' is nonzero. We have for $|\boldsymbol{a}| < d$

$$F(B')\,e^{-\mathrm{i}\boldsymbol{a}\cdot\boldsymbol{p}}\,\chi(a\leq H<b)\,\psi = e^{-\mathrm{i}\boldsymbol{a}\cdot\boldsymbol{p}}\,F(B'-\boldsymbol{a})\,\chi(a\leq H<b)\,\psi = 0, \tag{1.186}$$

since $B'-\boldsymbol{a} \subset B$. Next we consider for all $\boldsymbol{a} \in \mathbb{R}^3$ the function

$$h(\boldsymbol{a}) = (\phi_{B'}, e^{-\mathrm{i}\boldsymbol{a}\cdot\boldsymbol{p}}\,\chi(a \le \boldsymbol{H} < b)\,\psi)$$
$$= \int e^{-\mathrm{i}\boldsymbol{a}\cdot\boldsymbol{q}}\,\chi(a \le \lambda(\boldsymbol{q}) < b)\,d(\phi_{B'}, E_{\boldsymbol{p}}(\boldsymbol{q})\psi) \equiv \int e^{-\mathrm{i}\boldsymbol{a}\cdot\boldsymbol{q}}\,d\mu(\boldsymbol{q}), \quad (1.187)$$

where $E_{\boldsymbol{p}}(\boldsymbol{q})$ is the spectral family of $\boldsymbol{p}$. The support of the measure $d\mu(\boldsymbol{q})$ is contained in $\{\boldsymbol{q} \in \mathbb{R}^3 \mid a \le \lambda(\boldsymbol{q}) \le b\}$ which is compact. According to the Paley-Wiener-Schwartz theorem, it's Fourier transform $h(\boldsymbol{a})$ is an analytic function. Since $h(\boldsymbol{a}) = 0$ for $|\boldsymbol{a}| < d$, we have $h(\boldsymbol{a}) = 0$ for all $\boldsymbol{a}$. Choose a partition of the interval $[0, \infty)$ into subintervals $[\lambda_{k-1}, \lambda_k)$ of finite length. Then

$$(\phi, F(B')\,e^{-\mathrm{i}\boldsymbol{a}\cdot\boldsymbol{p}}\,\psi) = \big(\phi_{B'}, e^{-\mathrm{i}\boldsymbol{a}\cdot\boldsymbol{p}} \sum \chi(\lambda_{k-1} \le H < \lambda_k)\,\psi\big) = 0, \quad (1.188)$$

for all ϕ and $\boldsymbol{a}$. Hence we must have $F(B'-\boldsymbol{a})\,\psi = 0$ for all $\boldsymbol{a}$, which is only possible for $\psi = 0$. □

In the Hilbert space $\mathfrak{H} = \mathfrak{H}_{\mathrm{pos}}$ the assumptions of the theorem are easily verified for $F(B) = \chi(\boldsymbol{x}_{\mathrm{NW}} \in B)$ (the spectral measure of the Newton-Wigner operator) and $\lambda(\boldsymbol{p}) = (c^2\boldsymbol{p}^2 + m^2c^4)^{1/2}$. The generator of translations is the momentum operator $\boldsymbol{p} = -\mathrm{i}\nabla$, we have $e^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{a}}\,\boldsymbol{x}_{\mathrm{NW}}\,e^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{a}} = \boldsymbol{x}_{\mathrm{NW}} + \boldsymbol{a}$. Assumption i) is implied by (1.170), ii) by (1.173).

1.8.2 Violation of Einstein Causality

Let us discuss a special case of Theorem 1.6. Take $F(B)$ as the spectral measure of some position operator in $\mathfrak{H} = \mathfrak{H}_{\mathrm{pos}}$. As we have discussed in Sect. 1.7.3 there are states $\psi \in \mathfrak{H}$, $\|\psi\| = 1$, satisfying $\big(\psi, F(B)\psi\big) \equiv \|F(B)\psi\|^2 = 1$, because $F(B)$ is a projection. One calls these states "localized in B". Now, take a state ψ localized in a proper subset B_0 of $\mathbb{R}^3$. Let B be another subset located far away from B_0. If d is the distance between B_0 and B then we would expect that ψ is localized outside B at least for the time d/c (the time a light signal needs to get from B_0 to B). But the probability of finding the system in B at time t is just given by (1.180), if $\boldsymbol{H}$ is the Hamiltonian of the system. Since this probability is nonzero for some arbitrarily small t, we have to admit that the system has a (small) probability of getting from B_0 to B in an arbitrary short time, thereby propagating with a superluminal speed.

Of course we expect the effects of this "instantaneous spreading" to be immeasurably small in physically reasonable situations. Nevertheless, we cannot neglect it in a discussion of localization properties because according to our quantum mechanical interpretation the accuracy of measurements of one single observable is not limited *a priori*. We may conclude that the notion of localization as defined, e.g., in Sect. 1.7.3 is in contradiction to the principles of the theory of relativity.

1.8.3 Support Properties of Wavefunctions

If we restrict the operator $\chi(\boldsymbol{x} \in B)$ as in Sect. 1.7.1,

$$\tilde{\chi}(\boldsymbol{x} \in B) \equiv P_{\text{pos}}\, \chi(\boldsymbol{x} \in B)\, P_{\text{pos}} + P_{\text{neg}}\, \chi(\boldsymbol{x} \in B)\, P_{\text{neg}}, \tag{1.189}$$

then the result would not be a projection operator because $\tilde{\chi}(\boldsymbol{x} \in B)^2 \neq \tilde{\chi}(\boldsymbol{x} \in B)$. Consequently, $\tilde{\chi}(\boldsymbol{x} \in B)$ is not the spectral measure of any self-adjoint operator. We have

$$(\psi, \tilde{\chi}(\boldsymbol{x} \in B)\psi) = \int_B \{\|\psi_{\text{pos}}(\boldsymbol{x})\|^2 + \|\psi_{\text{neg}}(\boldsymbol{x})\|^2\}\, d^3\boldsymbol{x}, \tag{1.190}$$

which in general is different from $\int_B d^3\boldsymbol{x} \|\psi(\boldsymbol{x})\|^2$, unless $B = \mathbb{R}^3$. However,

$$(\psi_{\text{pos}}, \tilde{\chi}(\boldsymbol{x} \in B)\psi_{\text{pos}}) = \int_B \|\psi_{\text{pos}}(\boldsymbol{x})\|^2\, d^3\boldsymbol{x}, \tag{1.191}$$

and similar for ψ_{neg}. Therefore, also $\tilde{\chi}(\boldsymbol{x} \in B)$ satisfies the assumptions of the theorem.

Now, *assume* that $(\psi_{\text{pos}}, \tilde{\chi}(\boldsymbol{x} \in B)\psi_{\text{pos}}) = 1$ for some proper subset B of $\mathbb{R}^3$. Because of (1.191), ψ_{pos} vanishes almost everywhere outside of B_0. According to the Dirac equation the wavefunction ψ_{pos} spreads according to

$$\psi_{\text{pos}}(t, \boldsymbol{x}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} S(t, \boldsymbol{x} - \boldsymbol{y})\, \psi_{\text{pos}}(\boldsymbol{y})\, d^3\boldsymbol{y} \tag{1.192}$$

with finite speed, because the integral kernel S is zero for $|\boldsymbol{x} - \boldsymbol{y}| > c|t|$. This is clearly a contradiction to the infinite propagation speed required by Theorem 1.6.

Therefore it is impossible for a wavefunction with positive energy to be initially localized in a proper subset of $\mathbb{R}^3$. Any wavefunction with positive energy has to be spread over all of space for all times. Of course, a similar consideration is also valid for ψ_{neg}. Thus we have proven

Corollary 1.7. Let ψ be an arbitrary state in $\mathfrak{H}_{\text{pos}}$ (or $\mathfrak{H}_{\text{neg}}$). Then

$$\text{supp}(\psi) \equiv \text{closure of } \{\boldsymbol{x} \in \mathbb{R}^3 \mid \psi(\boldsymbol{x}) \neq 0\} = \mathbb{R}^3. \tag{1.193}$$

Part of this corollary can easily be shown directly. $P_{\text{pos}}\psi = \psi$ implies for the Fourier transform $\phi = \mathcal{F}\psi$ of any positive energy wavefunction a relation between upper and lower components, namely

$$\begin{pmatrix} \phi_3(\boldsymbol{p}) \\ \phi_4(\boldsymbol{p}) \end{pmatrix} = \frac{c\boldsymbol{\sigma} \cdot \boldsymbol{p}}{\sqrt{c^2p^2 + m^2c^4} + mc^2} \begin{pmatrix} \phi_1(\boldsymbol{p}) \\ \phi_2(\boldsymbol{p}) \end{pmatrix}. \tag{1.194}$$

Now if ψ had support in a compact subset B_0 of $\mathbb{R}^3$ then, according to the Paley-Wiener-Schwartz theorem $\phi_1, \ldots, \phi_4$ all had to be entire analytic functions in $\boldsymbol{p}$, which is impossible because of the square root in (1.194).

1.8.4 Localization and Positive Energies

We may summarize the results obtained so far as follows. If we choose $\mathfrak{H}_{\text{pos}}$ to be the Hilbert space of a free electron the observables have to be represented by operators which leave this Hilbert space invariant. Then there are essentially two possibilities:

a) We can retain the interpretation of $|\psi(\boldsymbol{x})|^2$ as a position probability density even after restriction to the positive energy subspace. But then the position is not a quantum mechanical observable in the usual sense. This is because by Corollary 1.7 there are no strictly localized states and consequently there is no self-adjoint operator in $\mathfrak{H}_{\text{pos}}$ whose spectral measure is related with the position probability. The probability of finding the particle in a set B is still a well defined concept, although there are no states for which this probability is 1 if $B \neq \mathbb{R}^3$.

b) On the other hand, we could insist on a quantum mechanical position observable (i.e., a self-adjoint operator which leaves $\mathfrak{H}_{\text{pos}}$ invariant). But then we have to face the violation of Einstein causality as predicted by Theorem 1.6.

Obviously, for particles with positive energy there is no possibility of having a relativistic notion of position, which is analogous to the nonrelativistic concept and satisfies the causality requirements of a relativistic theory.

Fortunately, to most of the mathematical results obtained below — as well as to practical measurements — it seems to be irrelevant which interpretation is preferred. For the purpose of this book we keep calling $|\psi(\boldsymbol{x})|^2$ a position probability density.

Difficulties with the strict localization of an electron are not quite unexpected. Restricting an electron to a finite region, which is necessary in order to prepare a localized state, would require an infinite potential barrier and thus a lot of energy so that pair production is likely to happen. But this effect cannot be described by the Dirac equation alone.

1.9 Approximate Localization

For most purposes in quantum mechanics the strict localization properties are irrelevant. It is often sufficient to specify an approximate localization region and to estimate the probability of finding the particle outside. The mathematical results of this section will be needed for Chapter 8.

1.9.1 The Non-Stationary Phase Method

The time evolution of a free particle with positive energy $\lambda(\boldsymbol{p}) = \sqrt{c^2p^2 + m^2c^4}$ can be written as

$$\psi(t,\boldsymbol{x}) = \frac{1}{(2\pi)^{3/2}} \int e^{\mathrm{i}(\boldsymbol{x}\cdot\boldsymbol{p} - \lambda(\boldsymbol{p})t)} \big(\mathcal{F}\psi\big)(\boldsymbol{p})\, d^3p$$

$$\equiv \frac{1}{(2\pi)^{3/2}} \int e^{\mathrm{i}\omega\phi(\boldsymbol{p})} \big(\mathcal{F}\psi\big)(\boldsymbol{p})\, d^3p, \tag{1.195}$$

where we have introduced

$$\omega = |\boldsymbol{x}| + c|t|, \qquad \phi(\boldsymbol{p}) = \omega^{-1}\big(\boldsymbol{x}\cdot\boldsymbol{p} - \lambda(\boldsymbol{p})\, t\big). \tag{1.196}$$

We want to estimate (1.195) for large values of $|\boldsymbol{x}|$ and/or $|t|$. Note that the estimate $|\phi(\boldsymbol{p})| \le 2\lambda(\boldsymbol{p})/c$ is independent of ω. If ω is very large, small variations of $\boldsymbol{p}$ will eventually cause the exponential function $\exp(\mathrm{i}\omega\phi(\boldsymbol{p}))$ to oscillate very rapidly, so that due to frequent cancellations there is only a small contribution to the integral. Only in the neighborhood of points with $\nabla\phi(\boldsymbol{p}) = 0$ ("points of stationary phase") the function ϕ changes slowly with $\boldsymbol{p}$ and hence there are no oscillations. For large ω, the main contributions to the integral come from these points. If we want the integral to decay with increasing ω, we have to exclude these points by requiring that $\nabla\phi \neq 0$ on $\operatorname{supp}\phi$. The following theorem makes these ideas precise.

Theorem 1.8. Let K be a compact subset of $\mathbb{R}^n$, and $\phi : \mathbb{R}^n \to \mathbb{R}$ be $k+1$ times differentiable on a neighborhood of K, with $|\nabla\phi| \ge \epsilon > 0$ on K. Let $\hat{\psi}$ be k times differentiable with $\operatorname{supp}\hat{\psi} \subset K$. Then there exists a constant C, depending on r, ϕ and $\hat{\psi}$, such that for arbitrary $\omega \in \mathbb{R}$

$$\Big|\int_K e^{\mathrm{i}\omega\phi(\boldsymbol{p})}\, \hat{\psi}(\boldsymbol{p})\, d^3p\Big| \le C(1+|\omega|)^{-r}, \quad \text{all } r \le k. \tag{1.197}$$

Proof. By partial integration we find

$$\int e^{\mathrm{i}\omega\phi(\boldsymbol{p})}\, \hat{\psi}(\boldsymbol{p})\, d^3p = \frac{1}{\mathrm{i}\omega} \int \big(\nabla e^{\mathrm{i}\omega\phi(\boldsymbol{p})}\big) \cdot \frac{\nabla\phi(\boldsymbol{p})}{|\nabla\phi(\boldsymbol{p})|^2}\, \hat{\psi}(\boldsymbol{p})\, d^3p$$

$$= -\frac{1}{\mathrm{i}\omega} \int e^{\mathrm{i}\omega\phi(\boldsymbol{p})} \big(\mathcal{D}\hat{\psi}\big)(\boldsymbol{p})\, d^3p, \tag{1.198}$$

where $\mathcal{D}\hat{\psi} \equiv \nabla\cdot\big(\hat{\psi}\nabla\phi/|\nabla\phi|^2\big)$. Repeating this procedure gives

$$\Big(-\frac{1}{\mathrm{i}\omega}\Big)^r \int e^{\mathrm{i}\omega\phi(\boldsymbol{p})} \big(\mathcal{D}^r\hat{\psi}\big)(\boldsymbol{p})\, d^3p. \tag{1.199}$$

The function $\mathcal{D}^r\hat{\psi}$ is a sum of products of the factors

$$|\nabla\phi|^{-2}, \quad D^\alpha\phi, \quad D^\beta\hat{\psi}, \quad \text{where } |\alpha| < r+1,\ |\beta| < r. \tag{1.200}$$

We use the multiindex notation, $\alpha = (\alpha_1, \ldots, \alpha_n)$, where α_i are nonnegative integers, $|\alpha| = \sum_i \alpha_i$, and

$$D^\alpha = \frac{\partial^{|\alpha|}}{\partial_1^{\alpha_1} \cdots \partial_n^{\alpha_n}}. \tag{1.201}$$

Since ϕ and $\hat{\psi}$ are continuously differentiable, their derivatives are bounded uniformly on K. By assumption, $|\nabla\phi| \geq \epsilon$ on K, hence any finite product of the expressions (1.200) is bounded on K. We conclude that (1.199) is bounded by const.$|\omega|^{-r}$. Since the integral is regular for $\omega = 0$, the result follows. □

1.9.2 Propagation into the Classically Forbidden Region

With the help of the preceding theorem we can control the propagation of the wavefunction $\psi(\boldsymbol{x}, t)$. For our phase function ϕ defined in Eq. (1.196) the stationary points are given by

$$\boldsymbol{x} - \boldsymbol{u}(\boldsymbol{p})\, t = 0, \qquad \text{where} \quad \boldsymbol{u}(\boldsymbol{p}) = \frac{c^2 \boldsymbol{p}}{\lambda(\boldsymbol{p})}. \tag{1.202}$$

Note that $\boldsymbol{u}(\boldsymbol{p})$ is just the velocity of a classical relativistic particle with energy $\lambda(\boldsymbol{p})$. For a particle with negative energy everything is analogous, only $\boldsymbol{u}(\boldsymbol{p}) = -c^2\boldsymbol{p}/\lambda(\boldsymbol{p})$. Let K be a subset of $\mathbb{R}^3$. The set

$$\{\, \boldsymbol{x} \in \mathbb{R}^3 \mid \boldsymbol{x}/t = \boldsymbol{u}(\boldsymbol{p}) \text{ for some } \boldsymbol{p} \in K \,\} \tag{1.203}$$

describes the region in which a particle is localized according to the classical relativistic kinematics, provided its velocity is in the set

$$\{\, \boldsymbol{u} \in \mathbb{R}^3 \mid \boldsymbol{u} = \boldsymbol{u}(\boldsymbol{p}) \text{ with } \boldsymbol{p} \in K \,\}. \tag{1.204}$$

Therefore, the set (1.203) is called the "*classically allowed region*" for particles with momenta in K. In the classically *forbidden* region the condition $\boldsymbol{x}/t \neq \boldsymbol{u}(\boldsymbol{p})$ for all $\boldsymbol{p} \in \operatorname{supp} \mathcal{F}\psi$ avoids the points of stationary phase for (1.195). Theorem 1.8 states that the wave function decays fast in this region:

Corollary 1.9. Let ψ be a wavefunction with Fourier transform $\hat{\psi} \equiv \mathcal{F}\psi \in \mathcal{C}_0^\infty$ satisfying

$$\operatorname{supp} \hat{\psi} \subset \{\, \boldsymbol{p} \in \mathbb{R}^3 \mid 0 < u_0 \leq |\boldsymbol{u}(\boldsymbol{p})| \,\}. \tag{1.205}$$

Then for each $N > 0$ there is a constant C_N depending only on ψ such that

$$\| \, \chi(|\boldsymbol{x}| \leq u_0|t|/2)\, e^{-\mathrm{i}H_0 t}\, \psi \, \| \leq C_N\, (1 + |t|)^{-N}. \tag{1.206}$$

Proof. The situation here is different from Theorem 1.8 because the phase function ϕ depends also on ω, cf. Eq. (1.196). But for $\boldsymbol{x}$ in the ball $|\boldsymbol{x}| \leq u_0|t|/2$ we have

$$c|t| \leq \omega \leq (c + u_0/2)|t|, \tag{1.207}$$

and hence for $\boldsymbol{p}$ in $\operatorname{supp} \hat{\psi}$,

$$|(\nabla\phi)(\boldsymbol{p})| \geq \frac{|\boldsymbol{u}(\boldsymbol{p})t| - |\boldsymbol{x}|}{|\boldsymbol{x}| + c|t|} \geq \frac{u_0}{u_0 + 2c} > 0. \tag{1.208}$$

Moreover, $\phi(\boldsymbol{p})$ is infinitely differentiable on $\operatorname{supp} \hat{\psi}$ and all derivatives are bounded uniformly in $|t|$. Hence the proof of Theorem 1.8 applies to this situation as well. For $|\boldsymbol{x}| \leq u_0 t/2$ and each r we can estimate $\psi(t, \boldsymbol{x})$ by

$$\frac{\text{const}}{(1 + |\omega|)^r} \leq \frac{\text{const}'}{(1 + |t|)^r} \,. \tag{1.209}$$

Finally, the estimate

$$\begin{aligned} &\| \chi(|\boldsymbol{x}| \leq u_0|t|/2)\, e^{-\mathrm{i}H_0 t}\, \psi \|^2 \\ &\quad = \int_{|\boldsymbol{x}| \leq u_0|t|/2} |\psi(t, \boldsymbol{x})|^2 \, d^3\boldsymbol{x} \leq \frac{\hat{C}_N \, |t|^3}{(1 + |t|)^{2r}} \end{aligned} \tag{1.210}$$

proves the corollary. □

Remark. If a particle is in a state with minimum velocity larger than u_0, then after some time it will move away from the origin and the points $|\boldsymbol{x}| \leq u_0|t|/2$ will belong to the classically forbidden region. According to Corollary 1.9, the probability of finding the particle in this region decays rapidly in time. This result is very useful in scattering theory, cf. Chapter 8.

Appendix

1.A Alternative Representations of Dirac Matrices

Most calculations with Dirac matrices can be done without referring to a particular representation. For some considerations, however, an explicit form is useful. Here we list the most prominent representations. By $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ we denote the three Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{1.211}$$

which satisfy the properties

$$\{\sigma_i, \sigma_k\} = 2\delta_{ik}, \quad [\sigma_i, \sigma_k] = 2\mathrm{i} \sum_{m=1}^{3} \epsilon_{ikm}\sigma_m. \tag{1.212}$$

The following matrices are written in 2×2-block form, each entry is itself a 2×2-matrix.

1. Standard (or Dirac-Pauli) representation.

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \gamma_5 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{1.213}$$

2. Supersymmetric representation.

$$\beta_{\mathrm{s}} = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \boldsymbol{\alpha}_{\mathrm{s}} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad (\gamma_5)_{\mathrm{s}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{1.214}$$

This representation is related to the standard representation via the unitary matrix

$$T_{\mathrm{s}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \mathrm{i} \\ \mathrm{i} & 1 \end{pmatrix}, \tag{1.215}$$

i.e., $\beta_{\mathrm{s}} = T_{\mathrm{s}} \beta T_{\mathrm{s}}^{-1}$, etc.

3. Weyl (or spinor) representation.

$$\beta_{\mathrm{w}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\alpha}_{\mathrm{w}} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & -\boldsymbol{\sigma} \end{pmatrix}, \quad (\gamma_5)_{\mathrm{w}} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{1.216}$$

and the matrix giving the relation to the standard representation is

$$T_{\mathrm{w}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{1.217}$$

4. Majorana representation.

$$\beta_{\mathrm{m}} = \begin{pmatrix} 0 & \mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix}, \quad (\alpha_{\mathrm{m}})_{1,3} = \begin{pmatrix} \sigma_{1,3} & 0 \\ 0 & -\sigma_{1,3} \end{pmatrix}, \tag{1.218}$$

$$(\alpha_{\mathrm{m}})_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (\gamma_5)_{\mathrm{m}} = \begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix}. \tag{1.219}$$

Again, the Majorana representation is related to the standard representation by a unitary similarity transformation with

$$T_{\mathrm{m}} = \begin{pmatrix} 1 + \mathrm{i}\sigma_2 & 1 - \mathrm{i}\sigma_2 \\ -\mathrm{i} + \sigma_2 & \mathrm{i} + \sigma_2 \end{pmatrix}. \tag{1.220}$$

Sometimes also the representation with β_{m} replaced by

$$\tilde{\beta}_{\mathrm{m}} = \begin{pmatrix} \sigma_2 & 0 \\ 0 & \sigma_2 \end{pmatrix} \tag{1.221}$$

is referred to as the Majorana representation, corresponding to Majorana's original choice. In any case, the Majorana representation is characterized by the fact that the α-matrices are real, while $\overline{\beta} = -\beta$. Hence, in this representation, the charge conjugation C can simply be chosen as complex conjugation (cf. Sect. 1.4.6).

1.B Basic Properties of Dirac Matrices

$$\{\alpha_i, \alpha_k\} = 2\delta_{ik}, \quad \{\alpha_i, \beta\} = 0, \quad \beta^2 = 1, \tag{1.222}$$

$$[\alpha_i, \alpha_k] = 2(\alpha_i\alpha_k - \delta_{ik}) = 4\mathrm{i}\textstyle\sum_m \epsilon_{ikm} S_m, \tag{1.223}$$

$$S_i = -\tfrac{\mathrm{i}}{4}[\alpha_k, \alpha_m] = -\tfrac{\mathrm{i}}{2}\alpha_k\alpha_m = -2\mathrm{i}S_kS_m, \tag{1.224}$$

where (i, k, m) is a cyclic permutation of $(1, 2, 3)$,

$$[S_i, S_k] = \mathrm{i}\textstyle\sum_m \epsilon_{ikm} S_m, \quad \{S_i, S_k\} = \tfrac{1}{2}\delta_{ik}, \tag{1.225}$$

$$\alpha_i\alpha_k = \delta_{ik} + 2\mathrm{i}\epsilon_{ikm}S_m = 4S_iS_k, \tag{1.226}$$

$$\boldsymbol{S} \wedge \boldsymbol{A} = \frac{\mathrm{i}}{2}\big(\boldsymbol{A} - (\boldsymbol{\alpha}\cdot\boldsymbol{A})\boldsymbol{\alpha}\big), \tag{1.227}$$

$$(\boldsymbol{\alpha}\cdot\boldsymbol{A})(\boldsymbol{\alpha}\cdot\boldsymbol{B}) = \boldsymbol{A}\cdot\boldsymbol{B} + 2\mathrm{i}\boldsymbol{S}\cdot(\boldsymbol{A}\wedge\boldsymbol{B}) \quad \text{for any vectors } \boldsymbol{A}, \boldsymbol{B}, \tag{1.228}$$

$$-\mathrm{i}\alpha_1\alpha_2\alpha_3 \equiv \gamma_5, \quad (\gamma_5)^2 = 1, \tag{1.229}$$

$$\{\gamma_5, \beta\} = 0, \quad [\gamma_5, \boldsymbol{\alpha}] = 0, \quad \gamma_5\boldsymbol{\alpha} = 2\boldsymbol{S}. \tag{1.230}$$

1.C Commutators with H_0

We denote

$$\boldsymbol{S} \equiv \frac{\mathrm{i}}{4}\boldsymbol{\alpha}\wedge\boldsymbol{\alpha}, \quad \boldsymbol{L} \equiv \boldsymbol{x}\wedge\boldsymbol{p}, \quad \boldsymbol{J} \equiv \boldsymbol{L} + \boldsymbol{S}, \tag{1.231}$$

$$K \equiv \beta(2\boldsymbol{S}\cdot\boldsymbol{L} + 1), \quad B_0 \equiv \frac{2\mathrm{i}}{mc}K\boldsymbol{S}\cdot\boldsymbol{p} = \frac{1}{mc}\beta\boldsymbol{S}\cdot(\boldsymbol{p}\wedge\boldsymbol{L} - \boldsymbol{L}\wedge\boldsymbol{p}), \tag{1.232}$$

$$\boldsymbol{F} \equiv c\,\boldsymbol{\alpha} - c^2\boldsymbol{p}H_0^{-1}, \quad G \equiv \beta - mc^2H_0^{-1}, \tag{1.233}$$

$$\boldsymbol{N} \equiv \frac{1}{2}(H_0\boldsymbol{x} + \boldsymbol{x}H_0) = H_0\boldsymbol{x} + \frac{\mathrm{i}c}{2}\boldsymbol{\alpha} = \boldsymbol{x}H_0 - \frac{\mathrm{i}c}{2}\boldsymbol{\alpha}, \tag{1.234}$$

$$A \equiv \frac{1}{2}\left(H_0^{-1}\boldsymbol{p}\cdot\boldsymbol{x} + \boldsymbol{x}\cdot\boldsymbol{p}H_0^{-1}\right). \tag{1.235}$$

The following formal relations hold on a suitable dense domain, e.g., on $\mathcal{C}_0^\infty(\mathbb{R}^3)^4$.

$$\mathrm{i}[H_0, \boldsymbol{p}] = \mathrm{i}[H_0, \boldsymbol{J}] = \boldsymbol{0}, \quad \mathrm{i}[H_0, K] = \mathrm{i}[H_0, B_0] = \mathrm{i}[H_0, \boldsymbol{S}\cdot\boldsymbol{p}] = 0, \tag{1.236}$$

$$\mathrm{i}[H_0, \boldsymbol{\alpha}] = \mathrm{i}[H_0, \boldsymbol{F}] = 2\mathrm{i}H_0\boldsymbol{F}, \quad \mathrm{i}[H_0, \beta] = \mathrm{i}[H_0, G] = 2\mathrm{i}H_0G, \tag{1.237}$$

$$\mathrm{i}[H_0, \alpha_j\alpha_k] = 2c(\alpha_kp_j - \alpha_jp_k), \tag{1.238}$$

$$\mathrm{i}[H_0, \boldsymbol{L}] = -\mathrm{i}[H_0, \boldsymbol{S}] = \frac{1}{2\mathrm{i}H_0}\boldsymbol{F}\wedge\boldsymbol{p}, \tag{1.239}$$

$$\mathrm{i}[H_0, \boldsymbol{x}] = c\,\boldsymbol{\alpha}, \quad \mathrm{i}[H_0, c\,\boldsymbol{\alpha}\cdot\boldsymbol{x}] = 3c^2 + 2\mathrm{i}H_0\boldsymbol{F}\cdot\boldsymbol{x}, \quad \mathrm{i}[H_0, x^2] = 2c\,\boldsymbol{\alpha}\cdot\boldsymbol{x}, \tag{1.240}$$

$$\mathrm{i}[H_0, \boldsymbol{N}] = \tfrac{1}{2}(H_0\boldsymbol{\alpha} + \boldsymbol{\alpha}H_0) = c^2\boldsymbol{p}, \tag{1.241}$$

$$\mathrm{i}[H_0, A] = \tfrac{c}{2}\left(H_0^{-1}\boldsymbol{\alpha}\cdot\boldsymbol{p} + \boldsymbol{\alpha}\cdot\boldsymbol{p}H_0^{-1}\right) = c^2p^2H_0^{-2}. \tag{1.242}$$

1.D Distributions Associated with the Evolution Kernel

With $\lambda(p) = \sqrt{p^2 + m^2}$, $m > 0$, we define

$$\triangle_{\pm}(t, \boldsymbol{x}) = \mp \frac{\mathrm{i}}{(2\pi)^3} \int e^{\mathrm{i}p\cdot\boldsymbol{x}} \frac{e^{\mp \mathrm{i}\lambda(p)t}}{2\lambda(p)} d^3p, \tag{1.243}$$

$$\triangle(t, \boldsymbol{x}) = \triangle_+(t, \boldsymbol{x}) + \triangle_-(t, \boldsymbol{x}) = -\frac{1}{(2\pi)^3} \int e^{\mathrm{i}p\cdot\boldsymbol{x}} \frac{\sin\big(\lambda(p)t\big)}{\lambda(p)} d^3p, \tag{1.244}$$

where the integrals are Fourier transforms of distributions. Furthermore we define

$$\triangle_{\mathrm{ret}}(t, \boldsymbol{x}) = \theta(t)\, \triangle(t, \boldsymbol{x}), \tag{1.245}$$

$$\triangle_{\mathrm{av}}(t, \boldsymbol{x}) = -\theta(-t)\, \triangle(t, \boldsymbol{x}), \tag{1.246}$$

$$\triangle_{\mathrm{f}}(t, \boldsymbol{x}) = \theta(t)\, \triangle_+(t, \boldsymbol{x}) - \theta(-t)\, \triangle_-(t, \boldsymbol{x}), \tag{1.247}$$

$$\triangle_{\mathrm{f}^*}(t, \boldsymbol{x}) = \theta(t)\, \triangle_-(t, \boldsymbol{x}) - \theta(-t)\, \triangle_+(t, \boldsymbol{x}). \tag{1.248}$$

The tempered distributions $\triangle_k$, where k = ret, av, f, or f*, are fundamental solutions of the Klein-Gordon equation,

$$\left(-\frac{\partial^2}{\partial t^2} + \triangle - m^2\right) \triangle_k(t, \boldsymbol{x}) = \delta(t)\, \delta(\boldsymbol{x}). \tag{1.249}$$

For a distribution $\triangle(t, \boldsymbol{x})$ we define

$$\tilde{\triangle}(E, \boldsymbol{p}) = \int e^{\mathrm{i}(Et - \boldsymbol{p}\cdot\boldsymbol{x})}\, \triangle(t, \boldsymbol{x})\, d^3x\, dt. \tag{1.250}$$

Then

$$\tilde{\triangle}_{\pm}(E, \boldsymbol{p}) = \mp 2\pi\mathrm{i}\, \theta(\pm E)\, \delta(p^2 - m^2), \tag{1.251}$$

$$\tilde{\triangle}(E, \boldsymbol{p}) = \mp 2\pi\mathrm{i}\, \mathrm{sgn}(E)\, \delta(p^2 - m^2), \tag{1.252}$$

$$\tilde{\triangle}_{\substack{\mathrm{ret} \\ \mathrm{av}}}(E, \boldsymbol{p}) = -\frac{1}{\lambda(p)^2 - (E \pm \mathrm{i}0)^2}, \tag{1.253}$$

$$\tilde{\triangle}_{\substack{\mathrm{f} \\ \mathrm{f}^*}}(E, \boldsymbol{p}) = \frac{1}{p^2 - m^2 \pm \mathrm{i}0}. \tag{1.254}$$

Fundamental solutions of the free Dirac equation are obtained from the $\triangle$'s by differentiation,

$$S_k(t, \boldsymbol{x}) = \mathrm{i}\Big(\mathrm{i}\frac{\partial}{\partial t} - \mathrm{i}\boldsymbol{\alpha}\cdot\nabla + \beta m\Big) \triangle_k(t, \boldsymbol{x}), \quad k = \mathrm{ret}, \mathrm{av}, \mathrm{f}, \mathrm{f}^*, \tag{1.255}$$

$$\Big(\mathrm{i}\frac{\partial}{\partial t} + \mathrm{i}\boldsymbol{\alpha}\cdot\nabla - \beta m\Big) S_k(t, \boldsymbol{x}) = \mathrm{i}\delta(t)\delta(\boldsymbol{x}). \tag{1.256}$$

The distribution

$$S_{\mathrm{F}}(t, \boldsymbol{x}) \equiv -\mathrm{i}S_{\mathrm{f}}(t, \boldsymbol{x})\beta \tag{1.257}$$

is usually called Feynman propagator (see, e.g., the book of Bjorken and Drell [BD 64]. Feynman [Fe 61] uses the notation $I_+(t,\boldsymbol{x}) \equiv -\triangle_{\mathrm{f}}(t,\boldsymbol{x})$, and $K_+(2,1) = S_{\mathrm{f}}(t_2-t_1,\boldsymbol{x}_2-\boldsymbol{x}_1)\beta)$. As we have seen in Sect. 1.5 the Schrödinger picture evolution operator is given by the integral kernel

$$S(t,\boldsymbol{x}) = \mathrm{i}\Big(\mathrm{i}\frac{\partial}{\partial t} - \mathrm{i}\boldsymbol{\alpha}\cdot\nabla + \beta m\Big)\triangle(t,\boldsymbol{x}) = S_+(t,\boldsymbol{x}) + S_-(t,\boldsymbol{x}). \tag{1.258}$$

The distribution $S_{\mathrm{f}}(t,\boldsymbol{x})$ satisfies

$$S_{\mathrm{f}}(t,\boldsymbol{x}) = \theta(t)\,S_+(t,\boldsymbol{x}) - \theta(-t)\,S_-(t,\boldsymbol{x}), \quad \text{for } t \neq 0, \tag{1.259}$$

from which we see that it is just the integral kernel of the operator

$$\theta(t)\,e^{-\mathrm{i}H_0 t}\,P_{\mathrm{pos}} - \theta(-t)\,e^{-\mathrm{i}H_0 t}\,P_{\mathrm{neg}}. \tag{1.260}$$

1.E Explicit Form of the Resolvent Kernel

The resolvent $(H_0 - z)^{-1}$ of the free Dirac operator H_0 is defined for all $z \in \mathbb{C} \setminus \sigma(H_0)$,

$$\big((H_0 - z)^{-1}\,\psi\big)(\boldsymbol{x}) = \int_{\mathbb{R}^3} K(\boldsymbol{x}-\boldsymbol{y},z)\,\psi(\boldsymbol{y})\,d^3y. \tag{1.261}$$

The integral kernel K can be obtained from the well known resolvent kernel of the Laplace operator $p^2 = -\Delta$ because

$$\begin{aligned}(H_0 - z)^{-1} &= (H_0 + z)(H_0^2 - z^2)^{-1} \\ &= \frac{1}{c^2}\left(c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2 + z\right)\left(p^2 - \left[\frac{z^2}{c^2} - m^2c^2\right]\right)^{-1}.\end{aligned} \tag{1.262}$$

We find

$$\begin{aligned}K(\boldsymbol{x},z) &= \frac{1}{c^2}\left(-\mathrm{i}c\boldsymbol{\alpha}\cdot\nabla + \beta mc^2 + z\right)\frac{1}{4\pi}\,\frac{e^{\mathrm{i}k(z)|\boldsymbol{x}|}}{|\boldsymbol{x}|} \\ &= \left(\mathrm{i}c\,\frac{\boldsymbol{\alpha}\cdot\boldsymbol{x}}{|\boldsymbol{x}|^2} + ck(z)\,\frac{\boldsymbol{\alpha}\cdot\boldsymbol{x}}{|\boldsymbol{x}|} + \beta mc^2 + z\right)\frac{e^{\mathrm{i}k(z)|\boldsymbol{x}|}}{4\pi c^2|\boldsymbol{x}|},\end{aligned} \tag{1.263}$$

where $k(z) = \sqrt{z^2/c^2 - m^2c^2}$, and the branch of the square root has been chosen such that $\operatorname{Im} k(z) > 0$.

1.F Free Plane-Wave Solutions

For $\boldsymbol{p} \in \mathbb{R}^3$ with $p = (p_1^2 + p_2^2 + p_3^2)^{1/2} \neq 0$ and $p \neq p_3$ we define

$$h_+(\boldsymbol{p}) = \frac{1}{\sqrt{2p(p-p_3)}}\begin{pmatrix} p_1 - \mathrm{i}p_2 \\ p - p_3 \end{pmatrix}, \tag{1.264}$$

$$h_-(\boldsymbol{p}) = \frac{1}{\sqrt{2p(p-p_3)}} \begin{pmatrix} p_3 - p \\ p_1 + \mathrm{i}p_2 \end{pmatrix}, \tag{1.264}$$

For $p = p_3$ we simply set $h_+(p) = \binom{1}{0}$, $h_-(p) = \binom{0}{1}$. Then we have

$$\boldsymbol{\sigma} \cdot \boldsymbol{p}\, h_\pm(\boldsymbol{p}) = \pm p\, h_\pm(\boldsymbol{p}). \tag{1.265}$$

It is obvious from Sect. 1.4.1 that (with $a_\pm$ as in (1.44))

$$\omega_{\mathrm{pos},\pm}(\boldsymbol{p}) \equiv \mathrm{u}(\boldsymbol{p})^{-1} \begin{pmatrix} h_\pm(\boldsymbol{p}) \\ \binom{0}{0} \end{pmatrix} = \begin{pmatrix} a_+(p)\, h_\pm(\boldsymbol{p}) \\ \pm a_-(p)\, h_\pm(\boldsymbol{p}) \end{pmatrix} \quad \text{and} \tag{1.266}$$

$$\omega_{\mathrm{neg},\pm}(\boldsymbol{p}) \equiv \mathrm{u}(\boldsymbol{p})^{-1} \begin{pmatrix} \binom{0}{0} \\ h_\pm(\boldsymbol{p}) \end{pmatrix} = \begin{pmatrix} \mp a_-(p)\, h_\pm(\boldsymbol{p}) \\ a_+(p)\, h_\pm(\boldsymbol{p}) \end{pmatrix} \tag{1.267}$$

are eigenvectors of the matrix $\mathrm{h}(\boldsymbol{p})$ corresponding to the eigenvalues $\pm\lambda(p)$, where $\lambda(p) = (c^2p^2 + m^2c^4)^{1/2}$. Hence

$$\omega_{\substack{\mathrm{pos} \\ \mathrm{neg}},\pm}(\boldsymbol{p}, \boldsymbol{x}) \equiv \omega_{\substack{\mathrm{pos} \\ \mathrm{neg}},\pm}(\boldsymbol{p})\, e^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}} \tag{1.268}$$

are generalized (i.e., not square-integrable) eigenfunctions of the free Dirac operator H_0 with positive or negative energy $\pm\lambda(p)$. Moreover,

$$\omega_{\mathrm{pos},\pm}(\boldsymbol{p})\, e^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x} - \mathrm{i}\lambda(p)t}, \quad \omega_{\mathrm{neg},\pm}(\boldsymbol{p})\, e^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x} + \mathrm{i}\lambda(p)t}, \tag{1.269}$$

are "*plane-wave solutions*" of the Dirac equation.

The functions ω are simultaneously eigenfunctions of the "*helicity operator*" $\boldsymbol{S}\cdot\boldsymbol{p}/p$ which projects the spin into the direction of the momentum. The helicity is conserved for free particles, because $\boldsymbol{S} \cdot \boldsymbol{p}$ commutes with H_0. Using (1.265) we find

$$\frac{\boldsymbol{S}\cdot\boldsymbol{p}}{p}\, \omega_{\substack{\mathrm{pos} \\ \mathrm{neg}},+}(\boldsymbol{p}) = \tfrac{1}{2}\, \omega_{\substack{\mathrm{pos} \\ \mathrm{neg}},+}(\boldsymbol{p}), \tag{1.270}$$

$$\frac{\boldsymbol{S}\cdot\boldsymbol{p}}{p}\, \omega_{\substack{\mathrm{pos} \\ \mathrm{neg}},-}(\boldsymbol{p}) = -\tfrac{1}{2}\, \omega_{\substack{\mathrm{pos} \\ \mathrm{neg}},-}(\boldsymbol{p}), \tag{1.271}$$

Denoting the projections onto positive/negative helicity by $P_\pm$, i.e.,

$$P_\pm = \frac{1}{2}(\mathbf{1} \pm \frac{2\boldsymbol{S}\cdot\boldsymbol{p}}{p}) \tag{1.272}$$

we can write the Hilbert space as an orthogonal direct sum of four subspaces

$$\mathfrak{H}_{\substack{\mathrm{pos} \\ \mathrm{neg}},\pm} = P_{\substack{\mathrm{pos} \\ \mathrm{neg}}}\, P_\pm\, \mathfrak{H}. \tag{1.273}$$

It is clear from (1.49) that the plane-wave solutions can be used to form square-integrable wavepackets. For example, with $f \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$,

$$\psi(t, \boldsymbol{x}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x} - \mathrm{i}\lambda(p)t}\, \omega_{\mathrm{pos},-}(\boldsymbol{p})\, f(\boldsymbol{p})\, d^3p \;\in\; \mathfrak{H}_{\mathrm{pos},-} \tag{1.274}$$

is a square integrable solution of the free Dirac equation with positive energy and negative helicity.

If we let the mass m tend to zero, then $a_{\pm}(p) \to 1/\sqrt{2}$, and the ω's become eigenvectors of the "*chirality matrix*" $\gamma_5 \equiv -\mathrm{i}\alpha_1\alpha_2\alpha_3$ which for $m = 0$ commutes with the free Dirac operator

$$H_0(m{=}0) = c\boldsymbol{\alpha}\cdot\boldsymbol{p} = 2c\gamma_5\boldsymbol{S}\cdot\boldsymbol{p}, \qquad [H_0(m{=}0), \gamma_5] = 0. \tag{1.275}$$

$$\gamma_5\omega_{\mathbf{pos},\pm} = \pm\omega_{\mathbf{pos},\pm}, \qquad \gamma_5\omega_{\mathbf{neg},\pm} = \mp\omega_{\mathbf{neg},\pm}, \qquad (m = 0). \tag{1.276}$$

2 The Poincaré Group

In Chapter 1 the Dirac equation was defined in such a way that it automatically satisfies the energy-momentum relation as required by classical relativistic mechanics — at least in a particular inertial frame. According to the principles of relativity, different inertial frames are related by Poincaré transformations (Sect. 2.1). In this chapter we are going to prove that the Dirac equation — and the quantum theory developed in Chapter 1 — is invariant under Poincaré transformations. This is perhaps obscured by the fact that the position is represented by an operator, whereas time remains a parameter. After all, this is not quite in the spirit of the theory of relativity, where space and time coordinates are mixed up by Lorentz transformations.

A quantum mechanical theory is relativistically invariant if the Poincaré group has a representation by symmetry transformations. The pure states of a quantum system are uniquely described by the one-dimensional subspaces ("rays") of the Hilbert space. The set of all rays forms a projective space and symmetry transformations are to be defined in this space. Hence we are looking for a "projective representation" of the Poincaré group.

By the Wigner-Bargmann theorem any symmetry transformation in the projective space of states can be described as a unitary or antiunitary operator in the Hilbert space of the system. The connectedness of the proper Poincaré group implies that it has a projective unitary representation. Antiunitary operators can only appear in representations of the discrete Lorentz transformations (Sect. 2.2). Any unitary representation of a Lie group also defines a projective representation, but it is not true that a projective representation is always given by a unitary representation (problem of lifting representations). The analysis in Sect. 2.4 shows that under suitable assumptions (which we show to be fulfilled for the proper Poincaré group) the projective representations of a connected Lie group can be derived from the unitary representations of the universal covering group.

A representation of the Poincaré covering group is obtained as follows: On the basis of Chapter 1 it is easy to obtain a representation of the Lie algebra of the Poincaré group in the Hilbert space of a Dirac particle. The infinitesimal generators are simply given by the Dirac operator, the momentum and angular momentum operators and the center of energy operator (Sect. 1.3). Exponentiating this Lie algebra representation we obtain with the help of Nelson's theorem a unitary representation of the simply connected Poincaré covering group. It is interesting to note that in the Hilbert space of the Dirac electron we cannot obtain a unitary representation of the Poincaré group itself (Sect. 2.3). Nevertheless, the existence of a unitary representation of the Poincaré covering group provides us with the desired projective representation of the Poincaré group and is therefore sufficient to prove the relativistic invariance of the Dirac theory.

These results motivate a detailed investigation of the Poincaré covering group. We describe its 4-dimensional representations which are most important for the Dirac theory in Sect. 2.5. It turns out that 4 dimensions are indeed necessary for a linear representation of the parity transform. In this context the Dirac matrices arise in a natural way.

2.1 The Lorentz and Poincaré Groups

This is a preparatory section where we define the relativistic symmetry groups and describe some of their properties which are needed later.

2.1.1 The Minkowsky Space

An "event" is something that happens at a definite time at a definite place (e.g., the emission of a photon, the detection of a particle, etc.). Events in space-time are described with respect to an "inertial frame" by coordinates[1] $x = (x^0, \boldsymbol{x})^\top \in \mathbb{R}^4$, where $\boldsymbol{x} = (x^1, x^2, x^3)^\top$ are the space coordinates, and $x^0 = ct$ is the time coordinate of the event. The factor c denotes the velocity of light. It gives x^0 the dimension of a length. The principle of relativity states that all inertial frames are equivalent for the description of nature. The coordinate transformations $I \to I'$ between all possible inertial frames are called Poincaré transformations.

In the vector space $\mathbb{R}^4$ we define the "*Lorentz metric*"

$$\langle y, x\rangle = y^0x^0 - y^1x^1 - y^2x^2 - y^3x^3, \quad \text{all } x, y \in \mathbb{R}^4. \tag{2.1}$$

The bilinear form $\langle\cdot,\cdot\rangle$ is symmetric and nondegenerate[2], but not positive definite. With the 4×4 matrix

$$\mathrm{g} = (g_{\mu\nu}) = (g^{\mu\nu}) = \begin{pmatrix} 1 & 0^\top \\ 0 & -\mathbf{1}_3 \end{pmatrix} \tag{2.2}$$

(where 0 is the three-dimensional zero column vector) we can write (2.1) in the form

$$\langle y, x\rangle = y^\top \mathrm{g}\, x = \sum_{\mu,\nu=0}^{4} g_{\mu\nu}\, y^\mu x^\nu. \tag{2.3}$$

The vector space $\mathbb{R}^4$ endowed with the Lorentz metric is called "*Minkowsky space*".

Remark. With the help of the Lorentz metric we can associate a unique element y' of the dual space of $\mathbb{R}^4$ with a given vector $y \in \mathbb{R}^4$ by writing $y'(x) = \langle y, x\rangle$, for all x. The components of the linear form y' with respect to the canonical basis in the dual space are $(y^0, -y^1, -y^2, -y^3)$. Usually one denotes by y^μ the components of the vector y in the Minkowsky space and by y_μ the components of the linear form y' in the dual space. By the summation convention one automatically takes the sum over an index which appears twice in an expression, once as a lower index and once as an upper index, e.g.,

$$y_\mu = g_{\mu\nu}y^\nu, \qquad \langle y, x\rangle = y^\mu x_\mu = y_\mu x^\mu. \tag{2.4}$$

[1] "$\top$" denotes the transposed of a vector or a matrix. We would like to consider x a column vector.

[2] i.e., for all $y \neq 0$ there exists an x such that $\langle y, x\rangle \neq 0$.

2.1.2 Definition of the Lorentz Group

Definition 2.1. *A (homogeneous) Lorentz transformation of* $\mathbb{R}^4$ *is a linear map* $\Lambda : \mathbb{R}^4 \to \mathbb{R}^4$ *with*

$$\langle \Lambda y, \Lambda x \rangle = \langle y, x \rangle \quad \textit{for all } x,\ y \in \mathbb{R}^4. \tag{2.5}$$

The elements of the matrix of Λ *are denoted by* $\Lambda^\mu{}_\nu$.

Eq. (2.5) is obviously equivalent to

$$\Lambda^\top \mathrm{g} \Lambda = \mathrm{g}, \quad \text{or} \quad \Lambda^\mu{}_\rho\, g_{\mu\nu}\, \Lambda^\nu{}_\tau = g_{\rho\tau}, \tag{2.6}$$

which consists of ten independent quadratic equations for the components of Λ, e.g.,

$$(\Lambda^0{}_0)^2 - (\Lambda^1{}_0)^2 - (\Lambda^2{}_0)^2 - (\Lambda^3{}_0)^2 = 1. \tag{2.7}$$

This implies for all Lorentz transformations

$$\Lambda^0{}_0 \geq 1 \quad \text{or} \quad \Lambda^0{}_0 \leq -1. \tag{2.8}$$

The composition of two Lorentz transformations is again a Lorentz transformation. We find

$$1 = -\det \mathrm{g} = -\det \Lambda^\top \mathrm{g} \Lambda = -\det \Lambda^\top \det \mathrm{g} \det \Lambda = (\det \Lambda)^2 \tag{2.9}$$

and hence $\det \Lambda = \pm 1$ for any Lorentz transformation Λ. Therefore Λ is invertible and the set of all Lorentz transformations forms a group, the "*Lorentz group*", denoted by

$$\mathcal{L} = O(3,1). \tag{2.10}$$

Eq. (2.6) shows that only six of the 16 matrix elements of Λ can be chosen independently. Therefore, six real numbers suffice to characterize any Lorentz transformation uniquely. The set of all Lorentz transformations forms a six-dimensional manifold. By (2.6), $\mathcal{L}$ is a closed subgroup of the general linear group and hence is a Lie group. Eq. (2.8) shows that the group manifold is not connected.

2.1.3 Examples of Lorentz Transformations

Example 2.2. Rotations. Let $\mathbf{R} \in SO(3)$, the group of orthogonal real 3×3 matrices with determinant $+1$. Then

$$\Lambda = \begin{pmatrix} 1 & 0^\top \\ 0 & \mathbf{R} \end{pmatrix}, \tag{2.11}$$

is a Lorentz transformation. The rotation $\mathbf{R} = (R_{ik})$ can be most intuitively characterized by the rotation vector $\boldsymbol{\varphi} = \varphi \boldsymbol{n}$ where the parameter $\varphi \in [0, \pi)$

specifies the angle of the rotation, and the unit vector $\boldsymbol{n}$ gives the axis (the sense of rotation is determined by the right-hand rule),

$$R_{ik} = \delta_{ik}\cos\varphi + n_i n_k(1-\cos\varphi) - \sum_{m=1}^{3} \epsilon_{ikm} n_m \sin\varphi. \tag{2.12}$$

The set of all rotations is a subgroup of the Lorentz group. It is obviously isomorphic to $SO(3)$.

Remark. The group manifold of the Lie group $SO(3)$ is connected, but not simply connected[3]. This can be understood as follows. By the association of $\boldsymbol{\varphi}$ to each rotation the Lie group $SO(3)$ is mapped homeomorphically to the ball B with radius π in $\mathbb{R}^3$. However, we must identify antipodal points on the surface of B, because they correspond to the same rotation. Obviously, the resulting manifold is connected, but not simply connected, because there are closed paths which cannot be continuously shrunk to a point. Take, for example, any diameter joining two antipodal points.

The rotations around a fixed axis form a one-parameter subgroup. If we choose the rotation angle as the parameter, then the composition of two rotations is described by addition (mod 2π) of the angles.

Example 2.3. Boosts. With $\boldsymbol{v} \in \mathbb{R}^3$ (column vector), $v \equiv |\boldsymbol{v}| < 1$, define

$$\gamma(v) = \frac{1}{\sqrt{1-v^2}}. \tag{2.13}$$

Then one can check that

$$\Lambda = \begin{pmatrix} \gamma(v) & \gamma(v)\boldsymbol{v}^\top \\ \gamma(v)\boldsymbol{v} & 1_3 + \frac{\gamma(v)-1}{v^2}\boldsymbol{v}\boldsymbol{v}^\top \end{pmatrix} \tag{2.14}$$

is a Lorentz transformation. Here $(\boldsymbol{v}\boldsymbol{v}^\top)_{ik} = v_i v_k$.

Eq. (2.14) describes an "active" velocity transformation in the following sense. Consider a free classical particle which is at rest in some inertial frame. Thus for subsequent times t_1, t_2 it has the coordinates $(t_1, \boldsymbol{x})$, $(t_2, \boldsymbol{x})$. The boost Λ applied to these points gives $(s_1, \boldsymbol{y}_1)$, $(s_2, \boldsymbol{y}_2)$. Using (2.14) we find that the velocity of the particle after the transformation is just $\boldsymbol{v}$.

The subset of boosts is *not* a subgroup of $\mathcal{L}$, but it forms a submanifold of $\mathcal{L}$. Nevertheless, the set of boosts in a fixed direction $\boldsymbol{v}/|\boldsymbol{v}|$ forms a one-parameter subgroup. If we choose the parametrization

$$\boldsymbol{v} \equiv \tanh(\omega)\,\boldsymbol{v}/|\boldsymbol{v}|, \quad \omega \in [0, \infty), \tag{2.15}$$

then the composition of two boosts with parameters ω_1 and ω_2 gives a boost in the same direction with parameter $\omega_1 + \omega_2$. Similar to the rotation vector

[3] [Ch 46], Chapter II, Sects. IV and XI.

φ we may define a boost vector $\omega = \omega v/|v| \in \mathbb{R}^3$. Therefore the manifold of boosts is homeomorphic to $\mathbb{R}^3$ and hence simply connected and noncompact.

For $m > 0$ define the hyperboloid

$$M_{\text{pos}} \equiv \{ p \in \mathbb{R}^4 \mid \langle p, p \rangle = m^2,\ p^0 > 0 \}$$

$$= \{ (\sqrt{\boldsymbol{p}^2 + m^2}, \boldsymbol{p}) \in \mathbb{R}^4 \mid \boldsymbol{p} \in \mathbb{R}^3 \}. \tag{2.16}$$

which is usually called the "*mass shell*". It contains in particular the point $q = (m, 0, 0, 0)$. We associate to each $p \in M_{\text{pos}}$ a boost Λ_p which is uniquely determined by the condition $\Lambda_p q = p$. The transformation Λ_p is given by (2.14) where v is uniquely determined by p,

$$v = \frac{\boldsymbol{p}}{\sqrt{\boldsymbol{p}^2 + m^2}}, \qquad \boldsymbol{p} = m\gamma(v)v. \tag{2.17}$$

Hence the mass shell can be identified with the submanifold of boosts.

Example 2.4. Discrete transformations. The matrices

$$P = \begin{pmatrix} 1 & 0^\top \\ 0 & -1_3 \end{pmatrix}, \quad T = \begin{pmatrix} -1 & 0^\top \\ 0 & 1_3 \end{pmatrix}, \quad PT = -1_4. \tag{2.18}$$

define the "*discrete*" Lorentz transformations. P is called "*space inversion*" or "*parity transform*", T "*time reversal*". Together with the 4×4 unit matrix 1_4 the discrete transformations form a subgroup of the Lorentz group.

2.1.4 Basic Properties of the Lorentz Group

The Lorentz group $\mathcal{L} = O(3,1)$ is a Lie group with a six dimensional group manifold consisting of four connected components

$$\mathcal{L}_+^\uparrow \equiv \{ \Lambda \in \mathcal{L} \mid \Lambda^0{}_0 \geq 1, \det\Lambda = +1 \}, \tag{2.19}$$

$$\mathcal{L}_-^\uparrow \equiv \{ \Lambda \in \mathcal{L} \mid \Lambda^0{}_0 \geq 1, \det\Lambda = -1 \} = P\mathcal{L}_+^\uparrow, \tag{2.20}$$

$$\mathcal{L}_-^\downarrow \equiv \{ \Lambda \in \mathcal{L} \mid \Lambda^0{}_0 \leq 1, \det\Lambda = -1 \} = T\mathcal{L}_+^\uparrow, \tag{2.21}$$

$$\mathcal{L}_+^\downarrow \equiv \{ \Lambda \in \mathcal{L} \mid \Lambda^0{}_0 \leq 1, \det\Lambda = +1 \} = PT\mathcal{L}_+^\uparrow. \tag{2.22}$$

The connected component of the identity $\mathcal{L}_+^\uparrow$ is a Lie subgroup, called the proper Lorentz group. It is noncompact, because it contains the subset of boosts which is homeomorphic to $\mathbb{R}^3$. It is not simply connected, because the subgroup of rotations is not simply connected. Indeed, all group elements of $\mathcal{L}_+^\uparrow$ can be obtained from boosts and rotations: For any $\Lambda \in \mathcal{L}_+^\uparrow$ we can write

$$\Lambda = \Lambda(v)\,\Lambda(\varphi), \tag{2.23}$$

where $\Lambda(v)$ is a boost with velocity v and $\Lambda(\varphi)$ is a rotation with rotation vector φ. We find

$$v^\top = (\Lambda^0{}_1, \Lambda^0{}_2, \Lambda^0{}_3)/\Lambda^0{}_0, \tag{2.24}$$

and a little calculation gives the rotation matrix $\mathbf{R}$ in $\Lambda(\varphi)$ in terms of the matrix elements of Λ,

$$R_{ik} = \begin{cases} \Lambda^i{}_k, & \text{if } v = 0, \\ \Lambda^i{}_k - (\Lambda^0{}_0 - 1)\,\Lambda^i{}_0 \Lambda^0{}_k \left(\sum_{n=0}^3 (\Lambda^0{}_n)^2\right)^{-1}, & \text{if } v \neq 0. \end{cases} \tag{2.25}$$

Other Lie subgroups of the Lorentz group are

$$\mathcal{L}_+ \equiv \mathcal{L}_+^\uparrow \cup \mathcal{L}_+^\downarrow = SO(3,1), \qquad \mathcal{L}^\uparrow \equiv \mathcal{L}_+^\uparrow \cup \mathcal{L}_-^\uparrow. \tag{2.26}$$

Remark. The topological properties of $\mathcal{L}_+^\uparrow$ are of central importance in quantum mechanics. The multiple connectedness will force us to use representations of the simply connected covering group ("spinor representations") and can be regarded as the group theoretical reason for half-integer angular momenta (spin-1/2). The noncompactness prevents the existence of nontrivial unitary representations in a finite dimensional space. As a consequence, the spinor components of Dirac wavefunctions have to be transformed with the help of non-unitary matrices.

2.1.5 The Poincaré Group

The Poincaré group is obtained by combining Lorentz transformations and space-time translations.

Definition 2.5. *A Poincaré transformation* $\Pi = (a, \Lambda)$, *where* $\Lambda \in \mathcal{L}$ *and* $a \in \mathbb{R}^4$, *is a mapping from* $\mathbb{R}^4$ *to* $\mathbb{R}^4$ *which is defined as*

$$\Pi(x) = \Lambda x + a. \tag{2.27}$$

The set $\mathcal{P}$ of all Poincaré transformations is a group with the composition law

$$(a_1, \Lambda_1)(a_2, \Lambda_2) = (a_1 + \Lambda_1 a_2, \Lambda_1 \Lambda_2). \tag{2.28}$$

Hence the Poincaré group $\mathcal{P}$ is the semidirect product of the Lorentz group and the group of space-time translations (i.e., the additive group $\mathbb{R}^4$)

$$\mathcal{P} = \mathbb{R}^4 \odot \mathcal{L}. \tag{2.29}$$

The subgroup of translations is an abelian normal subgroup of $\mathcal{P}$.

Remark 1. The semidirect product of two arbitrary Lie groups $(\mathcal{H}, \cdot)$ and $(\mathcal{T}, \circ)$ can be defined if there is an action of $\mathcal{H}$ on $\mathcal{T}$. We say that a group $\mathcal{H}$ acts on a set $\mathcal{T}$, if for every $h \in \mathcal{H}$ there is a bijective map $\Lambda_h : \mathcal{T} \to \mathcal{T}$, which satisfies

a) $\Lambda_e = \mathrm{id}_{\mathcal{T}}$ (e is the neutral element of $\mathcal{H}$),
b) $\Lambda_g(\Lambda_h(t)) = \Lambda_{g \cdot h}(t)$, for all $g, h \in \mathcal{H}$, and all $t \in \mathcal{T}$.

Furthermore we assume that each Λ_h is a Lie group automorphism of $\mathcal{T}$, i.e.,

c) $\Lambda_h : \mathcal{T} \to \mathcal{T}$ is analytic,
d) $\Lambda_h(s \circ t) = \Lambda_h(s) \circ \Lambda_h(t)$, for all $h \in \mathcal{H}$, and all $s, t \in \mathcal{T}$.

Then the "semidirect product" of $\mathcal{T}$ and $\mathcal{H}$ is the Lie group $\mathcal{T} \odot \mathcal{H}$ which as a set is the cartesian product

$$\mathcal{T} \times \mathcal{H} = \{ (t, h) \mid t \in \mathcal{T},\ h \in \mathcal{H} \}, \tag{2.30}$$

and on which the group multiplication is defined as

$$(s, g)(t, h) = (s \circ \Lambda_g(t), g \cdot h). \tag{2.31}$$

Note that in a "direct product" $\mathcal{T} \otimes \mathcal{H}$ one would have the multiplication law

$$(s, g) \times (t, h) = (s \circ t, g \cdot h). \tag{2.32}$$

Remark 2. The connected component of the identity of $\mathcal{P}$ is called the proper Poincaré group

$$\mathcal{P}_+^{\uparrow} = \mathbb{R}^4 \odot \mathcal{L}_+^{\uparrow}. \tag{2.33}$$

The proper Poincaré group is regarded as the fundamental symmetry group of physics. Different inertial systems are connected by Poincaré transformations. The principle of relativity states that all laws of nature are independent of the inertial system chosen for their description.

2.1.6 The Lie Algebra of the Poincaré Group

Since the Poincaré group $\mathcal{P}$ is a Lie group, we can introduce local coordinates, say

$$q = (a, \omega, \varphi) \in \mathbb{R}^{10}, \tag{2.34}$$

in a neighborhood of the identity element e, to which we associate the origin O in $\mathbb{R}^{10}$. For our choice of coordinates on $\mathcal{P}$ the coordinate lines $q_j(t) = (0, \ldots, t, \ldots, 0)$ (with t on the j-th place) are in fact one-parameter subgroups of the proper Poincaré group $\mathcal{P}_+^{\uparrow}$, such that group multiplication is described by addition of the parameters

$$q_j(s) \circ q_j(t) = q_j(s + t). \tag{2.35}$$

There are ten one-parameter groups obtained in this way. The infinitesimal generators, defined by

$$A_j = \frac{d}{dt} q_j(t)\Big|_{t=0}, \tag{2.36}$$

are denoted as follows:

$-P_0 \equiv -\frac{1}{c}H_0$	generator of x^0-translations,
P_1, P_2, P_3	generators of space translations,
$-\frac{1}{c}N_1, -\frac{1}{c}N_2, -\frac{1}{c}N_3$	generators of boosts,
J_1, J_2, J_3	generators of rotations.

The sign convention is consistent with our quantum mechanical notation in Chapter 1. We can use the following formula for the Lie bracket of A_j and A_k

$$[A_j, A_k] = \frac{d}{ds}\frac{d}{dt} q_j(s)\, q_k(t)\, q_j(s)^{-1}\Big|_{s=t=0} \tag{2.37}$$

to determine the Lie algebra,

$$\begin{aligned}
&[P_j, P_k] = [P_j, H_0] = [J_j, H_0] = 0,\\
&[N_j, P_k] = -\delta_{jk} H_0, \qquad [N_j, H_0] = -c^2 P_j,\\
&[J_j, P_k] = -\sum_m \epsilon_{jkm} P_m, \qquad [J_j, J_k] = -\sum_m \epsilon_{jkm} J_m,\\
&[N_j, N_k] = c^2 \sum_m \epsilon_{jkm} J_m, \qquad [J_j, N_k] = -\sum_m \epsilon_{jkm} N_m.
\end{aligned} \tag{2.38}$$

Here j, k, and m run from 1 to 3.

Remark 1. The last three equations in (2.38) form the Lie-algebra of the Lorentz group. For groups of matrices the infinitesimal generators are also given by matrices and the Lie bracket (2.37) becomes the commutator. It is interesting to note that the Pauli matrices $N_k = \frac{1}{2}\sigma_k$, $J_k = \frac{i}{2}\sigma_k$ satisfy the Lorentz-Lie algebra, as can be seen immediately from Eq. (1.212).

Remark 2. The generators of symmetry transformations of a physical theory are related to the basic observables of the theory (like energy, momentum, center of energy, angular momentum). Conversely, the existence of self-adjoint operators which represent the Poincaré Lie algebra can be used to prove the relativistic invariance of the Dirac theory. This strategy will be pursued in the next sections.

2.2 Symmetry Transformations in Quantum Mechanics

The principle of relativity states that the behavior of physical systems should not depend on the inertial frame chosen for the preparation and description of the experiment. The state of any physical system S is described with respect to a given inertial frame I in terms of coordinates $x \in \mathbb{R}^4$. If we prepare a system of the same kind identically with respect to another (equivalent) coordinate system I', then an observer in I' would describe the system exactly as before, but this time the numbers x refer to the new frame I'. From the point of view of an observer in the old frame I the state of S is changed during that procedure. We say that the system S is transformed. Hence the coordinate transformation $I \to I'$ is reflected by a corresponding transformation in the state space of the physical system. In the following sections we investigate, how these transformations could be represented in the state space (Hilbert space) of a quantum mechanical system. The predictions of a quantum theory are given as transition probabilities (Sect. 1.2.3). Hence the basic requirement for the invariance of a quantum mechanical theory with respect to the description in different inertial frames is that the transition probability between two states ϕ and ψ should be the same as between the corresponding transformed states ϕ' and ψ'.

2.2.1 Phases and Rays

It is clear that there is no one-to-one correspondence between states of a physical system and vectors ψ in a Hilbert space. If ψ and ϕ are unit vectors differing only by a complex number of modulus one, then they obviously describe the same state, because they lead to the same observable predictions (probability measures, expectation values). Hence all vectors in the one-dimensional subspace ("ray")

$$\hat{\psi} = \{\lambda\psi \mid \lambda \in \mathbb{C}\} \tag{2.39}$$

correspond to the same state. The set of all $\hat{\psi}$ forms a projective space, denoted by $\hat{\mathfrak{H}}$.

Remark. Let ψ_n, $n = 0, 1, 2, \ldots$, be an orthonormal basis in the Hilbert space of a quantum mechanical system. Of course, for each n, the vectors ψ_n and $\lambda_n\psi_n$ (with $|\lambda_n| = 1$) represent the same state. However, the vectors ψ and ψ', where

$$\psi = \sum_{n=1}^{\infty} a_n\psi_n, \qquad \psi' = \sum_{n=1}^{\infty} a_n\lambda_n\psi_n, \tag{2.40}$$

represent in general different states.

The ambiguity in the description of states complicates the description of symmetry transformations which we are now going to define.

2.2.2 The Wigner-Bargmann Theorem

The transition probability from a state $\hat{\phi}$ to a state $\hat{\psi}$ is given by

$$\langle \hat{\psi}, \hat{\phi} \rangle \equiv |(\psi, \phi)|^2, \tag{2.41}$$

where ϕ and ψ are arbitrary unit vectors in the subspaces $\hat{\phi}$ and $\hat{\psi}$, respectively.

Definition 2.6. *A bijective map $T: \hat{\mathfrak{H}} \to \hat{\mathfrak{H}}$ is called a symmetry transformation, if for all $\hat{\psi}$, $\hat{\phi}$*

$$\langle T\hat{\psi}, T\hat{\phi} \rangle = \langle \hat{\psi}, \hat{\phi} \rangle. \tag{2.42}$$

The set of all symmetry transformations forms a group with respect to composition. Obviously, any unitary (or antiunitary[4]) operator U in $\mathfrak{H}$ defines a symmetry transformation $\hat{U}$ by

$$\hat{U}\hat{\psi} \equiv (U\psi)\hat{}. \tag{2.43}$$

The converse result is the following fundamental theorem.

Theorem 2.7 (Wigner-Bargmann). Every symmetry transformation T in $\hat{\mathfrak{H}}$ is of the form

$$T = \hat{U}, \quad \text{with } U \text{ unitary or antiunitary in } \mathfrak{H}. \tag{2.44}$$

If U_1 and U_2 are operators with $T = \hat{U}_1 = \hat{U}_2$ then

$$U_2 = e^{i\theta} U_1, \quad \text{for some } \theta \in [0, 2\pi). \tag{2.45}$$

In particular, the operators U satisfying (2.44) are either all unitary or all antiunitary.

2.2.3 Projective Representations

Since inertial frames are linked by Poincaré transformations, we expect that any Poincaré transformation should correspond to a symmetry transformation of the quantum system. We call a quantum system "relativistically invariant", if the Poincaré group can be implemented as a group of symmetry transformations in the projective space of states. We require this implementation to form a "projective representation".

Definition 2.8. *Let $\mathcal{G}$ be a Lie group with unit element e. A projective representation of $\mathcal{G}$ in $\hat{\mathfrak{H}}$ is a mapping ρ of $\mathcal{G}$ into the group of symmetry transformations such that*

[4] An antiunitary transformation A is antilinear, $A(\alpha\psi + \beta\phi) = \overline{\alpha}A(\psi) + \overline{\beta}A(\phi)$, and satisfies $(A\psi, A\phi) = (\phi, \psi)$, whereas a unitary transformation U is linear, and $(U\psi, U\phi) = (\psi, \phi)$.

a) $\rho(gh) = \rho(g)\rho(h)$, *for all* $g, h \in \mathcal{G}$,
b) $\rho(e) = \hat{1}$ *(identity in* $\hat{\mathfrak{H}}$*),*
c) $g_n \to g$ *in* $\mathcal{G}$ *implies* $\rho(g_n) \to \rho(g)$.

(We say that $\hat{U}_n \to \hat{U}$ *if* $(U_n\psi)\hat{} \to (U\psi)\hat{}$ *for all* $\psi \in \mathfrak{H}$*). Each* $\rho(g)$, $g \in \mathcal{G}$, *is of the form* $\rho(g) = \hat{\pi}(g)$, *where* $\pi(g)$ *is either unitary or antiunitary and* $\hat{\pi}(g)$ *is the symmetry transformation associated with* $\pi(g)$ *by (2.43). If, in addition,*

d) $\pi(g)$ *is unitary for all* $\pi(g)$ *with* $\rho(g) = \hat{\pi}(g)$,

then ρ *is called a projective unitary representation.*

In order to prove the relativistic invariance of the Dirac theory, we have to show that there is a projective representation of the Poincaré group in $\hat{\mathfrak{H}}$. Any projective representation is given by a set of (anti)unitary operators in the underlying Hilbert space which are only unique up to a phase. We are going to investigate carefully the relations between projective group representations and their possible realizations as operators $\pi(g)$. As a first result we note

Theorem 2.9. Any projective representation of a *connected* Lie group is a projective unitary representation.

Proof. Let ρ be an arbitrary projective representation of a connected Lie group. Every element g of a connected Lie group is element of a one-parameter subgroup $\{h(t) \mid t \in \mathbb{R}\}$, i.e., $g = h(t_0)$. Hence g is the square of the element $h(t_0/2)$. By the Wigner-Bargmann Theorem $\rho(g) = \hat{\pi}(g)$, where $\pi(g)$ is the square of a unitary or antiunitary operator. Hence $\pi(g)$ is always unitary. □

2.2.4 Representations in a Hilbert Space

Given a projective representation ρ we can choose operators $\pi(g)$ with $\rho(g) = \hat{\pi}(g)$. Now Def. 2.8.a implies together with (2.45)

$$\pi(g)\pi(h) = \omega(g,h)\,\pi(gh), \quad \text{all } g, h \in \mathcal{G}, \tag{2.46}$$

with some suitable phase factor $\omega(g,h) \in U(1) = \{e^{i\theta} \mid \theta \in \mathbb{R}\}$. The ω's cannot be chosen completely arbitrary, e.g., the associativity law of the group multiplication $[fg]h = f[gh]$ implies for all $f, g, h \in \mathcal{G}$

$$\omega(fg,h)\,\omega(f,g) = \begin{cases} \omega(f,gh)\,\omega(g,h), & \text{if } \pi(f) \text{ is unitary,} \\ \omega(f,gh)\,\overline{\omega(g,h)}, & \text{if } \pi(f) \text{ is antiunitary.} \end{cases} \tag{2.47}$$

The ω's are further restricted by the requirement that the operators $\pi(g)$ should depend continuously on g. It is a difficult problem to decide whether one can choose the operators $\pi(g)$ with all the ω's being equal to one (Sect. 2.4.2). If this is the case, then (2.46) becomes the usual representation property.

Definition 2.10. *A representation π of a Lie group $\mathcal{G}$ in a Hilbert space $\mathfrak{H}$ is a mapping π of $\mathcal{G}$ into the set of bounded linear (or antilinear) operators such that*

a) $\pi(gh) = \pi(g)\pi(h)$, *for all* $g, h \in \mathcal{G}$,
b) $\pi(e) = \mathbf{1}$ *(identity in* $\mathfrak{H}$*),*
c) $g_n \to g$ *in* $\mathcal{G}$ *implies for all* $u \in \mathfrak{H}$ *that* $\pi(g_n)u \to \pi(g)u$ *in* $\mathfrak{H}$ *(strong continuity).*

Each $\pi(g)$ *is bounded invertible by a) and b). If, in addition,*

d) $\pi(g)^* = \pi(g^{-1}) = \pi(g)^{-1}$,

then π *is called a unitary representation.*

Remark. It is well known that the Lorentz group has no finite dimensional **unitary** representations except the trivial one $\pi(g) = \mathbf{1}$, **all** g.

Definition 2.11. *A representation π of a group $\mathcal{G}$ is irreducible, if there are no proper subspaces of $\mathfrak{H}$ which remain invariant under all operators $\pi(g)$. Otherwise the representation is reducible.*

Lemma 2.12 (Schur). A unitary representation π of a group $\mathcal{G}$ is irreducible if and only if the only operators commuting with all $\pi(g)$, $g \in \mathcal{G}$, are scalar multiples of the identity operator.

Proof. Almost any book on representation theory, see for example [BR 86], Chapter 5, Sect. 3. □

2.2.5 Lifting of Projective Representations

It is clear that every representation of a group by unitary or antiunitary operators defines also a projective representation. Conversely, if for a projective representation ρ there exists a representation π with $\hat{\pi} = \rho$, then we say that ρ admits a lifting π (this means that all $\omega(g, h) = 1$). The following example shows that the lifting of a projective representation is not always possible.

Example 2.13. Let $\mathcal{G}$ be the (abelian) subgroup of discrete Lorentz-transformations id, P, T, and PT defined in Sect. 2.1.3, and let $\mathfrak{H} = \mathbb{C}^2$. The projective space of one-dimensional subspaces is the complex projective line $\hat{\mathfrak{H}} = P\mathbb{C}$. It's elements are of the form

$$\hat{\psi} = \{ (\lambda z_1, \lambda z_2) \mid \lambda \in \mathbb{C} \} \quad \text{for } \psi = (z_1, z_2) \in \mathbb{C}^2. \tag{2.48}$$

We define a projective representation of $\mathcal{G}$ in $\hat{\mathfrak{H}}$ by

$$\rho(P) = \hat{\sigma}_1, \quad \rho(T) = \hat{\sigma}_2, \quad \rho(PT) = \hat{\sigma}_3, \tag{2.49}$$

where σ_i are the Pauli matrices. Because of

$$\sigma_i\sigma_k = \delta_{ik} + \mathrm{i}\epsilon_{ikm}\sigma_m \tag{2.50}$$

it is easy to verify Def. 2.8.a). The associated operators

$$\pi(P) = \sigma_1, \quad \pi(T) = \sigma_2, \quad \pi(PT) = \sigma_3, \quad \pi(\mathrm{id}) = \mathbf{1}_2, \tag{2.51}$$

do not form a representation in $\mathbb{C}^2$, instead we obtain from (2.50)

$$\pi(P)\pi(T) = \mathrm{i}\pi(PT), \quad \pi(T)\pi(P) = -\mathrm{i}\pi(PT), \quad \text{etc.}, \tag{2.52}$$

which violates the representation property Def. 2.10.a. By Theorem 2.2 the operators π are determined uniquely up to a phase by the given projective representation ρ. Hence we could try to repair the representation property by multiplying each σ_k with a suitable chosen phase $\lambda_k \in U(1)$, i.e.,

$$\pi'(P) = \lambda_1\sigma_1, \quad \text{etc.} \tag{2.53}$$

It is clear that $\hat{\pi}'(P) = \hat{\pi}(P) = \rho(P)$, etc. Now (2.52) can be replaced by

$$\pi'(P)\pi'(T) = \mathrm{i}\lambda_1\lambda_2\lambda_3^{-1}\pi'(PT), \quad \pi'(T)\pi'(P) = -\mathrm{i}\lambda_1\lambda_2\lambda_3^{-1}\pi'(PT). \tag{2.54}$$

In order to obtain the representation property Def. 2.10.a) for the operators π' we have to require that both $\mathrm{i}\lambda_1\lambda_2\lambda_3^{-1}$ and $-\mathrm{i}\lambda_1\lambda_2\lambda_3^{-1}$ should be equal to one. But this is clearly impossible. Hence this group has a projective representation which cannot be lifted to a Hilbert space representation by a suitable choice of phases.

Example 2.14. The proper Poincaré group $\mathcal{P}_+^\uparrow$ is a connected (but not simply connected) Lie group. By Theorem 1.2 any projective representation ρ is projective unitary. In Sect. 2.3.4 we will find unitary operators π in $L^2(\mathbb{R}^3)^4$ such that $\hat{\pi}$ is a projective representation of $\mathcal{P}_+^\uparrow$. But as we shall see the operators π cannot be chosen to form a representation of $\mathcal{P}_+^\uparrow$ in this Hilbert space because both $\pi = 1$ and $\pi = -1$ correspond to the identity transformation in $\mathcal{P}_+^\uparrow$. Hence there is a projective unitary representation of $\mathcal{P}_+^\uparrow$ which does not admit a lifting. (It can, however, be lifted to a representation of the simply connected covering group, Sect. 2.4).

2.3 Lie Algebra Representations

In the previous section we have seen that a quantum theory could have a symmetry group which is not represented by a group of (anti)unitary operators in the Hilbert space of the system, because it is not possible to adjust the arbitrary phases properly. Next, we are going to investigate the proper Poincaré group (the connected component of the identity) by "integrating" a representation of of its Lie algebra. We will obtain a representation of the Poincaré covering group, but not a representation of the Poincaré group itself.

2.3.1 The Lie Algebra and the Gårding Domain

We first show that a unitary representation of a Lie group defines a unique representation of the Lie algebra in terms of self-adjoint operators.

Let π be a unitary representation of a Lie group $\mathcal{G}$ in a Hilbert space $\mathfrak{H}$. Any one-parameter subgroup $h(t) = \exp(\mathbf{A}t)$ corresponds to a strongly continuous one parameter group of unitary operators $\pi(h(t))$. By Stone's theorem (Sect. 1.2) we must have

$$\pi(h(t)) = e^{-\mathrm{i}At}, \tag{2.55}$$

where the operator A is self-adjoint. Clearly, the operator A corresponds to the Lie algebra element $\mathbf{A}$.

Theorem 2.15. There is a dense linear subspace $\mathfrak{D}_G$ (the Gårding domain) of $\mathfrak{H}$ which is a common invariant domain for all generators, i.e.,

$$\mathfrak{D}_G \subset \mathfrak{D}(A), \qquad A\mathfrak{D}_G \subset \mathfrak{D}_G, \tag{2.56}$$

whenever $\exp(-\mathrm{i}At)$ represents a one-parameter subgroup of $\mathcal{G}$. On the Gårding domain, the Lie bracket operation is represented by i times the commutator of the corresponding (essentially) self-adjoint operators.

Proof. The construction of the Gårding domain uses the existence of a (left invariant) Haar measure dg and the possibility of defining differentiable functions with compact support on the group manifold. For $\psi \in \mathfrak{H}$ and $f \in \mathcal{C}_0^\infty(\mathcal{G})$ define

$$\psi_f = \int_{\mathcal{G}} f(g)\, \pi(g)\, \psi \, dg, \tag{2.57}$$

where π is any representation of $\mathcal{G}$ in $\mathfrak{H}$. The integral may be considered a Riemann integral. It extends only over the support of f. The Gårding domain $\mathfrak{D}_G$ consists of all possible linear combinations of the vectors ψ_f with $\psi \in \mathfrak{H}$ and $f \in \mathcal{C}_0^\infty(\mathcal{G})$. $\mathfrak{D}_G$ is dense because for all $\psi \in \mathfrak{H}$ we can find a sequence $\psi_{f_n} \in \mathfrak{D}_G$ which converges to ψ, as $n \to \infty$: Simply choose $f_n \in \mathcal{C}_0^\infty(\mathcal{G})$ with

$$f_n \to 0, \qquad \int f_n(g)\, dg = 1, \quad \text{for all } n, \tag{2.58}$$

and such that $\mathrm{supp}(f_n)$ shrinks to $e \in \mathcal{G}$, as $n \to \infty$. Furthermore, the Gårding domain is an invariant domain for all generators of one-parameter subgroups. Let $h(t)$ be any one-parameter subgroup of $\mathcal{G}$, $\pi(h(t)) = \exp(-\mathrm{i}At)$, i.e.,

$$A\psi = \mathrm{i} \lim_{t \to 0} \frac{\pi(h(t)) - 1}{t}\, \psi, \tag{2.59}$$

for all ψ for which this limit exists. For ψ_f in the Gårding domain we have

$$\frac{\pi(h(t)) - 1}{t}\, \psi_f = \int \frac{1}{t} f(g)\, \{\pi(h(t)g) - \pi(g)\}\, \psi \, dg$$

$$= \int \frac{1}{t} \{f(h(t)^{-1}g) - f(g)\} \pi(g) \psi \, dg, \tag{2.60}$$

where we have used the left-invariance of the Haar measure,

$$d(h^{-1}g) = dg. \tag{2.61}$$

Let A denote the Lie algebra element corresponding to the one-parameter subgroup $h(t) = \exp(\mathrm{A}t)$. Then $h(t)^{-1} = h(-t)$ is generated by $-\mathrm{A}$. The tangent vector A acts as a derivation on differentiable functions $f \in \mathcal{C}_0^\infty(\mathcal{G})$. $\mathrm{A}f$ is again a differentiable function in $\mathcal{C}_0^\infty(\mathcal{G})$ and its value at g is given by

$$(-\mathrm{A}f)(g) = \frac{d}{dt} f\big(h(t)^{-1}g\big)\Big|_{t=0}. \tag{2.62}$$

Hence we obtain from (2.60) (by interchanging the integral sign with the limit $t \to 0$)

$$\mathrm{i}A\,\psi_f = \int (\mathrm{A}f)(g)\, \pi(g)\, \psi \, dg = \psi_{\mathrm{A}f}. \tag{2.63}$$

This shows that A leaves the Gårding domain invariant. (2.63) also defines a representation of the Lie algebra of $\mathcal{G}$ by operators $\mathrm{i}A$ in the Hilbert space, where A is self-adjoint. Let A and B be infinitesimal generators and

$$\pi(e^{\mathrm{A}t}) = e^{-\mathrm{i}At}, \quad \pi(e^{\mathrm{B}t}) = e^{-\mathrm{i}Bt}. \tag{2.64}$$

Then

$$\begin{aligned} \psi_{[\mathrm{A},\mathrm{B}]f} &= \psi_{\mathrm{AB}f - \mathrm{BA}f} = \psi_{\mathrm{AB}f} - \psi_{\mathrm{BA}f} \\ &= \mathrm{i}A(\mathrm{i}B)\psi_f - \mathrm{i}B(\mathrm{i}A)\psi_f. \end{aligned} \tag{2.65}$$

Hence the Lie bracket $\mathrm{C} = [\mathrm{A}, \mathrm{B}]$ defines via (2.63) an operator C which is i times the commutator of the self-adjoint operators A and B

$$C = \mathrm{i}[A, B]. \tag{2.66}$$

Due to the invariance of $\mathfrak{D}_G$ this commutator is well defined and symmetric on $\mathfrak{D}_G$. In fact, C is essentially self-adjoint on $\mathfrak{D}_G$ because $\mathfrak{D}_G$ is an invariant domain for the unitary group $\pi(\exp(\mathrm{C}t))$ whose generator is by construction a self-adjoint extension of the operator C (see [RS 72], Theorem VIII.11). □

2.3.2 The Poincaré Lie Algebra

Let us assume that the Poincaré group (or any group with the same Lie algebra) has a unitary representation in some Hilbert space. According to Theorem 2.15 the ten infinitesimal generators

$$\{ -\tfrac{1}{c}\mathrm{H}_0,\ \mathrm{p}_k,\ \mathrm{J}_k,\ -\tfrac{1}{c}\mathrm{N}_k\ ;\ k = 1, 2, 3\} \tag{2.67}$$

of the Poincaré group, which were defined in Sect. 2.1.6, correspond to self-adjoint operators

$$\{-\tfrac{1}{c}H_0,\ p_k,\ J_k,\ -\tfrac{1}{c}N_k\ ;\ k=1,\ 2,\ 3\} \tag{2.68}$$

which are well defined on the Gårding domain in the Hilbert space of the representation.

Remark. In particular, the self-adjoint generator of time translations is denoted by $-H_0$. The minus sign is chosen for consistency with our earlier notation. In this chapter we describe Poincaré transformations from the "active" point of view. Hence a time translation puts the system in the future and is described with respect to a fixed coordinate system in $\mathbb{R}^4$, i.e., by an observer which is at rest at the origin of the Minkowsky space: If this observer prepares a system in the state ψ then

$$\pi(e^{-\mathbf{H}_0 t}) = e^{\mathrm{i}H_0 t} \tag{2.69}$$

puts this state into the future at time t. In quantum mechanics (Chapter 1), $\psi(t) = \exp(-\mathrm{i}H_0 t)\psi$ is the state observed at time t. Hence $\exp(-\mathrm{i}H_0 t)$ describes the change seen by a human observer which (sometimes against his own will) moves through the time towards the future (this "passive" point of view coincides with the Schrödinger picture of quantum mechanics). It is clear that an active Poincaré transformations is the inverse of the same transformation in the passive interpretation.

The self-adjoint operators (2.68) form a representation of the Lie algebra of the Poincaré group. From (2.38) we obtain with (2.63) and (2.66) the following commutation relations.

$$\begin{aligned}
&[p_j, p_k] = [p_j, H_0] = [J_j, H_0] = 0,\\
&[N_j, p_k] = \mathrm{i}\delta_{jk}H_0, \qquad [N_j, H_0] = \mathrm{i}c^2 p_j,\\
&[J_j, p_k] = \sum_m \mathrm{i}\epsilon_{jkm}p_m, \qquad [J_j, J_k] = \sum_m \mathrm{i}\epsilon_{jkm}J_m,\\
&[N_j, N_k] = -\sum_m \mathrm{i}c^2\epsilon_{jkm}J_m, \qquad [J_j, N_k] = \sum_m \mathrm{i}\epsilon_{jkm}N_m.
\end{aligned} \tag{2.70}$$

Here j, k, and m run from 1 to 3. The commutators are well defined on the Gårding domain.

The relations (2.70) are valid for all unitary representations of the Poincaré group. So far we haven't found any. Therefore, let us consider the converse problem, namely to start with a representation of the Lie algebra in order to find a group representation by exponentiating. In fact, it is much easier to find a representation of the Lie algebra because the generators of symmetry transformations have a direct physical meaning. The generator of time translations, is the energy of the system, $\boldsymbol{p}$ is the momentum, $\boldsymbol{J}$ the angular momentum, and $\boldsymbol{N}$ is usually associated with the center of energy. If the given Hilbert space is

the state space of some physical system, then one usually has some idea how these operators should look like.

Example 2.16. It is clear that in the Hilbert space $L^2(\mathbb{R}^3)^4$ of a Dirac electron the time translations are generated by the Dirac operator H_0. The choice of $\boldsymbol{p}$ and $\boldsymbol{J}$ for translations and rotations is also more or less obvious, at least in view of the correspondence to nonrelativistic quantum mechanics. For $\boldsymbol{N}$ we symmetrize the classical expression $H_0\boldsymbol{x}$. Hence we choose the following operators in order to represent the Poincaré Lie algebra:

$$\boldsymbol{p} = -\mathrm{i}\nabla, \qquad H_0 = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2,$$

$$\boldsymbol{J} = \boldsymbol{x}\wedge\boldsymbol{p} - \frac{\mathrm{i}}{4}\boldsymbol{\alpha}\wedge\boldsymbol{\alpha}, \qquad \boldsymbol{N} = \frac{1}{2}(H_0\boldsymbol{x} + \boldsymbol{x}H_0). \tag{2.71}$$

Obviously $C_0^\infty(\mathbb{R}^3)^4$ is a common dense invariant domain, on which the operators (2.71) are symmetric. We can verify that these operators satisfy indeed the commutation relations (2.70) of the Poincaré Lie algebra. (This requires some commutator gymnastics using the formulas in the Appendix of Chapter 1). Hence the operators (2.71) form a representation of the Poincaré Lie algebra.

We want to stress that this representation of the Poincaré Lie algebra was obtained here by an "educated guess" and not by a derivation from a unitary representation of the Poincaré group. We shall see that a unitary representation of the Poincaré group from which this particular Lie algebra representation can be derived does not exist[5]. In the next section we give a criterion for obtaining a unitary group representation from a Lie algebra representation.

2.3.3 Integration of Lie Algebra Representations

Can we always construct a unitary representation of the whole group from the self-adjoint representation of the generators? The answer is no.

Example 2.17. Let M be the Riemann surface of $\sqrt{z}$. In $L^2(M)$ consider the operators $p_x = -\mathrm{i}\partial/\partial x$, and $p_y = -\mathrm{i}\partial/\partial y$, which are essentially self-adjoint on $C_0^\infty(M\setminus\{0\})$ and satisfy $[p_x, p_y] = 0$ on this domain. Hence they represent the Lie algebra of the abelian translation group $(\mathbb{R}^2, +)$. The unitary groups generated by p_x and p_y in $L^2(M)$ describe finite translations in x- and y-direction on the Riemann surface (not on $\mathbb{R}^2$). Therefore $\exp(-\mathrm{i}ap_x)\exp(-\mathrm{i}bp_y) \neq \exp(-\mathrm{i}bp_y)\exp(-\mathrm{i}ap_x)$, because finite translations on the Riemann surface do not commute.

This counterexample shows that what we know so far about the operators (2.71) representing the Poincaré Lie algebra does not guarantee that these operators generate a unitary representation of a Lie group. A sufficient condition for the existence of a group representation is given in the next theorem.

[5] Don't worry! All we need is a *projective* unitary representation.

Theorem 2.18 (Nelson's Theorem). Let $A_1, \ldots, A_n$ be symmetric operators defined on a dense linear subset $\mathfrak{D}$ in a Hilbert space $\mathfrak{H}$. We assume that these operators represent the Lie algebra $L_{\mathcal{G}}$ of some Lie group $\mathcal{G}$,

$$A_j \mathfrak{D} \subset \mathfrak{D}, \quad j = 1, \ldots, n, \tag{2.72}$$

$$[A_j, A_k] = \sum_m c_{jkm} A_m \quad \text{on } \mathfrak{D}, \quad j, k = 1, \ldots, n. \tag{2.73}$$

If the operator

$$Q = \sum_{m=1}^{n} A_m^2 \tag{2.74}$$

is essentially self-adjoint on $\mathfrak{D}$, then there is on $\mathfrak{H}$ a unique unitary representation π of the simply connected Lie group $\tilde{\mathcal{G}}$ (see below), which has $L_{\mathcal{G}}$ as its Lie-algebra. If $\mathrm{A}_1, \ldots, \mathrm{A}_n$ form a basis of the Lie-algebra of $\mathcal{G}$, then the group element $\exp(t_1 \mathrm{A}_1 + \cdots + t_n \mathrm{A}_n)$ is represented by

$$\pi\left(e^{t_1 \mathrm{A}_1 + \cdots + t_n \mathrm{A}_n}\right) = e^{-\mathrm{i}(t_1 A_1 + \cdots + t_n A_n)}. \tag{2.75}$$

Remark 1. If $\mathcal{G}$ is connected, then $\tilde{\mathcal{G}}$ is the universal covering group of $\mathcal{G}$. The universal covering group of $\mathcal{G}$ can be understood as the "smallest" Lie group which covers $\mathcal{G}$ and which is simply connected. See [Ch 46] for a precise definition. The universal covering group of the proper Poincaré group will be described explicitly in Sect. 2.5 below. In Nelson's theorem the covering group appears for the following reason: The representation of the Lie-algebra defines only a local homomorphism of a neighborhood of e in $\mathcal{G}$ into the group of unitary operators in $\mathfrak{H}$. This local representation can only be extended uniquely to a global representation if the group is simply connected.

Remark 2. If $\mathcal{G}$ is not connected, then $\tilde{\mathcal{G}}$ is the universal covering group of the connected component of the neutral element in $\mathcal{G}$. In this case the theorem above tells nothing about the representation of the "discrete" group elements (like P, T, and PT in case of the Poincaré group).

Remark 3. The essential self-adjointness of Q together with the assumptions of the theorem imply the essential self-adjointness of the symmetric operators A_k, for $k = 1, \ldots, n$.

2.3.4 Integrating the Poincaré Lie Algebra

Nelson's theorem gives a useful criterion for the possibility of exponentiating a representation of the Lie algebra. In this section we shall prove that the assumptions of Nelson's theorem are fulfilled by the operators (2.71), namely, that

$$Q = \frac{1}{c^2}H_0^2 + p^2 + J^2 + \frac{1}{c^2}N^2 \tag{2.76}$$

is essentially self-adjoint on $\mathcal{C}_0^\infty(\mathbb{R}^3)^4$. Hence we obtain the following result with the help of Nelson's theorem.

Theorem 2.19. The operators H_0, $\boldsymbol{p}$, $\boldsymbol{J}$, and $\boldsymbol{N}$ (which are well defined and essentially self-adjoint on the common domain $\mathcal{C}_0^\infty(\mathbb{R}^3)^4$) are the generators of a uniquely determined unitary representation π of the simply connected covering group $\tilde{\mathcal{P}}_+^\uparrow$ of the proper Poincaré group.

The representation π will be obtained in Sect. 3.3.7 in a more explicit form and with the help of different techniques.

Remark 1. The operators (2.71) define a representation of the covering group, but they do *not* define a representation of the Poincaré group itself. This can be seen as follows. The subgroup of rotations around the x_3-axis is given by $\exp(-\mathrm{i}\varphi J_3)$. This implies that a rotation through 2π (which is identical to the neutral element in the Poincaré group) transforms a vector ψ into its negative,

$$e^{-\mathrm{i}2\pi J_3}\psi = e^{-\mathrm{i}2\pi S_3}e^{-\mathrm{i}2\pi L_3}\psi = e^{-\mathrm{i}2\pi S_3}\psi = -\psi. \tag{2.77}$$

Here we have used

$$e^{-\mathrm{i}\varphi L_3}\psi(x) = \psi(\mathbf{R}(\varphi)x), \tag{2.78}$$

$\mathbf{R}(\varphi)$ being the 3×3 orthogonal matrix corresponding to a rotation around the x_3-axis through an angle φ. This relation is perhaps familiar from the nonrelativistic quantum mechanics of spinless particles. It can be verified by showing that $\varphi \to \psi(\mathbf{R}(\varphi)x)$ is a strongly continuous one-parameter unitary group with generator L_3. Eq (2.77) now follows from

$$e^{-\mathrm{i}\varphi S_3} = \mathbf{1}\cos(\varphi/2) - 2\mathrm{i}S_3\sin(\varphi/2). \tag{2.79}$$

where we have used the expansion $\exp(-\mathrm{i}\varphi S_3) = \sum(\frac{-\mathrm{i}\varphi}{2})^n\frac{(2S_3)^n}{n!}$ together with $(2S_3)^2 = \mathbf{1}$. Hence the two operators $\mathbf{1}$ and $-\mathbf{1}$ both correspond to the neutral element e of the Poincaré group $\mathcal{P}_+^\uparrow$ which cannot be the case in a representation (see Definition 2.10.b). Of course, $\mathbf{1}$ and $-\mathbf{1}$ correspond to different elements e and h of the covering group $\tilde{\mathcal{P}}_+^\uparrow$ (see Sect. 2.5.8).

Remark 2. A representation of the Poincaré covering group which does not define a representation of the Poincaré group itself is sometimes called a *spinor representation.*

Remark 3. The representation π of Theorem 2.19 is reducible. The Hilbert space $L^2(\mathbb{R}^3)^4$ decomposes into two invariant subspaces because all generators commute with the sign of the energy

$$\operatorname{sgn}(H_0) = H_0/\sqrt{H_0^2}. \tag{2.80}$$

In particular, $[N_j, \operatorname{sgn}(H_0)] = 0$. These invariant subspaces are just the spectral subspaces $\mathfrak{H}_{\text{pos}}$, $\mathfrak{H}_{\text{neg}}$ corresponding to positive and negative energies, respectively. (See Chapter 1).

Finally, we prove the lemma which verifies the assumptions of Nelson's theorem for the generators (2.71).

Lemma 2.20. The operator $Q = H_0^2/c^2 + p^2 + J^2 + N^2/c^2$ defined with the help of (2.71) is essentially self-adjoint on $\mathcal{C}_0^\infty(\mathbb{R}^3)^4$.

Proof. We set $c = 1$ for the purpose of this proof. On $\mathfrak{D} = \mathcal{C}_0^\infty(\mathbb{R}^3)^4$ we obtain by an elementary computation of commutators the formulas

$$J^2 = L^2 + 2\boldsymbol{L}\cdot\boldsymbol{S} + \tfrac{3}{4}, \tag{2.81}$$

$$L^2 = \boldsymbol{x}\cdot p^2\boldsymbol{x} - (\boldsymbol{x}\cdot\boldsymbol{p})(\boldsymbol{p}\cdot\boldsymbol{x}), \tag{2.82}$$

$$2\boldsymbol{L}\cdot\boldsymbol{S} = \mathrm{i}\boldsymbol{x}\cdot\boldsymbol{p} - \mathrm{i}(\boldsymbol{\alpha}\cdot\boldsymbol{x})(\boldsymbol{\alpha}\cdot\boldsymbol{p}), \tag{2.83}$$

$$N^2 = \boldsymbol{x}\cdot p^2\boldsymbol{x} + m^2x^2 - \tfrac{3}{4} + \mathrm{i}\boldsymbol{x}\cdot\boldsymbol{p} - \mathrm{i}(\boldsymbol{\alpha}\cdot\boldsymbol{x})(\boldsymbol{\alpha}\cdot\boldsymbol{p}) - \mathrm{i}m(\boldsymbol{\alpha}\beta)\cdot\boldsymbol{x}. \tag{2.84}$$

Hence on $\mathfrak{D}$ we may write $Q = X + Y + R$, where

$$X = 2p^2 + m^2x^2, \quad Y = 2J^2 + (\boldsymbol{x}\cdot\boldsymbol{p})(\boldsymbol{p}\cdot\boldsymbol{x}), \quad R = mi\beta\boldsymbol{\alpha}\cdot\boldsymbol{x} + m^2 - \tfrac{3}{2}. \tag{2.85}$$

The operator X is equal to the Hamiltonian of a harmonic oscillator in nonrelativistic quantum mechanics. Hence we may define

$$A_k = mx_k + (\mathrm{i}\sqrt{2})p_k, \tag{2.86}$$

and obtain

$$X = \sum_k A_k^* A_k + (3\sqrt{2})m = \sum_k A_k A_k^* - (3\sqrt{2})m, \tag{2.87}$$

$$\|A_{k_1}^\times A_{k_2}^\times, \ldots A_{k_n}^\times \psi\| \le c_n \|X^{n/2}\psi\|, \quad \text{all } \psi \in \mathfrak{D}, \tag{2.88}$$

where $^\times$ means either "*" or "no *" and the c_n are suitable constants > 0. In order to prove the essential self-adjointness of Q we apply Konrady's trick[6]. First of all we define an operator

$$Z = kX^2 \quad \text{on } \mathfrak{D} \tag{2.89}$$

[6] [RS 75], Example 6 in Chapter X.2.

which is essentially self-adjoint for all $k > 0$. The operator Y can be written as a linear combination of terms of the form

$$BA_{k_1}A_{k_2}\dots A_{k_n}, \quad \text{B bounded}, \quad n \leq 4. \tag{2.90}$$

From (2.88) we see that Y is bounded relative to X^2. If we choose the constant k large enough, Y will have Z-bound < 1. The operator X is even infinitesimally bounded with respect to Z. We may use the theorem of Kato and Rellich to conclude that $Z + X + Y$ is essentially self-adjoint on $\mathfrak{D}$ (at least for k large enough). In our next step we prove that

$$(Z - R)^2 \leq (X + Y + Z)^2 + \text{const.} \tag{2.91}$$

(we say $A \leq B$ if $(\psi, A\psi) \leq (\psi, B\psi)$ for all $\psi \in \mathfrak{D}$). A little calculation shows

$$(X + Y + Z)^2 = (X + Y)^2 + Z^2 + 2kX^3 + 2kXYX + k[X,[X,Y]]. \tag{2.92}$$

Since $Y \geq O$ we conclude

$$(X + Y + Z)^2 \geq Z^2 + 2kX^3 + k[X,[X,Y]]. \tag{2.93}$$

or

$$(Z-R)^2 \leq (X+Y+Z)^2 - 2kX^3 + \{-k[X,[X,Y]] - (ZR+RZ) + R^2\}. \tag{2.94}$$

The operator $\{\dots\}$ is a finite linear combination of terms (2.90) with $n \leq 5$. Hence we conclude from (2.88) that

$$\{\dots\} \leq aX^{5/2} \quad \text{for some } a > 0. \tag{2.95}$$

This implies immediately that for all $\epsilon > 0$ there is a constant such that

$$\{\dots\} \leq \epsilon X^3 + \text{const}(\epsilon). \tag{2.96}$$

If we choose $\epsilon = 2k$ then (2.91) follows. Finally we use Wüst's theorem to conclude that $X + Y + R = (X + Y + Z) - (Z - R)$ is essentially self-adjoint on $\mathfrak{D}$. □

2.4 Projective Representations

2.4.1 Representations of the Covering Group

The results obtained so far are not yet completely satisfactory. We have postulated that the proper Poincaré group should be a symmetry group of the Dirac electron. Now, using Nelson's theorem, we have ended up with a unitary representation π of the universal covering group $\tilde{\mathcal{G}}$, which defines a projective unitary representation of $\tilde{\mathcal{G}}$. On the other hand, physical invariance requires a projective representation of the symmetry group $\mathcal{G} = \mathcal{P}_+^\uparrow$ and not of its covering group. Does our projective representation of $\tilde{\mathcal{G}}$ also define a projective

representation of $\mathcal{G}$? (The unitary representation of $\tilde{\mathcal{G}}$ obtained in Sect. 2.3.4 did not define a representation of $\mathcal{G}$).

In this section we show that under suitable assumptions the projective representations of a connected Lie group $\mathcal{G}$ can be derived from the unitary representations of the covering group $\tilde{\mathcal{G}}$ (and not from the representations of $\mathcal{G}$ itself).

Let $\mathcal{G}$ be a connected Lie group. We denote its covering group by $\tilde{\mathcal{G}}$,

$$\mathcal{G} \cong \tilde{\mathcal{G}}/\mathcal{H} = \{\tilde{g}\mathcal{H} \mid \tilde{g} \in \mathcal{G}\}, \tag{2.97}$$

$\mathcal{H}$ being a discrete central subgroup. The covering homomorphism $p : \tilde{\mathcal{G}} \to \mathcal{G}$ is defined by

$$p(\tilde{g}) = \tilde{g}\mathcal{H}. \tag{2.98}$$

If $\mathcal{G}$ is the symmetry group of a quantum mechanical system, then it is our goal to find a projective representation of $\mathcal{G}$ in $\hat{\mathfrak{H}}$. We assume that every projective representation of the covering group $\tilde{\mathcal{G}}$ admits a lifting to a unitary representation of $\tilde{\mathcal{G}}$. Under this condition the problem is equivalent to finding a suitable unitary representation in $\mathfrak{H}$ of the covering group $\tilde{\mathcal{G}}$. This can be seen as follows: Let ρ be a projective representation of $\mathcal{G}$. Then $\rho \circ p$ is a projective representation of $\tilde{\mathcal{G}}$ which by assumption admits a lifting, i.e.,

$$\rho(p(g)) = \hat{\pi}(g), \quad \text{for all } g \in \mathcal{G}, \tag{2.99}$$

where the operators $\pi(g)$ are unitary (because $\mathcal{G}$ is connected) and form a representation of $\tilde{\mathcal{G}}$ in the Hilbert space $\mathfrak{H}$. Because of $p(\tilde{g}_1) = p(\tilde{g}_2)$ we find

$$\hat{\pi}(\tilde{g}) = \hat{\pi}(\tilde{g}h) = \hat{\pi}(\tilde{g})\hat{\pi}(h), \tag{2.100}$$

hence we must have

$$\pi(h) = e^{i\theta(h)}\mathbf{1} \quad \text{for all } h \in \mathcal{H}. \tag{2.101}$$

Clearly, the operators $\pi(g)$ are unique up to a common phase factor.

Conversely, let π be a unitary representation of the covering group $\tilde{\mathcal{G}}$ in $\mathfrak{H}$ which satisfies (2.101). The symmetry transformations $\hat{\pi}(\tilde{g})$ clearly form a projective unitary representation of $\tilde{\mathcal{G}}$. They depend, however, only on the cosets $\tilde{g}\mathcal{H}$ because $\pi(\tilde{g}h) = \exp(i\theta(h))\pi(\tilde{g})$. Hence π defines a unique projective representation of $\mathcal{G}$ given by

$$\rho(\tilde{g}\mathcal{H}) = \rho(p(g)) = \hat{\pi}(g). \tag{2.102}$$

We have thus proven the following theorem.

Theorem 2.21. Let $\mathcal{G}$ be a connected Lie group and assume that every projective representation ρ of the covering group $\tilde{\mathcal{G}}$ admits a lifting, i.e., there is a unitary representation π of $\tilde{\mathcal{G}}$ such that $\hat{\pi}(\tilde{g}) = \rho(\tilde{g})$, for all $\tilde{g} \in \tilde{\mathcal{G}}$. Then there is a one-to-one correspondence between the projective representations of $\mathcal{G}$ and the unitary representations of $\tilde{\mathcal{G}}$ satisfying (2.101).

This explains the importance of covering groups in quantum mechanics: A group of symmetry transformations (acting on states) is usually realized as a group of unitary operators (acting on vectors in $\mathfrak{H}$) which form a representation of the universal covering group.

2.4.2 A Criterion for the Lifting

The next theorem states that the condition of Theorem 2.21 on the projective representations of the covering group $\tilde{\mathcal{G}}$ can be satisfied, if the Lie algebra of $\mathcal{G}$ (or equivalently of $\tilde{\mathcal{G}}$) has a simple property to be defined below. For the Poincaré Lie algebra we verify this property in the next section.

Theorem 2.22 (Bargmann). Let $\mathcal{G}$ be a simply connected Lie group with Lie algebra $L_{\mathcal{G}}$. Assume that the second cohomology group of the Lie algebra (with coefficients in $\mathbb{R}$) is trivial. Then any projective (and hence projective unitary) representation ρ of $\mathcal{G}$ admits a lifting.

Remark. The triviality of the second cohomology group means that for each bilinear form $\theta : L_{\mathcal{G}} \times L_{\mathcal{G}} \to \mathbb{R}$ satisfying

$$\theta(A,B) = -\theta(B,A), \tag{2.103}$$

$$\theta([A,B],C) + \theta([B,C],A) + \theta([C,A],B) = 0, \tag{2.104}$$

(all A, B, $C \in L_{\mathcal{G}}$) there exists a linear form $\omega : L_{\mathcal{G}} \to \mathbb{R}$ such that

$$\theta(A,B) = \omega([A,B]), \quad \text{for all } A,\, B \in L_{\tilde{\mathcal{G}}}. \tag{2.105}$$

Proof. If ρ is a projective representation, then for each $g \in \mathcal{G}$, $\rho(g)$ is a symmetry transformation which, by the Wigner-Bargmann theorem, is of the form $\rho(g) = \hat{\pi}(g)$, and each operator $\pi(g)$ is unitary (because $\mathcal{G}$ is connected). Each operator $\pi(g)$ is unique only up to a phase. One first has to prove, using the continuity property of the map $g \to \rho(g)$ that the operators $\pi(g)$ can be chosen such that the map $g \to \pi(g)$ is strongly continuous[7]. Still, π is not a representation because

$$\pi(g)\pi(h) = \omega(g,h)\,\pi(gh), \tag{2.106}$$

where ω is a phase factor. Note that ω depends continuously on (g,h) because the maps $(g,h) \to \pi(gh)$, $h \to \pi(h)$ are strongly continuous. By multiplying each $\pi(g)$ with a constant phase factor $\exp(\mathrm{i}\theta)$ we can achieve $\pi(e) = 1$ and hence $\omega(e,e) = 1$. If we can find phase factors $\lambda(g)$, with $g \to \lambda(g)$ continuous, and

$$\lambda(gh) = \omega(g,h)\lambda(g)\lambda(h), \tag{2.107}$$

then the operators

[7] see [Si 68], or [28], p.7

$$\pi'(g) = \lambda(g)\pi(g) \tag{2.108}$$

form a unitary representation of $\mathcal{G}$. To prove existence of suitable phase factors λ one uses a trick. The set $E^\omega = \mathcal{G} \times U(1)$, together with the multiplication

$$(g, \lambda)(h, \mu) = (gh, \omega(g, h)\lambda\mu), \quad \text{all } g,\ h \in \mathcal{G},\ \lambda,\ \mu \in U(1), \tag{2.109}$$

is a Lie group[8]. (In order to prove the associative law for (2.109) one has to use the property (2.47)). Now any continuous homomorphism $\mathcal{G} \to E^\omega$ of the form $g \to (g, \lambda(g))$ would provide us with the desired phase factors. For, let γ be such a homomorphism, then,

$$\begin{aligned}(gh, \lambda(gh)) &= \gamma(gh) = \gamma(g)\gamma(h) = (g, \lambda(g))(h, \lambda(h)) \\ &= (gh, \omega(g, h)\lambda(g)\lambda(h)).\end{aligned} \tag{2.110}$$

The elements in the Lie algebra L_{E^ω} are of the form (A, z), with $A \in L_\mathcal{G}$, and $z \in L_{U(1)} = \mathbb{R}$. Since $\mathcal{G}$ is simply connected, any Lie algebra homomorphism $\mu : L_\mathcal{G} \to L_{E^\omega}$ of the form $\mu(A) = (A, z_\mu)(A))$ defines a unique Lie group homomorphism $\gamma : \mathcal{G} \to E^\omega$ of the form $\gamma(g) = (g, \lambda(g))$, such that $\mu = \gamma'$. The construction of μ runs as follows. Choose any linear map $\beta : L_\mathcal{G} \to L_{E^\omega}$ such that $\beta(A) = (A, z_\beta(A))$. In general, β is not a Lie-algebra homomorphism. Therefore we define

$$\Theta(A, B) = [\beta(A), \beta(B)] - \beta([A, B]) \equiv (0, \theta(A, B)). \tag{2.111}$$

Then the real-valued bilinear form $\theta(A, B)$ satisfies (2.103) and (2.104). By assumption, we may write $\theta(A, B) = \omega([A, B])$. Define

$$\mu(A) = (0, \omega(A)) + \beta(A). \tag{2.112}$$

Then μ is a Lie algebra homomorphism because

$$\begin{aligned}[\mu(A), \mu(B)] &= [\beta(A), \beta(B)] = \Theta(A, B) + \beta([A, B]) \\ &= (0, \omega([A, B])) + \beta([A, B]) = \mu([A, B]).\end{aligned} \tag{2.113}$$

Moreover, $\mu(A) = (A, z_\beta(A) + \omega(A)) \equiv (A, z_\mu(A))$. This completes the proof of Bargmann's theorem. □

2.4.3 The Cohomology of the Poincaré Lie Algebra

The next theorem shows together with Theorem 2.22 that any projective representation of the Poincaré covering group $\tilde{\mathcal{P}}_+^\uparrow$ admits a lifting.

Theorem 2.23 (Bargmann). The Lie algebra $L_\mathcal{P}$ of the Poincaré group has a trivial second cohomology group (with coefficients in $\mathbb{R}$).

[8] This is a nontrivial result. We have to use the fact that a locally euclidean group is also a Lie group. See [176], [318].

Proof. Let θ be any real-valued bilinear form on $L_{\mathcal{P}}$ satisfying (2.103) and (2.104). We have to define a linear form ω such that $\theta(A,B) = \omega([A,B])$. It is sufficient to define ω on the basis $\mathcal{B} = \{-\mathrm{H}_0, \mathrm{p}_k, \mathrm{J}_k, -\mathrm{N}_k; k = 1,2,3\}$ of the Poincaré Lie algebra and extend it by linearity. A short inspection of (2.38) may convince the reader, that any $\mathrm{A} \in \mathcal{B}$ can be written as the Lie bracket of two other basis elements. Hence we define

$$\omega(\mathrm{A}) \equiv \theta(\mathrm{B},\mathrm{C}), \tag{2.114}$$

where B and C have been chosen from $\mathcal{B}$ such that $\mathrm{A} = [\mathrm{B},\mathrm{C}]$. We have to show that this definition does not depend on the particular choice of B and C, i.e.,

$$[\mathrm{B},\mathrm{C}] = [\mathrm{D},\mathrm{E}], \quad \text{implies} \quad \theta(\mathrm{B},\mathrm{C}) = \theta(\mathrm{D},\mathrm{E}). \tag{2.115}$$

It is sufficient to check (2.115) for $\mathrm{B}, \mathrm{C}, \mathrm{D}, \mathrm{E} \in \mathcal{B}$. Then the bilinearity of θ guarantees that (2.115) holds for all $\mathrm{B}, \mathrm{C}, \mathrm{D}, \mathrm{E} \in L_{\mathcal{P}}$. Inspection of (2.45) shows that for example the basis element J_k can be written in two ways as a commutator, namely

$$\mathrm{J}_n = [\mathrm{J}_j, \mathrm{J}_k] = \frac{1}{c^2}[\mathrm{N}_k, \mathrm{N}_j], \tag{2.116}$$

where (k,j,n) is a cyclic permutation of $(1,2,3)$.

$$\begin{aligned} c^2\theta(\mathrm{J}_j,\mathrm{J}_k) &= \theta([\mathrm{N}_r,\mathrm{N}_m],\mathrm{J}_k) = -\theta([\mathrm{N}_m,\mathrm{J}_k],\mathrm{N}_r) - \theta([\mathrm{J}_k,\mathrm{N}_r],\mathrm{N}_m) \\ &= \sum_{p=1}^{3}\{-\epsilon_{kmp}\theta(\mathrm{N}_p,\mathrm{N}_r) + \epsilon_{krp}\theta(\mathrm{N}_p,\mathrm{N}_m)\}, \end{aligned} \tag{2.117}$$

where (r,m,j) is a cyclic permutation of $(1,2,3)$. Since $k \neq j$ we must have $k = r$ or $k = m$. If $k = r$ then $\epsilon_{krp} = 0$. In the first summand only $p = j$ contributes, and $\epsilon_{rmj} = +1$. If $k = m$ only the term with $\epsilon_{krp} = \epsilon_{mrj} = -1$ survives. Hence

$$c^2\theta(\mathrm{J}_j,\mathrm{J}_k) = -\theta(\mathrm{N}_j,\mathrm{N}_k) = \theta(\mathrm{N}_k,\mathrm{N}_j). \tag{2.118}$$

As a second example consider

$$\begin{aligned} c^2\theta(\mathrm{p}_k,\mathrm{p}_j) &= \theta([\mathrm{N}_k,\mathrm{H}_0],\mathrm{p}_j) = -\theta([\mathrm{p}_j,\mathrm{N}_k],\mathrm{H}_0) \\ &= -\delta_{jk}\theta(\mathrm{H}_0,\mathrm{H}_0) = 0. \end{aligned} \tag{2.119}$$

In a similar way we can show using (2.103), (2.104) and (2.38) the relations

$$\begin{aligned} &\theta(\mathrm{p}_k,\mathrm{H}_0) = \theta(\mathrm{J}_k,\mathrm{H}_0) = 0, \\ &\theta(\mathrm{J}_k,\mathrm{p}_k) = \theta(\mathrm{J}_k,\mathrm{N}_k) = 0, \\ &\theta(\mathrm{N}_j,\mathrm{p}_k) = 0, \quad \theta(\mathrm{N}_j,\mathrm{p}_j) = \theta(\mathrm{N}_k,\mathrm{p}_k) = \theta(\mathrm{N}_m,\mathrm{p}_m), \\ &\theta(\mathrm{N}_m,\mathrm{H}_0) = c^2\theta(\mathrm{J}_j,\mathrm{p}_k) = c^2\theta(\mathrm{p}_j,\mathrm{J}_k), \\ &\theta(\mathrm{J}_j,\mathrm{N}_k) = \theta(\mathrm{N}_j,\mathrm{J}_k), \end{aligned} \tag{2.120}$$

where (j,k,m) is a cyclic permutation of $(1,2,3)$. We see that for ω defined as above, we have indeed $\theta(\mathrm{B},\mathrm{C}) = \omega([\mathrm{B},\mathrm{C}])$, all $\mathrm{B},\mathrm{C} \in L_{\mathcal{P}}$. □

2.4.4 Relativistic Invariance of the Dirac Theory

In this section we complete the proof of relativistic invariance of the Dirac theory. We want to show that there is a projective representation of the Poincaré group $\mathcal{P}_+^\uparrow$ in $\hat{\mathfrak{H}}$. We only have to apply Theorem 2.21 which says that a unitary representation of the covering group $\tilde{\mathcal{P}}_+^\uparrow$ corresponds to a unique projective representation of $\mathcal{G}$. We know already, that the Hilbert space $L^2(\mathbb{R}^3)^4$ carries a unitary representation of the covering group (which we obtained via Nelson's theorem) and that the condition of Theorem 2.21 on the lifting of projective representations is satisfied (as a consequence of Bargmann's Theorems 2.22, 2.23). It remains to check the condition (2.101).

In Sect. 2.5 we are going to investigate the Poincaré covering group in more detail. In particular we shall see that the Poincaré group $\mathcal{P}_+^\uparrow$ can be obtained from its covering group by factoring out the discrete group $\{e, h\}$ consisting of the neutral element and an element h which corresponds to a rotation through an angle 2π, i.e., $\mathcal{P}_+^\uparrow = \tilde{\mathcal{P}}_+^\uparrow / \{e, h\}$ (cf. Eq. (2.187)). From Sect. 2.3.4 we know that e and h are represented by $\pi(e) = \mathbf{1}$, and $\pi(h) = \exp(2\pi i J_3) = -\mathbf{1}$. Hence, the representation π satisfies Eq. (2.101), and Theorem 2.21 can be applied. It follows that $\hat{\pi}$ defines is a projective representation of $\mathcal{P}_+^\uparrow$ corresponding uniquely to the unitary representation π of $\tilde{\mathcal{P}}_+^\uparrow$ obtained by exponentiating the Poincaré Lie algebra. This shows that the proper Poincaré group is indeed a symmetry group for the quantum mechanical theory of the Dirac equation.

2.5 The Covering Group of the Lorentz Group

We have shown that the Dirac theory is relativistically invariant, because the Hilbert space of the system carries a representation of the Poincaré covering group. Here we are going to describe the covering group and its representation in the space of Dirac spinors in some detail. We know already from Eq. (2.77) that rotations of wavefunctions in $L^2(\mathbb{R}^3)^4$ are described by (1) transforming the argument and (2) multiplying the components by a 4×4 matrix. In this section we concentrate on the part of a Lorentz transformation acting on the components, i.e., we consider matrix representations of $\mathcal{L}$ (note that translations $\exp(i\boldsymbol{a} \cdot \boldsymbol{p})$ have a trivial matrix part). We start in the two-dimensional spinor space $\mathbb{C}^2$ which is used for the description of particles with zero rest mass. Here the matrix group $SL(2)$ can be defined in such a way that the isomorphism to $\tilde{\mathcal{L}}_+^\uparrow$ becomes obvious. In order to obtain a representation of the parity transformation, it will be necessary to switch to the representation space $\mathbb{C}^4$.

2.5.1 $SL(2)$ and Lorentz Group

The set of all complex Hermitian 2×2 matrices σ will be denoted by $H(2)$:

$$\sigma \in H(2) \quad \text{if and only if} \quad \sigma^{\top} = \overline{\sigma}, \tag{2.121}$$

where the superscript $^{\top}$ denotes the transposed, the bar the complex conjugated matrix. The multiplication of (each element of) a matrix in $H(2)$ with a real number as well as the addition of two matrices in $H(2)$ gives a matrix which is again in $H(2)$. Hence $H(2)$ is a vector space over the real numbers. This vector space is four-dimensional because the Pauli matrices $\sigma_0 \equiv \mathbf{1}_2$, σ_j, $j = 1,2,3$ defined in Sect. 1.1 form a basis of $H(2)$. Using

$$\{\sigma_i, \sigma_k\} = 2\delta_{ik}\mathbf{1}_2, \quad [\sigma_i, \sigma_k] = 2\mathrm{i}\sum_{m=1}^{3} \epsilon_{ikm}\sigma_m \mathbf{1}_2, \quad i,k = 1,2,3, \tag{2.122}$$

$$\operatorname{tr}\sigma_k = 0, \quad k = 1,2,3, \tag{2.123}$$

we see that every matrix σ in $H(2)$ has the representation

$$\sigma \equiv \sigma(x) = \sum_{\mu=0}^{3} x^{\mu}\sigma_{\mu} = \frac{1}{2}\sum_{\mu=0}^{3}(\operatorname{tr}\sigma\sigma_{\mu})\sigma_{\mu}, \quad \text{with } x \in \mathbb{R}^4. \tag{2.124}$$

Clearly, the association of x with $\sigma(x) \in H(2)$ defines an isomorphism of $\mathbb{R}^4$ onto $H(2)$. Another isomorphism is given by

$$x \to \sigma'(x) = x^0\sigma_0 - \sum_{k=1}^{3} x^k\sigma_k = \sum_{\mu=0}^{3} x_{\mu}\sigma_{\mu}. \tag{2.125}$$

It is easy to see that

$$\det\sigma(x) = \det\sigma'(x) = \langle x, x\rangle, \quad \sigma(x)\sigma'(x) = \sigma'(x)\sigma(x) = \langle x, x\rangle\mathbf{1}_2, \tag{2.126}$$

where $\langle\cdot,\cdot\rangle$ is the invariant Lorentz scalar product. With the parallelogram identity we find

$$\begin{aligned}&\tfrac{1}{2}\{\det[\sigma(x) + \sigma(y)] - \det\sigma(x) - \det\sigma(y)\}\\ &\quad = \tfrac{1}{4}\{\det[\sigma(x) + \sigma(y)] - \det[\sigma(x) - \sigma(y)]\} = \langle x, y\rangle.\end{aligned} \tag{2.127}$$

Next we consider the similarity transform of $\sigma(x)$ with a complex 2×2 matrix A,

$$\sigma(x) \to \sigma(y) = A\,\sigma(x)\,A^{*}. \tag{2.128}$$

($A^{*} = \overline{A^{\top}}$ denotes the adjoint matrix). The matrix $\sigma(y)$ is again Hermitian. Its components in the basis of Pauli matrices are determined from

$$y^{\nu} = \frac{1}{2}(\operatorname{tr}\sigma(y)\sigma_{\nu}) = \frac{1}{2}(\operatorname{tr}A\,\sigma(x)\,A^{*}\sigma_{\nu}) = \frac{1}{2}\sum_{\mu=0}^{3}(\operatorname{tr}A\sigma_{\mu}A^{*}\sigma_{\nu})\,x^{\mu}. \tag{2.129}$$

For any A we obtain in this way a linear mapping Λ_A: $x \to y$ of $\mathbb{R}^4$ into itself. Furthermore, if we assume that $\det A = 1$, then we find

$$\langle y, y\rangle = \det\sigma(y) = \det A \, \det\sigma(x) \, \det A^* = \det\sigma(x) = \langle x, x\rangle. \tag{2.130}$$

Because of (2.127) the mapping Λ_A leaves $\langle\cdot,\cdot\rangle$ invariant and defines therefore a Lorentz transformation.

The set of all complex 2×2 matrices A with $\det A = 1$ is a group with respect to matrix multiplication. It is denoted by $SL(2,\mathbb{C})$ or simply $SL(2)$. The vectors in the representation space $\mathbb{C}^2$ are usually called spinors.

Theorem 2.24. For $A \in SL(2)$ define Λ_A as above. The mapping $\Lambda : A \to \Lambda_A$ is a group homomorphism from $SL(2)$ onto $L_+^\uparrow$. Hence

$$\Lambda_{AB} = \Lambda_A \Lambda_B \quad \text{for all } A, B \in SL(2). \tag{2.131}$$

Both $\mathbf{1}_2$ and $-\mathbf{1}_2$ are mapped onto $\mathbf{1}_4$,

$$\Lambda^{-1}(\{\mathbf{1}_4\}) = \{\mathbf{1}_2, -\mathbf{1}_2\}. \tag{2.132}$$

Therefore we may write

$$\mathcal{L}_+^\uparrow = SL(2)/\{\mathbf{1}_2, -\mathbf{1}_2\}. \tag{2.133}$$

Proof. The kernel of the homomorphism Λ is given by

$$Z = \Lambda^{-1}(\{\mathbf{1}_4\}) = \{A \in SL(2) \mid A\sigma A^* = \sigma \text{ for all } \sigma \in H(2)\}. \tag{2.134}$$

Taking $\sigma = \mathbf{1}_2$ we see that $A \in Z$ is unitary. Hence we have $A \in Z$ if and only if $A\sigma = \sigma A$ for all $\sigma \in H(2)$. Hence, A must be a multiple of $\mathbf{1}_2$. But since A must also be unitary, we obtain $A = +\mathbf{1}_2$ or $A = -\mathbf{1}_2$. This proves (2.132). Furthermore $A = \pm B$ if and only if $\Lambda_A = \Lambda_B$, which is another way of writing (2.133). □

The group $\tilde{\mathcal{L}}_+^\uparrow \equiv SL(2)$ is a simply connected Lie group and hence it is isomorphic to the universal covering group of $\mathcal{L}_+^\uparrow$.

2.5.2 Rotations and Boosts

Any matrix A in $SL(2)$ can be written in the form

$$A = HU, \quad H = (A^*A)^{1/2}, \quad U = (A^*A)^{-1/2}A. \tag{2.135}$$

("Polar decomposition"). The square root of A^*A is most easily obtained in the basis of $\mathbb{C}^2$ with respect to which A^*A is diagonal. Since its eigenvalues are real and positive, the square root of A^*A is the diagonal matrix H with the square roots of these eigenvalues in its diagonal. Hence also H is Hermitian

and positive, $\det H = 1$. U is unitary. Hence H and U correspond each to a Lorentz transformation. We consider them separately.

a) Representation of boosts. Let H be any Hermitian 2×2 matrix with $\det H = 1$, i.e., $H \in SL(2)$. The ansatz

$$H = \cosh(\omega/2)\,\sigma_0 + \sum_{k=1}^{3} \sinh(\omega/2)\, n^k \sigma_k = e^{(\omega/2)\boldsymbol{n}\cdot\boldsymbol{\sigma}}, \tag{2.136}$$

with ω real and n^k being the components of a unit vector, automatically satisfies $\det H = 1$. The matrix elements of Λ_H can be read off from Eq. (2.129). If we compare this matrix with Eq. (2.14) we see that Λ_H is a pure boost with velocity

$$\frac{\boldsymbol{v}}{c} = \tanh(\omega)\boldsymbol{n}. \tag{2.137}$$

b) Representation of rotations. For any unitary matrix $U \in SU(2)$ (the group of complex unitary 2×2 matrices with determinant 1) we may write

$$U = \cos(\varphi/2)\,\sigma_0 - \mathrm{i}\sin(\varphi/2)\,\boldsymbol{n}\cdot\boldsymbol{\sigma} = e^{-\mathrm{i}(\varphi/2)\boldsymbol{n}\cdot\boldsymbol{\sigma}}. \tag{2.138}$$

with φ in $[0, 4\pi)$ and $\boldsymbol{n}$ being a three-dimensional real unit vector. Again we determine the matrix elements of Λ_U from Eq. (2.129). Comparison with (2.11) and (2.12) shows that Λ_U is a pure rotation around the axis $\boldsymbol{n}$ through an angle φ. If we replace $\varphi \to \varphi + 2\pi$, then $U \to -U$, but $\Lambda_U = \Lambda_{-U}$. In particular any "rotation through 2π" is represented by $-\mathbf{1}_2 \in SL(2)$.

The polar decomposition $A = HU$ of a $SL(2)$-matrix A obviously corresponds to the decomposition (2.23) of proper Lorentz transformations into boosts and rotations.

2.5.3 Nonequivalent Representations of $SL(2)$

When defining a correspondence between $SL(2)$ and Lorentz transformations, we have used the isomorphism $x \to \sigma(x)$ defined in (2.124). Let us now use the isomorphism $x \to \sigma'(x)$ of Eq. (2.125). Indeed,

$$\sigma'(x) \to \sigma'(y) = B\,\sigma'(x)\,B^*, \quad B \in SL(2), \tag{2.139}$$

defines again a Lorentz transformation. What is the connection between A and B if they correspond both to the same Lorentz transformation? With

$$\sigma'(x) = \sigma_2\,\overline{\sigma(x)}\,\sigma_2, \quad \overline{\sigma(x)} = \sigma_2\,\sigma'(x)\,\sigma_2, \tag{2.140}$$

we calculate

$$\sigma'(y) = \sigma_2\,\overline{A\,\sigma(x)\,A^*}\,\sigma_2 = (\sigma_2\overline{A}\sigma_2)\,\sigma'(x)\,(\sigma_2\overline{A}\sigma_2)^* = B\sigma'(x)B^*. \tag{2.141}$$

But for all $A \in SL(2)$

$$\sigma_2 \overline{A} \sigma_2 = (A^*)^{-1}, \tag{2.142}$$

hence

$$B = (A^*)^{-1}. \tag{2.143}$$

The map $A \to B$ is a group automorphism of $SL(2)$. The two representations of $SL(2)$ defined by the matrices A ("defining representation") resp. B are not equivalent. For equivalent representations A and $A' = TAT^{-1}$ we must have $\operatorname{tr} A' = \operatorname{tr} A$, all A. But with $A' = (A^*)^{-1}$ this condition is violated for the matrix

$$A = \begin{pmatrix} 2\mathrm{i} & 0 \\ 0 & -\mathrm{i}/2 \end{pmatrix}. \tag{2.144}$$

Remark 1. The automorphism $A \to B$ corresponds to space reflections. We have

$$\Lambda_{(A^*)^{-1}} = P \Lambda_A P^{-1}, \tag{2.145}$$

with P as in (2.18). In $SL(2)$ there is no element corresponding to P, i.e., the map $\sigma(x) \to \sigma'(x) = \sigma_2 \overline{\sigma(x)} \sigma_2 = \sigma(x)^{-1}$ cannot be described as $A \sigma(x) A^*$ with $A \in SL(2)$.

Remark 2. Another automorphism of $SL(2)$ is provided by $A \to \overline{A}$.

2.5.4 Linear Representation of the Space Reflection

The considerations above show that there is no possibility of covering the full Lorentz group with $SL(2)$ matrices, because the space reflection P cannot be described in this way. The fact that the space reflection P is given by the automorphism $A \leftrightarrow (A^*)^{-1}$ suggests to double the dimension of the representation space in order to obtain a matrix representation of P. In the linear space $\mathbb{C}^4$ we combine the matrices A and $(A^*)^{-1}$ into 4×4 matrices of the form

$$\mathbf{L}_A = \begin{pmatrix} A & 0 \\ 0 & (A^*)^{-1} \end{pmatrix}, \quad \text{with } A \in SL(2). \tag{2.146}$$

The automorphism $A \leftrightarrow (A^*)^{-1}$ can now be represented by the matrix

$$\mathbf{L}_P = \begin{pmatrix} 0 & \mathbf{1}_2 \\ \mathbf{1}_2 & 0 \end{pmatrix}, \tag{2.147}$$

which satisfies

$$\mathbf{L}_P \mathbf{L}_A \mathbf{L}_P^{-1} = \mathbf{L}_{(A^*)^{-1}} = (\mathbf{L}_A^*)^{-1}, \qquad \mathbf{L}_P^2 = \mathbf{1}_4. \tag{2.148}$$

The matrices $\mathbf{L}_A$ form a group with respect to matrix multiplication. This group is obviously isomorphic to the covering group $SL(2)$ of the proper Lorentz group $\mathcal{L}_+^\uparrow$. In fact, the map $A \to \mathbf{L}_A$ given by (2.146) defines an injective representation of $SL(2)$ which is reducible. There are two (and only two) invariant subspaces which are mapped on each other by the matrix $\mathbf{L}_P$. Hence, the matrix group

$$\tilde{\mathcal{L}}^\uparrow \equiv \{\mathbf{L}_A, \mathbf{L}_P \mathbf{L}_A \mid A \in SL(2)\} \tag{2.149}$$

acts irreducibly on $\mathbb{C}^4$. (2.148) shows that the element $\mathbf{L}_P$ represents a space reflection.

2.5.5 Gamma Matrices

In order to describe the connection of $\mathbf{L}_A$ with Lorentz transformations more precisely, we proceed similarly as in Sect. 2.4.1: We define a suitable 4×4 matrix $\gamma(x)$ for each $x \in \mathbb{R}^4$, such that a Lorentz transformation can be described as a similarity transformation of $\gamma(x)$. An obvious choice is

$$\gamma(x) \equiv \begin{pmatrix} 0 & \sigma(x) \\ \sigma'(x) & 0 \end{pmatrix}, \tag{2.150}$$

with $\sigma(x)$ and $\sigma'(x)$ defined as in (2.124) and (2.125), because with $B \equiv (A^*)^{-1}$ we obtain

$$\mathbf{L}_A \, \gamma(x) \, \mathbf{L}_A^{-1} = \begin{pmatrix} 0 & A\,\sigma(x)\,A^* \\ B\,\sigma'(x)\,B^* & 0 \end{pmatrix} = \gamma(\Lambda_A x), \tag{2.151}$$

$$\mathbf{L}_P \, \gamma(x) \, \mathbf{L}_P^{-1} = \begin{pmatrix} 0 & \sigma'(x) \\ \sigma(x) & 0 \end{pmatrix} = \gamma(Px), \tag{2.152}$$

where P is the parity transform defined in (2.18).

The bijective map

$$\gamma : x \leftrightarrow \gamma(x), \quad x \in \mathbb{R}^4, \tag{2.153}$$

is an isomorphism of the vector space $\mathbb{R}^4$ and the four dimensional real vector space of matrices of the form (2.150). The canonical basis $\{e_0, \ldots, e_3\}$ in $\mathbb{R}^4$ is mapped to the 4×4 matrices

$$\gamma_0 = \gamma(e_0) = \begin{pmatrix} 0 & \mathbf{1}_2 \\ \mathbf{1}_2 & 0 \end{pmatrix}, \quad \gamma_k = \gamma(e_k) = \begin{pmatrix} 0 & \sigma_k \\ -\sigma_k & 0 \end{pmatrix}. \tag{2.154}$$

($k = 1, 2, 3$). It is useful to combine the four γ matrices into a matrix four vector

$$\gamma = (\gamma^0, \gamma^1, \gamma^2, \gamma^3) = (\gamma_0, -\gamma_1, -\gamma_2, -\gamma_3), \tag{2.155}$$

and write

$$\gamma(x) = \sum_{\mu=0}^{3} \gamma_\mu x^\mu \equiv \langle \gamma, x \rangle = \gamma^0 x^0 - \gamma^1 x^1 - \gamma^2 x^2 - \gamma^3 x^3. \tag{2.156}$$

One easily finds using (2.122)

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\mu\nu}\mathbf{1}, \quad \mu, \nu = 0, 1, 2, 3. \tag{2.157}$$

Hence the matrices

$$\beta = \gamma^0, \quad \alpha^k = \gamma^0 \gamma^k = \begin{pmatrix} \sigma_k & 0 \\ 0 & -\sigma_k \end{pmatrix} \tag{2.158}$$

satisfy the anticommutation relations (1.6) of the Dirac matrices $\boldsymbol{\alpha}$ and β. Indeed, (2.158) are just the Dirac matrices in the Weil representation (see Appendix 1.A).

By construction, for every $\mathbf{L} \in \tilde{\mathcal{L}}^\uparrow$ there is a $\Lambda_{\mathbf{L}} \in \mathcal{L}^\uparrow$ such that

$$\mathbf{L}\langle \gamma, x \rangle \mathbf{L}^{-1} = \langle \gamma, \Lambda_{\mathbf{L}} x \rangle, \tag{2.159}$$

and the map $\mathbf{L} \to \Lambda_{\mathbf{L}}$ from $\tilde{\mathcal{L}}^\uparrow$ to $\mathcal{L}^\uparrow$ is onto and a homomorphism (the "covering homomorphism"). Hence $\tilde{\mathcal{L}}^\uparrow$ covers $\mathcal{L}^\uparrow$. If we define

$$(\Lambda_{\mathbf{L}} \gamma)^\nu = \sum_{\mu=0}^{3} (\Lambda_{\mathbf{L}})^\nu{}_\mu \gamma^\mu, \tag{2.160}$$

then, in view of (2.5),

$$\langle \Lambda_{\mathbf{L}} \gamma, \Lambda_{\mathbf{L}} x \rangle = \langle \gamma, x \rangle. \tag{2.161}$$

With (2.159) this implies

$$\mathbf{L}^{-1} \langle \gamma, x \rangle \mathbf{L} = \langle \gamma, \Lambda_{\mathbf{L}}^{-1} x \rangle = \langle \Lambda_{\mathbf{L}} \gamma, x \rangle \quad \text{for all } x, \tag{2.162}$$

therefore,

$$\Lambda_{\mathbf{L}} \gamma = \mathbf{L}^{-1} \gamma \mathbf{L}, \quad \text{all } \mathbf{L} \in \tilde{\mathcal{L}}^\uparrow. \tag{2.163}$$

The matrix $\Lambda_{\mathbf{L}}$ is given by

$$(\Lambda_{\mathbf{L}})^\mu{}_\nu = \tfrac{1}{4} \operatorname{tr} \mathbf{L}^{-1} \gamma^\mu \mathbf{L} \gamma_\nu. \tag{2.164}$$

Conversely, $\mathbf{L}$ is determined by Λ up to a sign, see Appendix 2.D.

2.5.6 Equivalent Representations

If $\gamma'^\mu = S\gamma^\mu S^{-1}$ with a (nonsingular) matrix S, then we could choose the matrices

$$\{S\mathbf{L}S^{-1} \mid \mathbf{L} \in \tilde{\mathcal{L}}^\uparrow\} \tag{2.165}$$

as an equivalent four dimensional representation of $\tilde{\mathcal{L}}^{\uparrow}$. The formulas (2.155)-(2.163) remain true if we write γ' instead of γ and $S\mathbf{L}S^{-1}$ instead of $\mathbf{L}$.

Lemma 2.25 (Pauli). Let γ'^{μ}, $\mu = 0, \ldots, 3$, be any other set of matrices satisfying (2.157). Then, with the γ matrices defined in (2.155),

$$\gamma'^{\mu} = S\gamma^{\mu}S^{-1}, \quad \mu = 0, 1, 2, 3, \tag{2.166}$$

with a nonsingular 4×4 matrix S which is unique except for a scalar factor.

Proof. We use the γ and γ'-matrices to form Γ and Γ' matrices as in Appendix 2.A. The basic idea is to choose

$$S = \sum_{k=1}^{16} \Gamma'_k F \Gamma_k \tag{2.167}$$

with a suitable 4×4 matrix F. First note, that for arbitrary F,

$$\Gamma'_j S \Gamma_j = \sum_{k=1}^{16} \Gamma'_j \Gamma'_k F \Gamma_k \Gamma_j = \sum_{m=1}^{16} \Gamma'_m F \Gamma_m = S, \tag{2.168}$$

where we have used Eqs. (2.206), (2.207) of Appendix 2.B. The matrix

$$T = \sum_{k=1}^{16} \Gamma_k G \Gamma'_k \tag{2.169}$$

has the same property for any 4×4 matrix G. Now, choose G such that T is nonzero. (This is possible, because if T were zero for all G, then we would have $\sum(\Gamma'_k)_{ij}\Gamma_k = 0$ by choosing appropriate matrices G. This contradicts the linear independence of the Γ-matrices). The matrix TS is now easily seen to satisfy

$$\Gamma_k TS = TS\Gamma_k. \tag{2.170}$$

Hence, by the lemma of Schur, TS must be a multiple of the unit matrix, $TS = k$. But now F can be chosen such that $k \neq 0$, otherwise we could construct the equation $\sum(T\Gamma'_k)\Gamma_k = 0$ by suitable choices of F which again contradicts the linear independence. The uniqueness follows because $S_1\gamma^{\mu}S_1^{-1} = S_2\gamma^{\mu}S_2^{-1}$ implies $S_2^{-1}S_1\Gamma_k = \Gamma_k S_2^{-1}S_1$ for all k, hence $S_2^{-1}S_1$ is a multiple of the unit matrix. □

Using γ matrices we can write the matrices $\mathbf{L}$ corresponding to boosts or rotations in a representation-independent way. Using (2.158) and (2.136), resp. (2.138), we find

$$\mathbf{L}_H = e^{(\omega/2)\boldsymbol{n}\cdot\boldsymbol{\alpha}}, \quad \text{boost with velocity } \boldsymbol{v} = c\tanh(\omega)\boldsymbol{n}, \tag{2.171}$$

$$\mathbf{L}_U = e^{-\mathrm{i}\varphi\boldsymbol{n}\cdot\boldsymbol{S}}, \quad \text{rotation through an angle } \varphi \text{ around } \boldsymbol{n}, \tag{2.172}$$

$$\mathbf{L}_P = \gamma^0 = \beta, \qquad \text{space reflection.} \tag{2.173}$$

The generators of rotations are obviously the components of the spin angular momentum operator $\boldsymbol{S}$, where each component $S_j = \sigma_j/2$ has eigenvalues $1/2$ and $-1/2$. Hence this representation of the rotation group is called a representation with spin-1/2. More on the classification of all finite dimensional representations of the rotation and Lorentz groups can be found, e.g., in [Ma 68].

Remark. The Hilbert space $\mathfrak{H}$ of the Dirac equation consists of $\mathbb{C}^4$-valued wavefunctions. In Sect. 2.3 we obtained a unitary representation of the Poincaré-covering group where the rotations are given by $e^{-\mathrm{i}\varphi\boldsymbol{n}\cdot\boldsymbol{J}} = e^{-\mathrm{i}\varphi\boldsymbol{n}\cdot\boldsymbol{L}} e^{-\mathrm{i}\varphi\boldsymbol{n}\cdot\boldsymbol{S}}$. Eq. (2.172) obviously describes the "matrix-part" of these transformations, i.e., the part acting on the spinor components of the wavefunctions without affecting their argument. It will become clear during the construction of the "covariant representation" in Chapter 3, that all matrices $\mathbf{L} \in \tilde{\mathcal{L}}^{\uparrow}$ describe the matrix part of the corresponding Poincaré transformation in $\mathfrak{H}$: The covariant representation π^{c} acts on solutions $\psi(x)$, $x = (x_0, \boldsymbol{x})$ of the Dirac equation by $[\pi^{\mathrm{c}}(\mathbf{L})\psi](x) = \mathbf{L}\,\psi(\Lambda_{\mathbf{L}}^{-1}x)$.

2.5.7 Time Reversal and Space Time Reflections

The vector space $\mathbb{C}^4$ is large enough to permit the description of time reversal and space-time reflections. For a time reversal we must have

$$\begin{aligned}\mathbf{L}_T\langle\gamma, x\rangle\mathbf{L}_T^{-1} &= \mathbf{L}_T \begin{pmatrix} 0 & \sigma'(x) \\ \sigma(x) & 0 \end{pmatrix} \mathbf{L}_T^{-1} \\ &\stackrel{!}{=} \begin{pmatrix} 0 & -\sigma(x) \\ -\sigma'(x) & 0 \end{pmatrix} = \langle\gamma, Tx\rangle. \end{aligned} \tag{2.174}$$

This is trivially achieved if we choose

$$\mathbf{L}_T \equiv \begin{pmatrix} 0 & -\mathrm{i}\mathbf{1}_2 \\ \mathrm{i}\mathbf{1}_2 & 0 \end{pmatrix} \tag{2.175}$$

which satisfies

$$\mathbf{L}_T^2 = \mathbf{1}_4. \tag{2.176}$$

The space-time reflection can be defined as

$$\mathbf{L}_{PT} \equiv \mathbf{L}_P\mathbf{L}_T = \begin{pmatrix} \mathrm{i}\mathbf{1}_2 & 0 \\ 0 & -\mathrm{i}\mathbf{1}_2 \end{pmatrix}. \tag{2.177}$$

One should not be irritated by the minus sign in the formulas

$$\mathbf{L}_P\mathbf{L}_T = -\mathbf{L}_T\mathbf{L}_P, \quad \mathbf{L}_{PT}^2 = -\mathbf{1}_4, \tag{2.178}$$

because $-\mathbf{1}_4$ corresponds like $+\mathbf{1}_4$ to the identity in the Lorentz group. The crucial relation, which shows that $\mathbf{L}_{PT}$ indeed corresponds to a space-time reflection, is

$$\mathbf{L}_{PT}\,\langle\gamma,x\rangle\,\mathbf{L}_{PT}^{-1} = -\langle\gamma,x\rangle = \langle\gamma,-x\rangle = \langle\gamma,PTx\rangle. \tag{2.179}$$

Hence the set of 4×4 matrices

$$\tilde{\mathcal{L}} \equiv \{\mathbf{L},\mathbf{L}_P\mathbf{L},\mathbf{L}_T\mathbf{L},\mathbf{L}_{PT}\mathbf{L} \mid \mathbf{L}\in\tilde{\mathcal{L}}_+^\uparrow\} \tag{2.180}$$

together with the matrix multiplication is a covering group of the full Lorentz group. The covering homomorphism is given by $\Lambda : \mathbf{L} \to \Lambda_{\mathbf{L}}$, where $\Lambda_{\mathbf{L}}$ is the unique Lorentz transformation given by

$$\mathbf{L}\langle\gamma,x\rangle\mathbf{L}^{-1} = \langle\gamma,\Lambda_{\mathbf{L}}x\rangle, \quad \text{all } \mathbf{L}\in\tilde{\mathcal{L}}. \tag{2.181}$$

Remark. The formula (2.179) remains true if we replace $\mathbf{L}_{PT}$ by $\mathbf{L}_T\mathbf{L}_P = -\mathbf{L}_{PT}$. This replacement would result in another covering group of the full Lorentz group. Since the full Lorentz group $\mathcal{L}$ is not connected, it has no unique covering group. In a covering group each of the three discrete elements can have its square equal to $\mathbf{1}$ or $-\mathbf{1}$ in $\tilde{\mathcal{L}}_+^\uparrow$ because both elements are mapped to the identity in $\tilde{\mathcal{L}}_+^\uparrow$ by the covering homomorphism. Indeed, one can choose, e.g.,

$$\mathbf{L}'_P = \mathrm{i}\begin{pmatrix} 0 & \mathbf{1}_2 \\ \mathbf{1}_2 & 0 \end{pmatrix} \tag{2.182}$$

for the space inversion while leaving $\mathbf{L}_T$ and $\mathbf{L}_{PT}$ unchanged. In this case ($\mathbf{L}_P'^2 = -\mathbf{1}_4$, i.e., two reflections correspond to a rotation trough an angle 2π. The resulting group is again a covering group of the Lorentz group, but it is not isomorphic to $\tilde{\mathcal{L}}$. In fact, there are eight non-isomorphic covering groups of $\mathcal{L}$. From the point of view of quantum mechanics it is a matter of convention which covering group is chosen, because they all lead to the same projective representation of the Poincaré group.

2.5.8 A Covering Group of the Full Poincaré Group

Given a covering group of the Lorentz group $\mathcal{L}$ it is easy to find a covering group of the Poincaré group P by forming the semidirect product with the translation group. To this purpose we define an action of $\tilde{\mathcal{L}}$ on $\mathbb{R}^4$ by $a \to \Lambda_{\mathbf{L}}a$, for $a\in\mathbb{R}^4$, where $\Lambda_{\mathbf{L}}$ is the Lorentz transformation corresponding to $\mathbf{L}\in\tilde{\mathcal{L}}$ via (2.181). Hence we may define the semidirect product (cf. Sect. 2.1.5)

$$\tilde{\mathcal{P}} = \mathbb{R}^4 \odot \tilde{\mathcal{L}} \tag{2.183}$$

consisting of pairs $(a,\mathbf{L})$ with the multiplication rule

$$(a,\mathbf{L}_1)(b,\mathbf{L}_2) = (a+\Lambda_{\mathbf{L}_1}b,\mathbf{L}_1\mathbf{L}_2). \tag{2.184}$$

$\tilde{\mathcal{P}}$ is the union of the four connected subsets

$$\tilde{\mathcal{P}}_+^\uparrow = \mathbb{R}^4 \odot \tilde{\mathcal{L}}_+^\uparrow, \qquad \tilde{\mathcal{P}}_-^\uparrow = (0, \mathbf{L}_P)\tilde{\mathcal{P}}_+^\uparrow, \tag{2.185}$$

$$\tilde{\mathcal{P}}_-^\downarrow = (0, \mathbf{L}_T)\tilde{\mathcal{P}}_+^\uparrow, \qquad \tilde{\mathcal{P}}_+^\downarrow = (0, \mathbf{L}_{PT})\tilde{\mathcal{P}}_+^\uparrow. \tag{2.186}$$

The connected component of the identity is the universal covering group of the proper Poincaré group. Denoting the neutral element $(0, \mathbf{1}_4)$ of $\tilde{\mathcal{P}}_+^\uparrow$ by e and $(0, -\mathbf{1}_4)$ by h, then it is clear from (2.133) that

$$\mathcal{P}_+^\uparrow = \tilde{\mathcal{P}}_+^\uparrow / \{e, h\}. \tag{2.187}$$

It is clear from Eq. (2.172) that $h = (0, -\mathbf{1}_4) = (0, e^{2\pi \mathrm{i} S_3})$ corresponds to a "rotation through an angle 2π".

Appendix

2.A Algebra of Gamma Matrices

From products of γ-matrices we can form the following 16 linearly independent matrices Γ_n, which form a basis in the space of complex 4×4 matrices. We give these matrices explicitly in the standard representation in 2×2 block matrix form, using the Pauli matrices σ_k together with the 2×2 unit matrix 1.

$$\Gamma_1 \equiv \mathbf{1}_4 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{2.188}$$

$$\Gamma_2 \equiv \gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.189}$$

$$\Gamma_3 \equiv \mathrm{i}\gamma^1 = \begin{pmatrix} 0 & \mathrm{i}\sigma_1 \\ -\mathrm{i}\sigma_1 & 0 \end{pmatrix}, \tag{2.190}$$

$$\Gamma_4 \equiv \mathrm{i}\gamma^2 = \begin{pmatrix} 0 & \mathrm{i}\sigma_2 \\ -\mathrm{i}\sigma_2 & 0 \end{pmatrix}, \tag{2.191}$$

$$\Gamma_5 \equiv \mathrm{i}\gamma^3 = \begin{pmatrix} 0 & \mathrm{i}\sigma_3 \\ -\mathrm{i}\sigma_3 & 0 \end{pmatrix}, \tag{2.192}$$

$$\Gamma_6 \equiv \gamma^0\gamma^1 \equiv -\mathrm{i}\sigma^{01} = \alpha_1 = \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix}, \tag{2.193}$$

$$\Gamma_7 \equiv \gamma^0\gamma^2 \equiv -\mathrm{i}\sigma^{02} = \alpha_2 = \begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix}, \tag{2.194}$$

$$\Gamma_8 \equiv \gamma^0\gamma^3 \equiv -\mathrm{i}\sigma^{03} = \alpha_3 = \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}, \tag{2.195}$$

$$\Gamma_9 \equiv \mathrm{i}\gamma^2\gamma^3 \equiv \sigma^{23} = \Sigma_1 = \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_1 \end{pmatrix}, \tag{2.196}$$

$$\Gamma_{10} \equiv \mathrm{i}\gamma^3\gamma^1 \equiv \sigma^{31} = \Sigma_2 = \begin{pmatrix} \sigma_2 & 0 \\ 0 & \sigma_2 \end{pmatrix}, \tag{2.197}$$

$$\Gamma_{11} \equiv \mathrm{i}\gamma^1\gamma^2 \equiv \sigma^{12} = \Sigma_3 = \begin{pmatrix} \sigma_3 & 0 \\ 0 & \sigma_3 \end{pmatrix}, \tag{2.198}$$

$$\Gamma_{12} \equiv \gamma^1\gamma^2\gamma^3 = -\mathrm{i}\gamma_5\gamma^0 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \tag{2.199}$$

$$\Gamma_{13} \equiv \mathrm{i}\gamma^0\gamma^2\gamma^3 = \gamma_5\gamma^1 = \begin{pmatrix} \sigma_1 & 0 \\ 0 & -\sigma_1 \end{pmatrix}, \tag{2.200}$$

$$\Gamma_{14} \equiv \mathrm{i}\gamma^0\gamma^3\gamma^1 = \gamma_5\gamma^2 = \begin{pmatrix} \sigma_2 & 0 \\ 0 & -\sigma_2 \end{pmatrix}, \tag{2.201}$$

$$\Gamma_{15} \equiv \mathrm{i}\gamma^0\gamma^1\gamma^2 = \gamma_5\gamma^3 = \begin{pmatrix} \sigma_3 & 0 \\ 0 & -\sigma_3 \end{pmatrix}, \tag{2.202}$$

$$\Gamma_{16} \equiv \mathrm{i}\gamma^0\gamma^1\gamma^2\gamma^3 = \gamma_5 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{2.203}$$

2.B Basic Properties of Gamma Matrices

The Γ-matrices are traceless (except Γ_1), Γ_k is Hermitian for all k, and

$$\Gamma_k^2 = 1, \qquad \Gamma_k^{-1} = \Gamma_k, \qquad \text{for all } k. \tag{2.204}$$

Multiply the equation $\sum_{k=1}^{16} \lambda_k \Gamma_k = 0$ by Γ_l and take the trace to obtain $\lambda_l = 0$. This shows that the Γ-matrices are linearly independent. Any complex 4×4 matrix M can be written as a linear combination

$$M = \sum_{k=1}^{16} m_k \Gamma_k, \qquad m_k = \frac{1}{4} \operatorname{tr}(\Gamma_k M). \tag{2.205}$$

For any two matrices Γ_j, Γ_k there is a unique matrix Γ_m, such that

$$\Gamma_j \Gamma_k = \epsilon_{jk} \Gamma_m, \quad \text{where } \epsilon_{jk} \in \{1, -1, \mathrm{i}, -\mathrm{i}\}. \tag{2.206}$$

If Γ_j is held fixed, then, as k ranges from 1 to 16, m must range also from 1 to 16. To see this, assume that for $l \neq k$, and with the same m as in (2.206) $\Gamma_j \Gamma_l = \epsilon_{jl} \Gamma_m$. Then $\Gamma_k = \epsilon_{jk} \Gamma_j \Gamma_m = \epsilon_{jk} \epsilon_{jl}^{-1} \Gamma_l$, which contradicts the assumed linear independence of Γ_k and Γ_l. Taking the inverse on both sides of Eq. (2.206) we find

$$\Gamma_k \Gamma_j = \epsilon_{jk}^{-1} \Gamma_m. \tag{2.207}$$

2.C Commutation Formulas

$$[\gamma^\mu, \gamma^\nu] = [\gamma_5\gamma^\mu, \gamma_5\gamma^\nu] = 2\gamma^\mu\gamma^\nu - 2g^{\mu\nu}\mathbf{1} = -2\mathrm{i}\sigma^{\mu\nu}, \tag{2.208}$$

$$[\sigma^{\mu\nu}, \gamma^\rho] = \mathrm{i}[\gamma^\mu\gamma^\nu, \gamma^\rho] = 2\mathrm{i}(\gamma^\mu g^{\nu\rho} - \gamma^\nu g^{\mu\rho}), \tag{2.209}$$

$$\begin{aligned}[\sigma^{\mu\nu}, \sigma^{\rho\tau}] &= -[\gamma^\mu\gamma^\nu, \gamma^\rho\gamma^\tau] \\ &= -2\mathrm{i}(\sigma^{\mu\rho}g^{\nu\tau} - \sigma^{\mu\tau}g^{\nu\rho} + \sigma^{\nu\tau}g^{\mu\rho} - \sigma^{\nu\rho}g^{\mu\tau}),\end{aligned} \tag{2.210}$$

$$[\gamma_5, \gamma^\mu] = 2\gamma_5\gamma^\mu, \tag{2.211}$$

$$[\gamma_5, \gamma^\mu\gamma_5] = 2\gamma^\mu, \tag{2.212}$$

$$[\gamma_5, \sigma^{\mu\nu}] = [\gamma_5, \gamma^\mu\gamma^\nu] = 0, \tag{2.213}$$

$$\{\gamma_5, \gamma^\mu\} = 0, \tag{2.214}$$

$$\{\sigma^{\mu\nu}, \gamma^\rho\} = -2\gamma_5\epsilon^{\mu\nu\rho\tau}\gamma_\tau. \tag{2.215}$$

2.D Dirac-Matrix Representation of Lorentz Transformations

Let $\mathbf{L} \in \tilde{\mathcal{L}}^\uparrow$. It satisfies

$$\mathbf{L}\,\gamma^0 = \gamma^0\,\mathbf{L}^{*-1}, \qquad \mathbf{L}\,\gamma_5 = \gamma_5\,\mathbf{L}. \tag{2.216}$$

The matrix

$$\Lambda^\mu{}_\nu = \tfrac{1}{4}(\mathrm{tr}\,\gamma^\mu\mathbf{L}\gamma_\nu\mathbf{L}^{-1}) \tag{2.217}$$

is the matrix of a Lorentz transformation in $\mathcal{L}^\uparrow$. Conversely,

$$\begin{aligned}\mathbf{L} = \pm\frac{1}{4\sqrt{G(\Lambda)}}\Big(&G(\Lambda) - \tfrac{\mathrm{i}}{2}\epsilon_{\mu\nu\rho\tau}\Lambda^{\mu\nu}\Lambda^{\rho\tau}\gamma_5 + \\ &+ \mathrm{i}\Lambda_{\kappa\rho}\Lambda^\rho_\tau\sigma^{\kappa\tau} - \mathrm{i}(2 + \mathrm{tr}\,\Lambda)\Lambda_{\mu\nu}\sigma^{\mu\nu}\Big),\end{aligned} \tag{2.218}$$

where

$$G(\Lambda) = 2(1 + \mathrm{tr}\,\Lambda) + \tfrac{1}{2}(\mathrm{tr}\,\Lambda)^2 - \tfrac{1}{2}(\mathrm{tr}\,\Lambda^2). \tag{2.219}$$

For boosts and rotations, (2.218) reduces to (2.171) and (2.172), respectively.

2.E Expansion of Products of Gamma Matrices

$$\gamma^\mu\gamma^\nu = g^{\mu\nu}\mathbf{1} - \mathrm{i}\sigma^{\mu\nu}, \tag{2.220}$$

$$\gamma_5\gamma^\mu\gamma_5 = -\gamma^\mu, \tag{2.221}$$

$$\sigma^{\mu\nu}\gamma_5 = \tfrac{\mathrm{i}}{2}\,\epsilon^{\mu\nu\rho\tau}\sigma_{\rho\tau}, \tag{2.222}$$

$$\gamma^\mu\gamma^\nu\gamma^\rho = g^{\mu\nu}\gamma^\rho - g^{\mu\rho}\gamma^\nu + g^{\nu\rho}\gamma^\mu + \mathrm{i}\epsilon^{\mu\nu\rho\sigma}\gamma_\sigma\gamma_5, \tag{2.223}$$

$$\gamma^\mu\gamma^\nu\gamma^5 = g^{\mu\nu}\gamma_5 - \tfrac{\mathrm{i}}{2}\,\epsilon^{\mu\nu\rho\sigma}\gamma_\rho\gamma_\sigma. \tag{2.224}$$

2.F Formulas with Traces

$$\operatorname{tr} \Gamma_k = 0, \quad k = 2, \ldots, 16, \tag{2.225}$$

$$\operatorname{tr} \Gamma_k \Gamma_l = 0, \quad \text{for } k \neq l, \text{ and } k, l = 1, \ldots, 16, \tag{2.226}$$

$$\operatorname{tr} \gamma^\mu \gamma^\nu = 4g^{\mu\nu}, \tag{2.227}$$

$$\operatorname{tr} \gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma = 4(g^{\mu\nu} g^{\rho\sigma} - g^{\mu\rho} g^{\nu\sigma} + g^{\mu\sigma} g^{\nu\rho}), \tag{2.228}$$

$$\operatorname{tr} \sigma^{\mu\nu} \sigma^{\rho\sigma} = 4(g^{\mu\rho} g^{\nu\sigma} - g^{\nu\rho} g^{\mu\sigma}), \tag{2.229}$$

$$\operatorname{tr} \gamma_5 \gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma = -4\mathrm{i}\epsilon^{\mu\nu\rho\sigma}, \tag{2.230}$$

$$\operatorname{tr} \gamma^{\mu_1} \ldots \gamma^{\mu_n} = 0, \qquad \text{for } n \text{ odd}, \tag{2.231}$$

$$\begin{aligned} \operatorname{tr} \gamma^{\mu_1} \ldots \gamma^{\mu_n} = {} & g^{\mu_1 \mu_2} (\operatorname{tr} \gamma^{\mu_3} \ldots \gamma^{\mu_n}) - g^{\mu_1 \mu_3} (\operatorname{tr} \gamma^{\mu_2} \gamma^{\mu_4} \ldots \gamma^{\mu_n}) + \\ & + g^{\mu_1 \mu_n} (\operatorname{tr} \gamma^{\mu_2} \ldots \gamma^{\mu_{n-1}}), \quad \text{for } n \text{ even}. \end{aligned} \tag{2.232}$$

3 Induced Representations

In this chapter we intend to illustrate the role of the Dirac equation in the general theory of unitary group representations. We show that the Dirac equation arises quite naturally in a construction of certain irreducible representations of the Poincaré covering group. Besides, we describe explicitly the behavior of wavefunctions $\psi(\boldsymbol{x}, t)$ under the transformations generated by H_0, $\boldsymbol{p}$, $\boldsymbol{J}$, and $\boldsymbol{N}$ (which represent the Poincaré Lie algebra, see Chapter 2).

A full classification of all unitary representations of the proper Poincaré group – and hence of all relativistically invariant quantum theories – can be obtained by the method of induced representations. A short introduction is given in Sect. 3.1. In order to find representations of a Lie group $\mathcal{G}$ one starts with a representation of a closed subgroup $\mathcal{K}$ (the inducing representation). In a suitable Hilbert space of functions defined on the factor set $\mathcal{G}/\mathcal{K}$ one can then obtain an induced representation of $\mathcal{G}$ in a canonical way.

The semidirect product structure of the Poincaré group can be used to show that the induced representations are irreducible, if the inducing representation of $\mathcal{K}$ is irreducible. Furthermore, all irreducible representations can be obtained in this way (Sect. 3.2). The subgroup $\mathcal{K}$ is chosen as the semidirect product of the translation subgroup and the isotropy group (or little group), which is isomorphic to $SU(2)$. For the representations which are of interest in connection with the Dirac equation the factor set $\mathcal{G}/\mathcal{K}$ can be identified with the mass shell in momentum space. There is a unitary irreducible representation of the proper Poincaré group for every value of the mass and for every irreducible representation of the isotropy group (i.e., for every spin).

The functions in the representation space of the induced representation satisfy an additional covariance condition. If one wants to get rid of this, one can pass to the so-called Wigner states which are functions on the mass shell with a characteristic behavior under group transformations. A second possibility is to introduce covariant states, which behave in a more transparent way under the action of the group. But the covariant representation can only be defined if the inducing representation is the restriction of a representation of the whole group.

In Sect. 3.3 we give a group theoretical "derivation" of the Dirac equation. We consider the covariant representation characterized by spin-1/2 and nonzero mass m of the particle. In order to define the inducing representation we start with the 4-dimensional representation of the Poincaré covering group obtained in Chapter 2. The restriction of this representation to the isotropy group (i.e., the inducing representation) is not irreducible in this case. The Dirac equation can be identified as a covariant projection to an irreducible subspace. Moreover, it is straightforward to introduce a new representation space in such a way that time translations are generated by a local differential operator, the Dirac operator. In this picture the Foldy-Wouthuysen transformation can be identified as the transition from covariant to Wigner states. The representation of the Poincaré group obtained in this way coincides with the one obtained in Chapter 2 by an exponentiation of the Poincaré Lie algebra.

In Sect. 3.4 we consider the problem of extending a unitary representation of the proper Poincaré covering group to a representation of the full Poincaré group with reflections. If we require that the subspaces with positive/negative energy remain invariant, then the time reversal has to be represented by an antiunitary operator. This leaves four possible unitary representations of the covering group with reflections, all leading to the same projective representation of the full Poincaré group.

3.1 Mackey's Theory of Induced Representations

3.1.1 Induced Representations of Lie Groups

Let $\mathcal{G}$ be a separable Lie group[1] with a left invariant measure dg (Haar measure). In order to define a representation of $\mathcal{G}$ we consider measurable functions ϕ on $\mathcal{G}$ with values in some (complex) Hilbert space $\mathfrak{X}$. The group $\mathcal{G}$ acts in a natural way on the set of these functions by left translation:

$$\pi(h)\,\phi(g) = \phi(h^{-1}g). \tag{3.1}$$

The existence of a Haar measure allows us to integrate these functions, the left invariance states that

$$\int_{\mathcal{G}} \phi(g)\,dg = \int_{\mathcal{G}} \phi(h^{-1}g)\,dg. \tag{3.2}$$

Let us assume that there exists a closed subgroup $\mathcal{K}$ of $\mathcal{G}$ for which a unitary representation τ in $\mathfrak{X}$ is known.

Example 3.1. Let $\mathcal{G} = \tilde{\mathcal{L}}^{\uparrow}$, given by Eq. (2.149), and $\mathfrak{X} = \mathbb{C}^4$. Then $\mathcal{K} = SU(2)$ is a closed subgroup, which has the unitary representation $\tau(U) = \mathbf{L}_U$ defined by Eq. (2.146). This representation is reducible. It is obtained as the restriction of an irreducible (but not unitary) four-dimensional representation of $\tilde{\mathcal{L}}^{\uparrow}$. An example of an irreducible representation is provided by the "defining representation" $\tau(U) = U$ of $SU(2)$ in $\mathfrak{X} = \mathbb{C}^2$.

Starting from the unitary representation τ of the subgroup $\mathcal{K}$ we can define in a natural way a unitary representation of the whole group $\mathcal{G}$. This representation will act on $\mathfrak{X}$-valued functions ϕ which satisfy the subsidiary condition

$$\phi(gk^{-1}) = \tau(k)\,\phi(g), \quad \text{all } g \in \mathcal{G} \text{ and all } k \in \mathcal{K}. \tag{3.3}$$

We can define a Hilbert space of functions satisfying (3.3), if there is an invariant[2] measure $d\mu$ on $\mathcal{G}/\mathcal{K}$. The factor set $\mathcal{G}/\mathcal{K}$ consists of cosets $\dot{g} = g\mathcal{K} = \{gk \mid k \in \mathcal{K}\}$ and by the invariance of the measure $d\mu$ we have

$$\int_{\mathcal{G}/\mathcal{K}} f(\dot{g})\,d\mu(\dot{g}) = \int_{\mathcal{G}/\mathcal{K}} f(\Lambda_h \dot{g})\,d\mu(\dot{g}), \quad \text{all } h \in \mathcal{G}, \tag{3.4}$$

where f is an arbitrary real-valued measurable function on $\mathcal{G}/\mathcal{K}$ and Λ_h is the natural left action of $\mathcal{G}$ on the cosets $\dot{g} = g\mathcal{K} \in \mathcal{G}/\mathcal{K}$,

---

[1] All the results of this section have a generalization to arbitrary separable locally compact topological groups $\mathcal{G}$. Every locally compact group has at least one Haar measure. A Lie group is always locally compact. It is separable iff it has a countable number of connected components. (The Poincaré group has four components).

[2] It would be sufficient to require the quasi-invariance of the measure $d\mu$, see, e.g., [Ma 68]. Our assumption of invariance makes the expressions look simpler and is fulfilled for the cases we are interested in.

$$\Lambda_h : \mathcal{G}/\mathcal{K} \to \mathcal{G}/\mathcal{K}, \qquad \Lambda_h(g\mathcal{K}) = hg\mathcal{K} \quad (= \text{coset of } hg). \tag{3.5}$$

For $\mathcal{X}$-valued functions ϕ satisfying the subsidiary condition (3.3) we may require the square integrability with respect to $d\mu$,

$$\int_{\mathcal{G}/\mathcal{K}} \|\phi(g)\|_{\mathcal{X}}^2 \, d\mu(\dot{g}) < \infty. \tag{3.6}$$

This makes sense because from the unitarity of τ and Eq. (3.3) it follows that $\|\phi(g)\|_{\mathcal{X}}^2 \equiv f(\dot{g})$ only depends on the coset $\dot{g} = g\mathcal{K}$.

Remark. If $f : \mathcal{G} \to \mathcal{X}$ is continuous and has compact support in $\mathcal{G}$, then

$$\phi(h) \equiv \int_{\mathcal{K}\subset\mathcal{G}} \tau(g)\, f(hg)\, dg \tag{3.7}$$

satisfies (3.3) and (3.6).

The set of (μ-equivalence classes of) functions ϕ on $\mathcal{G}$ with values in $\mathcal{X}$ satisfying (3.3) and (3.6) forms a Hilbert space $\mathfrak{M}$. The elements in this Hilbert space are sometimes called "Mackey states". The norm in $\mathfrak{M}$ is given by (3.6) and can be derived from the scalar product

$$(\phi_1, \phi_2) = \int_{\mathcal{G}/\mathcal{K}} \big(\phi_1(g), \phi_2(g)\big)_{\mathcal{X}} \, d\mu(\dot{g}), \tag{3.8}$$

where again the integrand depends only on the coset $\dot{g}$.

The left action (3.1) leaves this Hilbert space invariant because the function $g \to \pi(h)\phi(g) = \phi(h^{-1}g)$ satisfies again the condition (3.3). Hence the left action $\pi(h)$ defines a linear mapping of $\mathfrak{M}$ into itself which is again denoted by $\pi(h)$. The unitarity of $\pi(h)$ follows immediately from Eq. (3.4). The strong continuity of $h \to \pi(h)$ follows from the measurability of $h \to (\eta, \pi(h)\phi)$ (see, e.g., [HR 63], Sect. 22.20b).

Definition 3.2. *The representation $h \to \pi(h)$ in the Hilbert space $\mathfrak{M}$ is called the representation of $\mathcal{G}$ "induced" by the representation τ of $\mathcal{K}$.*

The importance of this concept comes from the fact that for a number of groups including the Poincaré group the irreducibility of the induced representation π follows from the irreducibility of the "inducing representation" τ.

3.1.2 A Strategy for Semidirect Products

In order to determine induced representations of the Poincaré group $\tilde{\mathcal{P}}^\uparrow$ we need a closed subgroup $\mathcal{K}$. Since $\tilde{\mathcal{P}}^\uparrow$ is a semidirect product $\mathbb{R}^4 \odot \tilde{\mathcal{L}}^\uparrow$ it is convenient to choose

$$\mathcal{K} = \mathbb{R}^4 \odot \mathcal{H}, \tag{3.9}$$

where $\mathcal{H}$ is a subgroup of $\tilde{\mathcal{L}}^{\uparrow}$. Then the factor set $\tilde{\mathcal{P}}^{\uparrow}/\mathcal{K}$ is simply given by

$$\tilde{\mathcal{P}}^{\uparrow}/\mathcal{K} = (\mathbb{R}^4 \odot \tilde{\mathcal{L}}^{\uparrow})/(\mathbb{R}^4 \odot \mathcal{H}) = \tilde{\mathcal{L}}^{\uparrow}/\mathcal{H}. \tag{3.10}$$

For any unitary representation τ of $\mathcal{K}$ in a Hilbert space $\mathfrak{X}$ the restrictions

$$\alpha(a) = \tau(a, \mathbf{1}), \quad a \in \mathbb{R}^4, \quad \text{and} \quad \sigma(\mathbf{L}) = \tau(0, \mathbf{L}), \quad \mathbf{L} \in \mathcal{H}, \tag{3.11}$$

are representations of the subgroups $\mathbb{R}^4$ and $\mathcal{H}$, respectively. From

$$(a, \mathbf{L}) = (a, \mathbf{1})(0, \mathbf{L}) = (0, \mathbf{L})(\Lambda_{\mathbf{L}}^{-1} a, \mathbf{1}) \tag{3.12}$$

(see (2.28)) we find

$$\tau(a, \mathbf{L}) = \alpha(a)\, \sigma(\mathbf{L}), \tag{3.13}$$

$$\sigma(\mathbf{L})^{-1}\, \alpha(a)\, \sigma(\mathbf{L}) = \alpha(\Lambda_{\mathbf{L}}^{-1} a), \quad \text{all } (a, \mathbf{L}) \in \mathcal{K}. \tag{3.14}$$

The mapping $a \to \gamma(a) \equiv \alpha(\Lambda_{\mathbf{L}}^{-1} a)$ again defines a representation of $\mathbb{R}^4$. (In the following two sections we are going to describe the map $\alpha \to \gamma$ as the dual action of the Poincaré group). Our strategy will be to choose the subgroup $\mathcal{H}$ such that

$$\alpha(\Lambda_{\mathbf{L}}^{-1} a) = \alpha(a) \quad \text{for all } \mathbf{L} \in \mathcal{H} \text{ and } a \in \mathbb{R}^4. \tag{3.15}$$

In this case the product of representation operators simplifies to

$$\tau(a, \mathbf{L}_1)\, \tau(b, \mathbf{L}_2) = \alpha(a + b)\, \sigma(\mathbf{L}_1 \mathbf{L}_2) \tag{3.16}$$

for all $(a, \mathbf{L}_1)$ and $(b, \mathbf{L}_2) \in \mathcal{K}$.

3.1.3 Characters and the Dual Group

We start by describing the irreducible representations of the subgroup of translations which is isomorphic to the additive group $\mathbb{R}^4$. This is quite simple because any irreducible representation of an abelian group is one-dimensional, as a consequence of Schur's Lemma: A unitary representation α of a group $\mathcal{G}$ in a Hilbert space $\mathfrak{H}$ is irreducible if and only if the only operators commuting with all the $\alpha(g)$ are of the form $\chi \mathbf{1}$, $\chi \in \mathbb{C}$. Now, if $\mathcal{G}$ is abelian, all operators $\alpha(g)$ commute and hence

$$\alpha(g) = \chi(g)\mathbf{1}, \tag{3.17}$$

where χ is a complex valued function on $\mathcal{G}$. Therefore every one-dimensional subspace of $\mathfrak{H}$ is invariant under α, i.e., α is irreducible if and only if $\dim \mathfrak{H} = 1$.

Definition 3.3. *A one-dimensional unitary representation of an abelian group $\mathcal{G}$ is called a "character". If ξ and χ are characters of $\mathcal{G}$ then $\xi\chi$ defined by $\xi\chi(g) = \xi(g)\chi(g)$ is again a one-dimensional unitary representation, i.e., a character. The set of characters of $\mathcal{G}$ endowed with this multiplication is a group which is called the "dual group".*

For each $p \in \mathbb{R}^4$, the map χ_p defined by

$$\chi_p(a) = e^{\mathrm{i}\langle p,a\rangle}, \quad \text{all } a \in \mathbb{R}^4. \tag{3.18}$$

is a character of the translation group in the Hilbert space $\mathfrak{H} = \mathbb{C}$. The set $N \equiv \{\chi_p \mid p \in \mathbb{R}^4\}$ with the multiplication

$$\chi_p \chi_q(a) = \chi_p(a)\chi_q(a) = \chi_{p+q}(a), \quad \text{all } a \in \mathbb{R}^4, \tag{3.19}$$

is the dual group N which in this case is again isomorphic to the additive group $\mathbb{R}^4$, the isomorphism being given by

$$\chi : p \to \chi_p, \quad \text{all } p \in \mathbb{R}^4. \tag{3.20}$$

(For a general abelian group $\mathcal{G}$ the dual group need not be isomorphic to $\mathcal{G}$).

Remark. We shall choose the inducing representation τ for the Poincaré group in such a way that the representation α of $\mathbb{R}^4$, defined in (3.11), is of the form

$$\alpha(a) = \chi_q(a)\mathbf{1}, \tag{3.21}$$

for some fixed $q \in \mathbb{R}^4$.

3.1.4 The Dual Action of the Poincaré Group

Any group $\mathcal{G}$ acts on itself as a group of inner automorphisms $I_h : \mathcal{G} \to \mathcal{G}$,

$$I_h(g) = hgh^{-1}. \tag{3.22}$$

It is natural to study the action of the Poincaré group on the abelian normal subgroup $\mathbb{R}^4$ (the subgroup of translations). We find

$$I_{(b,\mathbf{L})}(a,\mathbf{1}) = (b,\mathbf{L})\,(a,\mathbf{1})\,(b,\mathbf{L})^{-1} = (\Lambda_{\mathbf{L}}a,\mathbf{1}), \tag{3.23}$$

which we can simply write as $a \to \Lambda_{\mathbf{L}}a$. Now we can also define a "dual action" of the Poincaré group on the dual group N of $\mathbb{R}^4$,

$$\left(\hat{I}_{(b,\mathbf{L})}\chi_p\right)(a) \equiv \chi_p\left(\Lambda_{\mathbf{L}}^{-1}a\right) \equiv \chi_{\Lambda_{\mathbf{L}}p}(a). \tag{3.24}$$

Note that the action of the translation subgroup $\mathbb{R}^4$ on its dual is trivial, we have $\hat{I}_{(b,\mathbf{1})}\chi_p = \chi_p$ for all $b \in \mathbb{R}^4$.

Obviously, the isomorphism (3.20) preserves the action of the inner automorphism and we have the following commuting diagram

$$\begin{array}{ccc} p \cong (p,\mathbf{1}) & \to & \chi_p \\ \downarrow & & \downarrow \\ \Lambda_{\mathbf{L}}(p) \cong I_{(b,\mathbf{L})}(p,\mathbf{1}) & \to & \chi_{\Lambda_{\mathbf{L}}p} = \hat{I}_{(b,\mathbf{L})}\chi_p \end{array} \tag{3.25}$$

Remark. If we choose the inducing representation τ of the Poincaré group such that $\alpha(a) = \chi_q(a)\mathbf{1}$ (cf. Sect. 3.1.2), and if we assume that Eq. (3.15) should hold, then

$$\chi_q(a) = \chi_q(\Lambda_{\mathbf{L}}^{-1}a) = \chi_{\Lambda_{\mathbf{L}}q}(a), \quad \text{all } \mathbf{L} \in \mathcal{H},\ a \in \mathbb{R}^4, \tag{3.26}$$

suggests to choose $\mathcal{K} = \mathbb{R}^4 \odot \mathcal{H}$ as the subgroup whose dual action leaves the character χ_q invariant. A group with this property is called isotropy group. We shall discuss this concept in the next section.

3.1.5 Orbits and Isotropy Groups

Let $\mathcal{G}$ be a group which acts on a set M (Sect. 2.1.5), and let $q \in M$. The set

$$O_q \equiv \{\Lambda_h(q) \mid h \in \mathcal{G}\} \subset M \tag{3.27}$$

is called the *orbit* of q under the action of $\mathcal{G}$. Obviously, M is a disjoint union of orbits. Given an orbit O_q and some $p \in O_q$, we define

$$K_p \equiv \{h \in \mathcal{G} \mid \Lambda_h(q) = p\} \subset \mathcal{G}, \tag{3.28}$$

as the set of all group elements which map q onto p. Obviously, $\mathcal{G}$ is the union of the subsets K_p, $p \in O_q$. Two group elements h and k are both in K_p if and only if

$$\Lambda_h(q) = \Lambda_k(q) \quad \text{or} \quad \Lambda_{h^{-1}k}(q) = q,$$

i.e., if $h^{-1}k$ is in the set

$$\mathcal{G}_q = \{g \in \mathcal{G} \mid \Lambda_g(q) = q\}. \tag{3.29}$$

$\mathcal{G}_q$ is a subgroup of $\mathcal{G}$, called the "*isotropy group*" (or "*stability group*") of q under the given action of $\mathcal{G}$ on M. The isotropy group of q consists of all group elements which leave q invariant. If q' is any other point in the orbit of q, then the isotropy group $\mathcal{G}_{q'}$ is isomorphic to $\mathcal{G}_q$.

Example 3.4. $\mathcal{G} = \tilde{\mathcal{P}}^{\uparrow}$, $M = N$, the dual group of $\mathbb{R}^4$. From (3.24) it is clear that $\mathbb{R}^4$ is a subgroup of the isotropy group of any character χ_q under the dual action of $\tilde{\mathcal{P}}^{\uparrow}$ on N.

The set $\mathcal{G}/\mathcal{G}_q$ is defined as the collection of all cosets

$$g\mathcal{G}_q = \{gh \mid h \in \mathcal{G}_q\}, \quad g \in \mathcal{G}. \tag{3.30}$$

The coset $g\mathcal{G}_q$ coincides with K_p, where $p = \Lambda_g(q)$. Hence the elements of the factor set $\mathcal{G}/\mathcal{G}_q$ are in one-to-one correspondence to the points of the orbit O_q. Hereby the action Λ_h of $h \in \mathcal{G}$ on O_q corresponds to the left multiplication with h on the cosets $g\mathcal{G}_q$:

$$\begin{array}{ccc} p \in O_q & \to & \Lambda_h p \in O_q \\ \downarrow & & \downarrow \\ g\mathcal{G}_q \in \mathcal{G}/\mathcal{G}_q & \to & hg\mathcal{G}_q \in \mathcal{G}/\mathcal{G}_q \end{array} \tag{3.31}$$

The relation between factor sets and orbits is made precise in the following theorem.

Theorem 3.5. Let $\mathcal{G}$ be a separable Lie group which acts as a Lie transformation group on a manifold M (i.e., each $\Lambda_h : M \to M$ is a diffeomorphism). Then the isotropy group $\mathcal{G}_q$ of a point $q \in M$ is a closed subgroup of $\mathcal{G}$. The factor set $\mathcal{G}/\mathcal{G}_q$ has a unique analytic structure such that $\mathcal{G}$ with the action $g\mathcal{G}_q \to hg\mathcal{G}_q$ is a Lie transformation group on $\mathcal{G}/\mathcal{G}_q$. Moreover, $\mathcal{G}/\mathcal{G}_q$ is diffeomorphic to the orbit O_q, and the diffeomorphism is given by the map

$$g\mathcal{G}_q \leftrightarrow p = \Lambda_g(q). \tag{3.32}$$

Proof. See [He 78], Theorems 3.2, 4.2, and Proposition 4.3. □

3.1.6 Orbits of the Poincaré group

We fix a reference character by choosing $q \in \mathbb{R}^4$. The orbit of χ_q under the dual action of $\mathcal{G} = \tilde{\mathcal{P}}^\uparrow$ is the set

$$\hat{O}_q \equiv \{\hat{I}_h \chi_q \mid h = (a, \mathbf{L}) \in \tilde{\mathcal{P}}^\uparrow\}. \tag{3.33}$$

With the help of the isomorphism χ it can be identified with the subset

$$O_q \equiv \{\Lambda_{\mathbf{L}} q \mid \mathbf{L} \in \tilde{\mathcal{L}}^\uparrow\} = \{\Lambda q \mid \Lambda \in \mathcal{L}^\uparrow\} \tag{3.34}$$

of $\mathbb{R}^4$. The isotropy subgroup of χ_q under the action of $\tilde{\mathcal{P}}$ is

$$\tilde{\mathcal{P}}_q \equiv \{g \in \tilde{\mathcal{P}}^\uparrow \mid \hat{I}_g \chi_q = \chi_q\} = \{(a, \mathbf{L}) \in \tilde{\mathcal{P}}^\uparrow \mid \Lambda_{\mathbf{L}} q = q\}. \tag{3.35}$$

The subgroup of translations is obviously a subgroup of the isotropy group and we may write

$$\tilde{\mathcal{P}}_q = \mathbb{R}^4 \odot \tilde{\mathcal{L}}_q, \quad \tilde{\mathcal{L}}_q = \{\mathbf{L} \in \tilde{\mathcal{L}} \mid \Lambda_{\mathbf{L}} q = q\}. \tag{3.36}$$

The group $\tilde{\mathcal{L}}_q$ is called the little group of the character χ_q or simply the little group of q. The dual group $N \cong \mathbb{R}^4$ is a disjoint union of the following orbits:

1) $q = (\mu, 0, 0, 0)^\top$, $\mu > 0$: $O_q = \{p \in \mathbb{R}^4 \mid \langle p, p\rangle = \mu^2, p_0 > 0\} \equiv M_{\text{pos}}$,
2) $q = (-\mu, 0, 0, 0)^\top$, $\mu > 0$: $O_q = \{p \in \mathbb{R}^4 \mid \langle p, p\rangle = \mu^2, p_0 < 0\} \equiv M_{\text{neg}}$,
3) $q = (0, \mu, 0, 0)^\top$, $\mu > 0$: $O_q = \{p \in \mathbb{R}^4 \mid \langle p, p\rangle = -\mu^2\}$,
4) $q = (1, 1, 0, 0)^\top$: $O_q = \{p \in \mathbb{R}^4 \mid \langle p, p\rangle = 0, p_0 > 0\}$,
5) $q = (-1, 1, 0, 0)^\top$: $O_q = \{p \in \mathbb{R}^4 \mid \langle p, p\rangle = 0, p_0 < 0\}$,
6) $q = (0, 0, 0, 0)^\top$: $O_q = \{0\}$,

In the applications we shall deal exclusively with the orbits 1 and 2 because this leads to a description of particles with real mass $\mu/c = m > 0$. The orbit 3 has no clear physical significance (tachyons?), the orbits 4, 5, and 6 lead to particles with zero rest mass.

3.1.7 Invariant Measure and Little Group

Each orbit of the Poincaré group in the character group N carries an invariant measure. For $q = (\pm\mu, 0, 0, 0)^\top$, $\mu > 0$ (i.e., for the orbits 1 and 2 above) the invariant measure is given by

$$d\mu(p) = \frac{d^3p}{|p_0|}, \quad |p_0| = \sqrt{\mu^2 + \mathbf{p}^2}. \tag{3.37}$$

The stability subgroup of $q = (\pm\mu, 0, 0, 0)^\top$ obviously consists of all translations, all space rotations and the space reflection P, while any boost or time reversal would change the reference character q. Hence the little group of q is given by the following subgroup of $\tilde{\mathcal{L}}^\uparrow$

$$\tilde{\mathcal{L}}_q = \{\mathbf{L}_U, \mathbf{L}_P\mathbf{L}_U \mid U \in SU(2)\}, \qquad q = (\pm\mu, 0, 0, 0)^\top. \tag{3.38}$$

(See Sect. 2.5.4 for the relevant definitions).

Remark. The little group $\tilde{\mathcal{L}}_q$ is defined here as a subgroup of $\tilde{\mathcal{L}}^\uparrow$ which is a group of 4×4 matrices. The action of $\tilde{\mathcal{L}}_q$ in $\mathbb{C}^4$ is reducible, because apart from the unit matrix $\mathbf{1}$ also the matrix $\mathbf{L}_P = \beta$ commutes with all other matrices in $\tilde{\mathcal{L}}_q$. Hence, by Schur's Lemma, the 'defining representation' (3.38) cannot be irreducible. The matrices

$$Q^\pm = \frac{1}{2}(1 \pm \beta), \tag{3.39}$$

are obviously the projections onto the two irreducible subspaces $Q^\pm\mathbb{C}^4$, which are both isomorphic to $\mathbb{C}^2$. The vectors in $Q^+\mathbb{C}^4$ ($Q^-\mathbb{C}^4$) will be called the "even-parity (odd-parity) spinors".

3.1.8 Induced Representations of the Poincaré Group

Now we are ready to apply the results of Sect. 3.1.1 to the Poincaré group $\mathcal{G} = \tilde{\mathcal{P}}^\uparrow$. The closed subgroup $\mathcal{K}$ will be chosen as the isotropy group $\mathcal{K} = \tilde{\mathcal{P}}_q$ of a character χ_q defined in (3.36). $\mathcal{K}$ is precisely of the form (3.9) with $\mathcal{H} = \tilde{\mathcal{L}}_q$. We choose the inducing representation τ such that its restriction α to the subgroup of translations is of the form $\alpha = \chi_q\mathbf{1}$,

$$\tau(a, \mathbf{L}) = \chi_q(a)\,\sigma(\mathbf{L}), \quad a \in \mathbb{R}^4, \quad \mathbf{L} \in \tilde{\mathcal{L}}_q. \tag{3.40}$$

Then (3.15) is satisfied for any representation σ of $\tilde{\mathcal{L}}_q$. Moreover, the representations τ of $\tilde{\mathcal{P}}_q$ in a Hilbert space $\mathfrak{X}$ is irreducible if and only if σ is an irreducible representation of $\tilde{\mathcal{L}}_q$ in $\mathfrak{X}$. As in Sect. 3.1.1 we may hence define representations π induced by the representations (3.40) of the closed subgroups $\tilde{\mathcal{P}}_q$, the isotropy groups for the various choices of q. By Theorem 3.5 every factor set $\tilde{\mathcal{P}}^\uparrow/\tilde{\mathcal{P}}_q = \tilde{\mathcal{L}}^\uparrow/\tilde{\mathcal{L}}_q$ can be interpreted as the orbit O_q of χ_q (resp. q) under the

dual action $p \to \Lambda_{\mathbf{L}} p$ of $\tilde{\mathcal{P}}^{\uparrow}$. On each orbit exists a measure which is invariant with respect to this action. Therefore, an induced representation of $\tilde{\mathcal{P}}^{\uparrow}$ can be obtained for each orbit O_q and each unitary representation σ of the corresponding little group $\tilde{\mathcal{L}}_q$.

The Hilbert space $\mathfrak{M}_q$ for the representation consists of functions defined on $\mathcal{G} = \tilde{\mathcal{P}}^{\uparrow}$ with values in $\mathfrak{X}$ satisfying the condition

$$\phi\left((a,\mathbf{L})(b,\mathbf{L}')^{-1}\right) = e^{\mathrm{i}\langle q,b\rangle}\sigma(\mathbf{L}')\phi(a,\mathbf{L}), \tag{3.41}$$

for all $(a,\mathbf{L}) \in \tilde{\mathcal{P}}^{\uparrow}$ and all $(b,\mathbf{L}') \in \tilde{\mathcal{P}}_q$. The scalar product in $\mathfrak{M}_q$ is given by

$$(\phi,\eta) = \int_{O_q} \frac{d^3p}{|p_0|}\left(\phi(a,\mathbf{L}),\eta(a,\mathbf{L})\right)_{\mathfrak{X}}. \tag{3.42}$$

The integrand depends only on the point $p = \Lambda_{\mathbf{L}} q$ corresponding to the coset $(a,\mathbf{L})\tilde{\mathcal{P}}_q$. In special cases we shall obtain equivalent representations with more familiar scalar products.

3.2 Wigner's Realization of Induced Representations

So far we have obtained group representations in a Hilbert space of functions which are defined on the group itself and satisfy the condition (3.3). This is a rather unfamiliar situation. In order to get closer to the usual quantum mechanical formulations, we have to construct a more handsome Hilbert space. In this section we describe a possible way to get rid of the subsidiary condition (3.3). In case of the Poincaré group this will lead us to a Hilbert space of square-integrable functions which are defined on the mass shell.

3.2.1 Wigner States

We consider first the general case: Let $\mathcal{G}$ be a separable Lie group and let π be a representation of $\mathcal{G}$ which is induced from a unitary representation τ of a closed subgroup $\mathcal{K}$. The representation space consists of functions ϕ on $\mathcal{G}$ satisfying Eq (3.3). In order to eliminate this subsidiary condition we fix a mapping $s : \mathcal{G}/\mathcal{K} \to \mathcal{G}$ such that $s(g\mathcal{K}) \in g\mathcal{K}$ and such that the image

$$S = s(\mathcal{G}/\mathcal{K}) \subset \mathcal{G} \tag{3.43}$$

is a (Borel-) measurable set[3]. This simply means that we choose a representative s from each coset $\dot{g} = g\mathcal{K}$. Any $g \in \mathcal{G}$ has the unique form

$$g = sk^{-1}, \quad \text{where } s = s(\dot{g}), \text{ and } k \in \mathcal{K}. \tag{3.44}$$

The left action (3.5) of $\mathcal{G}$ on $\mathcal{G}/\mathcal{K}$ defines also a natural left action of $\mathcal{G}$ on S, we write

[3] According to the Mackey decomposition theorem such a mapping s exists on any separable locally compact group $\mathcal{G}$ with closed subgroup $\mathcal{K}$ (see [305], part I, Lemma 1.1)

$$\Lambda_h s \equiv s(hg\mathcal{K}) = s(\Lambda_h \dot{g}) \qquad \text{for all } s = s(\dot{g}) \in S. \tag{3.45}$$

The measure $d\mu(s) \equiv d\mu(\dot{g})$ on S is invariant with respect to this action, cf. Eq. (3.4).

The restriction of a function ϕ satisfying (3.3) to the set S defines a function ζ of $s \in S$. We have for all $g \in \mathcal{G}$ and $s = s(\dot{g})$

$$\zeta(s) \equiv \phi(s), \qquad \phi(g) = \phi(sk^{-1}) = \tau(k)\,\phi(s) = \tau(k)\,\zeta(s), \tag{3.46}$$

and the Hilbert space $\mathfrak{M}$ can be identified with the Hilbert space

$$\mathfrak{W} \equiv L^2(S, d\mu(s); \mathfrak{X}) \tag{3.47}$$

of square integrable $\mathfrak{X}$-valued functions ζ defined on $S \subset \mathcal{G}$. Here $\mathfrak{X}$ is the Hilbert space carrying the unitary representation τ, cf. Sect. 3.1.1.

The action of $\pi(h)$ on $\zeta(s)$ becomes

$$\pi^{\mathrm{w}}(h)\zeta(s) = \pi(h)\phi(s) = \phi(h^{-1}s). \tag{3.48}$$

The group element $h^{-1}s$ belongs to the coset $h^{-1}s\mathcal{K}$ which by (3.45) has the representative $\Lambda_h^{-1}s$. By Eq. (3.44) $h^{-1}s$ has the unique representation

$$h^{-1}s = (\Lambda_h^{-1}s)k^{-1} \quad \text{with some } k \in \mathcal{K}. \tag{3.49}$$

Hence we obtain with (3.3)

$$\pi^{\mathrm{w}}(h)\,\zeta(s) = \tau(k)\,\zeta(\Lambda_h^{-1}s) = \tau\big(s^{-1}h\,(\Lambda_h^{-1}s)\big)\,\zeta(\Lambda_h^{-1}s). \tag{3.50}$$

The operator $\pi(h)$ acts on elements of the Hilbert space $\mathfrak{W}$ which are not subject to any further restrictions. The elements in this Hilbert space are sometimes called "Wigner states".

3.2.2 Wigner States for the Poincaré Group

Let us now apply the abstract considerations of the previous section to the Poincaré group. Our first task is to find a representative s for each coset in $\mathcal{G}/\mathcal{K} = \tilde{\mathcal{P}}^{\uparrow}/\tilde{\mathcal{P}}_q$. Since by Theorem 3.5 each $\dot{g} \in \tilde{\mathcal{P}}^{\uparrow}/\tilde{\mathcal{P}}_q$ can be identified with a point $p \in O_q$ we can write $s = s(p)$. If $q = (\pm\mu, 0, 0, 0)$, $\mu > 0$, we choose

$$s(p) = (0, \mathbf{L}_p), \tag{3.51}$$

where $\mathbf{L}_p$ denotes the 4×4 matrix corresponding to the unique boost mapping q to $p \in O_q$. The matrix $\mathbf{L}_p$ can be determined from

$$\Lambda_{\mathbf{L}_p}(q) = p, \tag{3.52}$$

and is Hermitian because it is of the form (2.146) with Hermitian A (see Sect. 2.5.4). By Eq. (2.159) we have

$$\langle \gamma, p\rangle = \mathbf{L}_p\,\langle \gamma, q\rangle\,\mathbf{L}_p^{-1} = q_0\,\mathbf{L}_p\,\gamma^0\,\mathbf{L}_p^{-1}, \tag{3.53}$$

where $q_0 = \pm\mu$. Using (2.216) and $\mathbf{L}_p^{*} = \mathbf{L}_p$ we obtain

$$\gamma^0 \mathbf{L}_p^{-1} = \mathbf{L}_p \gamma^0, \tag{3.54}$$

and hence

$$q_0 \mathbf{L}_p^2 = \langle \gamma, p \rangle \gamma^0. \tag{3.55}$$

From

$$\left(q_0 + \langle \gamma, p \rangle \gamma^0\right)^2 = 2(q_0 + p_0) \langle \gamma, p \rangle \gamma^0 \tag{3.56}$$

we finally obtain

$$\mathbf{L}_p = \frac{q_0 + \langle \gamma, p \rangle \gamma^0}{\sqrt{2q_0(q_0 + p_0)}} = \frac{q_0 + p_0 + \boldsymbol{\alpha} \cdot \boldsymbol{p}}{\sqrt{2q_0(q_0 + p_0)}}, \tag{3.57}$$

where the argument of the square root is always positive, because

$$p_0 = \pm\sqrt{\boldsymbol{p}^2 + \mu^2} \quad \text{for } q_0 = \pm\mu. \tag{3.58}$$

The mapping $p \to s(p)$ is one-to-one. It is just the homeomorphism identifying the mass shell O_q (which is M_{pos}, if $q_0 = +\mu$, and M_{neg}, if $q_0 = -\mu$) with the submanifold of Lorentz boosts (cf. Sect. 2.1.3). For each vector ϕ in the Hilbert space $\mathfrak{M}_q$ of the induced representation we define a Wigner state ζ as in (3.46). Identifying p with $s(p)$ we simply write

$$\zeta(p) \equiv \phi(0, \mathbf{L}_p), \quad \text{all } p \in O_q. \tag{3.59}$$

Next we calculate $\tau\left(s^{-1} h \left(\Lambda_h^{-1} s\right)\right)$ with $s = (0, \mathbf{L}_p)$, $h = (a, \mathbf{L}) \in \tilde{\mathcal{P}}$. The action of $\tilde{\mathcal{P}}$ on the representatives $(0, \mathbf{L}_p)$ is given by the action of $\tilde{\mathcal{P}}$ on $p \in O_q$, i.e.,

$$\Lambda_{(a,\mathbf{L})}(0, \mathbf{L}_p) = (0, \mathbf{L}_{\Lambda_{\mathbf{L}} p}). \tag{3.60}$$

Hence

$$s^{-1} h \left(\Lambda_h^{-1} s\right) = (0, \mathbf{L}_p)^{-1} (a, \mathbf{L}) (0, \mathbf{L}_{\Lambda_{\mathbf{L}}^{-1} p}) = (\Lambda_{\mathbf{L}_p}^{-1} a, \mathbf{L}_p^{-1} \mathbf{L} \mathbf{L}_{\Lambda_{\mathbf{L}}^{-1} p}) \tag{3.61}$$

and

$$\tau(s^{-1} h \left(\Lambda_h^{-1} s\right)) = \exp(\mathrm{i} \langle q, \Lambda_{\mathbf{L}_p}^{-1} a \rangle) \sigma(\mathbf{L}_p^{-1} \mathbf{L} \mathbf{L}_{\Lambda_{\mathbf{L}}^{-1} p}). \tag{3.62}$$

With

$$\langle q, \Lambda_{\mathbf{L}_p}^{-1} a \rangle = \langle \Lambda_{\mathbf{L}_p} q, a \rangle = \langle p, a \rangle \tag{3.63}$$

and (3.50) we finally arrive at

$$\left(\pi^{\mathbf{w}}(a, \mathbf{L}) \zeta\right)(p) = e^{\mathrm{i}\langle p, a \rangle} \sigma(\mathbf{L}_p^{-1} \mathbf{L} \mathbf{L}_{\Lambda_{\mathbf{L}}^{-1} p}) \zeta(\Lambda_{\mathbf{L}}^{-1} p). \tag{3.64}$$

The Wigner states ζ form a Hilbert space $\mathfrak{W}_q$ with the scalar product

$$(\zeta, \xi) = \int_{O_q} \frac{d^3 p}{|p_0|} \left(\zeta(p), \xi(p)\right)_{\mathfrak{X}}. \tag{3.65}$$

Now the integrand depends explicitly on p (cf. Eq. (3.42)).

3.2.3 Irreducibility of the Induced Representation

Theorem 3.6. For each orbit O_q and each irreducible representation σ of the corresponding little group $\mathcal{H}$ the induced representation (3.64) of the Poincaré group $\tilde{\mathcal{P}}^{\uparrow}$ is irreducible.

Proof. In the Hilbert space

$$\mathfrak{W}_q = L^2(O_q, d\mu(\boldsymbol{p}), \mathfrak{X}) \cong L^2(O_q, d\mu(p)) \otimes \mathfrak{X} \tag{3.66}$$

the translations are represented by

$$\pi^{\mathrm{w}}(a, \mathbf{1}) = e^{\mathrm{i}\langle p, a\rangle} \otimes \mathbf{1}, \tag{3.67}$$

i.e., they act trivially on $\mathfrak{X}$ and as a multiplication operator on $L^2(O_q)$. Let B be any bounded operator in $\mathfrak{W}_q$ which commutes with all the representation operators $\pi^{\mathrm{w}}(a, \mathbf{L})$. In particular, the part of B acting in $L^2(O_q)$ commutes with $\exp(\mathrm{i}\langle p, a\rangle)$ for all $a \in \mathbb{R}^4$. Therefore[4], it is an operator of multiplication by a bounded function of p. We conclude that B must be of the form,

$$(B\zeta)(p) = B(p)\zeta(p), \tag{3.68}$$

where each $B(p)$ is a bounded operator in $\mathfrak{X}$. $B\zeta$ and ζ can be extended to functions on the whole group by applying (3.3). We write $\zeta(p) \equiv \zeta(0, \mathbf{L}_p)$ and denote the elements of $\mathcal{K}$ by $(a, \mathbf{U})$. Then (3.68) becomes

$$\big(B\zeta\big)\big((0, \mathbf{L}_p)(a, \mathbf{U})^{-1}\big) = B(p)\zeta\big((0, \mathbf{L}_p)(a, \mathbf{U})^{-1}\big), \tag{3.69}$$

because the action of B depends only on the coset given by p. Using (3.3) this can be written as

$$e^{\mathrm{i}\langle q, a\rangle}\, \sigma(\mathbf{U})\, (B\zeta)(p) = B(p)\, e^{\mathrm{i}\langle q, a\rangle}\, \sigma(\mathbf{U})\, \zeta(p), \tag{3.70}$$

or

$$\sigma(\mathbf{U})\, B(p) = B(p)\, \sigma(\mathbf{U}), \quad \text{all } \mathbf{U} \in \mathcal{H}. \tag{3.71}$$

Since σ is irreducible it follows from Schur's lemma that

$$B(p) = b(p)\mathbf{1}, \tag{3.72}$$

where $b(p)$ is a bounded complex valued function. Finally, since B commutes with all representation operators $\pi^{\mathrm{w}}(0, \mathbf{L})$, we have

$$B(p) = \pi^{\mathrm{w}}(0, \mathbf{L})\, B(p)\, \pi^{\mathrm{w}}(0, \mathbf{L})^{-1} = B(\Lambda_{\mathbf{L}} p), \quad \text{all } \mathbf{L} \in \tilde{\mathcal{L}}^{\uparrow}, \tag{3.73}$$

i.e., $b(p)$ has the same value for all values of p on the orbit O_q. This shows that B is a multiple of the identity in $\mathfrak{W}_q$. The lemma of Schur now states that the representation π is irreducible. □

[4] Although this result is folklore, it is mathematically highly nontrivial. One can prove it, e.g., by noting that the generators $p_0, \ldots, p_3$ of $\pi(a, \mathbf{1})$ form a complete set of commuting operators in $L^2(O_q)$. (See Def. IV.5.2 in [Pr 71]). Any operator commuting with a complete set must be a function of these operators (Theorem IV.5.6 of [Pr 71]).

3.2.4 Classification of Irreducible Representations

Theorem 3.7. Every irreducible unitary representation of $\tilde{\mathcal{P}}^{\uparrow}$ is equivalent to a representation of the form (3.64) induced by (3.40), where σ is an irreducible unitary representation of $\mathcal{H}$. The representation σ is determined up to equivalence and the orbit O_q is determined uniquely.

Proof. This theorem (together with Theorem 3.6) is a special case of more general results of Mackey [Ma 68]. □

This result provides a complete classification of the unitary irreducible representations of the Poincaré group. In the physical applications the orbit O_q determines the mass of the particle, while the chosen inducing representation of the little group determines the spin of the particle. In the following we are going to consider the representations with nonzero mass and spin-1/2.

3.2.5 The Defining Representation of the Little Group

In order to be more explicit we consider here the 'defining' representation

$$\sigma(\mathbf{L}) = \mathbf{L} \qquad (\text{all } \mathbf{L} \in \tilde{\mathcal{L}}_q) \tag{3.74}$$

of the little group $\mathcal{H} = \tilde{\mathcal{L}}_q$ of $q = (\pm\mu, 0, 0, 0)$, $\mu > 0$. According to our results in Sect. 3.1.7, the action of $\mathcal{H}$ is *not* irreducible in the Hilbert space $\mathfrak{X} = \mathbb{C}^4$. The subspaces of even and odd-parity spinors,

$$\mathfrak{X}^{\pm} = Q^{\pm}\mathbb{C}^4 \cong \mathbb{C}^2, \tag{3.75}$$

where $Q^{\pm} = \frac{1}{2}(1 \pm \beta)$, remain invariant under all linear transformations in $\mathcal{H}$. The representation $\sigma(\mathbf{L}) = \mathbf{L}$ of $\mathcal{H}$ restricted to $\mathfrak{X}^+$ (or $\mathfrak{X}^-$) is irreducible.

Next we investigate the representation induced by σ in the Hilbert space of Wigner states $\mathfrak{W}_q$. This representation is, like σ, reducible, and $Q^{\pm}\mathfrak{W}_q$ are invariant subspaces: From (3.64) and the fact that all $\mathbf{L}$ in the little group commute with β and hence with $Q^{\pm}$ we find

$$\pi^{\mathrm{w}}(a, \mathbf{L})\,(Q^{\pm}\zeta)(p) = Q^{\pm}\,\pi^{\mathrm{w}}(a, \mathbf{L})\,\zeta(p). \tag{3.76}$$

The invariant subspace $Q^{+}\mathfrak{W}_q$ consists of Wigner functions with values in $\mathfrak{X}^+$. Hence π^{w} restricted to $Q^{+}\mathfrak{W}_q$ equals the representation induced from σ^{+} ($\equiv \sigma$, restricted to $\mathfrak{X}^+$). This shows that π^{w} acts irreducibly on $Q^{+}\mathfrak{W}_q$.

For particles with nonzero rest mass, we obtain as a whole four irreducible representations in the Hilbert spaces

$$\mathfrak{W}^{\epsilon}_{q_\delta} \equiv Q^{\epsilon}\,\mathfrak{W}_{q_\delta}, \qquad \epsilon, \delta = + \text{ or } -, \qquad q_{\pm} = (\pm\mu, 0, 0, 0). \tag{3.77}$$

The index δ distinguishes between particles with positive (+) or negative (−) rest energy. The index ϵ corresponds to two possibilities of implementing the parity transform. We want to stress that the spaces $\mathfrak{W}^{\pm}_q$ do not consist of states with even or odd parity. The action of the parity transform is the restriction

of $\pi^{\mathrm{w}}(0, \mathbf{L}_P)$ to $\mathfrak{W}_q^{\pm}$, and can be evaluated with the help of Eq. (3.64), using $\mathbf{L}_P = \beta$. It is only at the point $p = q$ that we find $\pi^{\mathrm{w}}(0, \mathbf{L}_P)\, \zeta^{\pm}(q) = \pm\zeta^{\pm}(q)$ for $\zeta^{\pm} \in \mathfrak{W}_q^{\pm}$.

3.3 Covariant Realizations and the Dirac Equation

3.3.1 Covariant States

Let $\mathcal{G}$ be a separable Lie group, $\mathcal{K}$ a closed subgroup, and τ a unitary representation of $\mathcal{K}$ in a Hilbert space $\mathfrak{X}$. In this section we describe a second possibility of eliminating the subsidiary condition (3.3). Let us assume that the unitary representation τ of $\mathcal{K}$ is the restriction of a representation $\tilde{\tau}$ in $\mathfrak{X}$ of the whole group $\mathcal{G}$. It is not necessary to assume that $\tilde{\tau}(g)$ be unitary for those elements $g \in \mathcal{G}$ which are not in $\mathcal{K}$. For any function ϕ on $\mathcal{G}$ satisfying the condition (3.3) we can define a new function

$$\tilde{\psi}(g) \equiv \tilde{\tau}(g)\, \phi(g). \tag{3.78}$$

This function has the nice property

$$\tilde{\psi}(gk^{-1}) \equiv \tilde{\tau}(gk^{-1})\phi(gk^{-1}) = \tilde{\tau}(gk^{-1})\tau(k)\phi(g) = \tilde{\tau}(g)\phi(g) \equiv \tilde{\psi}(g), \tag{3.79}$$

i.e., $\tilde{\psi}$ depends only on the coset $g\mathcal{K}$ of g and it is sufficient to know $\tilde{\psi}$ on a representative of this coset,

$$\tilde{\psi}(h) = \tilde{\psi}(s) = \tilde{\tau}(s)\, \zeta(s) \quad \text{for all } h \in g\mathcal{K} \text{ and } s = s(g\mathcal{K}). \tag{3.80}$$

(s is the map chosen in order to define the Wigner states, see Sect. 3.2.1). We define a Hilbert space $\mathfrak{C}$ of functions $\tilde{\psi}$ defined on $S = s(\mathcal{G}/\mathcal{K})$ by introducing the scalar product

$$(\tilde{\psi}_1, \tilde{\psi}_2) \equiv \int_S \left(\tilde{\tau}(s)^{-1}\tilde{\psi}_1(s)\,, \tilde{\tau}(s)^{-1}\tilde{\psi}_2(s) \right)_{\mathfrak{X}} d\mu(s). \tag{3.81}$$

With this definition, the mapping $\zeta \to \tilde{\psi}$ defined by (3.80) is an isometric isomorphism of $\mathfrak{W}$ and $\mathfrak{C}$. In the new Hilbert space $\mathfrak{C}$ a representation π^{c} of $\mathcal{G}$ can be defined with (3.50) as follows:

$$\begin{aligned} \tilde{\psi}(s) &= \tilde{\tau}(s)\, \zeta(s) \\ &\to \tilde{\tau}(s) \left(\pi^{\mathrm{w}}(h)\zeta\right)(s) = \tilde{\tau}(s)\, \tilde{\tau}\left(s^{-1}h(\Lambda_h^{-1}s)\right) \zeta(\Lambda_h^{-1}s) \\ &= \tilde{\tau}(s)\, \tilde{\tau}(s^{-1})\, \tilde{\tau}(h)\, \tilde{\tau}(\Lambda_h^{-1}s)\, \zeta(\Lambda_h^{-1}s) = \tilde{\tau}(h)\, \tilde{\psi}(\Lambda_h^{-1}s), \end{aligned} \tag{3.82}$$

i.e.,

$$\left(\pi^{\mathrm{c}}(h)\, \tilde{\psi}\right)(s) = \tilde{\tau}(h)\, \tilde{\psi}(\Lambda_h^{-1}s). \tag{3.83}$$

The operator $\pi^{\mathrm{c}}(h) : \mathfrak{C} \to \mathfrak{C}$ is unitary for all $h \in \mathcal{G}$ whenever $\pi^{\mathrm{w}}(k) : \mathfrak{W} \to \mathfrak{W}$ is unitary for all $k \in \mathcal{K}$. Clearly, the representation π^{c} is equivalent to the representation π^{w}. Hence the irreducibility of π^{c} depends on the irreducibility of the restriction τ of $\tilde{\tau}$. The elements of the representation space $\mathfrak{C}$ are called "covariant states" and π^{c} "covariant representation".

3.3.2 Covariant States for the Poincaré Group

In the following we investigate the covariant representation defined by the orbits of $q = q_+$ or $q = q_-$, where

$$q_\pm = (\pm\mu, 0, 0, 0)^\top \quad \mu > 0, \tag{3.84}$$

and the representation

$$\tau(a, \mathbf{L}) = e^{\mathrm{i}\,\langle q,a\rangle}\mathbf{L}, \quad \text{all } (a, \mathbf{L}) \in \tilde{\mathcal{P}}_q, \tag{3.85}$$

of the corresponding isotropy group $\mathcal{K} = \tilde{\mathcal{P}}_q$ in the Hilbert space $\mathfrak{X} = \mathbb{C}^4$. (See (3.36) and (3.38) for a definition of $\tilde{\mathcal{P}}_q$). Clearly, τ is the restriction of the representation

$$\tilde{\tau}(a, \mathbf{L}) = e^{\mathrm{i}\,\langle q,a\rangle}\mathbf{L}, \quad \text{all } (a, \mathbf{L}) \in \tilde{\mathcal{P}}^\uparrow, \tag{3.86}$$

to the isotropy subgroup. The representation $\tilde{\tau}$ of $\tilde{\mathcal{P}}^\uparrow$ is not unitary because the matrices corresponding to boosts are only Hermitian (cf. Sect. 2.5). But the restriction τ of $\tilde{\tau}$ is unitary and we can define the two representations of $\tilde{\mathcal{P}}^\uparrow$ induced by τ in the two Hilbert spaces $\mathfrak{W}_{q_+}$ and $\mathfrak{W}_{q_-}$. Both representations are reducible because the restriction τ of $\tilde{\tau}$ is reducible in $\mathbb{C}^4$ (see Sect. 3.2.5).

Starting from Wigner states we define the covariant states

$$\tilde{\psi}(p) \equiv \tilde{\tau}(0, \mathbf{L}_p)\zeta(p) = \mathbf{L}_p\zeta(p), \quad \text{all } \zeta \in \mathfrak{W}_q. \tag{3.87}$$

as in the previous section. Although the matrix $\mathbf{L}_p$ in (3.87) is not unitary, the map $\zeta(p) \to \tilde{\psi}(p)$ is unitary (isometric) from $\mathfrak{W}_q$ to $\mathfrak{C}_q$. Here the matrix $\mathbf{L}_p$ is given by (3.57). The covariant states form a Hilbert space $\mathfrak{C}_q$ of $\mathbb{C}^4$-valued functions with the scalar product

$$(\tilde{\psi}_1, \tilde{\psi}_2) = \int_{O_q} \frac{d^3p}{|p_0|} \left(\mathbf{L}_p^{-1}\tilde{\psi}_1(p), \mathbf{L}_p^{-1}\tilde{\psi}_2(p)\right)_{\mathbb{C}^4}. \tag{3.88}$$

The covariant representation is given by the unitary operators

$$\pi^{\mathrm{c}}(a, \mathbf{L})\,\tilde{\psi}(p) = e^{i\langle p,a\rangle}\,\mathbf{L}\tilde{\psi}(\Lambda_{\mathbf{L}}^{-1}p), \quad \text{all } (a, \mathbf{L}) \in \tilde{\mathcal{P}}^\uparrow \text{ and } \tilde{\psi} \in \mathfrak{C}_q. \tag{3.89}$$

3.3.3 Invariant Subspaces

From Sect. 3.2.5 we know that the subspaces $Q^\pm\mathfrak{W}_q$, with

$$Q^\pm = \frac{1}{2}(1 \pm \beta), \tag{3.90}$$

are invariant and irreducible under π^{w}. In (3.90) β denotes the Dirac β-matrix. The Wigner states ζ in the invariant subspaces satisfy

$$\zeta(p) = Q^\pm\zeta(p) \quad \text{if } \zeta \in Q^\pm\mathfrak{W}_q. \tag{3.91}$$

and for the corresponding covariant states $\tilde{\psi} = \mathbf{L}_p\zeta$ we obtain

$$\tilde{\psi}(p) = \mathbf{L}_p(Q^{\pm}\zeta)(p) = (\mathbf{L}_p Q^{\pm}\mathbf{L}_p^{-1})\mathbf{L}_p\zeta(p) = (\mathbf{L}_p Q^{\pm}\mathbf{L}_p^{-1})\tilde{\psi}(p). \tag{3.92}$$

Therefore, also $\mathfrak{C}_q$ splits into the two invariant subspaces

$$\mathfrak{C}_q^{\pm} = (\mathbf{L}_p Q^{\pm}\mathbf{L}_p^{-1})\mathfrak{C}_q = \mathbf{L}_p Q^{\pm}\mathfrak{W}_q. \tag{3.93}$$

The corresponding projection operators are multiplication by a matrix-valued function of p which can be obtained from (3.53),

$$Q^{\pm}(p) \equiv \mathbf{L}_p Q^{\pm}\mathbf{L}_p^{-1} = \frac{1}{2}(1 \pm \mathbf{L}_p\beta\mathbf{L}_p^{-1}) = \frac{1}{2q_0}(q_0\mathbf{1} \pm \langle\gamma, p\rangle). \tag{3.94}$$

The condition

$$Q^{\pm}(p)\tilde{\psi}(p) = \tilde{\psi}(p), \quad \text{all } \tilde{\psi} \in \mathfrak{C}_q^{\pm}, \tag{3.95}$$

is equivalent to

$$\langle\gamma, p\rangle\tilde{\psi}(p) = \pm q_0\tilde{\psi}(p), \quad \text{all } \tilde{\psi} \in \mathfrak{C}_q^{\pm}. \tag{3.96}$$

We want to stress that the covariant states $\tilde{\psi}(p)$ are not eigenstates of the parity matrix $\mathbf{L}_P = \beta$.

3.3.4 The Scalar Product in the Invariant Subspaces

Using

$$\mathbf{L}_p^{-1}\tilde{\psi} = \pm\beta\mathbf{L}_p^{-1}\tilde{\psi}, \quad \text{for } \tilde{\psi} \in \mathfrak{C}_q^{\pm}, \tag{3.97}$$

and (2.216), i.e.,

$$\mathbf{L}_p^{*-1}\beta\mathbf{L}_p^{-1} = \beta, \tag{3.98}$$

we obtain

$$\big(\mathbf{L}_p^{-1}\tilde{\psi}_1(p), \mathbf{L}_p^{-1}\tilde{\psi}_2(p)\big)_{\mathbb{C}^4} = \pm\big(\tilde{\psi}_1(p), \beta\tilde{\psi}_2(p)\big)_{\mathbb{C}^4}, \quad \text{for } \tilde{\psi}_1, \tilde{\psi}_2 \in \mathfrak{C}_q^{\pm}. \tag{3.99}$$

Hence the scalar product (3.88) in $\mathfrak{C}_q^{\pm}$ becomes Covariant states — scalar product

$$(\tilde{\psi}_1, \tilde{\psi}_2) = \pm\int_{O_q} \frac{d^3p}{|p_0|}\,\big(\tilde{\psi}_1(p), \beta\tilde{\psi}_2(p)\big)_{\mathbb{C}^4}, \quad \tilde{\psi}_1, \tilde{\psi}_2 \in \mathfrak{C}_q^{\pm}. \tag{3.100}$$

For $\tilde{\psi} \in \mathfrak{C}_q^{\pm}$ we obtain (using $\beta = \gamma_0$) from (3.96) the relation

$$\big(\tilde{\psi}(p), \beta p_0\,\tilde{\psi}(p)\big) = \big(\tilde{\psi}(p), \{\pm q_0\}\tilde{\psi}(p)\big) + \big(\tilde{\psi}(p), \sum_{k=1}^{3}\gamma_k p_k\,\tilde{\psi}(p)\big). \tag{3.101}$$

Since the Dirac matrices γ_1, γ_2, γ_3 are antihermitian, the last summand is purely imaginary, while the other expressions are real. Hence we must have

$$(\tilde{\psi}(p), \beta\tilde{\psi}(p)) = \pm\frac{q_0}{p_0}(\tilde{\psi}(p), \tilde{\psi}(p)), \quad \text{for all } \tilde{\psi} \in \mathfrak{C}_q^{\pm}, \tag{3.102}$$

and therefore, using (3.100) and $q_0/p_0 = \mu/|p_0|$,

$$(\tilde{\psi}, \tilde{\psi}) = \|\tilde{\psi}\|^2 = \int_{O_q} d^3p\, \frac{\mu}{p_0^2}\, \|\tilde{\psi}(p)\|_{\mathbb{C}^4}^2, \quad \text{all } \tilde{\psi} \in \mathfrak{C}_q^{\pm}. \tag{3.103}$$

With the parallelogram identity this finally gives

$$(\tilde{\psi}_1, \tilde{\psi}_2) = \int_{O_q} d^3p\, \frac{\mu}{p_0^2}\, (\tilde{\psi}_1(p), \tilde{\psi}_2(p))_{\mathbb{C}^4}, \quad \text{all } \tilde{\psi}_1, \tilde{\psi}_2 \in \mathfrak{C}_q^{\pm}. \tag{3.104}$$

3.3.5 Covariant Dirac Equation

Eq. (3.96) is a condition for the generators of the space-time translations in the Hilbert spaces $\mathfrak{C}_q^{\pm}$. From

$$\pi^c(a, \mathbf{1})\,\tilde{\psi}(p) = e^{i\,(p,a)}\tilde{\psi}(p), \quad \text{all } \tilde{\psi} \in \mathfrak{C}_q^{\pm}, \tag{3.105}$$

it is clear that the operator of multiplication by p_0 is the self-adjoint generator of time translations, whereas p_k, $k = 1, 2, 3$, generate space translations. Multiplying (3.96) from the left with $\gamma_0 = \beta$ and using $\alpha_k = \beta\gamma_k$ we obtain

$$p_0\,\tilde{\psi}(p) = \Big\{\sum_{k=1}^{3} \alpha_k p_k \pm \beta q_0\Big\}\tilde{\psi}(p) \quad \text{for all } \tilde{\psi} \in \mathfrak{C}_q^{\pm}. \tag{3.106}$$

While this relation holds for all $\tilde{\psi} \in \mathfrak{C}_q^{\pm}$, it is clear that the domain of the operator of multiplication by p_0 in the Hilbert spaces $\mathfrak{C}_q^{\pm}$ consists only of those $\tilde{\psi}$ for which also $p_0\tilde{\psi} \in \mathfrak{C}_q^{\pm}$. In all these expressions, $q = q_+$ or $q = q_-$, as in (3.84). For $\tilde{\psi}$ in $\mathfrak{C}_{q_+}^{+}$ (i.e., $q_0 = +\mu$) and for $\tilde{\psi} \in \mathfrak{C}_{q_-}^{-}$ (i.e., $q_0 = -\mu$) the expression $\{\ldots\}$ in Eq. (3.106) coincides with the Dirac operator $H_0/c = \boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta mc$ in momentum space (see Sect. 1.4). Here we have identified μ with mc, m being the mass of the particle. Eq. (3.96) becomes

$$\langle\gamma, p\rangle\,\tilde{\psi}(p) - mc\,\tilde{\psi}(p) = 0, \quad \text{for } \tilde{\psi} \in \mathfrak{C}_{q_+}^{+} \text{ or } \tilde{\psi} \in \mathfrak{C}_{q_-}^{-}, \tag{3.107}$$

and is called the Dirac equation in covariant form.

Remark. For $\tilde{\psi}$ in $\mathfrak{C}_{q_+}^{-}$ or $\mathfrak{C}_{q_-}^{+}$ Eq. (3.106) leads to a Dirac operator H_0' with β-matrix having the opposite sign. It is unitarily equivalent to H_0 because $H_0' = \gamma_5 H_0 \gamma_5$.

The argument $p = (p_0, \boldsymbol{p})$ of the covariant functions $\tilde{\psi} \in \mathfrak{C}_{q_+}^{\pm}$ can vary on the orbit $O_{q_+} = \{\, p \in \mathbb{R}^4 \mid p_0 = \sqrt{\boldsymbol{p}^2 + m^2c^2}\,\}$. Hence

$$p_0\,\tilde{\psi}(p) = \frac{\lambda(p)}{c}\,\tilde{\psi}(p), \quad \text{if } \tilde{\psi} \in \mathfrak{C}_{q_+}^{\pm}, \tag{3.108}$$

where $\lambda(p) \equiv (c^2\boldsymbol{p}^2 + m^2c^4)^{(1/2)}$. Similarly,

$$p_0\,\tilde{\psi}(p) = -\frac{\lambda(p)}{c}\,\tilde{\psi}(p), \quad \text{if } \tilde{\psi} \in \mathfrak{C}^{\pm}_{q_-}, \tag{3.109}$$

Therefore (3.106) defines a positive operator in $\mathfrak{C}^{\pm}_{q_+}$, and a negative operator on $\mathfrak{C}^{\pm}_{q_-}$.

3.3.6 The Configuration Space

Let

$$M = O_{q_+} \cup O_{q_-}, \quad q_\pm = (\pm mc, 0, 0, 0)^{\tilde{}}, \quad mc > 0 \tag{3.110}$$

be the two-sheeted mass hyperboloid and assume

$$\tilde{\psi} \in \mathfrak{C}^{+}_{q_+} \oplus \mathfrak{C}^{-}_{q_-}. \tag{3.111}$$

Hence $\tilde{\psi}$ is a function defined on M such that

$$\int_M d^3p\,\frac{mc}{p_0^2}\,(\tilde{\psi}(p), \tilde{\psi}(p))_{\mathbb{C}^4} < \infty, \tag{3.112}$$

and such that (3.107) holds. The Hilbert space $\mathfrak{C}^{+}_{q_+} \oplus \mathfrak{C}^{-}_{q_-}$ is the direct sum of two $\tilde{\mathcal{P}}^{\uparrow}$-invariant subspaces.

The covariant functions $\tilde{\psi}(p)$ do not really depend on four variables, because p is restricted to M. In order to make this explicit we define two functions $\hat{\psi}_{\text{pos,neg}}$ on $\mathbb{R}^3$ by

$$\frac{\sqrt{mc}}{p_0}\,\tilde{\psi}(p) \equiv \begin{cases} \hat{\psi}_{\text{pos}}(\boldsymbol{p}), & \text{if } p \in O_{q_+}, \\ \hat{\psi}_{\text{neg}}(\boldsymbol{p}), & \text{if } p \in O_{q_-}. \end{cases} \tag{3.113}$$

The functions $\hat{\psi}_{\text{pos,neg}}$ are square integrable and orthogonal in the Hilbert space $L^2(\mathbb{R}^3, d^3p, \mathbb{C}^4) \equiv L^2(\mathbb{R}^3, d^3p)^4$. The generators of space and time translations act as matrix multiplication operators on the functions $\hat{\psi}$. After an inverse Fourier transformation these generators will be represented by differential operators. Assume that $\hat{\psi}_{\text{pos,neg}}$ are smooth functions in $\mathcal{S}(\mathbb{R}^3)^4$, and with $x = (x_0, \boldsymbol{x}) = (ct, \boldsymbol{x})$ define

$$\begin{aligned} \psi(x) &= \sqrt{\frac{mc}{8\pi^3}} \int_M \frac{d^3p}{p_0}\, e^{-\mathrm{i}\,\langle p,x\rangle}\tilde{\psi}(p) \\ &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} d^3p\, e^{\mathrm{i}\,\boldsymbol{p}\cdot\boldsymbol{x}} \left\{ e^{-\mathrm{i}\,\lambda(p)t}\hat{\psi}_{\text{pos}}(\boldsymbol{p}) + e^{\mathrm{i}\,\lambda(p)t}\hat{\psi}_{\text{neg}}(\boldsymbol{p}) \right\}. \end{aligned} \tag{3.114}$$

It is easy to see that ψ is a solution of the Dirac equation because (3.107) implies

$$0 = \sqrt{\frac{mc}{8\pi^3}} \int_M \frac{d^3p}{p_0}\, e^{-\mathrm{i}\,\langle p,x\rangle} \{p_0 - \boldsymbol{\alpha}\cdot\boldsymbol{p} - \beta mc\}\,\tilde{\psi}(p)$$

$$= \{\mathrm{i}\frac{\partial}{\partial x_0} - \boldsymbol{\alpha}\cdot(-\mathrm{i}\nabla) - \beta mc\}\,\psi(x),$$

i.e.,

$$\mathrm{i}\frac{\partial}{\partial t}\,\psi(x) = \{-\mathrm{i}\,c\boldsymbol{\alpha}\cdot\nabla + \beta mc^2\}\,\psi(x). \tag{3.115}$$

For each fixed $x_0 = ct$ and smooth functions $\tilde{\psi}_1,\ \tilde{\psi}_2 \in \mathfrak{C}^+_{q_+} \oplus \mathfrak{C}^-_{q_-}$ we find for the corresponding functions $\psi_1,\ \psi_2$ that

$$\int_M d^3p\,\frac{mc}{p_0^2}\,(\tilde{\psi}_1(p), \tilde{\psi}_2(p))_{\mathbb{C}^4} = \int_{\mathbb{R}^3} d^3x\,(\psi_1(x_0,\boldsymbol{x}), \psi_2(x_0,\boldsymbol{x}))_{\mathbb{C}^4}, \tag{3.116}$$

i.e., the mapping $\tilde{\psi} \to \psi$ extends to a unitary mapping from $\mathfrak{C}^+_{q_+} \oplus \mathfrak{C}^-_{q_-}$ onto $\mathfrak{H} = L^2(\mathbb{R}^3, d^3x)^4$. From Sect. 1.4 we know that $\mathfrak{H}$ decomposes into a direct sum $\mathfrak{H} = \mathfrak{H}_{\mathrm{pos}} \oplus \mathfrak{H}_{\mathrm{neg}}$ of spectral subspaces belonging to positive and negative energies, respectively. $\mathfrak{H}_{\mathrm{pos}}$ is the image of $\mathfrak{C}^+_{q_+}$ under the isomorphism $\tilde{\psi} \to \psi$, and $\mathfrak{H}_{\mathrm{neg}}$ is the image of $\mathfrak{C}^-_{q_-}$.

3.3.7 Poincaré Transformations in Configuration Space

Using (3.114), the Poincaré transformation (3.89) of a covariant state $\tilde{\psi}(p)$ can be represented in the configuration space $\mathfrak{H} = L^2(\mathbb{R}^3, d^3x)^4$ as follows.

$$\begin{aligned}
\psi(x) \to \sqrt{\frac{mc}{8\pi^3}} \int_M \frac{d^3p}{p_0}\, e^{-\mathrm{i}\,\langle p,x\rangle}\, e^{\mathrm{i}\,\langle p,a\rangle}\, \mathbf{L}\,\tilde{\psi}(\Lambda_{\mathbf{L}}^{-1}p) \\
= \mathbf{L}\sqrt{\frac{mc}{8\pi^3}} \int_M \frac{d^3p}{p_0}\, e^{-\mathrm{i}\,\langle p,x-a\rangle}\,\tilde{\psi}(\Lambda_{\mathbf{L}}^{-1}p) \\
= \mathbf{L}\sqrt{\frac{mc}{8\pi^3}} \int_M \frac{d^3p}{p_0}\, e^{-\mathrm{i}\,\langle \Lambda_{\mathbf{L}}p,x-a\rangle}\,\tilde{\psi}(p) \\
= \mathbf{L}\sqrt{\frac{mc}{8\pi^3}} \int_M \frac{d^3p}{p_0}\, e^{-\mathrm{i}\,\langle p,\Lambda_{\mathbf{L}}^{-1}(x-a)\rangle}\,\tilde{\psi}(p) \\
= \mathbf{L}\,\psi\big(\Lambda_{\mathbf{L}}^{-1}(x-a)\big).
\end{aligned} \tag{3.117}$$

We collect these results in the following theorem

Theorem 3.8. In the Hilbert space $\mathfrak{H} = L^2(\mathbb{R}^3, d^3x)^4$ let H_0 be the free Dirac operator and denote

$$\psi(t,\boldsymbol{x}) = e^{-\mathrm{i}H_0 t}\,\psi(\boldsymbol{x}), \qquad \text{all } \psi \in \mathfrak{H},\ \boldsymbol{x} \in \mathbb{R}^3. \tag{3.118}$$

The transformations $(a, \mathbf{L})$ of the Poincaré covering group $\tilde{\mathcal{P}}^\uparrow$ are represented by unitary operators

$$\pi(a,\mathbf{L})\,\psi(t,\boldsymbol{x}) = \mathbf{L}\,\psi(t',\boldsymbol{x}'), \tag{3.119}$$

where $(ct', \boldsymbol{x}') \equiv x' = \Lambda_{\mathbf{L}}^{-1}(x-a)$, $x = (ct, \boldsymbol{x})$. In particular,

$$e^{-\mathrm{i}H_0 t} = \pi(a, \mathbf{1}), \qquad \text{where } a = (-t, 0, 0, 0). \tag{3.120}$$

The next theorem states that this representation coincides with the representation obtained in Sect. 2.3 by integrating the Lie algebra representation.

Theorem 3.9. The infinitesimal generators of the representation

$$\{\pi(a, \mathbf{L})\psi\}(x) = \mathbf{L}\,\psi\big(\Lambda_{\mathbf{L}}^{-1}(x - a)\big) \tag{3.121}$$

of $\tilde{\mathcal{P}}_+^\uparrow$ in $L^2(\mathbb{R}^3, d^3x)^4$ are just the operators H_0, $\boldsymbol{p}$, $\boldsymbol{J}$, and $\boldsymbol{N}$ of Theorem 2.14.

Proof. As a typical example we calculate the generator of a boost in the x_1 direction. The other generators can be found similarly. The (active) boost is given by

$$\begin{aligned} &x^0 \to x^0 \cosh\omega + x^1 \sinh\omega, \quad x^1 \to x^0 \sinh\omega + x^1 \cosh\omega, \\ &x^2 \to x^2, \qquad\qquad x^3 \to x^3. \end{aligned} \tag{3.122}$$

Hence, using (2.136) we find that at time $x^0 = 0$ the covariant representation (3.121) of this boost is given by

$$\{\pi(0, \mathbf{L}_H)\psi\}(0, \boldsymbol{x}) = e^{(\omega/2)\alpha_1}\psi(-x^1 \sinh\omega, x^1 \cosh\omega, x^2, x^3). \tag{3.123}$$

By construction, this transformation is unitary, and we write it as $\exp(\mathrm{i}\,\omega N_1/c)$. Its self-adjoint generator N_1 is obtained by differentiation with respect to ω,

$$\begin{aligned} &-\mathrm{i}\,\frac{d}{d\omega} e^{(\omega/2)\alpha_1}\psi(-x^1 \sinh\omega, x^1 \cosh\omega, x^2, x^3) \\ &= -e^{(\omega/2)\alpha_1}\left\{\mathrm{i}\,\frac{\alpha_1}{2} - x^1 \cosh\omega\,\mathrm{i}\,\partial_0 + x^1 \sinh\omega\,\mathrm{i}\,\partial_1\right\}\psi(\ldots). \end{aligned} \tag{3.124}$$

But any ψ in the representation space satisfies (3.115), i.e., $\mathrm{i}\,\partial_0\psi = (H_0/c)\psi$, where H_0 is the free Dirac operator. Evaluating (3.124) at $\omega = 0$ gives therefore

$$\frac{N_1}{c} = -\mathrm{i}\,\frac{\alpha_1}{2} + x_1\frac{H_0}{c} = \frac{1}{2c}(H_0 x_1 + x_1 H_0). \tag{3.125}$$

But this result coincides with the usual definition of N_1, cf. (2.71). □

3.3.8 Invariance of the Free Dirac Equation

The Dirac equation is invariant under Poincaré transformations in the following sense. If we apply a Poincaré transformation to a solution $\psi(x^0, \boldsymbol{x})$ of the Dirac equation (3.115), then $\{\pi(a, \mathbf{L})\psi\}(x^0, \boldsymbol{x})$, given by (3.121), is another solution of the Dirac equation. This is an immediate consequence of our construction of the Dirac equation as the projection onto an irreducible subspace. It is, however, useful to verify the invariance of the Dirac equation by a direct calculation. In configuration space, we assume

$$mc\,\psi(x) = \mathrm{i}\gamma^\mu \frac{\partial}{\partial x^\mu}\,\psi(x) \tag{3.126}$$

with ψ being continuously differentiable in all variables. We denote $x' = \Lambda^{-1}(x-a)$ and perform a Poincaré transformation on both sides of (3.126). Using the summation convention we have

$$mc\,\mathbf{L}\psi(x') = \mathbf{L}\,\mathrm{i}\gamma^\mu \frac{\partial}{\partial x'^\mu}\,\psi(x') = \mathbf{L}\,\mathrm{i}\gamma^\mu \frac{\partial}{\partial x^\lambda}\,\psi(x')\,\frac{\partial x^\lambda}{\partial x^\mu} =$$

$$\mathbf{L}\,\mathrm{i}\Lambda^\lambda{}_\mu\gamma^\mu \frac{\partial}{\partial x^\lambda}\,\psi(x') = \mathbf{L}\,\mathrm{i}\Lambda^\lambda{}_\mu\gamma^\mu\mathbf{L}^{-1}\mathbf{L}\frac{\partial}{\partial x^\lambda}\,\psi(x'). \tag{3.127}$$

Finally, using (2.163) we obtain

$$mc\,\mathbf{L}\psi\big(\Lambda^{-1}(x-a)\big) = \mathrm{i}\gamma^\lambda \frac{\partial}{\partial x^\lambda}\,\mathbf{L}\psi\big(\Lambda^{-1}(x-a)\big). \tag{3.128}$$

Hence the Poincaré transformed wavefunction $\psi'(x) = \mathbf{L}\psi\big(\Lambda^{-1}(x-a)\big)$ is again a solution of the Dirac equation.

Remark. In a practical calculation one wants to determine the transformed wavefunction of an electron which is boosted with some velocity $\boldsymbol{v}$ or rotated through an angle φ around some axis $\boldsymbol{n}$. Usually, only the matrix Λ is given, e.g., by Eqs. (2.11), (2.14), or (2.18), and one has to determine first the matrix $\mathbf{L}$ which transforms the spinor components of ψ. This can be done for any $\Lambda \in \mathcal{L}^\uparrow$ with the help of Eq. (2.215). If Λ is already given as the product of a boost, a rotation, and a space reflection (any $\Lambda \in \mathcal{L}^\uparrow$ can be written in this way), then it is easier to use the matrices $\mathbf{L}$ given explicitly by Eqs. (2.168), (2.169), and (2.170) in terms of the boost-velocity $\boldsymbol{v}$, or rotation-vector $\boldsymbol{\varphi}$. In Sect. 3.4 below we are going to show how to deal with a time-reversal or space-time reflection.

3.3.9 The Foldy-Wouthuysen Transformation

Multiplication with the matrix

$$\mathbf{L}_p = \frac{q_0 + p_0 + \boldsymbol{\alpha}\cdot\boldsymbol{p}}{\sqrt{2q_0(q_0+p_0)}}. \tag{3.129}$$

is applied to Wigner states in $\mathfrak{W}_{q_\pm}$, $q_\pm = (\pm mc, 0, 0, 0)^\top$, when transforming to the covariant representation in (3.87). For Wigner states ζ in $Q^+\mathfrak{W}_{q_+} \oplus Q^-\mathfrak{W}_{q_-}$, we replace q_0 in (3.129) by $mc\,\mathrm{sgn}(p_0)$ and use

$$\beta\zeta(p) = \mathrm{sgn}(p_0)\,\zeta(p) = \frac{\lambda(p)}{cp_0}\zeta(p). \tag{3.130}$$

Hence

$$\tilde{\psi}(p) = \mathbf{L}_p\zeta(p) = \frac{mc^2 + \lambda(p) - \beta c\boldsymbol{\alpha}\cdot\boldsymbol{p}}{\sqrt{2mc^2(mc^2+\lambda(p))}}\,\mathrm{sgn}(p_0)\,\zeta(p)$$

$$= u(\boldsymbol{p})^{-1} \sqrt{\frac{\lambda(p)}{mc^2}}\, \mathrm{sgn}(p_0)\, \zeta(p), \tag{3.131}$$

where $u(\boldsymbol{p})$ is the unitary matrix defined in Eq. (1.43). We obtain

$$\frac{1}{\sqrt{|p_0|}}\, \zeta(p) = u(\boldsymbol{p})\, \frac{\sqrt{mc}}{p_0}\, \tilde{\psi}(p) = \begin{cases} u(\boldsymbol{p})\hat{\psi}_{\mathrm{pos}}(\boldsymbol{p}), & \text{if } p \in O_{q_+}, \\ u(\boldsymbol{p})\hat{\psi}_{\mathrm{neg}}(\boldsymbol{p}), & \text{if } p \in O_{q_-}. \end{cases} \tag{3.132}$$

Applying an inverse Fourier transformation and using $U_{\mathrm{FW}} = \mathcal{F}^{-1} u(\boldsymbol{p}) \mathcal{F}$ we find that a Foldy-Wouthuysen transformation maps a state $\psi(\boldsymbol{x})$ onto a state

$$(U_{\mathrm{FW}}\psi)(\boldsymbol{x}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} d^3p\, e^{\mathrm{i}p\cdot\boldsymbol{x}}\, \frac{1}{\sqrt{|p_0|}}\, \zeta(p). \tag{3.133}$$

In this way the Foldy-Wouthuysen transformation links the Hilbert space of covariant states with the Hilbert space of Wigner states.

3.4 Representations of Discrete Transformations

We have obtained a unitary representation of the Poincaré covering group $\tilde{\mathcal{P}}^{\uparrow}$, but in quantum mechanics we are mainly interested in a projective representation (Chapter 2). Hence there arises some ambiguity in the representation of the discrete transformations. For example, if we had started with the group $\tilde{\mathcal{P}}'^{\uparrow}$, where the matrix $\mathbf{L}_P$ is replaced by $\mathbf{L}'_P = \mathrm{i}\mathbf{L}_P$, and which is also a covering group of $\mathcal{P}^{\uparrow}$, then we would have obtained the same projective representation of $\mathcal{P}^{\uparrow}$. One could even represent the discrete group elements by antiunitary operators. In the following we describe some restrictions on the number of possible choices which arise from mathematical and physical considerations.

3.4.1 Projective Representations of the Poincaré Group

Any projective representation of the full Poincaré group contains a projective unitary representation of the proper Poincaré group corresponding to a unitary representation π of the covering group $\tilde{\mathcal{P}}^{\uparrow}_{+}$. This representation has the property (2.98), i.e.,

$$\pi(0, \pm\mathbf{1}_4) \in U(1) \equiv \{e^{\mathrm{i}\theta}\mathbf{1} \mid \theta \in \mathbb{R}\}, \tag{3.134}$$

and from Definition 2.10.b we find

$$\pi(0, \mathbf{1}_4) = \mathbf{1}, \quad \pi(0, -\mathbf{1}_4) = \pm 1. \tag{3.135}$$

Consider any extension of this unitary representation of $\tilde{\mathcal{P}}^{\uparrow}_{+}$ by three additional unitary or antiunitary operators

$$\pi(0, \mathbf{L}_X) \equiv \pi_X, \quad \text{where } X = P,\ T, \text{ or } PT, \tag{3.136}$$

which describe the discrete Poincaré transformations. Let us assume (for X, $Y = P$, T, or PT)

$$\pi_X \pi_Y = \omega(X,Y)\,\pi(0, \mathbf{L}_X \mathbf{L}_Y), \quad \text{with } \omega(X,Y) \in U(1), \tag{3.137}$$

$$\pi_X \pi(a,\mathbf{L}) = \omega_X(a,\mathbf{L})\,\pi(Xa, \mathbf{L}_X \mathbf{L} \mathbf{L}_X^{-1})\,\pi_X, \quad \text{with } \omega_X(a,\mathbf{L}) \in U(1), \tag{3.138}$$

where $(a,\mathbf{L}) \in \tilde{\mathcal{P}}_+^\uparrow$, and hence

$$(Xa, \mathbf{L}_X \mathbf{L} \mathbf{L}_X^{-1}) = (0,\mathbf{L}_X)\,(a,\mathbf{L})\,(0,\mathbf{L}_X)^{-1} \in \tilde{\mathcal{P}}_+^\uparrow. \tag{3.139}$$

Next, define operators

$$\pi(Xa, \mathbf{L}_X \mathbf{L}) \equiv \pi_X\,\pi(a,\mathbf{L}), \quad A \in SL(2), \tag{3.140}$$

to obtain unitary or antiunitary operators also for the Poincaré transformations $(Xa, \mathbf{L}_X\mathbf{L})$ in the other connected components $(0,\mathbf{L}_X)\tilde{\mathcal{P}}_+^\uparrow$ of $\tilde{\mathcal{P}}$. The relations (3.137) and (3.138) assure that the symmetry transformations

$$\rho(a,\Lambda_{\mathbf{L}}) \equiv \pi(a,\mathbf{L}), \quad \text{for } (a,\mathbf{L}) \in \tilde{\mathcal{P}}, \tag{3.141}$$

form a projective representation of the full Poincaré group. However, the phase factors are not completely arbitrary.

First of all, we have

$$\pi_X^2 = \omega(X,X)\,\pi(0,\pm\mathbf{1}_4) = \pm\omega(X,X) \equiv e^{\mathrm{i}\phi}. \tag{3.142}$$

If π_X is antiunitary, we can write it in the form

$$\pi_X = UK, \tag{3.143}$$

where U is unitary and K is the antiunitary operator of complex conjugation in a suitable basis of the Hilbert space $\mathfrak{H}$. But then

$$\begin{aligned} e^{\mathrm{i}\phi} &= UKUK = U\overline{U}K^2 = U\overline{U} = U^\top \overline{U} U \overline{U} \\ &= U^\top \overline{U}\,\overline{\overline{U}}\,\overline{U} = U^\top e^{-\mathrm{i}\phi}\overline{U} = e^{-\mathrm{i}\phi} \end{aligned} \tag{3.144}$$

shows that

$$\pi_X^2 = \pm 1, \quad \text{if } \pi_X \text{ is antiunitary.} \tag{3.145}$$

On the other hand, if π_X is unitary we can always achieve $\pi_X^2 = 1$ instead of (3.142) by multiplying π_X with $\exp(-\mathrm{i}\phi/2)$. We also note that multiplying an antiunitary operator by a phase does not change its square because

$$(e^{\mathrm{i}\phi}\pi_X)^2 = e^{\mathrm{i}\phi} UK e^{\mathrm{i}\phi} UK = e^{\mathrm{i}\phi} e^{-\mathrm{i}\phi} UKUK = \pi_X^2. \tag{3.146}$$

Next, for $(a,\mathbf{L}) \in \tilde{\mathcal{P}}_+^\uparrow$ consider

$$\pi_X\,\pi(a,\mathbf{L})\,\pi_X^{-1} = \omega_X(a,\mathbf{L})\,\pi\big((0,X)\,(a,\mathbf{L})\,(0,X)\big). \tag{3.147}$$

Hence, if we multiply (3.147) by

$$\pi_X\,\pi(a',\mathbf{L}')\,\pi_X^{-1}, \quad (a',\mathbf{L}') \in \tilde{\mathcal{P}}_+^{\uparrow}, \tag{3.148}$$

we find, using the representation property

$$\pi(a,\mathbf{L})\,\pi(a',\mathbf{L}') = \pi\big((a,\mathbf{L})\,(a',\mathbf{L}')\big), \tag{3.149}$$

that the phase factors ω_X form a one-dimensional unitary representation of the group $\tilde{\mathcal{P}}_+^{\uparrow}$:

$$\omega_X(a,\mathbf{L})\,\omega_X(a',\mathbf{L}') = \omega_X\big((a,\mathbf{L})\,(a',\mathbf{L}')\big). \tag{3.150}$$

But the only finite dimensional unitary representation of the proper Poincaré group is the trivial representation. Hence we find

$$\omega_X(a,\mathbf{L}) = 1 \quad \text{for all } (a,\mathbf{L}) \in \tilde{\mathcal{P}}_+^{\uparrow} \tag{3.151}$$

and thus

$$\pi_X\,\pi(a,\mathbf{L})\,\pi_X^{-1} = \pi\big((0,\mathbf{L}_X)\,(a,\mathbf{L})\,(0,\mathbf{L}_X)\big). \tag{3.152}$$

3.4.2 Antiunitarity of the Time Reversal Operator

As in Sect. 2.3.2 we denote the self-adjoint generators of space-time translations by $p = (H_0/c, \boldsymbol{p})$, i.e.,

$$\pi(a,\mathbf{1}_4) \equiv \exp\big(\mathrm{i}H_0 a^0/c - \mathrm{i}\boldsymbol{p}\cdot\boldsymbol{a}\big) \equiv e^{\mathrm{i}\langle p,a\rangle}, \quad \text{for } a \in \mathbb{R}^4. \tag{3.153}$$

Theorem 3.10. If we require that $\mathfrak{H}_{\mathrm{pos}}$ and $\mathfrak{H}_{\mathrm{neg}}$ remain invariant with respect to all transformations of a representation of the full Poincaré group, i.e.,

$$\pi(a,\mathbf{L})\,(\operatorname{sgn} H_0)\,\pi(a,\mathbf{L})^{-1} = \operatorname{sgn} H_0, \quad \text{all } (a,\mathbf{L}) \in \tilde{\mathcal{P}}, \tag{3.154}$$

then the time reversal $(0,\mathbf{L}_T)$ must be represented by an antiunitary operator π_T, whereas the operator π_P corresponding to the parity transform has to be unitary.

Proof. Using (3.152) we find

$$\pi_X\,e^{\mathrm{i}\langle p,a\rangle}\,\pi_X^{-1} = e^{\mathrm{i}\langle p,Xa\rangle} = e^{\mathrm{i}\langle Xp,a\rangle}. \tag{3.155}$$

Choose $a = (ct,0,0,0)$. Then $\exp(\mathrm{i}\langle p,a\rangle) = \exp(\mathrm{i}H_0 t)$. If π_X is unitary, then by the spectral theorem

$$\pi_X\,e^{\mathrm{i}H_0 t}\,\pi_X^{-1} = \exp(\mathrm{i}\pi_X H_0\,\pi_X^{-1}\,t), \tag{3.156}$$

whereas if π_X is antiunitary,

$$\pi_X e^{\mathrm{i}H_0 t}\pi_X^{-1} = \exp(-\mathrm{i}\pi_X H_0\, \pi_X^{-1}\, t). \tag{3.157}$$

If $X = P$, then $\langle Xp, a\rangle = +H_0 t$, if $X = T$ or PT, then $\langle Xp, a\rangle = -H_0 t$. Hence we have to choose π_P unitary and the operators π_T and π_{PT} antiunitary in order to achieve $\pi_X H_0 \pi_X^{-1} = H_0$ in all cases. □

Let π be a representation of the group $\tilde{\mathcal{P}}$ with an antiunitary time reversal operator as required by the theorem. By a suitable choice of phase we can make the unitary operator π_P satisfy $\pi_P^2 = \mathbf{1}$. Furthermore, choose phases for π_T and π_{PT} such that $\pi_P\pi_T = \pi_{PT}$, where the square of the antiunitary operators π_T and π_{PT} remains $\pm\mathbf{1}$. Hence the representations of $\tilde{\mathcal{P}}$ with antiunitary time reversal can be labelled by $(\operatorname{sgn}\pi_T^2, \operatorname{sgn}\pi_{PT}^2)$. There are four possible combinations, $(+,+)$, $(+,-)$, $(-,+)$, and $(-,-)$. Each possibility obviously leads to the same projective representation of $\tilde{\mathcal{P}}$.

Example 3.11. In the Hilbert space of a Dirac electron,

$$\big(\pi_P\psi\big)(\boldsymbol{x}) = \mathbf{L}_P\, \psi(-\boldsymbol{x}) = \beta\psi(-\boldsymbol{x}), \tag{3.158}$$

$$\big(\pi_T\psi\big)(\boldsymbol{x}) = \beta\,\overline{\psi(\boldsymbol{x})}. \tag{3.159}$$

The last equation implies together with (3.157) and $\pi_T H_0 \pi_T^{-1} = H_0$

$$\big(\pi_T\psi\big)(t,\boldsymbol{x}) = e^{-\mathrm{i}H_0 t}\,\big(\pi_T\psi\big)(\boldsymbol{x}) = \pi_T e^{\mathrm{i}H_0 t}\,\psi(\boldsymbol{x}) = \beta\,\overline{\psi(-t,\boldsymbol{x})}. \tag{3.160}$$

For this choice we have $\operatorname{sgn}\pi_T^2 = \operatorname{sgn}\pi_{PT}^2 = 1$.

4 External Fields

In this chapter we introduce an external potential as an operator V of multiplication with a Hermitian 4×4 matrix-valued function of the space-time variable x. According to their behavior under Poincaré transformations the fields can be classified as scalar or pseudoscalar, vector potentials or pseudovector potentials, tensor or pseudotensor forces (Sects. 4.1 and 4.2). Vector potentials describe electromagnetic forces, scalar potentials can be used as a model for quark confinement, and tensor forces are needed to describe the behavior of particles with anomalous electric and magnetic moments.

In order to make the Dirac operator well defined and to ensure the existence of unique solutions for the initial value problem, the potential function $V(x)$ must have a certain regularity. In Sect. 4.3 we formulate conditions establishing the self-adjointness of the Dirac operator $H = H_0 + V$. Concerning the local behavior, potentials with $1/r$-singularities are admitted only for coupling constants γ less than $c/2$. Stronger singularities can only be dealt with for special matrix potentials. In the case of an electrostatic Coulomb potential γ/r one can find physically distinguished self-adjoint extensions for $\gamma < c$ (nuclear charges < 137). The behavior of the potentials at infinity is not restricted, in contrast to the Schrödinger case. This can be understood as a consequence of the finite propagation speed of Dirac particles. In Sect. 4.3.4 we show that the Dirac operator in an external field has the same essential spectrum as the free Dirac operator, provided the potential vanishes at infinity.

For static potentials the self-adjointness of the Dirac operator is sufficient to solve the initial value problem by Stone's theorem. For time-dependent potentials we need some additional assumptions. A short discussion of these problems is given in Sect. 4.4. The situation is particularly simple if the time dependence is the result of a gauge or symmetry transformation.

The limitations of the theory are most clearly indicated by the Klein paradox. This phenomenon occurs whenever the interaction is so strong as to cause transitions from electron states to positron states. We show that in the presence of high potential steps the Dirac equation has solutions which violate the principle of charge conservation. This paradoxical situation has no completely satisfactory physical explanation within a one particle interpretation.

The explicit solution of the Dirac equation with an external field is of course largely facilitated by the presence of symmetries. Most important for applications (e.g., the hydrogen atom) are spherically symmetric potentials, which we treat in Sect. 4.6. In this case the Hilbert space can be decomposed into an orthogonal direct sum of partial wave subspaces, which are the simultaneous eigenspaces of the angular momentum operators J^2, J_3 and the operator K which describes the spin-orbit coupling. On each subspace the Dirac equation is equivalent to a two dimensional system of ordinary differential equations of first order (the radial Dirac equation). Some general results on the spectral properties of the radial Dirac operator are reviewed in Sect. 4.6.6.

In Sect. 4.7 we present some results on the behavior of eigenvalues. We prove the relativistic virial theorem, which gives simple criteria for the absence of embedded eigenvalues in certain regions of the continuous spectrum.

4.1 Transformation Properties of External Fields

4.1.1 The Potential Matrix

A theory of particles in an "external" field is a first step towards a description of a true interaction. External fields have an influence on the motion of particles without being perturbed by the presence of particles. This is an idealized concept because in reality the particles interact with the field generating mechanism. In quantum mechanics, external forces are taken into account by adding to the free Hamiltonian a term describing the interaction energy.

For our purposes the external field is given by a 4×4 matrix-valued function V,

$$V(x) = (V_{ij}(x))_{\substack{i=1,\dots,4 \\ j=1,\dots,4}}, \quad x = (ct, \boldsymbol{x}), \tag{4.1}$$

which acts as a multiplication operator in $L^2(\mathbb{R}^3)^4$ for each t. The potential matrix is added to the free Dirac operator H_0 to obtain the *"Dirac operator in an external field"*

$$H = H_0 + V, \qquad H_0 = -\mathrm{i}\, c\boldsymbol{\alpha} \cdot \nabla + \beta mc^2. \tag{4.2}$$

We shall require that (for each t) the Dirac operator H is self-adjoint on a suitable domain. In particular, the matrix $V(x)$ has to be Hermitian for all $x \in \mathbb{R}^4$. Regularity conditions on the functions V_{ij} implying the self-adjointness of H and the existence of a unitary time evolution will be discussed in Sects. 4.3 and 4.4.

4.1.2 Poincaré Covariance of the Dirac Equation

In order to investigate the behavior of the perturbed Dirac equation under Poincaré transformations, we have to transform not only the particles, but also the whole mechanism generating the external field.

From (4.2) we obtain the perturbed Dirac equation in covariant form if we multiply $\mathrm{i}\frac{d}{dt}\psi = H\psi$ from the left with $\frac{1}{c}\beta$,

$$\left\{\mathrm{i}\,\langle \gamma, \partial\rangle - mc - V_{\mathrm{cov}}(x)\right\}\psi(x) = 0, \quad \text{where} \quad \partial = \left(\frac{\partial}{\partial x^0}, -\frac{\partial}{\partial x^k}\right). \tag{4.3}$$

Here we have defined (with $\gamma^0 \equiv \beta$)

$$V_{\mathrm{cov}}(x) \equiv \tfrac{1}{c}\gamma^0 V(x). \tag{4.4}$$

Following the calculation in Sect. 3.3.8, we find that a Poincaré transformation $(a, \mathbf{L}) \in \tilde{\mathcal{P}}^\uparrow$ converts (4.3) into

$$\left\{\mathrm{i}\,\langle \gamma, \partial\rangle - mc - V'_{\mathrm{cov}}(x)\right\}\mathbf{L}\psi(\Lambda_{\mathbf{L}}^{-1}(x-a)) = 0, \tag{4.5}$$

where

$$V'_{\mathrm{cov}}(x) = \mathbf{L}\, V_{\mathrm{cov}}(\Lambda_{\mathbf{L}}^{-1}(x-a))\, \mathbf{L}^{-1}. \tag{4.6}$$

If the external field (i.e., the field generating mechanism) undergoes a Poincaré transformation, then $V_{\mathrm{cov}}(x)$ must change into $V'_{\mathrm{cov}}(x)$, given by (4.6). From the transformation law (4.6) we deduce with the help of Eq. (4.4) and the relation $\gamma^0 \mathbf{L} \gamma^0 = \mathbf{L}^{*-1}$ the corresponding transformation law for the potential matrix V.

Theorem 4.1. Assume that the function $\psi(x)$ satisfies the Dirac equation (in Hamiltonian form) with the potential $V(x)$. Let $(a, \mathbf{L}) \in \tilde{\mathcal{P}}^{\uparrow}$. Then the Poincaré transformed wavefunction $\mathbf{L}\psi\big(\Lambda_{\mathbf{L}}^{-1}(x-a)\big)$ is a solution of the Dirac equation with the Poincaré transformed potential

$$V'(x) = \mathbf{L}^{*-1}\, V\big(\Lambda_{\mathbf{L}}^{-1}(x-a)\big)\, \mathbf{L}^{-1}. \tag{4.7}$$

4.2 Classification of External Fields

The 4×4 matrix $V_{\mathrm{cov}}(x)$ is a linear combination (with real coefficients) of the 16 Γ-matrices defined in Appendix A of Chapter 2. Concerning the behavior under Poincaré transformations we can distinguish among several special cases.

4.2.1 Scalar Potential

Let ϕ_{sc} be a real-valued function of $x = (ct, \boldsymbol{x})$. Define

$$V_{\mathrm{cov}}(x) = \tfrac{1}{\mathrm{c}}\phi_{\mathrm{sc}}(x)\mathbf{1}, \qquad V(x) = \beta\phi_{\mathrm{sc}}(x), \qquad (\beta \equiv \gamma^0). \tag{4.8}$$

A Poincaré transformation $V_{\mathrm{cov}} \to V'_{\mathrm{cov}}$ according to Eq. (4.6) requires the replacement

$$\phi_{\mathrm{sc}}(x) \to \phi_{\mathrm{sc}}(\Lambda^{-1}(x-a)), \quad \text{for all } \Lambda \in \mathcal{L},\ a \in \mathbb{R}^4. \tag{4.9}$$

We see that ϕ_{sc} must behave like a scalar under Poincaré transformations. The Dirac operator with a scalar potential reads $H = -\mathrm{i}c\,\boldsymbol{\alpha}\cdot\nabla + \beta\big(mc^2 + \phi_{\mathrm{sc}}(x)\big)$, i.e., ϕ_{sc} is like an x-dependent rest mass.

4.2.2 Electromagnetic Vector Potential

With the help of four real-valued functions $A = (A^{\mu}) = (\phi_{\mathrm{el}}, \boldsymbol{A})$ which are arranged as a four vector we define the potential matrix

$$V_{\mathrm{cov}}(x) = \langle \gamma, A(x) \rangle = \sum_{\mu=0}^{3} \gamma^{\mu} A_{\mu}(x), \tag{4.10}$$

$$V(x) = \phi_{\mathrm{el}}(x) - \boldsymbol{\alpha}\cdot\boldsymbol{A}(x). \tag{4.11}$$

Using Eqs. (4.6) and (2.159) we find that under a Poincaré transformation,

$$\langle \gamma, A(x) \rangle = V_{\mathrm{cov}}(x) \to V'_{\mathrm{cov}}(x) = \langle \gamma, \Lambda A\big(\Lambda^{-1}(x-a)\big) \rangle. \tag{4.12}$$

In order to achieve relativistic covariance we have to assume that the external field described by $A(x)$ behaves in such a way that

$$A(x) \to A'(x) = \Lambda A\big(\Lambda^{-1}(x-a)\big), \tag{4.13}$$

whenever the field generating mechanism is subject to a Poincaré transformation. This is precisely the behavior of electromagnetic potentialsHence, for the applications, ϕ_{el} is an electric potential, and $\boldsymbol{A}$ is the magnetic vector potential. The electric and magnetic field strengths which satisfy Maxwell's equations are given by (where $x = (ct, \boldsymbol{x})$)

$$\boldsymbol{E}(x) = -\mathrm{grad}_{\boldsymbol{x}} \phi_{\mathrm{el}}(x) - \frac{\partial \boldsymbol{A}(x)}{\partial ct}, \qquad \boldsymbol{B}(x) = \mathrm{rot}_{\boldsymbol{x}} \mathbf{A}(x). \tag{4.14}$$

If we perform a Poincaré transformation of the electromagnetic potentials according to (4.13), then the corresponding new field strengths $\boldsymbol{E}'$ and $\boldsymbol{B}'$ will again satisfy Maxwells equations.

The Dirac operator (4.2) with an electromagnetic field reads

$$H = c\,\boldsymbol{\alpha} \cdot \big(\boldsymbol{p} - \tfrac{e}{c}\boldsymbol{A}(ct, \boldsymbol{x})\big) - \beta mc^2 + e\phi_{\mathrm{el}}(ct, \boldsymbol{x}). \tag{4.15}$$

Here the coupling constant e has been introduced to describe the charge of the particle.

Remark. In classical mechanics, the forces by which the field strengths act on particles are given by the following rule ("principle of minimal coupling"): If $H(\boldsymbol{p})$ is the Hamilton function (energy) of a free classical particle, then $H(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}(x)) + e\phi_{\mathrm{el}}(x)$ is the Hamilton function of a charged particle in the given electromagnetic field. We see that Eq. (4.15) is obtained if we apply the minimal coupling principle to the free Dirac operator.

4.2.3 Anomalous Magnetic Moment

With the help of six real-valued functions we form an antisymmetric 4×4 matrix $F_{\mu\nu} = -F_{\nu\mu}$, where $\mu, \nu = 0, \ldots, 3$. Define

$$V_{\mathrm{cov}}(x) = \frac{\mu_{\mathrm{a}}}{2c} \sum_{\mu,\nu=0}^{3} \sigma^{\mu\nu} F_{\mu\nu}(x). \tag{4.16}$$

If we perform a Poincaré transformation $V_{\mathrm{cov}} \to V'_{\mathrm{cov}}$, then the required behavior of $F_{\mu\nu}$ can be read off from the following calculation (where we set $\boldsymbol{x}' = \Lambda^{-1}(x-a)$ and apply the summation convention)

$$\mathbf{L}\sigma^{\mu\nu} F_{\mu\nu}(x')\,\mathbf{L}^{-1} = \mathrm{i}\,\mathbf{L}\gamma^{\mu}\mathbf{L}^{-1}\mathbf{L}\gamma^{\nu}\mathbf{L}^{-1} F_{\mu\nu}(x')$$

$$= \mathrm{i}\,(\Lambda^{-1})^{\mu}{}_{\rho}\,\gamma^{\rho}\,(\Lambda^{-1})^{\nu}{}_{\tau}\,\gamma^{\tau}\,F_{\mu\nu}(x')$$
$$= \mathrm{i}\,\gamma^{\rho}\gamma^{\tau}\Lambda_{\rho}{}^{\mu}\Lambda_{\tau}{}^{\nu}F_{\mu\nu}(x') = \sigma^{\rho\tau}F'_{\rho\tau}(x). \tag{4.17}$$

The relativistic covariance of the Dirac equation with this kind of potential requires $F_{\mu\nu}$ to behave under a Poincaré transformation like

$$F_{\mu\nu}(x) \to F'_{\rho\tau}(x) = \Lambda_{\rho}{}^{\mu}\Lambda_{\tau}{}^{\nu}F_{\mu\nu}\big(\Lambda^{-1}(x-a)\big). \tag{4.18}$$

Hence $F_{\mu\nu}$ must be a tensor field. We can take for $F_{\mu\nu}$ the "electromagnetic field tensor"

$$F = \begin{pmatrix} 0 & -E_1 & -E_2 & -E_3 \\ E_1 & 0 & -B_3 & B_2 \\ E_2 & B_3 & 0 & -B_1 \\ E_3 & -B_2 & B_1 & 0 \end{pmatrix}, \tag{4.19}$$

where E_j and B_j are the components of the electric and magnetic field strengths.

Physically, the potential matrix given by (4.16) and (4.19) describes a particle with an additional anomalous magnetic moment. The magnitude of the anomalous moment is given by the coupling constant μ_{a} in units of the Bohr-magneton $|e|/2mc$.

For the potential matrix V in the standard representation we obtain, using

$$\frac{1}{2}\sum_{\mu,\nu=0}^{3}\beta\sigma^{\mu\nu}F_{\mu\nu} = \mathrm{i}\,\beta\boldsymbol{\alpha}\cdot\boldsymbol{E} - 2\beta\boldsymbol{S}\cdot\boldsymbol{B}, \tag{4.20}$$

and the explicit formulas of Appendix A of Chapter 2

$$V = \mu_{\mathrm{a}}\begin{pmatrix} -\boldsymbol{\sigma}\cdot\boldsymbol{B} & \mathrm{i}\,\boldsymbol{\sigma}\cdot\boldsymbol{E} \\ -\mathrm{i}\,\boldsymbol{\sigma}\cdot\boldsymbol{E} & \boldsymbol{\sigma}\cdot\boldsymbol{B} \end{pmatrix}. \tag{4.21}$$

4.2.4 Anomalous Electric Moment

As before, we use a tensor field $F_{\mu\nu}$ to define

$$V_{\mathrm{cov}}(x) = -\mathrm{i}\,\frac{\delta_{\mathrm{a}}}{2c}\sum_{\mu,\nu=0}^{3}\gamma_5\sigma^{\mu\nu}F_{\mu\nu}(x). \tag{4.22}$$

We can use Eq. (2.246) to obtain (summation convention!)

$$-\mathrm{i}\,\gamma_5\sigma^{\mu\nu}F_{\mu\nu} = \sigma_{\rho\tau}\hat{F}^{\rho\tau}, \tag{4.23}$$

where $\hat{F}$ is the Hodge dual of F. If F is the field strength tensor (4.19), then

$$\hat{F}^{\rho\tau} = \frac{1}{2}\epsilon^{\rho\tau\mu\nu}F_{\mu\nu} = \begin{pmatrix} 0 & -B_1 & -B_2 & -B_3 \\ B_1 & 0 & E_3 & -E_2 \\ B_2 & -E_3 & 0 & E_1 \\ B_3 & E_2 & -E_1 & 0 \end{pmatrix}. \tag{4.24}$$

Hence we obtain the potential matrix

$$V = \delta_a\{\mathrm{i}\,\beta\boldsymbol{\alpha}\cdot\boldsymbol{B} + 2\beta\boldsymbol{S}\cdot\boldsymbol{E}\} = \delta_a \begin{pmatrix} \boldsymbol{\sigma}\cdot\boldsymbol{E} & \mathrm{i}\,\boldsymbol{\sigma}\cdot\boldsymbol{B} \\ -\mathrm{i}\,\boldsymbol{\sigma}\cdot\boldsymbol{B} & -\boldsymbol{\sigma}\cdot\boldsymbol{E} \end{pmatrix}, \tag{4.25}$$

which describes the energy of a particle with an anomalous electric moment in an electromagnetic field. The magnitude of the anomalous moment is given by δ_a, which again is measured in units of Bohr magnetons.

Using the Weyl representation of γ_5, Eq. (1.216), and of the matrix $\mathbf{L}$ which corresponds to a proper Lorentz transformation, Eq. (2.146), we see that γ_5 is a scalar under *proper* Lorentz transformations,

$$\mathbf{L}\,\gamma_5\,\mathbf{L}^{-1} = \gamma_5, \quad \text{for all } \mathbf{L} \in \tilde{\mathcal{L}}_+^{\uparrow}. \tag{4.26}$$

But for the parity transformation (Sect.2.5.4) we have

$$\mathbf{L}_P\,\gamma_5\,\mathbf{L}_P^{-1} = -\gamma_5. \tag{4.27}$$

We find that the Dirac equation is $\tilde{\mathcal{L}}^{\uparrow}$-covariant, if the quantity $F_{\mu\nu}$ in Eq. (4.22) is a pseudotensor. However, the electromagnetic field strength tensor does not change sign under a space reflection. Therefore the Dirac equation with the potential (4.25) is not covariant with respect to a parity transformation.

4.2.5 Pseudovector Potential

The pseudovector potential is formed with the help of four real-valued functions (A_{pv}^{μ}),

$$V_{\mathrm{cov}}(x) = \gamma_5\langle\gamma, A_{\mathrm{pv}}(x)\rangle. \tag{4.28}$$

In order to obtain $\mathcal{P}^{\uparrow}$-covariance of the Dirac equation, A_{pv} must behave as a vector potential, as far as proper Poincaré transformations are concerned. Because of (4.27), A_{pv} must change sign under a space reflection, if the Dirac equation is required to be parity covariant,

$$A_{\mathrm{pv}}(x) \to -PA_{\mathrm{pv}}(Px). \tag{4.29}$$

For the electromagnetic vector potential we simply have, according to Eq. (4.13), $A(\boldsymbol{x}) \to PA(P\boldsymbol{x})$.

4.2.6 Pseudoscalar Potential

With a real-valued scalar function ϕ_{ps} of the space-time variable x we define

$$V_{\mathrm{cov}}(x) = \tfrac{1}{\mathrm{c}}\gamma_5\phi_{\mathrm{ps}}(x)\mathbf{1}, \qquad V(x) = \beta\gamma_5\phi_{\mathrm{ps}}(x). \tag{4.30}$$

It is clear from Eqs. (4.26) and (4.27) that under a Poincaré transformation the field ϕ_{ps} must behave like a scalar potential, see Eq. (4.9), except that under a space reflection $\phi_{\mathrm{ps}}(x) \to -\phi_{\mathrm{ps}}(Px)$.

4.3 Self-Adjointness and Essential Spectrum

If H_0 is the free Dirac operator and V is some potential matrix, does $H_0 + V$ define a unique self-adjoint operator? The answer is yes, if we can prove the essential self-adjointness of $H_0 + V$ on some convenient dense domain. The unique self-adjoint extension is then given by the closure of $H_0 + V$.

4.3.1 Local Singularities

The following simple theorem is based on the Kato-Rellich theorem (see, e.g., [RS 75], Sect. X.2) and is sufficient for many applications of physical interest.

Theorem 4.2. Let V be a multiplication operator with a Hermitian 4×4 matrix such that each component V_{ik} is a function satisfying the estimate

$$|V_{ik}(\boldsymbol{x})| \leq a \frac{c}{2|\boldsymbol{x}|} + b, \quad \text{all } \boldsymbol{x} \in \mathbb{R}^3 \setminus \{\mathrm{O}\}, \quad i,k = 1,\ldots,4, \tag{4.31}$$

for some constants $b > 0$, and $a < 1$. Then the operator $H = H_0 + V$, where H_0 is the free Dirac operator defined in Eq. (1.11), is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3 \setminus \{\mathrm{O}\})^4$ and self-adjoint on $\mathfrak{D}(H_0) = H^1(\mathbb{R}^3)^4$.

Proof. From Hardy's inequality ($r \equiv |\boldsymbol{x}|$)

$$\int_{\mathbb{R}^3} \frac{1}{4r^2} |\psi(\boldsymbol{x})|^2 \, d^3x \leq \int_{\mathbb{R}^3} |\nabla\psi(\boldsymbol{x})|^2 \, d^3x, \quad \psi \in C_0^\infty(\mathbb{R}^3), \tag{4.32}$$

we conclude the same inequality for spinor valued $\psi \in C_0^\infty(\mathbb{R}^3)^4$ by adding the results for the components. Next we note that

$$|-\mathrm{i}\,c\boldsymbol{\alpha}\cdot\nabla\psi(\boldsymbol{x})|^2 = c^2|\nabla\psi(\boldsymbol{x})|^2 \equiv c^2 \sum_{i,k=1}^{4} |\partial\psi_i(\boldsymbol{x})/\partial x_k|^2, \tag{4.33}$$

and find that the multiplication operator $c/2r$ is bounded relative to $\mathrm{i}c\boldsymbol{\alpha}\cdot\nabla$. From (4.31) we obtain for all $\psi \in C_0^\infty(\mathbb{R}^3)^4$

$$\|V\psi\| \leq a\|-\mathrm{i}\,c\boldsymbol{\alpha}\cdot\nabla\psi\| + b\|\psi\| \leq a\|H_0\psi\| + (b + amc^2)\|\psi\|. \tag{4.34}$$

Since the possible singularity of V_{ik} at the origin is square integrable we have $\mathfrak{D}(V) \supset \mathfrak{D}(H_0) = H^1(\mathbb{R}^3)^4$. The operator V is symmetric since the matrix $(V_{ik}(\boldsymbol{x}))$ is Hermitian for all $\boldsymbol{x}$. (Essential) self-adjointness of H finally follows from the (essential) self-adjointness of H_0 by the Kato-Rellich Theorem, because $a < 1$. □

Remark. For the result on essential self-adjointness, $a = 1$ would be also admitted by Wüst's theorem ([RS 75], Thm. X.14). One can show that there are matrix-valued potentials satisfying

$$|V_{ik}(\boldsymbol{x})| \leq \frac{1/2+\epsilon}{|\boldsymbol{x}|}, \quad \text{with } \epsilon > 0 \text{ arbitrarily small,}$$

for which the Dirac operator is not essentially self-adjoint. In this sense the result of Theorem 4.2 is optimal.

4.3.2 Behavior at Infinity

Theorem 4.3. Assume that each element of the Hermitian potential matrix V is an infinitely differentiable function,

$$V_{ik} \in C^\infty(\mathbb{R}^3) \quad \text{for all } i, k = 1, \ldots, 4. \tag{4.35}$$

Then $H = H_0 + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)^4$.

Proof. Since V is Hermitian, $H = H_0 + V$ is symmetric on $C_0^\infty(\mathbb{R}^3)^4$. By the basic criterion for essential self-adjointness ([RS 72], corollary to Theorem VIII.3, p. 257), it is sufficient to show that $(H \pm \mathrm{i})\psi = 0$ for some $\psi \in L^2(\mathbb{R}^3)^4$ implies $\psi = 0$. The operator $H \pm \mathrm{i}$ is an elliptic differential operator of first order with variable C^∞ coefficients. (A differential operator $\sum_{|\alpha| \leq k} a_\alpha(x) D^\alpha$ is called elliptic at x_0, if $\sum_{|\alpha|=k} a_\alpha(x_0) p^\alpha \neq 0$ for all $p \neq 0$). By the local regularity property of elliptic operators ([RS 75], Sect. IX.6) we conclude that any L^2 solution of $(H + \mathrm{i})\psi = 0$ is infinitely differentiable. Let ψ be such a solution. Choose a function $f \in C_0^\infty(\mathbb{R}^3)$ with $f(x) = 1$ for $|x| \leq 1$ and set $f_n(x) = f(\frac{x}{n})$. Then we find

$$(H + \mathrm{i}) f_n \psi = -\mathrm{i}\, c\boldsymbol{\alpha} \cdot (\nabla f_n)\psi, \tag{4.36}$$

and from $(\nabla f_n)(x) = \frac{1}{n}(\nabla f)(\frac{x}{n})$

$$\|f_n\psi\|^2 + \|H f_n \psi\|^2 = \|(H + \mathrm{i}) f_n \psi\|^2 = \|(\nabla f_n)\psi\|^2$$

$$\leq \tfrac{1}{n^2} \sup_x |(\nabla f)(x)|^2 \, \|\psi\|^2. \tag{4.37}$$

As n tends to infinity, we have $\|f_n\psi\| \to \|\psi\|$ and with (4.37) we obtain $\psi = 0$. The same argument works for a solution of $(H - \mathrm{i})\psi = 0$. □

Remark 1. A physically interesting example of a potential which is described by this theorem is the constant magnetic field $\boldsymbol{B}(\boldsymbol{x}) = (0, 0, B)$, for which we can choose $\boldsymbol{A}(\boldsymbol{x}) = (B/2)(-x_2, x_1, 0)$

Remark 2. Theorem 4.3 states that the Dirac operator is essentially self-adjoint on C_0^∞ irrespective of the growth of the potential at infinity. This is not true for Schrödinger operators because a force field which increases too fast, as $|\boldsymbol{x}| \to \infty$, could accelerate a particle so much that it escapes to infinity in a finite time. In this case the unitarity of the time evolution and hence the

self-adjointness of its generator breaks down. This situation clearly cannot happen for a Dirac particle, because the relativistic bound on the velocity prevents a finite travelling time to infinity.

4.3.3 The Coulomb Potential

An electron in the field of a point nucleus is described by the Coulomb potential

$$\phi_{\mathrm{el}}(\boldsymbol{x}) = \frac{\gamma}{|\boldsymbol{x}|}. \quad \text{In atomic units, } \gamma = e^2 Z/\hbar,\ Z \text{ nuclear charge.} \tag{4.38}$$

For coupling constants $|\gamma| < c/2$ ($Z \leq 68$) the Coulomb potential is covered by the assumptions of Theorem 4.2. In this case the Dirac operator $H = H_0 + \phi_{\mathrm{el}}\mathbf{1}$ is well defined and self-adjoint on $\mathfrak{D}(H_0)$. The restriction on γ is quite unfamiliar from the nonrelativistic theory. It is not only due to the method of proof. The essential self-adjointness indeed breaks down, if $|\gamma| > c\sqrt{3}/2$ ($Z > 118$), see Example 4.17 in Sect. 4.6.6 below. Fortunately, this problem arises only for point-like nuclei which do not occur in reality. Besides, if one takes into account the anomalous magnetic moment of the electron, the situation changes completely (see Sect. 5.3.2).

The following theorem covers also non-spherically symmetric potentials. We refer to the literature cited in the notes for the proof and further information.

Theorem 4.4. Assume that the electrostatic potential $V = \phi_{\mathrm{el}}\mathbf{1}$ satisfies the condition

$$\sup_{\boldsymbol{x}\in\mathbb{R}^3\setminus\{\mathrm{O}\}} |\,\boldsymbol{x}\,\phi_{\mathrm{el}}(\boldsymbol{x})\,| < \gamma. \tag{4.39}$$

Then for $\gamma < c\sqrt{3}/2$ the Dirac operator $H = H_0 + \phi_{\mathrm{el}}\mathbf{1}$ is essentially self-adjoint on $\mathfrak{D} = C_0^\infty(\mathbb{R}^3 \setminus \{\mathrm{O}\})$ and self-adjoint on $\mathfrak{D}(H) = \mathfrak{D}(H_0)$. For $\gamma < c$ the Dirac operator H, defined on $\mathfrak{D}$, has a self-adjoint extension $\tilde{H}$ which is uniquely characterized by the property

$$\mathfrak{D}(\tilde{H}) \subset \mathfrak{D}(|H_0|^{1/2}) \quad \text{or equivalently} \quad \mathfrak{D}(\tilde{H}) \subset \mathfrak{D}(|V|^{1/2}). \tag{4.40}$$

4.3.4 Invariance of the Essential Spectrum and Local Compactness

The essential spectrum $\sigma_{\mathrm{ess}}(H)$ of an operator H consists of all accumulation points of $\sigma(H)$ and of the infinitely degenerate eigenvalues of H. For the free Dirac operator H_0, the essential spectrum is clearly given by

$$\sigma_{\mathrm{ess}}(H_0) = \sigma(H_0) = (-\infty, -mc^2] \cup [mc^2, \infty). \tag{4.41}$$

The essential spectrum is very stable under perturbations.

Theorem 4.5. Let H and H_0 be self-adjoint operators such that for one (and hence all) $z \in \mathbb{C} \setminus \mathbb{R}$ the operator

$$(H - z)^{-1} - (H_0 - z)^{-1} \quad \text{is compact.} \tag{4.42}$$

Then $\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H_0)$.

Proof. This is a famous theorem of H. Weyl. It is proven, e.g., in [RS 78], Thm. XIII.14 and Corollary 1. □

Since the product of a compact operator with a bounded operator is compact, Eq. (4.42) implies that

$$\big((H - z)^{-1} - (H_0 - z)^{-1}\big)\, \chi(|\boldsymbol{x}| < R) \quad \text{is compact for all } R > 0. \tag{4.43}$$

Here $\chi(|\boldsymbol{x}| < R)$ is the (bounded) multiplication operator with the characteristic function of the ball with radius R. On the other hand, if the resolvent difference has decay at infinity, i.e., if

$$\lim_{R \to \infty} \| \big((H - z)^{-1} - (H_0 - z)^{-1}\big)\, \chi(|\boldsymbol{x}| \geq R) \| = 0, \tag{4.44}$$

then (4.43) implies (4.42) because

$$(H - z)^{-1} - (H_0 - z)^{-1} \tag{4.45}$$

$$= \big((H - z)^{-1} - (H_0 - z)^{-1}\big)\, \chi(|\boldsymbol{x}| < R) \tag{4.46}$$

$$+ \big((H - z)^{-1} - (H_0 - z)^{-1}\big)\, \chi(|\boldsymbol{x}| \geq R). \tag{4.47}$$

By (4.44), the summand (4.47) vanishes, as $R \to \infty$, and the resolvent difference (4.45) is the norm limit of a sequence of compact operators. This implies compactness of (4.45).

Compactness of the operator in (4.43) is almost always true and can easily be verified. In our applications we shall even find that each of the summands in Eq. (4.43) is compact. A self-adjoint operator H is said to have the "*local compactness property*", if the operator $(H - z)^{-k}\, \chi(|x| < R)$ is compact for all $R > 0$, some $z \in \mathbb{C} \setminus \mathbb{R}$ and some $k > 0$ (if this is the case, the operator is compact for all $z \in \mathbb{C} \setminus \mathbb{R}$ and all $k > 0$)[1].

Lemma 4.6. The free Dirac operator H_0 has the local compactness property. In particular the operators $|H_0|^{-k}\, \chi(|x| < R)$ are compact for all $k > 0$, $R > 0$.

Proof. Since $|H_0|^k (H_0 - z)^{-k}$ is a bounded operator with bounded inverse, compactness of $(H_0 - z)^{-k}\, \chi(|x| < R)$ is equivalent to compactness of the operator $|H_0|^{-k}\, \chi(|x| < R)$. In momentum space, $|H_0|^{-k} = (c^2 p^2 + m^2 c^4)^{-k/2}$ is a bounded function which vanishes, as $p^2 \to \infty$. Now the lemma follows from the following general result: If $f : [0, \infty) \to \mathbb{C}$ and $g : [0, \infty) \to \mathbb{C}$ are

[1] [Pe 83], Proposition 2.2

bounded with $\lim_{r\to\infty} f(r) = \lim_{r\to\infty} g(r) = 0$, then the operator $g(p^2)\, f(x^2)$ is compact[2]. □

Let H be a Dirac operator in an external field and assume that H is self-adjoint on a domain with the property

$$\mathfrak{D}(H) \subset \mathfrak{D}(|H_0|^{1/2}), \tag{4.48}$$

(cf. Theorem 4.4). Then the operator $|H_0|^{1/2}(H - z)^{-1}$ is bounded[3], and the lemma implies compactness of

$$\chi(|x| < R)\,(H - z)^{-1} = \chi(|x| < R)\,|H_0|^{-1/2}\,|H_0|^{1/2}\,(H - z)^{-1} \tag{4.49}$$

($\chi(|x| < R)\,|H_0|^{-1/2}$ is the adjoint of $|H_0|^{-1/2}\,\chi(|x| < R)$ and hence compact). Hence we see that Dirac operators have the local compactness property under the extremely weak condition (4.48), roughly speaking, whenever they are defined properly.

In order to show that the essential spectrum of the Dirac operator $H = H_0 + V$ is given by (4.41) it remains to prove the decay at infinity of the resolvent difference (4.44). If V is relatively bounded (which is the case for Coulomb potentials), we can use the resolvent equation

$$(H - z)^{-1} - (H_0 - z)^{-1} = -(H - z)^{-1}\, V\, (H_0 - z)^{-1}, \tag{4.50}$$

to simplify the condition (4.44). We obtain the following result.

Theorem 4.7. Let $H = H_0 + V$ be self-adjoint, and V be H_0-bounded with

$$\lim_{R\to\infty} \| V\,(H_0 - z)^{-1}\,\chi(|\boldsymbol{x}| \geq R) \| = 0. \tag{4.51}$$

Then

$$\sigma_{\mathrm{ess}}(H) = (-\infty, -mc^2] \cup [mc^2, \infty). \tag{4.52}$$

Remark 1. Eq. (4.51) is a very weak decay condition on the potential. If V is a multiplication operator, it is equivalent to

$$\lim_{R\to\infty} \| V\,\chi(|\boldsymbol{x}| \geq R)\,(H_0 - z)^{-1} \| = 0. \tag{4.53}$$

In order to prove that (4.53) implies (4.51), let $f_R : [0, \infty) \to [0, 1]$ be differentiable, such that $f_R(r) = 0$ for $r < R/2$, $f_R(r) = 1$ for $r > R$, and $\sup_r f_R'(r) < 4/R$. Then $\chi(|\boldsymbol{x}| \geq R) = f_R(|\boldsymbol{x}|)\,\chi(|\boldsymbol{x}| \geq R)$ and

$$\begin{aligned} &\| V\,(H_0 - z)^{-1}\,\chi(|\boldsymbol{x}| \geq R) \| \\ &\quad \leq \| V\,(H_0 - z)^{-1}\, c\boldsymbol{\alpha} \cdot (\nabla f_R)\,(H_0 - z)^{-1} \| \qquad (4.54) \\ &\quad + \| V\, f_R\,(H_0 - z)^{-1} \|. \qquad (4.55) \end{aligned}$$

[2] [Pe 83], Proposition 2.2b.

[3] This is a consequence of the closed graph theorem, see [We 80], Thm. 5.9.

In (4.54) we have used

$$[(H_0 - z)^{-1}, f_R] = (H_0 - z)^{-1}[f_R, H_0 - z](H_0 - z)^{-1}, \tag{4.56}$$

$$[f_R, H_0 - z] = [f_R, c\boldsymbol{\alpha} \cdot \boldsymbol{p}] = ic\boldsymbol{\alpha} \cdot (\nabla f_R). \tag{4.57}$$

(4.54) vanishes, as $R \to \infty$, because the norm of the matrix multiplication operator $\boldsymbol{\alpha} \cdot (\nabla f_R)$ is given by

$$\| \boldsymbol{\alpha} \cdot (\nabla f_R) \| = \sup_{r \in [R/2, R]} f'(r) = \frac{\text{const.}}{R}. \tag{4.58}$$

(4.55) is bounded by $\| V \chi(|\boldsymbol{x}| \geq R/2) (H_0 - z)^{-1} \|$ which by Eq. (4.53) vanishes, as $R/2 \to \infty$. Similarly one proves that (4.51) implies (4.53).

Remark 2. Any potential matrix, with $V(x) \to 0$, as $|\boldsymbol{x}| \to \infty$ satisfies

$$\| V \chi(|\boldsymbol{x}| \geq R) \| = \sup_{|\boldsymbol{x}| > R} |V(\boldsymbol{x})| \to 0, \quad \text{as } R \to \infty, \tag{4.59}$$

and hence (4.53). But the conditions (4.51) and (4.53) are more general than (4.59) because they admit singularities of the potential even at large distances.

Remark 3. The condition (4.51) is not optimal, mainly because there are potentials which tend to infinity, as $|\boldsymbol{x}| \to \infty$, and still (4.52) holds. In particular, this occurs for unisotropic potentials as well as for magnetic fields in three dimensions, see Chapter 7.

4.4 Time Dependent Potentials

4.4.1 Propagators

If the potential matrix V is time-dependent, then the time evolution is in general not given by a one-parameter unitary group. Instead, we have to live with two-parameter families.

Definition 4.8. *A two-parameter family $U(s,t)$, $(s,t) \in \mathbb{R}^2$, of bounded operators in a Hilbert space $\mathfrak{H}$ is called a unitary propagator, if*

a) $U(s,t)$ is unitary for all s and t,
b) $U(t,t) = \mathbf{1}$ for all t,
c) $U(r,s)U(s,t) = U(r,t)$ for all r, s and t,
d) the mapping $(s,t) \to U(s,t)\psi$ is continuous for all $\psi \in \mathfrak{H}$.

The following theorems are not specific to relativistic quantum mechanics, therefore we quote them without proofs.

Theorem 4.9. Let $H(t)$ be a family of operators which are self-adjoint on a common domain $\mathfrak{D}(H(t)) = \mathfrak{D}_0$ and assume that for any compact interval I the mapping

$$(s,t) \to \frac{1}{s-t}\Big(\big(H(s)-z\big)\,\big(H(t)-z\big)^{-1} - 1\Big)\,\psi, \qquad z \in \bigcap_{t\in\mathbb{R}} \rho(H(t)), \tag{4.60}$$

from $I \times I$ into $\mathfrak{H}$ is continuous for all $\psi \in \mathfrak{H}$. Then there exists a unitary propagator $U(s,t)$, and if $\psi \in \mathfrak{D}_0$, then $U(s,t)\psi$ is in $\mathfrak{D}_0$ for all t and is a solution of the equations

$$\mathrm{i}\,\frac{\partial}{\partial t}\,U(t,s)\,\psi = H(t)\,U(t,s)\,\psi, \tag{4.61}$$

$$\mathrm{i}\,\frac{\partial}{\partial s}\,U(t,s)\,\psi = -U(t,s)\,H(s)\,\psi. \tag{4.62}$$

Proof. See, e.g., [RS 75], Theorem X.70. □

Theorem 4.10. Let H_0 be self-adjoint. The assumptions of Theorem 4.9 are satisfied for $H(t) = H_0 + V(t)$, if $V(t)$ is bounded and self-adjoint for each t, and if the mapping $t \to V(t)\psi$ is continuous for all ψ. In this case we have

$$\tilde{U}(t,s) = \sum_{n=0}^{\infty} (-\mathrm{i})^n \int_s^t dt_1 \int_s^{t_1} dt_2 \cdots \int_s^{t_{n-1}} dt_n\, \tilde{V}(t_1)\cdots\tilde{V}(t_n), \tag{4.63}$$

where

$$\tilde{U}(t,s) = e^{\mathrm{i}H_0 t}\,U(t,s)\,e^{-\mathrm{i}H_0 s}, \qquad \tilde{V}(t) = e^{\mathrm{i}H_0 t}\,V(t)\,e^{-\mathrm{i}H_0 t}. \tag{4.64}$$

Proof. See, e.g., [RS 75], Theorem X.69. □

4.4.2 Time Dependence Generated by Unitary Operators

The time dependence is trivial, if the Hamiltonians at different times are connected by unitary transformations,

$$H(t+s) = e^{\mathrm{i}At}\,H(s)\,e^{-\mathrm{i}At}. \tag{4.65}$$

We assume that $\mathfrak{D}(H(0))$ is left invariant by $\exp(-\mathrm{i}At)$, all t, i.e., A is well defined and essentially self-adjoint on this domain[4]. This is, e.g., the case if A is the generator of some Poincaré transformation. If $U(t,s)$ is the propagator generated by $H(t)$, then

$$\mathrm{i}\,\frac{d}{dt}\,e^{-\mathrm{i}As}\,U(t+s,s)\,e^{\mathrm{i}As} = H(t)\,e^{-\mathrm{i}As}\,U(t+s,s)\,e^{\mathrm{i}As}, \tag{4.66}$$

[4] [RS 72], Theorem VIII.11.

which shows

$$e^{-\mathrm{i}As}\,U(t+s,s)\,e^{\mathrm{i}As} = U(t,0). \tag{4.67}$$

Hence the operators $\exp(-\mathrm{i}At)\,U(t,0)$, $t \in \mathbb{R}$ form a one-parameter group of unitary operators. We may write

$$e^{-\mathrm{i}At}\,U(t,0) \equiv e^{-\mathrm{i}Gt}, \tag{4.68}$$

where G is a self-adjoint extension of the operator $H(0)+A$ on $\mathfrak{D}(H(0))$. The solution of the evolution equation with Hamiltonian $H(t)$ and initial condition $\psi(0)=\psi_0$ is hence given by

$$\psi(t) = e^{\mathrm{i}At}\,e^{-\mathrm{i}(H(0)+A)t}\,\psi_0. \tag{4.69}$$

In a special case, a time dependence of the more general form $H(t) = W(t,s)H(s)W(s,t)$, where W is a unitary propagator, will be considered in Chapter. 9.

4.4.3 Gauge Transformations

Gauge transformations could be another trivial source of time dependence in the Dirac equation. It is well known from the theory of electromagnetism that the vector potential A is not uniquely determined by the field strengths. Let $F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x)$ be the electromagnetic field strength tensor. We denote $x = (x^\mu) = (ct, \boldsymbol{x})$ and $\partial_\mu = \partial/\partial x^\mu$. If we replace A_μ by $A_\mu + \partial_\mu g$, where g is a smooth function of x, then the field strength tensor $F_{\mu\nu}$ remains unchanged. Note that the function g may depend on time. If we write $A = (\phi_{\mathrm{el}}, \boldsymbol{A})$, then the gauge transformation becomes

$$\phi_{\mathrm{el}} \to \phi_{\mathrm{el}} + \frac{1}{c}\frac{\partial g}{\partial t}, \qquad \boldsymbol{A} \to \boldsymbol{A} - \nabla g. \tag{4.70}$$

Since only the field strength and not the potential is regarded as a physically observable quantity, this replacement should lead to an equivalent mathematical description of the physical system ("gauge invariance"). In quantum mechanics, the transition from the theory in terms of A_μ to a theory formulated with the vector potential $A_\mu + \partial_\mu g$ can be accomplished by the (possibly time-dependent) unitary transformation $\psi(x) \to e^{-\mathrm{i}g(x)}\psi(x)$. We find

$$e^{-\mathrm{i}g}(-\mathrm{i}\nabla - \boldsymbol{A})e^{\mathrm{i}g} = -\mathrm{i}\nabla - \boldsymbol{A} + \nabla g. \tag{4.71}$$

Eq. (4.71) shows that two Dirac operators with different vector potentials belonging to the same magnetic field B are unitarily equivalent. Hence we obtain the following lemma.

Lemma 4.11. We assume that the Dirac operator $H = H_0 + V$ is well defined and essentially self-adjoint on the domain $\dot{\mathfrak{D}} \equiv C_0^\infty(\mathbb{R}^3 \setminus \{\mathrm{O}\})^4$. Let $g(t,\cdot) \in C^\infty(\mathbb{R}^3 \setminus \{\mathrm{O}\})$ be real-valued for each $t \in \mathbb{R}$. Then the multiplication operator

$\exp(-\mathrm{i}\,g)\mathbf{1}$ is unitary for each t and leaves $\mathring{\mathfrak{D}}$ invariant. The Dirac operator on this domain is unitarily equivalent to the operator

$$H(t) = e^{\mathrm{i}\,g(t,\cdot)}\,(H_0 + V)\,e^{-\mathrm{i}\,g(t,\cdot)} = H_0 + V - c\boldsymbol{\alpha}\cdot\nabla g(t,\cdot), \tag{4.72}$$

and if $\psi(t)$ is a solution of the Dirac equation with the potential matrix V, then $e^{\mathrm{i}\,g(t,\cdot)}\,\psi(t)$ solves the Dirac equation with the potential

$$V(t) = V + \frac{\partial g(t,\cdot)}{\partial t}\,\mathbf{1} - c\boldsymbol{\alpha}\cdot\nabla g(t,\cdot). \tag{4.73}$$

Remark. If we set $V = 0$ and $g = 1/(n|\boldsymbol{x}|^n)$ with arbitrary $n > 0$, then we find that the Dirac operator with the very singular potential $V(x) = (\boldsymbol{\alpha}\cdot\boldsymbol{x})/r^{n+2}$ is essentially self-adjoint on $\mathring{\mathfrak{D}}$.

The unitary equivalence of quantum theories with different vector potentials for a given field strength is the mathematical formulation of the statement that "physics" does not depend on the "choice of gauge" (i.e., the choice of a particular vector potential A).

4.5 Klein's Paradox

The Dirac operator H with an external field usually does not commute with the sign of H_0. Therefore, a particle which initially has positive kinetic energy can be found in a state with negative kinetic energy at time t: $P^0_{\mathrm{neg}} e^{-\mathrm{i}Ht} P^0_{\mathrm{pos}} \neq 0$ where $P^0_{\mathrm{pos,neg}}$ are the spectral projections of the free Dirac operator H_0 (Sect. 1.4.2). In scattering theory with time-independent fields one can show that at least asymptotically the sign of the kinetic energy is a conserved quantity (Chapter 8). However, if the external field is time dependent or if the potential does not vanish at infinity, a permanent transition from electron to positron states might occur. This effect is called the Klein's paradox. It will be demonstrated for the one-dimensional Dirac equation (cf. Eq. (1.14)) with an electrostatic step potential

$$\mathrm{i}\frac{\partial}{\partial t}\,\psi(t,x) = H(\phi_{\mathrm{el}})\,\psi(t,x), \tag{4.74}$$

$$H(\phi_{\mathrm{el}}) = -\mathrm{i}\,\sigma_1\frac{\partial}{\partial x} + \sigma_3\,mc^2 + \phi_{\mathrm{el}}(x)\,\mathbf{1}, \tag{4.75}$$

$$\phi_{\mathrm{el}}(x) = \begin{cases} \phi_0 & \text{for } x \geq R, \\ \text{measurable, bounded} & \text{for } x \in (-R,R), \\ 0 & \text{for } x \leq -R. \end{cases} \tag{4.76}$$

The asymptotic motion is described by the Dirac operator $H(\phi_0)$ for particles moving to the right, and by $H(0) = H_0$ for particles moving to the left, respectively. The functions

$$\underset{\rightarrow}{\omega}(E,x) = \begin{pmatrix} \sqrt{E+mc^2} \\ \sqrt{E-mc^2} \end{pmatrix} \frac{\exp\{\frac{i}{c}\sqrt{E^2-m^2c^4}\,(\operatorname{sgn} E)\,x\}}{\sqrt{4\pi c}\,(E^2-m^2c^4)^{1/4}}, \tag{4.77}$$

$$\underset{\leftarrow}{\omega}(E,x) = \sigma_3\,\underset{\rightarrow}{\omega}(E,-x), \tag{4.78}$$

with $E \in \sigma(H_0) = (-\infty, -mc^2] \cup [mc^2, \infty)$ are eigenfunctions of $H(0)$ in a distributional sense. Similarly, $\underset{\rightarrow}{\omega}(E-\phi_0,x)$ and $\underset{\leftarrow}{\omega}(E-\phi_0,x)$ are eigenfunctions of $H(\phi_0)$. In this case we have $E \in \sigma(H(\phi_0)) = \sigma(H_0)+\phi_0$. Let $\underset{\rightarrow}{\Phi}$, $\underset{\leftarrow}{\Phi} \in C_0^\infty(\mathbb{R})$ have support in $\sigma(H_0)$ but away from $\pm mc^2$. The wavepackets of the form

$$\psi(x) = \int_{\sigma(H_0)} \{\underset{\rightarrow}{\Phi}(E)\,\underset{\rightarrow}{\omega}(E,x) + \underset{\leftarrow}{\Phi}(E)\,\underset{\leftarrow}{\omega}(E,x)\}\,dE. \tag{4.79}$$

are dense in the Hilbert space $\mathfrak{H} = L^2(\mathbb{R},dx)^2$. The mapping $(\underset{\rightarrow}{\Phi},\underset{\leftarrow}{\Phi}) \to \psi$ is unitary from $L^2(\sigma(H_0),dE)^2$ to $\mathfrak{H}$. For the wavepackets formed with "$\rightarrow$" alone the classical velocity $c^2pH_0^{-1}$ is easily seen to be a positive operator because $\underset{\rightarrow}{\omega}$ has momentum $(\operatorname{sgn} E)\,\frac{1}{c}\sqrt{E^2-m^2c^4}$. Hence these states correspond to particles moving to the right. Similarly the states obtained from $\underset{\leftarrow}{\omega}$ correspond to particles moving to the left. We denote the corresponding subspaces of $\mathfrak{H}$ by $\underset{\rightarrow}{\mathfrak{H}}$ and $\underset{\leftarrow}{\mathfrak{H}}$ with projection operators $\underset{\rightarrow}{P}$, $\underset{\leftarrow}{P}$, respectively. The Klein paradox occurs if $\phi_0 > 2mc^2$. In this case the positive part of $\sigma(H_0)$ intersects with the lower part of $\sigma(H(\phi_0))$. Hence a particle with energies in $(mc^2, -mc^2+\phi_0)$ can propagate on both sides of the potential step, as an electron on the left side, and as a positron on the right side.

Remark. In nonrelativistic quantum mechanics, a particle with this energy can propagate only at the left side ($E > \phi$), the wavefunction decays exponentially in regions with $\phi > E$ (inside the step). Therefore a particle coming in from the left is reflected with probability one, when it hits the potential step.

Assume $\phi_0 > 2mc^2$ and $mc^2 < E < -mc^2 + \phi_0$. Then $H(\phi_{el})$ given by (4.75) has distributional eigenfunctions given by

$$u_1(E,x) = \begin{cases} \underset{\rightarrow}{\omega}(E,x) + R^l(E)\,\underset{\leftarrow}{\omega}(E,x) & \text{for } x \le -R, \\ T(E)\,\underset{\rightarrow}{\omega}(E-\phi_0,x) & \text{for } x \ge R, \end{cases} \tag{4.80}$$

$$u_2(E,x) = \begin{cases} T(E)\,\underset{\leftarrow}{\omega}(E,x) & \text{for } x \le -R, \\ \underset{\leftarrow}{\omega}(E-\phi_0,x) + R^r(E)\,\underset{\rightarrow}{\omega}(E-\phi_0,x) & \text{for } x \ge R. \end{cases} \tag{4.81}$$

Here the functions $R^{l,r}(E)$ are called reflection coefficients, $T(E)$ is the transmission coefficient. They satisfy for all $E \in (mc^2, -mc^2+\phi_0)$

$$|T(E)|^2 + |R^l(E)|^2 = 1, \qquad |R^l(E)| = |R^r(E)|, \tag{4.82}$$

$$T(E)\,\overline{R^l(E)} + \overline{T(E)}\,R^r(E) = 0. \tag{4.83}$$

In general the transmission coefficient is nonzero as can be seen from an explicit calculation of some examples (e.g., the rectangular potential step). A solution of the Dirac equation of the form

$$\psi(t,x) = \int_{mc^2}^{-mc^2+\phi_0} \Phi(E)\, u_1(E,x)\, e^{-\mathrm{i}\,Et}\, dE \tag{4.84}$$

describes a wavepacket which comes from the left, moves towards the potential step, where part of it is reflected, another part being transmitted. The transmitted part moves to the right and behaves like a solution with negative energy of the Dirac equation. Similarly, there is a L^2-solution obtained from $u_2(x,E)$. It describes a positron coming in from the right. When it hits the potential step it is split into a reflected part, moving to the right, and a transmitted part, which can be detected as an ordinary electron with positive energy at the left side.

4.6 Spherical Symmetry

One cannot expect to find explicit solutions of the Dirac equation unless there are some additional symmetries. The physically most important example are spherically symmetric potentials for which the Dirac operator can be largely simplified. The requirement of spherical symmetry restricts not only the dependence on x, but also the matrix-structure of the potential.

4.6.1 Assumptions on the Potential

Definition 4.12. *A spherically symmetric potential is a Hermitian 4×4 matrix multiplication operator V which remains unchanged under a rotation in $\tilde{\mathcal{L}}_+^\uparrow$.*

In the Hilbert space $L^2(\mathbb{R}^3)^4$ the $SU(2)$-rotations are represented by

$$e^{-\mathrm{i}\,\varphi \boldsymbol{J}\cdot\boldsymbol{n}}\,\Psi(x) = e^{-\mathrm{i}\,\varphi \boldsymbol{S}\cdot\boldsymbol{n}}\,\Psi(\mathbf{R}^{-1}x), \quad \varphi\in[0,4\pi), \tag{4.85}$$

where $\mathbf{R}$ is the orthogonal 3×3 matrix corresponding to a rotation $(\varphi,\boldsymbol{n})$. The matrix V has to be rotated according to Eq. (4.7). Note that the Dirac β-matrix commutes with $\boldsymbol{S}$ and hence with $\exp(-\mathrm{i}\,\varphi \boldsymbol{S}\cdot\boldsymbol{n})$. Hence, V is spherically symmetric, if and only if

$$e^{\mathrm{i}\,\varphi \boldsymbol{S}\cdot\boldsymbol{n}}\, V(\mathbf{R}^{-1}x)\, e^{-\mathrm{i}\,\varphi \boldsymbol{S}\cdot\boldsymbol{n}} = V(x). \tag{4.86}$$

The potential matrix should be sufficiently regular, so that

$$\dot{\mathfrak{D}} \equiv C_0^\infty(\mathbb{R}^3\setminus\{\mathrm{O}\})^4 \subset \mathfrak{D}(V). \tag{4.87}$$

The domain $\dot{\mathfrak{D}}$ consists of smooth four component functions with compact support away from the origin O. It is dense in $L^2(\mathbb{R}^3)^4$ and invariant under rotations.

Condition (4.87) is fulfilled if each component of V is locally square integrable on $\mathbb{R}^3\setminus\{\mathrm{O}\}$.

$$V_{ij} \in L^2_{\mathrm{loc}}(\mathbb{R}^3\setminus\{\mathrm{O}\})^4, \quad i,j=1,\ldots,4. \tag{4.88}$$

In this case, the operator $H = H_0 + V$ is well defined and symmetric on $\dot{\mathfrak{D}}$.

It is easy to find potentials V which are spherically symmetric. First we note that if a scalar function ϕ satisfies $\phi(\boldsymbol{x}) = \phi(\mathbf{R}^{-1}\boldsymbol{x})$ for all rotation matrices $\mathbf{R}$, then ϕ can only depend on $r = |\boldsymbol{x}|$. Since the 4×4 unit matrix and β commute with $\exp(-\mathrm{i}\,\varphi \boldsymbol{S} \cdot \boldsymbol{n})$, we find that

$$V(\boldsymbol{x}) = \phi_{\mathrm{sc}}(r)\,\beta + \phi_{\mathrm{el}}(r)\,\mathbf{1}_4 \tag{4.89}$$

is a spherically symmetric potential. Here we assume that ϕ_{sc} and ϕ_{el} are real-valued functions describing a scalar and electric potential, respectively. Another physically interesting example is

$$V(\boldsymbol{x}) = \mathrm{i}\beta\,\boldsymbol{\alpha} \cdot \boldsymbol{e}_r\,\phi_{\mathrm{am}}(r) \tag{4.90}$$

where again ϕ_{am} is real-valued, and $\boldsymbol{e}_r = \boldsymbol{x}/r$. To see that (4.90) is spherically symmetric we use (2.159), (2.173), with $\gamma = (\beta, \beta\boldsymbol{\alpha})$ to obtain

$$e^{\mathrm{i}\,\varphi \boldsymbol{n}\cdot\boldsymbol{S}}\,\beta\boldsymbol{\alpha} \cdot (\mathbf{R}^{-1}\boldsymbol{x})\,e^{-\mathrm{i}\,\varphi \boldsymbol{n}\cdot\boldsymbol{S}} = \beta\boldsymbol{\alpha} \cdot \boldsymbol{x}. \tag{4.91}$$

If we compare Eq. (4.90) with Eq. (4.20) we see that a potential matrix of this form can be used to describe a particle with an anomalous magnetic moment. If the particle has charge e and anomalous moment μ_{a}, and if there is only a spherically symmetric electric field $\boldsymbol{E}(\boldsymbol{x}) = -\nabla\phi_{\mathrm{el}}(r)$, then, according to (4.20),

$$V(\boldsymbol{x}) = e\phi_{\mathrm{el}}(r) - \mathrm{i}\,\mu_{\mathrm{a}}\beta\,\boldsymbol{\alpha} \cdot \nabla\,\phi_{\mathrm{el}}(r) = e\phi_{\mathrm{el}}(r) - \mathrm{i}\,\mu_{\mathrm{a}}\beta\,\frac{\boldsymbol{\alpha} \cdot \boldsymbol{x}}{r}\,\frac{d\phi_{\mathrm{el}}(r)}{dr}. \tag{4.92}$$

A term like (4.90) could also be used to describe a particle with an anomalous electric moment in the spherically symmetric field of a magnetic monopole, see Eq. (4.25).

4.6.2 Transition to Polar Coordinates

On $\mathbb{R}^3 \setminus \{\mathrm{O}\}$ we introduce polar coordinates

$$\begin{aligned} x_1(r,\vartheta,\varphi) &= r\,\sin\vartheta\,\cos\varphi, \qquad & r &= |\boldsymbol{x}| \in (0,\infty), \\ x_2(r,\vartheta,\varphi) &= r\,\sin\vartheta\,\sin\varphi, & \vartheta &= \arccos(x_3/|\boldsymbol{x}|) \in [0,\pi), \\ x_3(r,\vartheta,\varphi) &= r\,\cos\vartheta, & \varphi &= \pi\,\theta(-x_1)\,\mathrm{sgn}\,(x_2) \\ & & & \quad + \arctan(x_2/x_1) \in [-\pi,\pi). \end{aligned} \tag{4.93}$$

(The definition of φ has to be extended by continuity for $x_1 \to 0$ and is ambiguous on the half-plane $x_1 \leq 0$, $x_2 = 0$. This is because coordinates on a sphere cannot be defined globally. If necessary, one has to choose another set of local spherical coordinates). Next we define the unit vectors in the directions of the polar coordinate lines

$$\boldsymbol{e}_r = (\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta) = \frac{\boldsymbol{x}}{r},$$

$$e_\vartheta = (\cos\vartheta\cos\varphi, \cos\vartheta\sin\varphi, -\sin\vartheta) = \frac{\partial e_r}{\partial\vartheta},$$

$$e_\varphi = (-\sin\varphi, \cos\varphi, 0) = \frac{1}{\sin\vartheta}\frac{\partial e_r}{\partial\varphi}, \tag{4.94}$$

For all Ψ in the Hilbert space $L^2(\mathbb{R}^3)$ we write

$$\psi(r,\vartheta,\varphi) = r\Psi\big(x_1(r,\vartheta,\varphi), \ldots, x_3(r,\vartheta,\varphi)\big) \tag{4.95}$$

We consider ψ an element of the Hilbert space

$$L^2((0,\infty), dr; L^2(S^2)) \cong L^2((0,\infty), dr) \otimes L^2(S^2). \tag{4.96}$$

For each $r \in (0,\infty)$ the function $\psi(r,\cdot)$ of the angular variables is square integrable on the unit sphere S^2. The mapping $\Psi \to \psi$ is a unitary isomorphism from $L^2(\mathbb{R}^3)$ onto $L^2((0,\infty), dr) \otimes L^2(S^2)$.

For the Hilbert space $L^2(\mathbb{R}^3)^4$ we introduce an analogous transformation to polar coordinates by applying the transformation (4.95) to every component of the wavefunction. In this way we obtain the decomposition

$$L^2(\mathbb{R}^3)^4 \cong L^2((0,\infty), dr) \otimes L^2(S^2)^4. \tag{4.97}$$

Similarly, the transformation (4.95) maps the domain $\mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{O\})^4$ onto $\mathcal{C}_0^\infty(0,\infty) \otimes \mathcal{C}^\infty(S^2)$.

The decomposition of the Hilbert space into a "radial" and an "angular" part is useful because the angular momentum operators $\boldsymbol{L}$ and $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$ act only on the angular part $L^2(S^2)^4$ in a nontrivial way. Using the expression for ∇ in polar coordinates,

$$\nabla = e_r\frac{\partial}{\partial r} + \frac{1}{r}\left(e_\vartheta\frac{\partial}{\partial\vartheta} + e_\varphi\frac{1}{\sin\vartheta}\frac{\partial}{\partial\varphi}\right), \tag{4.98}$$

we obtain

$$\boldsymbol{L} = \mathrm{i}\,e_\vartheta\frac{1}{\sin\vartheta}\frac{\partial}{\partial\varphi} - \mathrm{i}\,e_\varphi\frac{\partial}{\partial\vartheta}, \tag{4.99}$$

$$L^2 = -\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) - \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}, \tag{4.100}$$

where the differentiation applies to each component of the wavefunction. In view of the decomposition (4.97) it would be more correct to write, e.g., $L_3 = \mathbf{1} \otimes (-\mathrm{i}\,\partial/\partial\varphi)$ in order to indicate that the angular momentum operator acts like the identity in $L^2(0,\infty,dr)$. Since this notation is a little bit clumsy, we use the same letter for the angular momentum operators L_3, etc., and for their restriction to $L^2(S^2)$.

4.6.3 Operators Commuting with the Dirac Operator

We rewrite the Dirac operator on $\dot{\mathfrak{D}}$ using polar coordinates. With (4.98) and (4.99) we obtain

$$-\mathrm{i}\nabla = -\mathrm{i}e_r \tfrac{\partial}{\partial r} - \tfrac{1}{r}(\boldsymbol{e}_r \wedge \boldsymbol{L}), \tag{4.101}$$

where $L = \boldsymbol{x} \wedge (-\mathrm{i}\nabla)$ is the orbital angular momentum. Hence we find the following identities on $\dot{\mathfrak{D}}$.

$$\begin{aligned} -\mathrm{i}\,\boldsymbol{\alpha}\cdot\nabla &= -\mathrm{i}(\boldsymbol{\alpha}\cdot\boldsymbol{e}_r)\tfrac{\partial}{\partial r} - \tfrac{1}{r}\boldsymbol{\alpha}\cdot(\boldsymbol{e}_r \wedge \boldsymbol{L}) \\ &= -\mathrm{i}(\boldsymbol{\alpha}\cdot\boldsymbol{e}_r)\tfrac{\partial}{\partial r} + \tfrac{\mathrm{i}}{r}(\boldsymbol{\alpha}\cdot\boldsymbol{e}_r)(2\boldsymbol{S}\cdot\boldsymbol{L}). \end{aligned} \tag{4.102}$$

In the last step we have used the formula

$$(\boldsymbol{\alpha}\cdot\boldsymbol{A})(2\boldsymbol{S}\cdot\boldsymbol{B}) = \mathrm{i}\gamma_5\boldsymbol{A}\cdot\boldsymbol{B} - \mathrm{i}\,\boldsymbol{\alpha}\cdot(\boldsymbol{A}\wedge\boldsymbol{B}) \tag{4.103}$$

which follows easily from Eqs. (1.228) and (1.230) in Appendix 1.B. Finally we arrive at

$$H_0 = -\mathrm{i}c(\boldsymbol{\alpha}\cdot\boldsymbol{e}_r)\left(\tfrac{\partial}{\partial r} + \tfrac{1}{r} - \tfrac{1}{r}\beta K\right) + \beta mc^2. \tag{4.104}$$

Here we have introduced the "spin-orbit operator"

$$K = \beta(2\boldsymbol{S}\cdot\boldsymbol{L} + 1) = \beta(J^2 - L^2 + \tfrac{1}{4}). \tag{4.105}$$

The operators H_0, $\boldsymbol{J}$, $\boldsymbol{L}$, $J^2 = J_1^2 + J_2^2 + J_3^2$, and $L^2 = L_1^2 + L_2^2 + L_3^2$ and hence also K are all essentially self-adjoint on the domain $\dot{\mathfrak{D}} \equiv \mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{\mathrm{O}\})^4$. We know already that H_0 commutes with each of the angular momentum operators $\boldsymbol{J}_k$ because H_0 and J_k are generators of a representation of the Poincaré group.

$$[H_0, J_k] = 0, \quad \text{on } \dot{\mathfrak{D}}, \text{ for } k = 1, 2, 3. \tag{4.106}$$

A little calculation shows

$$\{\boldsymbol{S}\cdot\boldsymbol{L}, \boldsymbol{\alpha}\cdot\boldsymbol{e}_r\} = -\boldsymbol{\alpha}\cdot\boldsymbol{e}_r. \tag{4.107}$$

Hence $\{2\boldsymbol{S}\cdot\boldsymbol{L} + 1, \boldsymbol{\alpha}\cdot\boldsymbol{e}_r\} = 0$. Since the Dirac matrix β commutes with $\boldsymbol{S}\cdot\boldsymbol{L}$ and anticommutes with $\boldsymbol{\alpha}\cdot\boldsymbol{e}_r$ we conclude that

$$[K, \boldsymbol{\alpha}\cdot\boldsymbol{e}_r] = 0. \tag{4.108}$$

From (4.104) it is clear that K commutes with the free Dirac operator H_0, at least on $\dot{\mathfrak{D}}$. At the same time, K commutes with rotations and hence with J^2 and J_3.

4.6.4 Angular Momentum Eigenfunctions

The operators J^2, J_3, and K defined in the Hilbert space $L^2(S^2)^4$ have a pure discrete spectrum. There is a complete system of orthonormal eigenvectors Φ_{m_j,κ_j} such that

$$\begin{aligned} J^2\,\Phi_{m_j,\kappa_j} &= j(j+1)\,\Phi_{m_j,\kappa_j}, & j &= \tfrac{1}{2},\tfrac{3}{2},\tfrac{5}{2},\ldots, \\ J_3\,\Phi_{m_j,\kappa_j} &= m_j\,\Phi_{m_j,\kappa_j}, & m_j &= -j,-j+1,\ldots,+j, \\ K\,\Phi_{m_j,\kappa_j} &= -\kappa_j\,\Phi_{m_j,\kappa_j}, & \kappa_j &= -(j+\tfrac{1}{2}),+(j+\tfrac{1}{2}). \end{aligned} \tag{4.109}$$

For each set of eigenvalues j, m_j and κ_j there are two orthogonal eigenvectors $\Phi^{\pm}_{m_j,\kappa_j}$ in $\mathcal{C}^\infty(S^2)^4$, hence

$$\Phi_{m_j,\kappa_j} = c^+\Phi^+_{m_j,\kappa_j} + c^-\Phi^-_{m_j,\kappa_j}, \tag{4.110}$$

with arbitrary complex constants c^+ and c^-. We have

$$\Phi^+_{m_j,\mp(j+1/2)} = \begin{pmatrix} \mathrm{i}\,\Psi^{m_j}_{j\mp1/2} \\ 0 \end{pmatrix}, \quad \Phi^-_{m_j,\mp(j+1/2)} = \begin{pmatrix} 0 \\ \Psi^{m_j}_{j\pm1/2} \end{pmatrix}, \tag{4.111}$$

$$\Psi^{m_j}_{j-1/2} = \frac{1}{\sqrt{2j}} \begin{pmatrix} \sqrt{j+m_j}\; Y^{m_j-1/2}_{j-1/2} \\ \sqrt{j-m_j}\; Y^{m_j+1/2}_{j-1/2} \end{pmatrix}, \tag{4.112}$$

$$\Psi^{m_j}_{j+1/2} = \frac{1}{\sqrt{2j+2}} \begin{pmatrix} \sqrt{j+1-m_j}\; Y^{m_j-1/2}_{j+1/2} \\ -\sqrt{j+1+m_j}\; Y^{m_j+1/2}_{j+1/2} \end{pmatrix}. \tag{4.113}$$

Here Y^m_l are the usual spherical harmonics. They are defined for $l = 0,1,2,\ldots$, and $m = -l,-l+1,\ldots,l$, with the help of the associated Legendre polynomials P^m_l,

$$Y^m_l(\vartheta,\varphi) = \sqrt{\tfrac{2l+1}{4\pi}\,\tfrac{(l-m)!}{(l+m)!}}\; e^{\mathrm{i}\,m\varphi}\, P^m_l(\cos\vartheta), \quad \text{for } m>0, \tag{4.114}$$

$$P^m_l(x) = \frac{(-1)^m}{2^l l!}\,(1-x^2)^{m/2}\,\frac{d^{m+l}}{dx^{m+l}}\,(x^2-1)^l, \tag{4.115}$$

$$Y^{-m}_l = (-1)^m\,\overline{Y^m_l}. \tag{4.116}$$

It is well known that the Y^m_l are the eigenfunctions of the operators L^2 and L_3 (orbital angular momentum) in the Hilbert space $L^2(S^2)$,

$$L^2\,Y^m_l = l(l+1)\,Y^m_l, \quad L_3\,Y^m_l = m\,Y^m_l, \tag{4.117}$$

and that the Y^m_l form a complete orthonormal set in $L^2(S^2)$. Moreover,

$$\begin{aligned} (L_1+\mathrm{i}\,L_2)\,Y^m_l &= \sqrt{(l+m+1)(l-m)}\;Y^{m+1}_l, \\ (L_1-\mathrm{i}\,L_2)\,Y^m_l &= \sqrt{(l-m+1)(l+m)}\;Y^{m-1}_l. \end{aligned} \tag{4.118}$$

One can verify all the statements (4.109) - (4.118) by a direct calculation using the explicit forms of the angular momentum operators in Eq. (4.99).

Remark. The functions $\Psi^{m_j}_{j\mp 1/2}$ defined in (4.112) and (4.113) are elements of the Hilbert space $L^2(S^2)^2$. They are simultaneous eigenfunctions of the operators L^2, L_3, $J^2 = L^2 + \boldsymbol{\sigma}\cdot\boldsymbol{L} + 3/4$, $J_3 = L_3 + \sigma_3/2$, and $\boldsymbol{\sigma}\cdot\boldsymbol{L} + 1$. (These operators are defined in an obvious way also in $L^2(S^2)^2$). The corresponding eigenvalues are denoted by $l(l+1)$, m_l, $j(j+1)$, m_j, and $-\kappa$, respectively. For $\Psi^{m_j}_{j-1/2}$ spin and orbital momentum are parallel, $l = j - 1/2 = 0, 1, \ldots$, and $\kappa = -l - 1 = -(j + 1/2) < 0$. For $\Psi^{m_j}_{j+1/2}$ we have $l = j + 1/2 = 1, 2, \ldots$, and $\kappa = l = (j + 1/2) > 0$, hence spin and orbital angular momenta are antiparallel. The functions $\Phi^{\pm}_{m_j,\kappa_j}$, however, are not eigenfunctions of L^2 or L_3. Such eigenfunctions can be obtained as special linear combinations of the $\Phi^{\pm}_{m_j,\kappa_j}$, but the corresponding subspaces are not left invariant by H_0, because the free Dirac operator does not commute with the orbital angular momentum.

The Hilbert space $L^2(S^2)^4$ is the orthogonal direct sum of two dimensional Hilbert spaces $\mathcal{K}_{m_j,\kappa_j}$, which are spanned by the simultaneous eigenfunctions $\Phi^{\pm}_{m_j,\kappa_j}$ of J^2, J_3, and K,

$$L^2(S^2)^4 = \bigoplus_{j=\frac{1}{2},\frac{3}{2},\ldots}^{\infty} \bigoplus_{m_j=-j}^{j} \bigoplus_{\kappa_j=\pm(j+\frac{1}{2})} \mathcal{K}_{m_j,\kappa_j}, \tag{4.119}$$

$$\mathcal{K}_{m_j,\kappa_j} = \{\, c^+\Phi^+_{m_j,\kappa_j} + c^-\Phi^-_{m_j,\kappa_j} \mid c^{\pm} \in \mathbb{C} \,\}. \tag{4.120}$$

The functions $\Psi^{m_j}_{j\pm 1/2}$ satisfy

$$\boldsymbol{\sigma}\cdot\boldsymbol{e}_r\, \Psi^{m_j}_{j\pm 1/2} = \Psi^{m_j}_{j\mp 1/2}, \tag{4.121}$$

and hence

$$\mathrm{i}\boldsymbol{\alpha}\cdot\boldsymbol{e}_r\, \Phi^{\pm}_{m_j,\kappa_j} = \mp\Phi^{\mp}_{m_j,\kappa_j}. \tag{4.122}$$

From this we conclude the following result.

Lemma 4.13. The subspaces $\mathcal{K}_{m_j,\kappa_j}$ are left invariant by the operators β and $\boldsymbol{\alpha}\cdot\boldsymbol{e}_r$. With respect to the basis $\{\Phi^+_{m_j,\kappa_j}, \Phi^-_{m_j,\kappa_j}\}$ defined by (4.110) - (4.116) these operators are represented by 2×2 matrices,

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad -\mathrm{i}\boldsymbol{\alpha}\cdot\boldsymbol{e}_r = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{4.123}$$

4.6.5 The Partial Wave Subspaces

The decomposition (4.119) of the angular Hilbert space implies a similar decomposition of $L^2(\mathbb{R}^3)^4$. Each "partial wave subspace" $L^2((0,\infty),dr) \otimes \mathfrak{K}_{m_j,\kappa_j}$ is isomorphic to $L^2((0,\infty),dr)^2$ if we choose the basis $\{\Phi^+_{m_j,\kappa_j}, \Phi^-_{m_j,\kappa_j}\}$ in $\mathfrak{K}_{m_j,\kappa_j}$. For $(f^+,f^-) \in L^2((0,\infty),dr)^2$,

$$\begin{aligned}\psi(r,\vartheta,\varphi) &= f^+(r)\,\Phi^+_{m_j,\kappa_j}(\vartheta,\varphi) + f^-(r)\,\Phi^-_{m_j,\kappa_j}(\vartheta,\varphi) \\ &= \begin{pmatrix} \mathrm{i}\, f^+(r)\, \Psi^{m_j}_{j+1/2}(\vartheta,\varphi) \\ f^-(r)\, \Psi^{m_j}_{j\pm 1/2}(\vartheta,\varphi) \end{pmatrix} \end{aligned} \tag{4.124}$$

defines a vector in $L^2((0,\infty),dr) \otimes \mathfrak{K}_{m_j,\kappa_j}$. By the isomorphism (4.95) this vector corresponds to $\Psi \in L^2(\mathbb{R}^3)^4$, where

$$\Psi(\boldsymbol{x}) = \frac{1}{r(\boldsymbol{x})}\, \psi(r(\boldsymbol{x}),\vartheta(\boldsymbol{x}),\varphi(\boldsymbol{x})), \tag{4.125}$$

with r, ϑ, and φ given as functions of $\boldsymbol{x}$ by (4.93). An arbitrary vector in $C_0^\infty(\mathbb{R}^3)^4$ is a linear combination of the form

$$\Psi(\boldsymbol{x}) = \sum_{j,m_j,\kappa_j} \frac{1}{r}\, f^+_{m_j,\kappa_j}(r)\, \Phi^+_{m_j,\kappa_j}(\vartheta,\varphi) + \frac{1}{r}\, f^-_{m_j,\kappa_j}(r)\, \Phi^-_{m_j,\kappa_j}(\vartheta,\varphi), \tag{4.126}$$

with coefficient functions $f^\pm \in C_0^\infty(0,\infty)$. Furthermore, if Φ is represented by a sequence (g_{m_j,κ_j}), then the scalar product of Ψ and Φ is given by

$$(\Psi,\Phi) = \sum_{j,m_j,\kappa_j} \int_0^\infty \left\{ \overline{f^+_{m_j,\kappa_j}(r)}\, g^+_{m_j,\kappa_j}(r) + \overline{f^-_{m_j,\kappa_j}(r)}\, g^-_{m_j,\kappa_j}(r) \right\} dr. \tag{4.127}$$

This shows that Eqs. (4.124) and (4.125) define a unitary isomorphism between the Hilbert space $L^2(\mathbb{R}^3)^4$ and the direct sum of the partial wave subspaces $L^2((0,\infty),dr)^2$. From the form (4.104) of the Dirac operator we find that the action of H_0 on differentiable states is easily calculated. Note that due to the factor r in (4.95) the operator $\frac{d}{dr} + \frac{1}{r}$ in $L^2(\mathbb{R}^3)$ simply becomes $\frac{d}{dr}$ in $L^2((0,\infty),dr)$.

Theorem 4.14. The Dirac operator with the potential

$$V(\boldsymbol{x}) = \phi_{\mathrm{sc}}(r)\beta + \phi_{\mathrm{el}}(r)\mathbf{1}_4 + \mathrm{i}\,\beta\,\boldsymbol{\alpha}\cdot\boldsymbol{e}_r\,\phi_{\mathrm{am}}(r) \tag{4.128}$$

leaves the partial wave subspaces $C_0^\infty(0,\infty) \otimes \mathfrak{K}_{m_j,\kappa_j}$ invariant. With respect to the basis $\{\Phi^+_{m_j,\kappa_j}, \Phi^-_{m_j,\kappa_j}\}$ the action of the Dirac operator on each subspace can be represented by the operator

$$h_{m_j,\kappa_j} = \begin{pmatrix} mc^2 + \phi_{\mathrm{sc}}(r) + \phi_{\mathrm{el}}(r) & c\{-\frac{d}{dr} + \frac{\kappa_j}{r}\} + \phi_{\mathrm{am}}(r) \\ c\{\frac{d}{dr} + \frac{\kappa_j}{r}\} + \phi_{\mathrm{am}}(r) & -mc^2 - \phi_{\mathrm{sc}}(r) + \phi_{\mathrm{el}}(r) \end{pmatrix} \tag{4.129}$$

which is well defined on $C_0^\infty(0,\infty)^2 \subset L^2((0,\infty),dr)^2$.

The Dirac operator H on $\mathcal{C}_0^\infty(\mathbb{R}^3)^4$ is unitarily equivalent to the direct sum of the "partial wave" Dirac operators h_{m_j,κ_j},

$$H \cong \bigoplus_{j=\frac{1}{2},\frac{3}{2},\ldots}^{\infty} \bigoplus_{m_j=-j}^{j} \bigoplus_{\kappa_j=\pm(j+\frac{1}{2})} h_{m_j,\kappa_j}. \tag{4.130}$$

Lemma 4.15. H is essentially self-adjoint on $\dot{\mathfrak{D}} \equiv \mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{\mathrm{O}\})^4$ if and only if all h_{m_j,κ_j} are essentially self-adjoint on $\mathcal{C}_0^\infty(0,\infty)$. If this is the case, then the spectrum of the corresponding self-adjoint operator H is the union of the spectra of self-adjoint operators h_{m_j,κ_j}.

Proof. By the basic criterion ([RS 72], corollary to Theorem VIII.3.) an operator T is essentially self-adjoint, if and only if $\mathrm{Ran}\,(T\pm\mathrm{i})$ is dense. Assume that for some m_j, κ_j the operator h_{m_j,κ_j} is not essentially self-adjoint. Hence there is a nonzero vector $f \in L^2(0,\infty)^2$ in the orthogonal complement of $\mathrm{Ran}\,(h_{m_j,\kappa_j}-\mathrm{i})$,

$$(f, (h_{m_j,\kappa_j}-\mathrm{i})g) = 0, \quad \text{for all } g \in \mathcal{C}_0^\infty(0,\infty)^2. \tag{4.131}$$

Define $\Psi \in L^2(\mathbb{R}^3)^4$ as in Eqs. (4.124) and (4.125). Clearly, Ψ is in the angular momentum subspace labelled by (j, m_j, κ_j). For any $\Phi \in \mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{\mathrm{O}\})^4$ the part of Φ in this angular momentum subspace can be represented by a function $g \in \mathcal{C}_0^\infty(0,\infty)^2$. From Eqs. (4.127) and (4.131) we find

$$(\Psi, H\Phi) = (f, h_{m_j,\kappa_j} g) = (f, \mathrm{i}g) = (\Psi, \mathrm{i}\Phi), \tag{4.132}$$

which shows that $\mathrm{Ran}\,(H-\mathrm{i})$ is not dense, hence H is not essentially self-adjoint. Conversely, if there exists a vector $0 \neq \Psi$ with

$$(\Psi, (H-\mathrm{i})\Phi) = 0, \quad \text{for all } \Phi \in \mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{\mathrm{O}\})^4, \tag{4.133}$$

then the relation $(f, h_{m_j,\kappa_j} g) = 0$ must hold for all $g \in \mathcal{C}_0^\infty(0,\infty)^2$ in any angular momentum subspace in which the component f of Ψ is nonzero (otherwise it is trivial). This implies that h_{m_j,κ_j} is not essentially self-adjoint.

The result on the spectrum follows from the fact that $(H-z)^{-1}$ is unitarily equivalent to the direct sum of the partial wave resolvents $(h_{m_j,\kappa_j}-z)^{-1}$. Hence z is in the resolvent set of H if and only if it is in the resolvent set of all operators h_{m_j,κ_j}. □

4.6.6 The Radial Dirac Operator

We want to give a short review of self-adjointness and spectral theory of the radial Dirac operator which is a self-adjoint extension of

$$h = \begin{pmatrix} 0 & -c\frac{d}{dr} \\ c\frac{d}{dr} & 0 \end{pmatrix} + V(r), \quad \text{on } \mathcal{C}_0^\infty(0,\infty), \tag{4.134}$$

where V is a symmetric matrix written in the form

$$V(r) = \begin{pmatrix} mc^2 + \phi_{\rm sc}(r) + \phi_{\rm el}(r) & c\frac{\kappa}{r} + \phi_{\rm am}(r) \\ c\frac{\kappa}{r} + \phi_{\rm am}(r) & -mc^2 - \phi_{\rm sc}(r) + \phi_{\rm el}(r) \end{pmatrix}, \tag{4.135}$$

with real-valued measurable and locally integrable functions $\phi_{\rm el}$, $\phi_{\rm sc}$, and $\phi_{\rm am}(r)$.

Theorem 4.16. The operator h is essentially self-adjoint if and only if for some $\lambda \in \mathbb{C}$ the equation $hf = \lambda f$ has a solution $f \notin L^2(0,R)^2$ for some $R > 0$, i.e., a solution which is not square integrable at the origin.

Proof. Ref. [467], Sätze **1**.4, 1.5, Korollar 5.2 □

This is a generalization of Weyl's limit-point criterion which is familiar for Sturm Liouville problems. It is remarkable that there is no condition for the behavior of the potential matrix or the solutions at infinity (Sect. 4.3.2).

Example 4.17. In the case of the Coulomb potential the potential matrix has the form

$$V(r) = \begin{pmatrix} mc^2 + \frac{\gamma}{r} & c\frac{\kappa}{r} \\ c\frac{\kappa}{r} & -mc^2 + \frac{\gamma}{r} \end{pmatrix}. \tag{4.136}$$

The bounded operator $\sigma_3 mc^2$ does not alter the self-adjointness properties of h, hence we can omit it in the following consideration. It is easy to see that the equation $hf = 0$ without the mass term has the solutions

$$f(r) = \begin{pmatrix} \gamma/c \\ -\kappa - s \end{pmatrix} r^s, \quad \text{where } s = \pm\sqrt{\kappa^2 - \gamma^2/c^2}. \tag{4.137}$$

The solution with s negative is not square integrable at zero if and only if $\gamma^2/c^2 \leq \kappa^2 - 1/4$. Therefore, according to Theorem 4.16 and Lemma 4.15, the Dirac-Coulomb operator $H = H_0 + \gamma/|\boldsymbol{x}|$ on $\mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{\mathrm{O}\})^4$ is essentially self-adjoint, if and only if $|\gamma| \leq c\sqrt{3}/2$.

Theorem 4.18. Assume that V can be written as $V(r) = V_1(r) + V_2(r)$ such that each component of V_1 is integrable in $[R,\infty)$, for some $R > 0$, V_2 is of bounded variation in $[R,\infty)$, and

$$\lim_{r\to\infty} V(r) = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}, \qquad a < b. \tag{4.138}$$

Then every self-adjoint extension of h has a purely absolutely continuous spectrum in $(-\infty, a) \cup (b, \infty)$.

Proof. Ref. [468], Satz 2.1. □

In particular, the theorem states that there are no eigenvalues embedded in the continuous spectrum. It is interesting to see that there are situations where the

Dirac operator has a purely absolutely continuous spectrum on the whole real axis. This occurs for electric potentials which tend to infinity, as $r \to \infty$.

Theorem 4.19. Assume that the potential matrix V is of the form

$$V(r) = \begin{pmatrix} mc^2 + \phi_{\text{el}}(r) & c\frac{\kappa}{r} \\ c\frac{\kappa}{r} & -mc^2 + \phi_{\text{el}}(r) \end{pmatrix}, \tag{4.139}$$

$$\lim_{r\to\infty} |\phi_{\text{el}}(r)| = \infty, \qquad \int_R^\infty \left| \frac{\phi'_{\text{el}}(r)}{\phi^2_{\text{el}}(r)} \right| dr < \infty \quad \text{for some } R > 0. \tag{4.140}$$

Then every self-adjoint extension of h has the whole real line as a purely absolutely continuous spectrum.

Proof. This theorem was proved in [447] under slightly more restrictive conditions on ϕ_{el}. These restrictions were removed in [130]. See also [135], Theorem 3 and Remark 5. □

This result is very remarkable. The Dirac equation with an electrostatic harmonic oscillator potential has no eigenvalue at all! This behavior is completely different from the Schrödinger equation, which for the potentials described in (4.140) has only discrete eigenvalues. The curious result for Dirac operators is related to Klein's paradoxw (Sect. 4.5). A qualitative explanation can be given as follows. Consider the Dirac equation with a positive harmonic oscillator potential ϕ_{el}. For any energy E we can find an oscillating (scattering) solution of the Dirac equation in the region where $\phi_{\text{el}}(r) - mc^2 > E$. Note that this region extends to infinity and corresponds to the classically allowed region for a positron, which is repelled by the potential. This explains why the essential spectrum must be the whole real line. The absence of bound states can be understood as follows. If a part of the wavefunction is "inside" the potential (i.e., in the "classically allowed region" for electrons at energy E, which is given by $\phi_{\text{el}}(r)+mc^2 < E$), then it can tunnel through the classically forbidden region to the region "outside". The wavefunction decays exponentially in the classically forbidden region, but the probability of penetrating into the positron region is nonzero. Hence what has been an electron bound state is now a resonance in a scattering process involving positrons.

4.7 Selected Topics from Spectral Theory

4.7.1 Potentials Increasing at Infinity

In Theorem 4.19 we stated that the Dirac operator with a radially symmetric electric potential $\phi_{\text{el}}(r)$ which tends to infinity, as $r \to \infty$ has a continuous spectrum $(-\infty, +\infty)$. Here we prove a similar result in a more general situation.

Theorem 4.20. Let B_n be a sequence of disjoint balls not containing the origin, with increasing radius $r_n \to \infty$, as $n \to \infty$. Assume that in each ball, the electric

potential $\phi_{\rm el}$ can be approximated by a continuous differentiable function v_n depending only on $r = |\boldsymbol{x}|$, such that, as n tends to infinity,

$$\min_{x \in B_n} |v_n(r)| \to \infty, \tag{4.141}$$

$$\frac{1}{r_n^3} \int_{B_n} \big(\phi_{\rm el}(\boldsymbol{x}) - v_n(r)\big)^2 d^3x \to 0. \tag{4.142}$$

$$\frac{1}{r_n^3} \int_{B_n} \Big[\frac{v_n'(r)}{v_n(r)}\Big]^2 d^3x \to 0, \tag{4.143}$$

Then the spectrum of the Dirac operator $H = H_0 + \phi_{\rm el}\mathbf{1}$ consists of $(-\infty, \infty)$.

Proof. Using Weyl's criterion (Theorem VII.12 in [RS 72]) we have to show that there is a sequence of orthonormal vectors $\Psi^{(n)}$ in $\mathfrak{D}(H)$ such that $\lim_{n\to\infty} \|(H-E)\Psi^{(n)}\| = 0$. We choose

$$\Psi^{(n)}(E, \boldsymbol{x}) = k_n \, e^{{\rm i}F_n(E,r)} \, v_n(r) \, j_n(\boldsymbol{x}) \, g_n(E, \boldsymbol{x}), \qquad r = |\boldsymbol{x}|. \tag{4.144}$$

The function F and the spinor g will be determined later. The function j_n is a smooth localization function with support in the ball B_n with center $\boldsymbol{x}_n$:

$$j_n(\boldsymbol{x}) = \begin{cases} 1, & |\boldsymbol{x} - \boldsymbol{x}_n| \le r_n - 1, \\ 0, & |\boldsymbol{x} - \boldsymbol{x}_n| \ge r_n, \end{cases} \qquad 0 \le j_n(\boldsymbol{x}) \le 1, \quad \text{for all } \boldsymbol{x}. \tag{4.145}$$

Furthermore we assume that $|\nabla j_n(\boldsymbol{x})|$ is bounded uniformly in n. Since the balls are disjoint, the sequence $\Psi^{(n)}$ consists of orthonormal vectors (the constant k_n is chosen such that $\|\Psi^{(n)}\| = 1$).

$$\begin{aligned}(H-E)\Psi^{(n)}(\boldsymbol{x}) &= \big(-{\rm ic}\boldsymbol{\alpha}\cdot\nabla + \beta mc^2 + \phi_{\rm el}(\boldsymbol{x}) - E\big)\,\Psi^{(n)}(\boldsymbol{x}) \\ &= \big({\rm c}\boldsymbol{\alpha}\cdot(\nabla F_n) + \beta mc^2 + v_n(r) - E\big)\,\Psi^{(n)}(\boldsymbol{x}) && (4.146) \\ &\quad + \big(\phi_{\rm el}(\boldsymbol{x}) - v_n(r)\big)\,\Psi^{(n)}(\boldsymbol{x}) && (4.147) \\ &\quad + k_n e^{{\rm i}F_n}\Big\{-ic\boldsymbol{\alpha}\cdot\Big[\big(\nabla v_n^{-1}\, j_n\big)\, g_n + v_n^{-1}\, j_n\,(\nabla g_n)\Big]\Big\}. && (4.148)\end{aligned}$$

The first summand (4.146) vanishes, if

$$\Big\{{\rm c}\,\frac{\boldsymbol{\alpha}\cdot\boldsymbol{x}}{r}\,F_n'(E,r) + \beta mc^2\Big\} g_n(E,\boldsymbol{x}) = \big(E - v_n(r)\big)\, g_n(E,\boldsymbol{x}). \tag{4.149}$$

The matrix on the left side has the eigenvalues $\pm(c^2 {F_n'}^2 + m^2c^4)^{1/2}$. If n is sufficiently large, (4.141) implies that either $E - v_n(r) > mc^2$ or $< -mc^2$. An eigenvector for the positive eigenvalue is given by the column vector ($^\top$ means "transposed")

$$g_n = \big(\,(c^2 {F_n'}^2 + m^2c^4)^{1/2} + mc^2\,,\, 0\,,\, c\tfrac{x_3}{r}F_n'\,,\, c\tfrac{x_1+{\rm i}x_2}{r}F_n'\,\big)^\top. \tag{4.150}$$

In the case $E - v_n(r) < -mc^2$ we choose instead

$$g_n = \big(-c\tfrac{x_1-{\rm i}x_2}{r}F_n'\,,\, {\rm c}\tfrac{x_3}{r}F_n'\,,\, 0\,,\, (c^2 {F_n'}^2 + m^2c^4)^{1/2} + mc^2\,\big)^\top. \tag{4.151}$$

In order to fulfill Eq. (4.149) we must have

$$c^2 F_n'^2(E,r) + m^2c^4 = \big(E - v_n(r)\big)^2. \tag{4.152}$$

Hence we take

$$F_n(E,r) = \frac{1}{c^2}\int_{|x_n|}^{r} \Big\{\big(E - v_n(s)\big)^2 - m^2c^4\Big\}^{\frac{1}{2}} ds. \tag{4.153}$$

With these definitions (4.146) vanishes, and we obtain

$$\begin{aligned} |g_n(E,r)|^2 &= \big\{\big(c^2F_n'^2(E,r) + m^2c^4\big)^{1/2} - mc^2\big\}^2 + c^2F_n'^2(E,r) \\ &= 2\big(E - v_n(r) \pm mc^2\big)\big(E - v_n(r)\big), \quad \text{if } v_n(r) \gtrless 0. \end{aligned} \tag{4.154}$$

Consequently, using assumption (4.141),

$$|\Psi^{(n)}(\boldsymbol{x})|^2 \le k_n^2 \int_{B_n} \frac{|g_n(\boldsymbol{x})|^2}{v_n^2(r)} d^3x \le \text{const.} k_n^2, \tag{4.155}$$

$$\text{const}_1\, k_n^2\,(r_n - 1)^3 \le \|\Psi^{(n)}\|^2 \le \text{const}_2\, k_n^2\, r_n^3. \tag{4.156}$$

We conclude that k_n must behave like const.$(r_n)^{-3/2}$, as $n \to \infty$, if we require $\|\Psi^{(n)}\| = 1$. Hence we can estimate (4.147) by

$$\|(\phi_{\text{el}} - v_n)\,\Psi^{(n)}\|^2 \le \text{const.} k_n^2 \int_{B_n} \big(\phi_{\text{el}}(\boldsymbol{x}) - v_n(r)\big)^2 d^3x, \tag{4.157}$$

which tends to zero, as $n \to \infty$, by assumption (4.142). A little calculation shows that

$$\begin{aligned} &|\boldsymbol{\alpha}\cdot\nabla g_n(\boldsymbol{x})|^2 \\ &= (v_n')^2 + \left\{\frac{-(E - v_n)v_n'}{\sqrt{(E - v_n)^2 - mc^2}} + \frac{2}{r}\sqrt{(E - v_n)^2 - mc^2}\right\}^2. \end{aligned} \tag{4.158}$$

This implies the estimate

$$k_n^2 \big\|c\boldsymbol{\alpha}\cdot\big[v_n^{-1}\, j_n\,(\nabla g_n)\big]\big\|^2 \le \text{const.} k_n^2 \int_{B_n} \left\{\left[\frac{v_n'(r)}{v_n(r)}\right]^2 - \frac{1}{r^2}\right\} d^3x. \tag{4.159}$$

By our condition (4.143) and the assumption on the balls B_n, this expression vanishes, as $n \to \infty$. It remains to estimate

$$\begin{aligned} k_n^2\big\|c\boldsymbol{\alpha}\cdot\big(\nabla v_n^{-1}\, j_n\big)\, g_n\big\|^2 &= k_n^2 \int_{B_n} \big\{(\nabla v_n^{-1})\, j_n + v_n^{-1}(\nabla j_n)\big\}^2 |g_n|^2 \\ &\le 2k_n^2 \int_{B_n} \big\{(\nabla v_n^{-1})^2 + v_n^{-2}(\nabla j_n)^2\big\}|g_n|^2 \\ &= \text{const.}\, k_n^2 \left\{\int_{B_n}\left[\frac{v_n'(r)}{v_n(r)}\right]^2 d^3x + \int_{B_n} |\nabla j_n(\boldsymbol{x})|^2\, d^3x\right\}. \end{aligned} \tag{4.160}$$

Since $\nabla j_n(\boldsymbol{x}) = 0$ in the ball with radius $r_n - 1$, the second integral is easily seen to be of order $k_n^2 r_n^2$, and hence tends to zero, as $n \to \infty$. The first integral vanishes in the limit of large n by assumption (4.143). Putting these results together proves that (4.148) and hence also $(H - E)\Psi^{(n)}$ tends to zero, as $n \to \infty$. Hence, by Weyl's criterion, E is in the essential spectrum of H. □

There are no bound states in an increasing electrostatic potential, as one would expect from nonrelativistic quantum mechanics. As discussed at the end of Sect. 4.6.6 this is a manifestation of the Klein paradox: An electron can tunnel to a region where it can exist as a positron. Instead of a bound state we observe a resonant positron scattering state.

Remark. Theorem 4.20 is not generally true in the presence of a scalar potential $V = \beta\phi_{\text{sc}}$. Scalar potentials can be attractive for electrons and positrons at the same time. Hence the Dirac operator with a scalar potential which increases at infinity is expected to have a discrete spectrum. This is indeed the case and can be seen most easily with the help of supersymmetric methods (Sect. 5.6.1).

4.7.2 The Virial Theorem

We prove the relativistic virial theorem under some simplifying domain assumptions

Theorem 4.21. Let V be a potential matrix such that $H = H_0 + V$ is self-adjoint on $\mathfrak{D}(H) \subset \mathfrak{D}(H_0) \cap \mathfrak{D}(V)$. Furthermore, we assume that for all $\theta > 1$

$$\mathfrak{D}(V(\theta\boldsymbol{x})) = \mathfrak{D}(V(\boldsymbol{x})), \tag{4.161}$$

$$\lim_{\theta \to 1} \frac{V(\theta\boldsymbol{x}) - V(\boldsymbol{x})}{\theta - 1} = \boldsymbol{x} \cdot \nabla V(\boldsymbol{x}) \quad \text{exists for all } \boldsymbol{x} \in \mathbb{R}^3 \setminus \{\mathrm{O}\}, \tag{4.162}$$

$$\mathfrak{D}(H) \subset \mathfrak{D}(\boldsymbol{x} \cdot \nabla V). \tag{4.163}$$

Then the following relation holds for any eigenvalue E of H with corresponding eigenfunction ψ.

$$(\psi, \boldsymbol{x} \cdot \nabla V\, \psi) = (\psi, c\boldsymbol{\alpha} \cdot \boldsymbol{p}\, \psi), \tag{4.164}$$

or, equivalently,

$$(\psi, \boldsymbol{x} \cdot \nabla V\, \psi) = (\psi, (E - \beta mc^2 - V)\, \psi). \tag{4.165}$$

Proof. Define the dilation operator

$$\big(U_\theta \psi\big)(\boldsymbol{x}) = \theta^{3/2} \psi(\theta\boldsymbol{x}), \tag{4.166}$$

which is unitary for real $\theta > 0$ and depends strongly continuously on θ. The proof of the virial theorem follows by evaluating the expectation value of the

commutator $[(H-E), U_\theta]$ in the state ψ, which must be zero if ψ is the eigenvector belonging to the eigenvalue E,

$$\big((H-E)\,\psi, U_\theta\psi\big) - \big(\psi, U_\theta(H-E)\,\psi\big) = 0. \tag{4.167}$$

It is easy to see that

$$U_\theta(H-E)\,\psi(\boldsymbol{x}) = \tfrac{1}{\theta}\big(-\mathrm{i}c\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{x}} + \theta(\beta mc^2 + V(\theta\boldsymbol{x}) - E)\big)U_\theta\psi(\boldsymbol{x}). \tag{4.168}$$

Using the self-adjointness of $-\mathrm{i}c\boldsymbol{\alpha}\cdot\nabla$ on $\mathfrak{D}(H) = \mathfrak{D}(H_0)$ we find that (4.167) equals

$$\big((\beta mc^2 + V(\boldsymbol{x}) - E), U_\theta\psi\big) - \big(\psi, \theta(\beta mc^2 + V(\theta\boldsymbol{x}) - E)U_\theta\psi\big) = 0, \tag{4.169}$$

which is equivalent to

$$\big((\beta mc^2 + V(\boldsymbol{x}) - E)\,\psi, U_\theta\psi\big) = -\theta\Big(\frac{V(\theta\boldsymbol{x}) - V(\boldsymbol{x})}{\theta - 1}\,\psi, U_\theta\psi\Big). \tag{4.170}$$

Our condition (4.161) implies for $\theta > 1$

$$\mathfrak{D}\Big(\frac{V(\theta\boldsymbol{x}) - V(\boldsymbol{x})}{\theta - 1}\Big) \supset \mathfrak{D}(H), \tag{4.171}$$

so that the left hand side of (4.170) is well defined. Since $\theta \to U_\theta\psi$ is continuous, and since also the limit $\boldsymbol{x}\cdot\nabla V$ defines an operator on $\mathfrak{D}(H)$, we can perform the limit $\theta \to 1$ on both sides of (4.170) to obtain

$$\big((\beta mc^2 + V(\boldsymbol{x}) - E)\,\psi, \psi\big) = -\big(\boldsymbol{x}\cdot\nabla V\,\psi, \psi\big) \tag{4.172}$$

which completes the proof of the theorem. □

As far as local singularities are concerned, Eqs. (4.161) and (4.163) are satisfied, if each component of the matrix V satisfies

$$\frac{|V_{ij}(\theta\boldsymbol{x}) - V_{ij}(\boldsymbol{x})|}{\theta - 1} \le \frac{c_1}{|\boldsymbol{x}|} + c_2, \quad \text{all } \theta \in (1, \theta_0),\ \boldsymbol{x} \in \mathbb{R}^3 \setminus \{\mathrm{O}\}, \tag{4.173}$$

for some $\theta_0 > 1$, and suitable constants $c_1,\ c_2 \ge 0$. In this case,

$$\mathfrak{D}\Big(\frac{V(\theta\boldsymbol{x}) - V(\boldsymbol{x})}{\theta - 1}\Big) \supset \mathfrak{D}\Big(\frac{1}{|\boldsymbol{x}|}\Big) \supset \mathfrak{D}(H_0) \supset \mathfrak{D}(H), \tag{4.174}$$

because $1/|\boldsymbol{x}|$ is bounded relative to H_0.

The virial theorem provides the simplest method of proving the absence of embedded eigenvalues.

Corollary 4.22. Let V satisfy the hypothesis of Theorem 4.21. Assume in addition that the matrix $V(\boldsymbol{x}) + \boldsymbol{x}\cdot\nabla V(\boldsymbol{x})$ has only non-positive eigenvalues for all $\boldsymbol{x} \in \mathbb{R}^3 \setminus \{\mathrm{O}\}$. Then we have $E \le mc^2$ for all eigenvalues E of H. Similarly, positivity of the matrix $V(\boldsymbol{x}) + \boldsymbol{x}\cdot\nabla V(\boldsymbol{x})$ implies $E \ge -mc^2$.

Proof. From (4.165) and the fact that β has the eigenvalues ± 1 we conclude immediately

$$E(\psi,\psi) = (\psi, (V + \boldsymbol{x}\cdot\nabla V + \beta mc^2)\psi) \leq mc^2(\psi,\psi), \tag{4.175}$$

whenever $(\psi, (V + \boldsymbol{x}\cdot\nabla V)\psi) \leq 0$. □

Remark. The Coulomb potential satisfies $V + \boldsymbol{x}\cdot\nabla V = 0$ and hence we conclude immediately that there are no eigenvalues in $\mathbb{R}\setminus[-mc^2, mc^2]$.

4.7.3 Number of Eigenvalues

Finally, we want to review some results on the number of eigenvalues in the spectral gap. We consider the Dirac operator with an electrostatic potential $H = H_0 + \gamma\phi_{\text{el}}\mathbf{1}$. A simple criterion for the finiteness of the spectrum in $(-mc^2, mc^2)$ is given in the following theorem.

Theorem 4.23. Assume that $|\phi_{\text{el}}(\boldsymbol{x})| \leq$ const. for $|\boldsymbol{x}| \geq R_0 > 0$. If

$$\lim_{R\to\infty} R\int_R^\infty |\phi_{\text{el}}(r,\vartheta,\varphi)|\, dr = 0, \quad \text{uniformly in } \vartheta,\varphi, \tag{4.176}$$

then the Dirac operator $H = H_0 + \phi_{\text{el}}\mathbf{1}$ has only finitely many eigenvalues with finite multiplicity in the interval $(-mc^2, mc^2)$.

If ϕ_{el} does not change sign, $|\phi_{\text{el}}(\boldsymbol{x})| \leq \epsilon < 2mc^2$ for $|\boldsymbol{x}| \geq R_0 > 0$, and

$$\lim_{R\to\infty} R\int_{|\boldsymbol{x}|\geq R} \frac{|\phi_{\text{el}}(\boldsymbol{x})|}{|\boldsymbol{x}|^2}\, d^3x = \infty, \tag{4.177}$$

then the number of points (counting multiplicity) of the spectrum of the Dirac operator in $(-mc^2, mc^2)$ is infinite.

Proof. Ref. [278], Thms. 5 and 6. □

Remark. It is well known [266] that the Dirac operator with the potential $\phi_{\text{el}}(\boldsymbol{x}) = \gamma(1+\boldsymbol{x}^2)^{-1}$ has finitely many eigenvalues in $(-mc^2, mc^2)$, if $\gamma < 1/8m$ and infinitely many eigenvalues for $\gamma > 1/8m$.

We expect that if the potential is negative and sufficiently regular, then, as the coupling constant γ is increased, eigenvalues will enter the gap at the threshold mc^2, move through the gap, and leave it at $-mc^2$. This is indeed the case for the spherically symmetric rectangular potential well, for which the Dirac equation can be solved explicitly. It is wrong for the Coulomb potential for which there are infinitely many eigenvalues at each value of the coupling constant (Sect. 7.4). In this case the lowest eigenvalue approaches $E = 0$ when the coupling constant constant becomes 1 and the Dirac operator ceases to be well defined. It is believed that an eigenvalue after diving into the continuous

spectrum at $-mc^2$ converts into a resonance for positron scattering. However, it seems to be impossible to give a physical explanation of these phenomena without quantum field theory. For the following we denote by $N^+(\gamma)$ the number of eigenvalues that enter the gap $(-mc^2, mc^2)$ at $+mc^2$, if we increase the coupling constant from 0 to γ. Similarly, $N^-(\gamma)$ is the number of eigenvalues leaving the gap at $-mc^2$. Klaus has proven the following result on the asymptotics of $N^{\pm}$.

Theorem 4.24. Let $\phi_{\mathrm{el}} \in L^3(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$, $\phi_{\mathrm{el}}(\boldsymbol{x}) \leq 0$. Then

$$\lim_{\gamma \to \infty} \frac{N^{\pm}(\gamma)}{\gamma^3} = \frac{1}{3\pi c^3} \int_{\mathbb{R}^3} |\phi_{\mathrm{el}}(\boldsymbol{x})|^3 \, d^3x. \tag{4.178}$$

Proof. Ref. [266]. □

Remark. All eigenvalues move from the right to the left if the coupling constant is increased (if $V \geq 0$ the eigenvalues enter the gap at $-mc^2$ and move to the right). It is not known whether every eigenvalue really leaves the gap for large values of γ. One can prove, however, that infinitely many eigenvalues pass through any given point E in the spectral gap, as $\gamma \to \infty$. If V is radially symmetric, this behavior occurs in each partial wave subspace. If some eigenvalue is supposed to get stuck at some energy E_0, it would be passed by infinitely many other eigenvalues. Hence there would be degenerate eigenvalues for some values of the coupling constant, which is impossible for the radial Dirac operator. We conclude that for spherically symmetric potentials the eigenvalues move through the gap, such that every eigenvalue also leaves the gap for sufficiently high coupling constants. It is, however, generally not true that all eigenvalues move one behind the other because an eigenvalue of some partial wave Dirac operator can (and will) be surpassed by an eigenvalue belonging to a different angular momentum.

5 Supersymmetry

The Dirac equation has a simple property that distinguishes it from most Schrödinger operators. This is the possibility of splitting the Dirac operator H into an "even" and an "odd" part, $H = H_{\text{even}} + H_{\text{odd}}$. We shall use this structure to define the concept of an abstract Dirac operator.

The above mentioned property turns out to be closely related with the general notion of supersymmetry. In fact, the abstract Dirac operator is a generalization of a supercharge. Therefore this chapter gives, among other things, an introduction to the basics of supersymmetric quantum mechanics.

In Sect. 5.3.1 we investigate the self-adjointness properties of H_{odd} by supersymmetric methods and treat H_{even} as a small perturbation. We obtain results for extremely singular perturbations of the free Dirac operator, assuming that the dominating singularities occur in the off-diagonal elements of the potential matrix. This is useful, e.g., for treating the Coulomb problem with anomalous moment interactions (Sect. 5.3.2).

A most interesting special case occurs if H_{even} anticommutes with H_{odd} (which is, e.g., the case for the free Dirac operator). In this case H is called a Dirac operator with supersymmetry (Sect. 5.4). In applications, however, Dirac operators have this property only in a few cases. These include the Dirac operator with an external (Lorentz-) scalar field, or a magnetic field, and the Dirac operator with anomalous moments in some special external field configurations (Sect. 5.5).

Supersymmetric Dirac operators can be brought to diagonal (or off-diagonal) form by a unitary transformation which can be given explicitly (Sect. 5.6). This will be the most abstract form of the Foldy-Wouthuysen (or Cini-Touschek) transformation (cf. Chapter 1). In this way one can reduce the spectral analysis of supersymmetric Dirac operators to the analysis of simpler operators which appear in the diagonal (or off-diagonal) of the transformed equation. In applications these operators are related to the nonrelativistic (or ultrarelativistic) limit of the corresponding supersymmetric Dirac operator.

A Dirac operator with supersymmetry has an essentially symmetric spectrum with respect to zero. The only possible asymmetry occurs at $\pm mc^2$. A measure for the amount of supersymmetry breaking is the index which counts the difference between the number of eigenvalues at $+mc^2$ and at $-mc^2$. For similar reasons one defines the spectral asymmetry (η invariant). The Dirac operators occurring in quantum mechanics usually do not have the Fredholm-property and therefore it is necessary to generalize the concept of an index. Various types of regularized indices and their relations, in particular the Witten index, are investigated in Sects. 5.7 and 5.8. A useful tool is Krein's spectral shift function, which is related to the phase shift of an associated supersymmetric scattering problem. The Witten index, the axial anomaly and the spectral asymmetry can be described in terms of Krein's function. In Sect. 5.10 we describe the connection with Fredholm determinants which can be used for explicit calculations of the index, especially in one-dimensional systems.

It turns out that the index is remarkably stable with respect to perturbations which preserve supersymmetry. The invariance of the regularized index under a supersymmetry preserving perturbation satisfying a relative trace class condition is considered in Sect. 5.9.

Finally, Sect. 5.11 lists some examples of supersymmetric Dirac operators for which the (Witten) index can be calculated explicitly.

5.1 Supersymmetric Quantum Mechanics

Here we describe the foundations of supersymmetric quantum mechanics in some detail, because these concepts play an important role in the remaining chapters.

5.1.1 The Unitary Involution τ

The abstract framework of supersymmetric quantum mechanics is given by some Hilbert space $\mathcal{H}$ in which a "unitary involution" is defined. An involution is a bounded operator τ in $\mathcal{H}$ satisfying $\tau^2 = 1$. It is easy to see that if an operator possesses any two of the properties "involutory", "unitary" and "self-adjoint", then it possesses the third. In the following τ always denotes a unitary (and hence self-adjoint) involution, i.e.,

$$\tau^* \tau = \tau \tau^* = \tau^2 = 1. \tag{5.1}$$

In connection with supersymmetry the operator τ is sometimes called "Klein's operator" or "grading operator".

Since $\tau^2 = 1$, only $+1$ and -1 can be eigenvalues of τ. In order to exclude trivialities like $\tau = 1$, we assume in the following that the spectrum of τ consists of both eigenvalues. We denote the corresponding eigenspaces by $\mathcal{H}_+$, resp. $\mathcal{H}_-$. The Hilbert space $\mathcal{H}$ decomposes into an orthogonal direct sum of these eigenspaces, $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$, and the operators

$$P_\pm \equiv \tfrac{1}{2}(1 \pm \tau) \tag{5.2}$$

are the orthogonal projections onto $\mathcal{H}_\pm$.

A simple example of a Hilbert space with a unitary involution is provided by $\mathcal{H} = L^2(\mathbb{R}^3)^4$ and $\tau = \beta$, the Dirac matrix defined in Eq. (1.9). Further examples of unitary involutions are given by γ_5, $\mathrm{i}\beta\gamma_5$, and $\operatorname{sgn} H_0 = H_0/|H_0|$, where H_0 is the free Dirac operator.

5.1.2 The Abstract Dirac Operator

Let $\mathcal{H}$ be a Hilbert space with a unitary involution τ. We define an "*abstract Dirac operator*" to be a self-adjoint operator H with a domain $\mathcal{D}(H)$ that is left invariant by τ, i.e., $\tau \mathcal{D}(H) = \mathcal{D}(H)$.

Lemma 5.1. Any abstract Dirac operator H can be uniquely written as the sum of two operators H_{odd} and H_{even}, both well defined and symmetric on $\mathcal{D}(H)$ (but not necessarily self-adjoint), such that H_{odd} anticommutes with τ, whereas H_{even} commutes with τ,

$$\{H_{\text{odd}}, \tau\} \equiv \tau H_{\text{odd}} + H_{\text{odd}} \tau = 0 \quad \text{on } \mathcal{D}(H), \tag{5.3}$$

$$[H_{\text{even}}, \tau] \equiv \tau H_{\text{even}} - H_{\text{even}} \tau = 0 \quad \text{on } \mathcal{D}(H). \tag{5.4}$$

Proof. Let $P_\pm$ be the projectors defined in Eq. (5.2). Since $P_\pm \mathfrak{D}(H) \subset \mathfrak{D}(H)$ we can write

$$H = (P_+ H P_+ + P_- H P_-) + (P_+ H P_- + P_- H P_+) \equiv H_{\text{even}} + H_{\text{odd}}, \tag{5.5}$$

and each summand is well defined on $\mathfrak{D}(H)$. Symmetry is easily verified and the commutation properties (5.3) and (5.4) follow from $\tau P_\pm = \pm P_\pm$. Uniqueness is established as follows. Let H_{ev} and H_{od} be two other operators satisfying the requirements of the lemma. Then $H_{\text{ev}} - H_{\text{even}} + H_{\text{od}} - H_{\text{odd}} = H - H = 0$ clearly commutes with τ and hence with $P_\pm$. By assumption, $H_{\text{ev}} - H_{\text{even}}$ commutes with τ and hence also $T \equiv H_{\text{od}} - H_{\text{odd}}$ commutes with τ. On the other hand, H_{od} and H_{odd} both anticommute with τ and hence $\tau T = T\tau = -\tau T$ on $\mathfrak{D}(H)$. This implies $T = 0$, i.e., $H_{\text{od}} = H_{\text{odd}}$ and hence $H_{\text{ev}} = H_{\text{even}}$. □

The symmetric operator H_{odd} is called the *odd* or *fermionic* part of H, and H_{even} is called the *even* or *bosonic* part. In most applications H_{odd} and H_{even} can be extended to self-adjoint operators.

An abstract Dirac operator Q for which $Q = Q_{\text{odd}}$ is called a *supercharge with respect to* τ. Thus a supercharge is a self-adjoint operator with

$$\tau \mathfrak{D}(Q) = \mathfrak{D}(Q), \qquad \{\tau, Q\} = 0 \quad \text{on } \mathfrak{D}(Q). \tag{5.6}$$

The positive operator Q^2 is usually called a *Hamiltonian with supersymmetry*. It commutes with τ and is therefore an even operator.

Concrete Dirac operators are given formally as a sum of a supercharge Q and an operator V which is symmetric and even, i.e.,

$$\tau \mathfrak{D}(V) = \mathfrak{D}(V), \qquad [\tau, V] = 0 \quad \text{on } \mathfrak{D}(V). \tag{5.7}$$

Very often V is an operator bounded perturbation of Q so that $H = Q + V$ is self-adjoint on $\mathfrak{D}(H) = \mathfrak{D}(Q)$ (see Sect. 5.3.1).

5.1.3 Associated Supercharges

Lemma 5.2. Let Q be a supercharge with respect to τ. Then the operator $Q' = \mathrm{i}Q\tau$, defined on $\mathfrak{D}(Q)$, is also a supercharge with respect to τ. It satisfies

$$Q'^2 = Q^2, \quad \{Q', Q\} = 0 \quad \text{on } \mathfrak{D}(Q^2), \tag{5.8}$$

$$(Q')' = Q, \quad \text{on } \mathfrak{D}(Q). \tag{5.9}$$

Proof. From (5.6) it is clear that Q' is defined on $\mathfrak{D}(Q)$, and that $\mathrm{i}Q\tau = -\mathrm{i}\tau Q$ on this domain. Hence $(\mathrm{i}Q\tau)^* = (-\mathrm{i}\tau Q)^* = \mathrm{i}Q^*\tau^* = \mathrm{i}Q\tau$, i.e., Q' is self-adjoint on $\mathfrak{D}(Q)$. Since Q' anticommutes with τ on $\mathfrak{D}(Q)$, we conclude that Q' is a supercharge with respect to τ. Eqs. (5.8) and (5.9) follow immediately from the definitions. □

5.2 The Standard Representation

The splitting of the Hilbert space in supersymmetric quantum mechanics makes it natural to write operators in matrix form. A mathematical correspondence between supercharges Q and closed operators D leads immediately to the polar decomposition theorem and to the spectral supersymmetry of D^*D and DD^*. This result will be used below in some explicit calculations (e.g., the solution of the Coulomb problem in Sect. 7.4).

5.2.1 Some Notation

Let τ be a unitary involution in a Hilbert space $\mathfrak{H}$, and let $\mathfrak{H}_\pm = P_\pm\mathfrak{H}$ with $P_\pm$ given by Eq. (5.2). The standard representation is defined by writing $\psi \in \mathfrak{H} = \mathfrak{H}_+ \oplus \mathfrak{H}_-$ as a column vector $\psi = (\psi^+, \psi^-)^\top$, where $\psi^+ \in \mathfrak{H}_+$, and $\psi^- \in \mathfrak{H}_-$. (Here "$^\top$" denotes the transposed of a matrix or a vector). We shall identify $\mathfrak{H}_+$ and $\mathfrak{H}_-$ with the set of vectors of the form $(\psi^+, 0)^\top$ and $(0, \psi^-)^\top$, respectively. With this notation the unitary involution τ is most naturally written as

$$\tau = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{in } \mathfrak{H} = \mathfrak{H}_+ \oplus \mathfrak{H}_-. \tag{5.10}$$

An abstract Dirac operator H is represented by the 2×2 matrix

$$H = P_+HP_+ + P_-HP_- + P_+HP_- + P_-HP_+ = \begin{pmatrix} H_+ & H_{+-} \\ H_{-+} & H_- \end{pmatrix}, \tag{5.11}$$

where, e.g.,

$$P_+HP_- \equiv \begin{pmatrix} 0 & H_{+-} \\ 0 & 0 \end{pmatrix} \quad \text{on } \mathfrak{H}_+ \oplus P_-\mathfrak{D}(H), \quad \text{etc.} \tag{5.12}$$

The operator H_{even} (H_{odd}) is just the diagonal (off-diagonal) part of the matrix operator H.

For an even operator V we obtain the representation

$$V = P_+VP_+ + P_-VP_- \equiv \begin{pmatrix} V_+ & 0 \\ 0 & V_- \end{pmatrix}. \tag{5.13}$$

I.e., V is the direct sum of the operators V_+ and V_-, hence[1] V is self-adjoint (essentially self-adjoint, symmetric, closed) if and only if the operators V_+ and V_- are both self-adjoint (essentially self-adjoint, symmetric, closed) on $\mathfrak{D}(V_\pm) \subset \mathfrak{H}_\pm$. The situation is slightly more complicated for odd operators which are the subject of the next section.

[1] [We 80], Ex. 5.43 on p. 128.

5.2.2 Nelson's Trick

A supercharge Q is an odd operator, hence it is an off diagonal matrix in the standard representation. The next lemma gives criteria for an odd operator to be symmetric, essentially self-adjoint, or self-adjoint.

Lemma 5.3. (Self-adjointness of a supercharge). Let $\mathfrak{H}_+$ and $\mathfrak{H}_-$ be Hilbert spaces, and assume that $D_+ : \mathfrak{D}_+ \subset \mathfrak{H}_+ \to \mathfrak{H}_-$ and $D_- : \mathfrak{D}_- \subset \mathfrak{H}_- \to \mathfrak{H}_+$ are densely defined closeable[2] operators. On $\mathfrak{D}_+ \oplus \mathfrak{D}_-$ define the operator

$$Q = \begin{pmatrix} 0 & D_- \\ D_+ & 0 \end{pmatrix}. \tag{5.14}$$

Then

$$Q^* = \begin{pmatrix} 0 & D_+^* \\ D_-^* & 0 \end{pmatrix}, \qquad Q^{**} = \begin{pmatrix} 0 & D_-^{**} \\ D_+^{**} & 0 \end{pmatrix}. \tag{5.15}$$

Proof. There exists a unitary isomorphism I between the Hilbert spaces $\mathfrak{H} = \mathfrak{H}_+ \oplus \mathfrak{H}_-$ and $\mathfrak{K} = \mathfrak{H}_- \oplus \mathfrak{H}_+$ given by $I(f,g)^\top = (g,f)^\top$, for $f \in \mathfrak{H}_+$ and $g \in \mathfrak{H}_-$. The operator Q can be written as PI, where

$$P = \begin{pmatrix} D_- & 0 \\ 0 & D_+ \end{pmatrix} : \mathfrak{D}_- \oplus \mathfrak{D}_+ \subset \mathfrak{K} \to \mathfrak{H}. \tag{5.16}$$

The notions closure, adjoint etc. of an operator immediately carry over to direct sums of operators. Thus the operator P is closeable (closed) iff both D_- and D_+ are closeable (closed). But from $Q = PI$ and the boundedness of I and $I^{-1} = I^*$ we conclude that Q is closeable (closed) iff P is closeable (closed)[3]. We have $Q^* = I^* P^*$ and since $I^{**} = I$ we find $Q^{**} = P^{**} I$. □

The lemma shows, that an odd operator Q is self-adjoint (i.e., $Q^* = Q$) if and only if D_+ is closed on $\mathfrak{D}_+$, and $D_- = D_+^*$ (which is equivalent to the statement that D_- is closed on $\mathfrak{D}_-$, and $D_+ = D_-^*$). Similarly, Q is essentially self-adjoint (i.e., $Q^{**} = Q^*$), if and only if $D_-^{**} = D_+^*$ or equivalently $D_+^{**} = D_-^*$. Q is symmetric (i.e., $Q^{**} \subset Q^*$)[4], iff $D_-^{**} \subset D_+^*$ or equivalently iff $D_+^{**} \subset D_-^*$.

Example 5.4. For the Dirac operator (4.15) with a magnetic field, the operator

$$D_+ = D_- = D \equiv c\boldsymbol{\sigma} \cdot (-\mathrm{i}\nabla - \tfrac{e}{c}\boldsymbol{A}) \quad \text{on } \mathcal{C}_0^\infty(\mathbb{R}^3)^2 \tag{5.17}$$

is symmetric, if each component of $\boldsymbol{A}$ is locally square integrable. A symmetric operator is always closeable. Hence Q is (essentially) self-adjoint, iff D is (essentially) self-adjoint.

---

[2] A densely defined linear operator T will be called "closeable" iff T^* is densely defined. In this case (closure of T) $= T^{**}$, and (closure of T)$^* = T^{***} =$ (closure of T^*) $= T^*$.

[3] [We 80], Ex. 5.12 on p. 96.

[4] For operators A and B, the notation $A \subset B$ means that $A = B$ on $\mathfrak{D}(A)$, which is a subset of $\mathfrak{D}(B)$

From the results above it is clear that there is a one-to-one correspondence between densely defined closed operators D and self-adjoint operators Q (supercharges) of the form

$$Q = \begin{pmatrix} 0 & D^* \\ D & 0 \end{pmatrix} \quad \text{on } \mathfrak{D}(Q) = \mathfrak{D}(D) \oplus \mathfrak{D}(D^*) \tag{5.18}$$

in a larger Hilbert space. Thus we can use well known theorems for self-adjoint operators to derive results for closed operators which are more difficult to obtain in a direct way. In an unpublished remark Edward Nelson has noticed that one can prove in this way a theorem of von Neumann: D^*D is densely defined and self-adjoint iff D is densely defined and closed. Just note that for any self-adjoint Q the operator Q^2 is densely defined and self-adjoint (by the spectral theorem). Another example where Nelson's trick is useful is the polar decomposition theorem for closed operators. These results are proven below because they are of general importance to supersymmetric quantum mechanics and necessary for calculations performed within the standard representation.

5.2.3 Polar Decomposition of Closed Operators

Theorem 5.5. If D is a densely defined, closed linear operator from $\mathfrak{D}(D) \subset \mathfrak{H}_+$ to $\mathfrak{H}_-$, then both D^*D and DD^* are densely defined, self-adjoint and positive, and $\mathfrak{D}(D^*D)$ (resp. $\mathfrak{D}(DD^*)$) is a core for D (resp. D^*). Moreover we can write

$$D = Q_- S = S Q_+, \tag{5.19}$$

with the self-adjoint and positive operators

$$Q_+ \equiv (D^*D)^{1/2}, \qquad Q_- \equiv (DD^*)^{1/2}, \tag{5.20}$$

defined on $\mathfrak{D}(Q_+) = \mathfrak{D}(D)$, $\mathfrak{D}(Q_-) = \mathfrak{D}(D)$, and with the partial isometry

$$S \equiv \begin{cases} Q_-^{-1} D = D Q_+^{-1} & \text{on } (\operatorname{Ker} D)^\perp \\ 0 & \text{on } \operatorname{Ker} D. \end{cases} \tag{5.21}$$

Here $\operatorname{Ker} D$ is the set $\{\psi \in \mathfrak{D}(D) \mid D\psi = 0\}$ (the "kernel" of D), and "$\perp$" denotes the orthogonal complement of a set.

Proof. Our proof uses Nelson's trick. A direct proof can be found in various textbooks, e.g., in [Ka 80], Sects. V.3.7 and VI.2.7, or in [We 80], Theorem 7.20. From D and D^* we may form the operator Q as in (5.18). By Lemma 5.3, Q is self-adjoint. By the spectral theorem for self-adjoint operators, Q^2 is self-adjoint on the dense domain

$$\mathfrak{D}(Q^2) = \{f \in \mathfrak{D}(Q) \mid Qf \in \mathfrak{D}(Q)\} = \mathfrak{D}(D^*D) \oplus \mathfrak{D}(DD^*), \tag{5.22}$$

and positive. Moreover, Q is essentially self-adjoint on $\mathfrak{D}(Q^2)$. This proves the first part of the theorem. For the second part we just note that (again by the spectral theorem) for any self-adjoint operator $Q = |Q| \operatorname{sgn} Q = \operatorname{sgn} Q\, |Q|$,

where $|Q| = (Q^2)^{1/2}$ is defined on $\mathfrak{D}(Q)$, and where $\operatorname{sgn} Q$ is a bounded, everywhere defined operator given by $Q|Q|^{-1} = |Q|^{-1}Q$ on $(\operatorname{Ker} Q)^\perp$ and 0 on $\operatorname{Ker} Q$. □

Remark. Note that for any supercharge given as in (5.18)

$$\operatorname{Ker} Q = \operatorname{Ker} D \oplus \operatorname{Ker} D^*. \tag{5.23}$$

By Nelson's trick, the formula

$$\operatorname{Ker} Q = \operatorname{Ker} Q^2 = (\operatorname{Ran} Q)^\perp \tag{5.24}$$

is equivalent to

$$\operatorname{Ker} D = \operatorname{Ker} D^*D = (\operatorname{Ran} D^*)^\perp = (\operatorname{Ran} D^*D)^\perp, \tag{5.25}$$

$$\operatorname{Ker} D^* = \operatorname{Ker} DD^* = (\operatorname{Ran} D)^\perp = (\operatorname{Ran} DD^*)^\perp. \tag{5.26}$$

The operator $\operatorname{sgn} Q$ is a unitary map from $(\operatorname{Ker} Q)^\perp$ onto $(\operatorname{Ker} Q)^\perp$, i.e., a partial isometry. In the standard representation it is given by

$$\operatorname{sgn} Q = \begin{pmatrix} 0 & S^* \\ S & 0 \end{pmatrix} \quad \text{on } (\operatorname{Ker} Q)^\perp. \tag{5.27}$$

Thus S is unitary from $(\operatorname{Ker} D)^\perp$ onto $(\operatorname{Ker} D^*)^\perp$.

Corollary 5.6. (Spectral supersymmetry). The operator D^*D on $(\operatorname{Ker} D)^\perp$ is unitarily equivalent to the operator DD^* on $(\operatorname{Ker} D^*)^\perp$. In particular, the spectra of D^*D and of DD^* are equal away from zero,

$$\sigma(DD^*) \setminus \{0\} = \sigma(D^*D) \setminus \{0\}. \tag{5.28}$$

Proof. The result follows immediately from the trivial calculation

$$\begin{pmatrix} D^*D & 0 \\ 0 & DD^* \end{pmatrix} = Q^2 = (\operatorname{sgn} Q)\, Q^2\, (\operatorname{sgn} Q) = \begin{pmatrix} S^*DD^*S & 0 \\ 0 & SD^*DS^* \end{pmatrix},$$

which holds on $(\operatorname{Ker} Q)^\perp$ and which shows that DD^* and D^*D are mapped onto each other by the isometry S. □

In particular, whenever $\lambda \neq 0$ is an eigenvalue of D^*D with eigenvector f, then Df is an eigenvector of DD^* belonging to the same eigenvalue:

$$DD^*(Df) = D(D^*Df) = D\lambda f = \lambda(Df). \tag{5.29}$$

Conversely, $DD^*g = \lambda g$, $\lambda \neq 0$, implies $g \in \mathfrak{D}(D^*)$, and $D^*D(D^*g) = \lambda(D^*g)$. Hence all eigenvectors g of DD^* can be written as $g = Df$, with f an eigenvector of D^*D belonging to the same eigenvalue. Furthermore, all eigenvalues $\lambda \neq 0$ of Q^2 are degenerate, $(f, 0)^\top$ and $(0, g)^\top$ are orthogonal eigenvectors.

5.2.4 Commutation Formulas

For any supercharge Q and any bounded continuous function f define on $\mathfrak{D}(Q)$ the operator

$$Q\,f(Q^2) = \int \lambda\, f(\lambda^2)\, dE_Q(\lambda) = f(Q^2)\, Q. \tag{5.30}$$

Since

$$f(Q^2) = \begin{pmatrix} f(D^*D) & 0 \\ 0 & f(DD^*) \end{pmatrix}, \tag{5.31}$$

we conclude from (5.24) and (5.18) that the following formulas hold on $\mathfrak{D}(D^*)$ resp. $\mathfrak{D}(D)$ for any densely defined closed operator D:

$$f(D^*D)\, D^* = D^*\, f(DD^*), \qquad f(DD^*)\, D = D\, f(D^*D). \tag{5.32}$$

5.3 Self-Adjointness Problems

5.3.1 Essential Self-Adjointness of Abstract Dirac Operators

In Sect. 4.3 we investigated singular perturbations of the free Dirac operator H_0, in cases where the perturbation V may be considered "small" compared to H_0. There are, however, important situations where the assumptions of Theorem 4.2 are violated (e.g., for electrons with an anomalous magnetic moment in a Coulomb field). In these cases we proceed as follows. Define

$$H_0 + V \equiv Q + W, \tag{5.33}$$

where $W = \beta mc^2 + V_{\text{even}}$ is even, and $Q = c\boldsymbol{\alpha} \cdot \boldsymbol{p} + V_{\text{odd}}$ is odd (with respect to the unitary involution $\tau = \beta$). In this section we shall obtain criteria for an odd operator Q to be essentially self-adjoint. These criteria are based on supersymmetry rather than on perturbation theory. The crucial observation is that in some cases W may be considered a small perturbation of the essentially self-adjoint operator Q although V is not a small perturbation of H_0.

Lemma 5.7. Define Q as in Lemma 5.3 and let Q be symmetric. Assume

a) $D_+\mathfrak{D}_+ \subset \mathfrak{D}(D_-^{**})$,
b) $D_-^{**}D_+$ is essentially self-adjoint on $\mathfrak{D}_+$.

Then Q is essentially self-adjoint on $\mathfrak{D}_+ \oplus \mathfrak{D}_-$.

Proof. We shall use the *basic criterion for essential self-adjointness*[5]: For a symmetric operator T the following three statements are equivalent: i) T is essentially self-adjoint, ii) $\mathrm{Ker}\,(T^* \pm \mathrm{i}) = \{0\}$, and iii) $\mathrm{Ran}\,(T \pm \mathrm{i})$ is dense.

[5] [RS 72], corollary to Theorem VIII.3.

Assume that for some $u \in \mathfrak{H}_+$ and $v \in \mathfrak{H}_-$

$$Q^* \begin{pmatrix} u \\ v \end{pmatrix} \equiv \begin{pmatrix} D_+^* v \\ D_-^* u \end{pmatrix} = \pm \mathrm{i} \begin{pmatrix} u \\ v \end{pmatrix}. \tag{5.34}$$

Then we have for all $\phi \in \mathfrak{D}_+$

$$\begin{aligned} (D_-^{**} D_+ \phi, u) &= (D_+ \phi, D_-^* u) = \pm \mathrm{i} (D_+ \phi, v) \\ &= \pm \mathrm{i} (\phi, D_+^* v) = -(\phi, u). \end{aligned} \tag{5.35}$$

This means $((D_-^{**} D_+ + 1)\phi, u) = 0$ and hence

$$u \in \mathrm{Ran}\,(D_-^{**} D_+ + 1)^{\perp}. \tag{5.36}$$

By the essential self-adjointness of $D_-^{**} D_+$ and the basic criterion we must have $u = 0$ and hence $v = 0$. But this implies that $\pm \mathrm{i}$ is not an eigenvalue of Q^*. Hence $\mathrm{Ker}\,(Q \pm \mathrm{i}) = \{0\}$ and Q is essentially self-adjoint. □

The same result holds if the roles of D_+ and of D_- in the conditions a) and b) of Lemma 5.7 are exchanged. Thus, if at least one of the operators $D_-^{**} D_+$ or $D_+^{**} D_-$ is well defined and essentially self-adjoint, then Q is essentially self-adjoint and by Lemma 5.3 its self-adjoint extension is given by

$$Q^{**} = \begin{pmatrix} 0 & D_-^{**} \\ D_-^* & 0 \end{pmatrix} = \begin{pmatrix} 0 & D_+^* \\ D_+^{**} & 0 \end{pmatrix}. \tag{5.37}$$

As in Theorem 5.5 we conclude that both $D_-^{**} D_-^*$ and $D_+^{**} D_+^*$ are densely defined, self-adjoint, and positive.

The assumptions of Lemma 5.7 are weaker than the requirement that Q^2 be essentially self-adjoint. This is illustrated in the following example.

Example 5.8. (The free radial Dirac operator for $\kappa_j = 1$). Let $\mathfrak{D}_\pm = \mathfrak{D} = C_0^\infty(0, \infty)$ and define

$$D_+ = \frac{d}{dr} + \frac{1}{r}, \qquad D_- = -\frac{d}{dr} + \frac{1}{r}. \tag{5.38}$$

These operators are closeable and they leave the domain $\mathfrak{D}$ invariant. Hence $D_-^{**} D_+ = D_- D_+$, and $D_+^{**} D_- = D_+ D_-$. We find

$$D_+ D_- = -\frac{d^2}{dr^2}, \qquad D_- D_+ = -\frac{d^2}{dr^2} + \frac{1}{r^2}. \tag{5.39}$$

Only $D_- D_+$ is essentially self-adjoint on $\mathfrak{D}$. By the lemma above Q is essentially self-adjoint on $C_0^\infty(0, \infty)^2$, while Q^2 is not. The self-adjoint operator $D_+^{**} D_+^*$ is the Friedrichs extension of $D_+ D_-$, and $D_-^{**} D_-^*$ is simply the closure of $D_- D_+$.

Together with Lemma 4.15 this example leads to another proof of the essential self-adjointness of the free Dirac operator H_0 on $C_0^\infty(\mathbb{R}^3 \setminus \{0\})^4$. This result does not extend to the nonrelativistic Schrödinger operator $-\Delta$.

Now, assume that W_+ and W_- are symmetric operators such that W_+^2 is form-bounded relative to $D_-^{**}D_+$, similar for W_- and $D_+^{**}D_-$. This means there exist constants a and b such that

$$(W_+u, W_+u) \leq a(D_-^*u, D_+u) + b(u,u), \tag{5.40}$$

$$(W_-v, W_-v) \leq a(D_+^*v, D_-v) + b(v,v). \tag{5.41}$$

for all $u \in \mathfrak{D}_+$ and $v \in \mathfrak{D}_-$. This implies, since $D_+ \subset D_+^{**} = D_-^*$,

$$\|W_+u\|^2 \leq a\|D_+u\|^2 + b\|u\|^2, \quad \text{for } u \in \mathfrak{D}_+, \tag{5.42}$$

(similar for W_-), i.e $W_\pm$ are (operator-) bounded relative to $D_\pm$. For Q as above and

$$W = \begin{pmatrix} W_+ & 0 \\ 0 & W_- \end{pmatrix} \tag{5.43}$$

we thus obtain immediately

$$\|W\psi\|^2 \leq a\|Q\psi\|^2 + b\|\psi\|^2, \quad \text{all } \psi \in \mathfrak{D}_+ \oplus \mathfrak{D}_-. \tag{5.44}$$

Now, if $a \leq 1$ we can apply the Kato-Rellich theorem (resp. Wüst's theorem for $a = 1$, see [RS 75], Thm. X.14) to conclude essential self-adjointness of $T = Q + W$ on $\mathfrak{D}_+ \oplus \mathfrak{D}_-$. For $a < 1$ the closure $H = T^{**}$ is self-adjoint on $\mathfrak{D}(Q^{**}) \subset \mathfrak{D}(W)$. This domain is left invariant by τ, as can be seen from (5.37). Therefore H defines an abstract Dirac operator. We summarize our results in the following theorem.

Theorem 5.9. Let Q, defined as in Lemma 1 be symmetric on some dense domain $\mathfrak{D}_+ \oplus \mathfrak{D}_-$. Assume that one of the operators $D_-^{**}D_+$ on $\mathfrak{D}_+$ or $D_+^{**}D_-$ on $\mathfrak{D}_-$ is well defined and essentially self-adjoint. Let $W_\pm$ be symmetric operators in $\mathfrak{H}_\pm$, such that $W_\pm^2$ are form-bounded relative to $D_-^{**}D_+$ resp. $D_+^{**}D_-$ with form bound $a \leq 1$. Then the operator

$$T = \begin{pmatrix} 0 & D_- \\ D_+ & 0 \end{pmatrix} + \begin{pmatrix} W_+ & 0 \\ 0 & W_- \end{pmatrix} \quad \text{on } \mathfrak{D}(T) = \mathfrak{D}_+ \oplus \mathfrak{D}_- \tag{5.45}$$

is essentially self-adjoint.

An application of this theorem is given in the next section.

5.3.2 Particles with an Anomalous Magnetic Moment

Let $\phi_{\mathrm{el}}(\boldsymbol{x}) \equiv \phi_{\mathrm{el}}(r)$, $r = |\boldsymbol{x}|$, be a rotationally symmetric electrostatic potential. We denote $\phi'_{\mathrm{el}}(r) \equiv d\phi_{\mathrm{el}}(r)/dr$. Then the Dirac operator for an electron with anomalous magnetic moment μ_{a} is unitarily equivalent to a direct sum of radial Dirac operators (cf. Sect. 4.6.5). The radial Dirac operators are defined on the basis of the following expressions

$$T = \begin{pmatrix} mc^2 + \phi_{\rm el}(r) & c\left(-\frac{d}{dr} + \frac{\kappa}{r}\right) - \mu_{\rm a}\phi'_{\rm el}(r) \\ c\left(\frac{d}{dr} + \frac{\kappa}{r}\right) - \mu_{\rm a}\phi'_{\rm el}(r) & -mc^2 + \phi_{\rm el}(r) \end{pmatrix}, \tag{5.46}$$

where $\kappa = \pm 1, \pm 2, \ldots$. If, for example, $\phi_{\rm el}(r)$ is a Coulomb potential γ/r, then $\phi'_{\rm el}(r)$ has a $1/r^2$-singularity which looks very bad in view of Sect. 4.3. It will nevertheless turn out that the existence of an anomalous magnetic moment has in fact a regularizing influence, so that the Dirac operator, as long as $\mu_{\rm a} \neq 0$, can be defined even for extremely singular potentials, like $\phi_{\rm el}(r) = \exp(1/r)$.

We want to define with the help of T a unique self-adjoint radial Dirac operator H in the Hilbert space $L^2(0,\infty)^2$. We assume that $\phi_{\rm el}$ is twice continuously differentiable with a possible singularity at the origin $r = 0$. Then the operators

$$D_\pm = c\left(\pm\frac{d}{dr} + \frac{\kappa}{r}\right) - \mu_{\rm a}\phi'_{\rm el}(r) \tag{5.47}$$

are well defined on $\mathfrak{D}_\pm = C_0^\infty(0,\infty)$ (the infinitely differentiable functions with compact support away from 0). Moreover $D_\pm \mathfrak{D}_\pm = C_0^1(0,\infty)$. Hence T may be defined on $C_0^\infty(0,\infty) \oplus C_0^\infty(0,\infty)$. By a partial integration we find $(f, D_- g) = (D_-^* f, g) = (D_+ f, g) = (f, D_+^* g)$ for all f and g in $C_0^\infty(0,\infty)$. Therefore D_+^* is a closed extension of D_- and hence $D_-^{**} \subset D_+^*$. Now we consider the operators $D_-^{**} D_+$ and $D_+^{**} D_-$ which are well defined on $C_0^\infty(0,\infty)$. We denote

$$V_{\rm eff}^\pm(r) \equiv \mu_{\rm a}^2 \phi'_{\rm el}(r)^2 + c\mu_{\rm a}\left\{-2\kappa\frac{\phi'_{\rm el}(r)}{r} \pm \phi''_{\rm el}(r)\right\} + c^2\frac{\kappa(\kappa \pm 1)}{r^2}, \tag{5.48}$$

then, on $C_0^\infty(0,\infty)$,

$$D_-^{**} D_+ = D_- D_+ = -c^2\frac{d^2}{dr^2} + V_{\rm eff}^+(r), \tag{5.49a}$$

$$D_+^{**} D_- = D_+ D_- = -c^2\frac{d^2}{dr^2} + V_{\rm eff}^-(r). \tag{5.49b}$$

According to Theorem 5.9, at least one of these operators, say $D_- D_+$ must be essentially self-adjoint on $C_0^\infty(0,\infty)$. From Lemma 5.7 of the previous section we may then conclude the essential self-adjointness of Q. Concerning the essential self-adjointness of the symmetric second order operators (5.36) many results exist in the literature on nonrelativistic quantum mechanics. We shall assume the following conditions on V:

(i) $\phi_{\rm el}$ is twice continuously differentiable on $(0,\infty)$,

(ii$_\pm$) $V_{\rm eff}^\pm(r) \geq \frac{3c^2}{4r^2} - kr^2 - k'$, for some real constants k, k',

(iii) $V_{\rm eff}^\pm(r) - \phi_{\rm el}^2(r) \geq -\frac{c^2}{4r^2} - b$, for some real constant b.

The conditions (i), and (ii$_+$) resp. (ii$_-$) imply essential self-adjointness of (5.49a) resp. (5.49b)[6]. They can be replaced, of course, by any other set of sufficient conditions. Note that in general only one of the operators (5.49a),

[6] see, e.g., [RS 75] p.200

(5.49b) is essentially self-adjoint (cf. Example 5.8). Note also that for $\mu_a \neq 0$ the conditions (i) - (iii) include rather singular potentials ϕ_{el} like

$$\phi_{el}(r) = r^{-b}, \quad \text{or} \quad \phi_{el}(r) = e^{b/r} - 1, \quad \text{any } b > 0. \tag{5.50}$$

On the other hand, if $\mu_a = 0$, the condition (iii) requires $|\phi_{el}(r)| \leq c/2r + b$, at least for $\kappa = \pm 1$. (In fact, electrons do have a small, but nonvanishing anomalous magnetic moment). Condition (iii) is needed for a perturbative treatment of the main diagonal part of T. For this we have to check, according to Theorem 5.31 (we may neglect the constants $\pm mc^2$ in a discussion of essential self-adjointness)

$$(\phi_{el}u, \phi_{el}u) \leq (D_-^* u, D_-^* u) + b(u,u), \tag{5.51}$$

which can be written as

$$\int_0^\infty dr\, \phi_{el}^2(r)\, |u(r)|^2 \leq \int_0^\infty dr \left(c^2 \left| \frac{du(r)}{dr} \right|^2 + \left(V_{\text{eff}}^+(r) + b \right) |u(r)|^2 \right). \tag{5.52}$$

Using assumption (iii) this condition can be satisfied if

$$\int_0^\infty dr \left(\frac{c^2}{4r^2} + b \right) |u(r)|^2 \leq \int_0^\infty dr \left(c^2 \left| \frac{du(r)}{dr} \right|^2 + b|u(r)|^2 \right), \tag{5.53}$$

or

$$\int_0^\infty dr\, \frac{1}{4r^2}\, |u(r)|^2 \leq \int_0^\infty dr \left| \frac{du(r)}{dr} \right|^2, \tag{5.54}$$

which is precisely Hardy's inequality[7]. This shows a remarkable fact: No matter how singular $\phi_{el}(r)$ is at $r = 0$, the Dirac operator is always well defined as long as $\mu_a \neq 0$.

The Coulomb-Dirac operator with $\mu_a \neq 0$ will be investigated further in Sect. 7.4.5.

5.4 Dirac Operators with Supersymmetry

5.4.1 Basic Definitions and Properties

As a particularly important special case of an abstract Dirac operator we define a "Dirac operator with supersymmetry". It has the form

$$H = Q + M\tau, \tag{5.55}$$

where Q is a supercharge with respect to τ, and M is a positive self-adjoint operator, which commutes with Q and τ (i.e., M is an even operator),

[7] see [RS 75], Sect. X.2, the lemma on p.169

$$M\mathfrak{D}(Q) \subset \mathfrak{D}(Q), \qquad [M,Q]=0 \quad \text{on } \mathfrak{D}(Q) \subset \mathfrak{D}(M). \tag{5.56}$$

$$\tau\mathfrak{D}(M) = \mathfrak{D}(M), \qquad [M,\tau]=0 \quad \text{on } \mathfrak{D}(M). \tag{5.57}$$

We assume for simplicity that M is invertible and that M and M^{-1} are bounded and defined on all of $\mathcal{H}$, from which we conclude

$$M : \mathfrak{D}(M) = \mathfrak{H} \to \mathfrak{H} \text{ is bijective, and } M\mathfrak{D}(Q) = \mathfrak{D}(Q). \tag{5.58}$$

In the applications, M is usually a positive constant, the rest mass of the particle.

Example 5.10. (The free Dirac operator). The operator $Q = -ic\boldsymbol{\alpha}\cdot\nabla$, where $\boldsymbol{\alpha}$ is the Dirac matrix defined in (1.9), is a supercharge with respect to β in the Hilbert space $L^2(\mathbb{R}^3)^4$. The Dirac operator $Q + mc^2\beta$ describing a free electron is a Dirac operator with supersymmetry. Further examples are given in Sect. 5.5.

Example 5.11. Let f be a bounded continuous real-valued function such that $f(\lambda) \geq k > 0$. For a given supercharge Q (with spectral family $E_Q(\lambda)$) define the bounded operator

$$f(Q^2) = \int_{-\infty}^{+\infty} f(\lambda^2)\, dE_Q(\lambda). \tag{5.59}$$

Then $Q + f(Q^2)\tau$ is a Dirac operator with supersymmetry.

Theorem 5.12. Let $H = Q + M\tau$ be a Dirac operator with supersymmetry. Then H is self-adjoint on $\mathfrak{D}(H) = \mathfrak{D}(Q)$. The operator H^2 is self-adjoint on $\mathfrak{D}(H^2) = \mathfrak{D}(Q^2)$, and

$$H^2 = Q^2 + M^2 \quad \text{on } \mathfrak{D}(Q^2). \tag{5.60}$$

Moreover, H^2 is strictly positive,

$$(\psi, H^2\psi) \geq \frac{1}{\|M^{-1}\|^2} \quad \text{for all } \psi \text{ with } \|\psi\| = 1. \tag{5.61}$$

Proof. The self-adjointness of H follows immediately from the boundedness of M. Since H is self-adjoint, the operator H^2 is densely defined, self-adjoint, and positive. For all $\psi \in \mathfrak{D}(Q^2)$ we may write $H^2\psi = (Q^2 + M\tau Q + Q\tau M + M^2)\psi$. On the domain $\mathfrak{D}(Q^2) \subset \mathfrak{D}(Q)$ we find $M\tau Q + Q\tau M = 0$, using (5.6), (5.56), and (5.57). $\mathfrak{D}(H^2)$ equals $\mathfrak{D}(Q^2)$, since M^2 is bounded. This proves (5.60). The strict positivity of H follows from $(\psi, H^2\psi) \geq (\psi, M^2\psi) = \|M\psi\|^2$, because $\|\psi\| = \|M^{-1}M\psi\| \leq \|M^{-1}\| \cdot \|M\psi\|$ implies $\|M\psi\| \geq \|\psi\|/\|M^{-1}\|$. □

The following commutation formulas follow immediately from the definitions.

$$M\mathfrak{D}(Q^2) = \mathfrak{D}(Q^2), \qquad MQ^2 = Q^2M \quad \text{on } \mathfrak{D}(Q^2), \tag{5.62}$$

$$\tau\mathfrak{D}(Q^2) = \mathfrak{D}(Q^2), \qquad \tau Q^2 = Q^2\tau \quad \text{on } \mathfrak{D}(Q^2), \tag{5.63}$$

$$M^2 Q = Q M^2 \quad \text{on } \mathfrak{D}(Q). \tag{5.64}$$

Therefore Q, as well as M, commute with $H^2 = Q^2 + M^2$, and we have

$$f(H^2)\, Q = Q\, f(H^2) \quad \text{on } \mathfrak{D}(Q), \qquad f(H^2)\, M = M\, f(H^2), \tag{5.65}$$

for any bounded, continuous function f.

5.4.2 Standard Representation

Let $H = Q + M\tau$ be a Dirac operator with supersymmetry. In the standard representation it has the form

$$H = \begin{pmatrix} M_+ & D^* \\ D & -M_- \end{pmatrix}, \tag{5.66}$$

The matrix elements of H do not commute with each other. However, from Eq. (5.56) we obtain

$$D^* M_- = M_+ D^* \quad \text{on } \mathfrak{D}(D^*), \qquad D M_+ = M_- D \quad \text{on } \mathfrak{D}(D), \tag{5.67}$$

and hence H^2 can be written as

$$H^2 = \begin{pmatrix} D^*D + M_+^2 & 0 \\ 0 & DD^* + M_-^2 \end{pmatrix}. \tag{5.68}$$

Denoting

$$H_+^2 \equiv D^*D + M_+^2, \qquad H_-^2 \equiv DD^* + M_-^2, \tag{5.69}$$

we obtain from (5.65) by Nelson's trick the formulas

$$f(H_+^2)\, D^* = D^*\, f(H_-^2) \quad \text{on } \mathfrak{D}(D^*), \tag{5.70}$$

$$f(H_-^2)\, D = D\, f(H_+^2) \quad \text{on } \mathfrak{D}(D). \tag{5.71}$$

for any bounded, continuous function f.

5.5 Examples of Supersymmetric Dirac Operators

5.5.1 Dirac Operator with a Scalar Field

Let $V = \beta\phi_{\mathrm{sc}}$ be a (Lorentz-) scalar potential (see Sect. 4.1.2). Using the "supersymmetric" representation of the Dirac matrices (see Appendix A to Chapter 1) the Dirac operator $H = H_0 + V$ has the form (5.66), with

$$M_+ = M_- = 0, \qquad D = -\mathrm{i}c\boldsymbol{\sigma}\cdot\nabla + \mathrm{i}(mc^2 + \phi_{\mathrm{sc}}), \tag{5.72}$$

$$\left.\begin{matrix} D^*D \\ DD^* \end{matrix}\right\} = -c^2\Delta \pm c\boldsymbol{\sigma}\cdot(\nabla\phi_{\mathrm{sc}}) + (mc^2 + \phi_{\mathrm{sc}})^2. \tag{5.73}$$

The unitary involution τ is now given by

$$\tau = \mathrm{i}\beta\gamma_5, \quad \text{where } \gamma_5 = -\mathrm{i}\alpha_1\alpha_2\alpha_3, \tag{5.74}$$

and H is a supercharge with respect to τ. This is just a special case of the following observation. If $\mathfrak{H}$ is a Hilbert space with a unitary involution, such that $\mathfrak{H}_+ = \mathfrak{H}_-$, and if H is an abstract Dirac operator of the form

$$H = \begin{pmatrix} V & D \\ D & -V \end{pmatrix}, \tag{5.75}$$

then H is unitarily equivalent to the supercharge

$$THT^{-1} = \begin{pmatrix} 0 & (D')^* \\ D' & 0 \end{pmatrix}, \quad T = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \mathrm{i} \\ \mathrm{i} & 1 \end{pmatrix}, \quad D' = D + \mathrm{i}V. \tag{5.76}$$

5.5.2 Supersymmetry in Electromagnetic Fields

Electron in a magnetic field: The Dirac operator for a spin-1/2 particle in a magnetic field reads

$$H = \begin{pmatrix} mc^2 & c\boldsymbol{\sigma}\cdot(-\mathrm{i}\nabla - \frac{\mathrm{e}}{\mathrm{c}}\boldsymbol{A}) \\ c\boldsymbol{\sigma}\cdot(-\mathrm{i}\nabla - \frac{\mathrm{e}}{\mathrm{c}}\boldsymbol{A}) & -mc^2 \end{pmatrix}. \tag{5.77}$$

We see that this is a Dirac operator with supersymmetry, because it has the form (5.66) if we set

$$M_+ = M_- = mc^2, \quad D = D^* = c\boldsymbol{\sigma}\cdot(-\mathrm{i}\nabla - \tfrac{\mathrm{e}}{\mathrm{c}}\boldsymbol{A}). \tag{5.78}$$

From the properties of the Pauli matrices $\boldsymbol{\sigma}$ we obtain

$$D^*D = DD^* = c^2(-\mathrm{i}\nabla - \tfrac{\mathrm{e}}{\mathrm{c}}\boldsymbol{A})^2 - ec\boldsymbol{\sigma}\cdot\boldsymbol{B} \equiv 2mc^2 H_{\mathrm{P}}, \tag{5.79}$$

where we have defined the Pauli Hamiltonian H_{P} which turns out to be the nonrelativistic limit of the Dirac operator (5.77) (cf. Chapter 6).

Particle with anomalous electric moment in a magnetic field: The influence of a magnetic field on the anomalous electric moment δ_{a} of a particle is described by a supersymmetric Dirac operator with

$$M_+ = M_- = mc^2, \qquad D = c\boldsymbol{\sigma}\cdot(-\mathrm{i}\nabla - \tfrac{\mathrm{e}}{\mathrm{c}}\boldsymbol{A}) - \mathrm{i}\delta_{\mathrm{a}}\,\boldsymbol{\sigma}\cdot\boldsymbol{B}. \tag{5.80}$$

Note that $D \neq D^*$ in this case. A little calculation shows

$$\left.\begin{matrix} D^*D \\ DD^* \end{matrix}\right\} = 2mc^2 H_{\mathrm{P}} \mp c\delta_{\mathrm{a}}\left\{\mathrm{i}\boldsymbol{\sigma}\cdot\mathrm{rot}\,\boldsymbol{B} + 2\boldsymbol{\sigma}\cdot\boldsymbol{B}\wedge(-\mathrm{i}\nabla - \tfrac{\mathrm{e}}{\mathrm{c}}\boldsymbol{A})\right\} + \delta_{\mathrm{a}}^2 B^2, \tag{5.81}$$

where H_{P} is defined as in (5.79). We have used that $\boldsymbol{B} = \mathrm{rot}\,\boldsymbol{A}$ and hence $\mathrm{div}\boldsymbol{B} = 0$, $\boldsymbol{B}\cdot\boldsymbol{A} = 0$.

Neutron in an electric field: The neutron is a neutral spin-1/2 particle with anomalous magnetic moment μ_a. In an electric field the Dirac operator is a Dirac operator with supersymmetry, where

$$M_+ = M_- = mc^2, \quad D = -\mathrm{i}c\boldsymbol{\sigma}\cdot\nabla - \mathrm{i}\mu_a\,\boldsymbol{\sigma}\cdot\boldsymbol{E}. \tag{5.82}$$

A similar calculation as for (5.81) shows

$$\left.\begin{matrix} D^*D \\ DD^* \end{matrix}\right\} = -c^2\Delta \mp c\mu_a\{\operatorname{div}\boldsymbol{E} + \mathrm{i}\boldsymbol{\sigma}\cdot\operatorname{rot}\boldsymbol{E} + 2\boldsymbol{\sigma}\cdot\boldsymbol{E}\wedge(-\mathrm{i}\nabla)\} + \mu_a^2E^2. \tag{5.83}$$

In case of electro*static* fields we have $\boldsymbol{E} = -\nabla\phi_{\mathrm{el}}$, and hence the term with $\operatorname{rot}\boldsymbol{E}$ vanishes.

Neutron in a magnetic field: If there is only a magnetic field then the Dirac operator for a neutron has the form (5.75). Applying the unitary transformation T defined in (5.76) the Dirac operator becomes a supercharge,

$$H = \begin{pmatrix} 0 & -\mathrm{i}c\boldsymbol{\sigma}\cdot\nabla - \mathrm{i}(mc^2 - \mu_a\boldsymbol{\sigma}\cdot\boldsymbol{B}) \\ -\mathrm{i}c\boldsymbol{\sigma}\cdot\nabla + \mathrm{i}(mc^2 - \mu_a\boldsymbol{\sigma}\cdot\boldsymbol{B}) & 0 \end{pmatrix}. \tag{5.84}$$

5.5.3 The Klein Gordon Equation

For a spin-0 particle with mass $m > 0$ in an external magnetic field described by the vector potential $\boldsymbol{A}(\boldsymbol{x})$ the Klein-Gordon equation reads

$$\left\{\frac{\partial^2}{\partial t^2} + \big(-\mathrm{i}\nabla - \boldsymbol{A}(\boldsymbol{x})\big)^2 + m^2\right\}u(\boldsymbol{x},t) = 0. \tag{5.85}$$

Writing this as a first order system we obtain

$$\mathrm{i}\frac{d}{dt}\psi(t) = H\psi(t), \qquad \psi(t) = \begin{pmatrix} u(\cdot,t) \\ \mathrm{i}\partial u(\cdot;t)/\partial t \end{pmatrix}, \tag{5.86}$$

$$H = \begin{pmatrix} 0 & 1 \\ T & 0 \end{pmatrix}, \qquad T = (-\mathrm{i}\nabla - \boldsymbol{A})^2 + m^2. \tag{5.87}$$

We shall define Hilbert spaces $\mathfrak{H}_+$, $\mathfrak{H}_-$ such that H becomes an abstract Dirac operator, even a supercharge, in a natural way.

The operator T is essentially a Schrödinger operator for a nonrelativistic particle in a magnetic field. Let (each component of) $\boldsymbol{A}$ be locally square integrable. Then $-\mathrm{i}\nabla - \boldsymbol{A}$ is well defined on $C_0^\infty(\mathbb{R}^3)$, symmetric and hence closeable. Denoting the closure of $-\mathrm{i}\nabla - \boldsymbol{A}$ by D we may write $T = D^*D + m^2$, and T is self-adjoint and strictly positive by Theorem 2.3. We define

$$\mathfrak{H}_+ \equiv \mathfrak{D}(T^{1/2}), \qquad \mathfrak{H}_- = L^2(\mathbb{R}^3). \tag{5.88}$$

The vector space $\mathfrak{H}_+$ is a Hilbert space with the scalar product

$$(u,v)_+ \equiv (T^{1/2}u, T^{1/2}v), \quad \text{where } (\cdot,\cdot) \equiv L^2\text{-scalar product.} \tag{5.89}$$

Note that ψ has finite norm in $\mathfrak{H}$ iff u has finite field energy,

$$\|\psi\|^2 = \int d^3x \left\{|(-\mathrm{i}\nabla - \boldsymbol{A})u|^2 + m^2|u|^2 + |\partial u/\partial t|^2\right\}. \tag{5.90}$$

In (5.87) the operator $\mathbf{1}$ denotes the identity, restricted to $\mathfrak{D}(T^{1/2})$,

$$1 : \mathfrak{D}(T^{1/2}) \subset \mathfrak{H}_- \to \mathfrak{H}_+. \tag{5.91}$$

It is just the adjoint of the operator

$$T : \mathfrak{D}(T) \subset \mathfrak{H}_+ \to \mathfrak{H}_-, \tag{5.92}$$

which can be seen as follows: The adjoint of a densely defined linear operator T from $\mathfrak{H}_+$ to $\mathfrak{H}_-$ is given on the domain

$$\mathfrak{D}(T^*) \equiv \{\, f \in \mathfrak{H}_- \mid \exists g \in \mathfrak{H}_+ : (f, Th) = (g, h)_+ \text{ for all } h \in \mathfrak{D}(T)\,\} \tag{5.93}$$

by $T^*f = g$. But from the self-adjointness of T we conclude $(f,h)_+ = (T^{1/2}f, T^{1/2}h) = (f, Th)$ for all $h \in \mathfrak{D}(T)$ and $f \in \mathfrak{D}(T^{1/2})$, and hence $T^*f = f$. This proves that H defined as in (5.87), (5.91), (5.92) is a supercharge.

5.6 Normal Forms of Supersymmetric Dirac Operators

5.6.1 The Abstract Foldy-Wouthuysen Transformation

The supersymmetric Dirac operator can be diagonalized by a suitable unitary transformation U_{FW}. For the free Dirac equation U_{FW} coincides with the Foldy-Wouthuysen transformation introduced in Sect. 1.4.

Theorem 5.13. Let $H = Q + M\tau$ be a supersymmetric Dirac operator. Define

$$U_{\mathrm{FW}} = a_+ + \tau\,(\operatorname{sgn} Q)a_-, \quad a_\pm = \frac{1}{\sqrt{2}}\sqrt{1 \pm M|H|^{-1}}, \tag{5.94}$$

Then U_{FW} is unitary and

$$U_{\mathrm{FW}} H U_{\mathrm{FW}}^* = \tau|H| = \tau\sqrt{Q^2 + M^2} \equiv H_{\mathrm{FW}}. \tag{5.95}$$

H_{FW} is an even operator and satisfies

$$H_{\mathrm{FW}}^2 = H^2. \tag{5.96}$$

In the standard representation U_{FW} diagonalizes the matrix operator H

$$U_{\mathrm{FW}} \begin{pmatrix} M_+ & D^* \\ D & -M_- \end{pmatrix} U_{\mathrm{FW}}^* = \begin{pmatrix} \sqrt{D^*D + M_+^2} & 0 \\ 0 & -\sqrt{DD^* + M_-^2} \end{pmatrix}. \tag{5.97}$$

Proof. On $(\operatorname{Ker} Q)^{\perp}$ the operator $M|H|^{-1}$ is self-adjoint and bounded with norm < 1. Hence $a_{\pm}$ can be defined as a norm-convergent series

$$\frac{1}{\sqrt{2}}\sqrt{1 \pm M|H|^{-1}} \equiv \frac{1}{\sqrt{2}}\left\{1 \pm M|H|^{-1} - \tfrac{3}{8}(M|H|^{-1})^2 \pm \ldots\right\}, \tag{5.98}$$

On $\operatorname{Ker} Q$ we simply have $a_+ = 1$, $a_- = 0$ so that $U_{\mathrm{FW}} = 1$ on $\operatorname{Ker} Q$. It is easy to verify the following formulas for the bounded operators $a_{\pm}$

$$a_+^2 + a_-^2 = 1, \quad a_+^2 - a_-^2 = M|H|^{-1}, \quad 2a_+a_- = |Q|\,|H|^{-1}. \tag{5.99}$$

Now the inverse transformation $U_{\mathrm{FW}}^* = U_{\mathrm{FW}}^{-1}$ is easily determined,

$$U_{\mathrm{FW}}^* = a_+ - \tau\,(\operatorname{sgn} Q)a_-. \tag{5.100}$$

Furthermore we note that $|H| = (Q^2 + M^2)^{1/2}$ commutes with τ and Q, and the following commutation relations hold on $\mathfrak{D}(H) = \mathfrak{D}(Q)$

$$[H, a_{\pm}] = [Q, a_{\pm}] = 0, \quad H\tau\,(\operatorname{sgn} Q) = -\tau\,(\operatorname{sgn} Q)\,H. \tag{5.101}$$

Now we can verify Eq. (5.95) in the following way

$$\begin{aligned} U_{\mathrm{FW}}HU_{\mathrm{FW}}^* &= (a_+ + \tau\,(\operatorname{sgn} Q)\,a_-)H(a_+ - \tau\,(\operatorname{sgn} Q)\,a_-) \\ &= (a_+^2 + 2\tau\,(\operatorname{sgn} Q)\,a_+a_- - a_-^2)H \\ &= (M|H|^{-1} + \tau\,(\operatorname{sgn} Q)\,|Q|\,|H|^{-1})H \\ &= (M + \tau Q)|H|^{-1}H = \tau(M\tau + Q)|H|^{-1}H \\ &= \tau H^2|H|^{-1} = \tau|H|. \end{aligned} \tag{5.102}$$

The matrix form of $\tau|H|$ immediately follows from (5.10), (5.68) and $|H| = \sqrt{H^2}$. □

Remark. Since the operator Q commutes with H^2 (cf. Sect. 5.4.1), we have in particular $[\operatorname{sgn} Q, H^2] = 0$ on $(\operatorname{Ker} Q)^{\perp}$. From this we conclude

$$DD^* + M_-^2 = S(D^*D + M_+^2)S^* \tag{5.103}$$

where S is the partial isometry defined in Eq. (5.21). In the special case where M is simply a constant we reformulate this result using the spectral mapping theorem.

Corollary 5.14. Let $H = Q + m\tau$ with some real constant $m > 0$. Then the spectrum of H is symmetric with respect to 0 (except possibly at $\pm m$), has a gap from $-m$ to $+m$, and is determined by the spectrum of D^*D (except at $-m$). The point $+m$ (or $-m$) is an eigenvalue of H, iff 0 is an eigenvalue of D (or D^*).

Example. We show that the Dirac operator with an increasing scalar potential has a purely discrete spectrum. If we assume that $\phi_{\mathrm{sc}}(\boldsymbol{x})$ tends to infinity,

as $x \to \infty$, such that $\phi_{\rm sc}$ and $\nabla\phi_{\rm sc}$ are infinitesimally bounded with respect to $-c^2\Delta + \phi_{\rm sc}^2$, then it follows from well known properties of Schrödinger operators that D^*D and DD^* in Eq. (5.73) have a purely discrete spectrum. By Corollary 5.14, the corresponding Dirac operator also has a purely discrete spectrum.

5.6.2 The Abstract Cini-Touschek Transformation

On $\operatorname{Ker} Q$ we have $a_+ = 1$, $a_- = 0$, hence $U_{\rm FW}$ is just the identity on $\operatorname{Ker} Q$. For $M = 0$, i.e., if H is a supercharge we can still define an abstract Foldy-Wouthuysen transformation. Setting $a_\pm = 1/\sqrt{2}$ on $(\operatorname{Ker} Q)^\perp$ we obtain

$$U_{\rm FW}(M{=}0) = \frac{1}{\sqrt{2}}(1 + \tau \operatorname{sgn} Q) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & S^* \\ -S & 1 \end{pmatrix}. \tag{5.104}$$

It is easy to see that

$$U_{\rm FW}(M{=}0)^*\, H_{\rm FW}\, U_{\rm FW}(M{=}0) = |H| \operatorname{sgn} Q. \tag{5.105}$$

Thus the unitary operator

$$U_{\rm CT} \equiv U_{\rm FW}(M=0)^* U_{\rm FW}, \quad \text{on } (\operatorname{Ker} Q)^\perp \tag{5.106}$$

transforms $H = Q + M\tau$ to an odd operator. For the free Dirac equation this transformation is known as the Cini-Touschek transformation. We state this result as a theorem.

Theorem 5.15. Let $H = Q + M\tau$ be a Dirac operator with supersymmetry. The operator $U_{\rm CT}$, defined as in (5.106) is unitary on the Hilbert space $(\operatorname{Ker} Q)^\perp$, and

$$U_{\rm CT} H U_{\rm CT}^* = |H| \operatorname{sgn} Q \equiv H_{\rm CT}. \tag{5.107}$$

In the Hilbert space $(\operatorname{Ker} Q)^\perp$ the operator $H_{\rm CT}$ is a supercharge with respect to τ and satisfies

$$(H_{\rm CT})^2 = H^2. \tag{5.108}$$

Hence H^2 is a Hamiltonian with supersymmetry. In the standard representation $U_{\rm CT}$ transforms H into off-diagonal form

$$U_{\rm CT} \begin{pmatrix} M_+ & D^* \\ D & -M_- \end{pmatrix} U_{\rm CT}^* = \begin{pmatrix} 0 & S^*\sqrt{DD^* + M_-^2} \\ S\sqrt{D^*D + M_+^2} & 0 \end{pmatrix}, \tag{5.109}$$

where $S = D|D^*D|^{-1/2}$, as defined in (5.21).

5.6.3 Connection with the Cayley Transform

For any self-adjoint operator A define the Cayley transform C as the unitary operator

$$C \equiv (\mathrm{i} - A)(\mathrm{i} + A)^{-1} = e^{2\mathrm{i} \arctan A}. \tag{5.110}$$

Conversely, if C is the Cayley transform of a self-adjoint operator A, then A is given by

$$\mathfrak{D}(A) = \mathrm{Ran}\,(1 + C), \qquad A = \mathrm{i}(1 - C)(1 + C)^{-1}. \tag{5.111}$$

Theorem 5.16. Let U_{FW} and U_{CT} be abstract Foldy-Wouthuysen and Cini-Touschek transformations, respectively. Then U_{FW}^4 is the Cayley transform of $(\mathrm{i}Q\tau)M^{-1}$ and on $(\mathrm{Ker}\,Q)^\perp$ the operator U_{CT}^4 is the Cayley transform of $M(\mathrm{i}Q\tau)^{-1}$. We have therefore the representations

$$U_{\mathrm{FW}} = \exp\{\tfrac{\mathrm{i}}{2} \arctan(\mathrm{i}Q\tau/M)\}, \tag{5.112}$$

$$U_{\mathrm{CT}} = \exp\{\tfrac{\mathrm{i}}{2} \arctan(M/\mathrm{i}Q\tau)\}, \quad \text{on } (\mathrm{Ker}\,Q)^\perp. \tag{5.113}$$

Moreover,

$$U_{\mathrm{FW}}^4 = -U_{\mathrm{CT}}^4, \quad \text{on } (\mathrm{Ker}\,Q)^\perp. \tag{5.114}$$

Proof. From the definitions in Sect. 5.4.1 we conclude that $\mathrm{i}Q\tau M^{-1}$ is a self-adjoint operator. Define

$$a_\pm(\lambda, m) = \frac{1}{\sqrt{2}} \sqrt{1 \pm \frac{m}{\sqrt{\lambda^2 + m^2}}} \tag{5.115}$$

A little calculation shows that for $\lambda \in \mathbb{R}$ and $m \neq 0$

$$\left\{ a_+(\lambda, m) + \mathrm{i}\frac{\lambda}{|\lambda|}\, a_-(\lambda, m) \right\}^4 = \frac{\mathrm{i} - \lambda m^{-1}}{\mathrm{i} + \lambda m^{-1}}. \tag{5.116}$$

This result also holds if we replace λ by the self-adjoint operator $Q' = \mathrm{i}Q\tau$, and m by the operator M, which commutes with Q'. Note that $\mathrm{i}Q'|Q'|^{-1} = -Q\tau|Q|^{-1} = \tau\,\mathrm{sgn}\,Q$ and $Q'^2 + M^2 = Q^2 + M^2 = H^2$. Hence the expression $\{\ldots\}$ in Eq. (5.116) simply becomes the operator U_{FW}. We obtain

$$U_{\mathrm{FW}}^4 = \frac{\mathrm{i} - Q'M^{-1}}{\mathrm{i} + Q'M^{-1}}. \tag{5.117}$$

With (5.110) this implies the result (5.112). The operator $Q'M^{-1}$ is injective on $(\mathrm{Ker}\,Q)^\perp$ and has dense range in this Hilbert space. We can therefore define the inverse MQ'^{-1} as a self-adjoint operator in $(\mathrm{Ker}\,Q)^\perp$. Hence we can also write

$$U_{\mathrm{FW}}^4 = -\frac{\mathrm{i} - MQ'^{-1}}{\mathrm{i} + MQ'^{-1}} \quad \text{on } (\mathrm{Ker}\, Q)^\perp. \tag{5.118}$$

On the other hand, since $U_{\mathrm{FW}}(M{=}0)^4 = -1$ and since $U_{\mathrm{FW}}(M{=}0)^*$ commutes with U_{FW} we have $U_{\mathrm{CT}}^4 = U_{\mathrm{FW}}(M{=}0)^{*4}\, U_{\mathrm{FW}}^4 = -U_{\mathrm{FW}}^4$. □

Example 5.17. For the free Dirac equation we have $\mathrm{i}Q\tau M^{-1} = -\frac{\mathrm{i}}{mc}\beta\boldsymbol{\alpha}\cdot\boldsymbol{p}$.

5.7 The Index of the Dirac Operator

5.7.1 The Fredholm Index

From Corollary 5.14 we know, that the supersymmetric Dirac operator

$$H = Q + m\tau = U_{\mathrm{FW}}^* \begin{pmatrix} \sqrt{D^*D + m^2} & 0 \\ 0 & -\sqrt{DD^* + m^2} \end{pmatrix} U_{\mathrm{FW}} \tag{5.119}$$

has a symmetric spectrum except at $\pm m$ because the spectra of the operators D^*D and DD^* coincide, except at 0. The asymmetry of the spectrum of H at $\pm m$ is studied by investigating the kernel of the operator Q (or equivalently the kernel of Q^2),

$$\mathrm{Ker}\, Q = \{\psi \in \mathfrak{H} \mid Q\psi = 0\} = \mathrm{Ker}\, Q^2. \tag{5.120}$$

An important special case occurs, if Q is a "*Fredholm operator*". A self-adjoint operator Q is a Fredholm operator if and only if $\mathrm{Ran}\, Q$ is closed, and $\dim \mathrm{Ker}\, Q < \infty$ (i.e., if the eigenvalue 0 of Q has finite multiplicity)[8].

Remark 1. The requirement that the range of Q has to be closed is included for the following reason. Denote by $\breve{Q}$ the restriction of Q to $(\mathrm{Ker}\, Q)^\perp \cap \mathfrak{D}(Q)$. Clearly $\mathrm{Ran}\, Q = \mathrm{Ran}\, \breve{Q}$. Moreover, since $\breve{Q}$ is injective and closed, we can define $\breve{Q}^{-1}$ on $\mathfrak{D}(\breve{Q}^{-1}) = \mathrm{Ran}\, Q$. The operator $\breve{Q}^{-1}$ is closed and has a closed domain, therefore it is bounded by the closed graph theorem. Hence we could define a self-adjoint Fredholm operator Q as an operator for which $\breve{Q}$ has a bounded inverse.

Remark 2. The self-adjoint operator Q is Fredholm if and only if Q^2 is. For the positive operator Q^2 the condition $\breve{Q}^2$ invertible is equivalent to $\inf \sigma_{\mathrm{ess}}(Q^2) > 0$.

For a supercharge Q the "*Fredholm index*" is defined as

$$\mathrm{ind}\, Q \equiv \dim \mathrm{Ker}\, D - \dim \mathrm{Ker}\, D^* = \dim \mathrm{Ker}\, D^*D - \dim \mathrm{Ker}\, DD^*, \tag{5.121}$$

[8] If Q is a supercharge, then our definition is equivalent to the usual definition of the Fredholm property for closed operators D [Ka 80], Sect. IV.5.

whenever this number exists. The integer $\operatorname{ind} Q$ is certainly well defined for Fredholm supercharges. Together with

$$\dim \operatorname{Ker} Q = \dim \operatorname{Ker} D + \dim \operatorname{Ker} D^* \tag{5.122}$$

the Fredholm index gives complete information about the dimensions of the kernels of D and D^*. For the Dirac operator (5.119), $\operatorname{ind} Q$ gives the difference between the multiplicities of the eigenvalues $+m$ and $-m$.

5.7.2 Regularized Indices

Fredholm operators are of limited use as supercharges in relativistic quantum mechanics, because the Schrödinger operators Q^2 usually have continuous spectrum $[0, \infty)$, hence Q cannot be a Fredholm operator (see the remark in Sect. 5.8.1). Here we describe some possibilities of defining an index for a supercharge Q even if Q is not Fredholm.

For a bounded operator A in a Hilbert space $\mathfrak{H}$, we define the trace

$$\operatorname{tr} A = \sum_{i=0}^{\infty} (\phi_i, A\phi_i), \quad \text{with } \{\phi_i\} \text{ an orthonormal base in } \mathfrak{H}, \tag{5.123}$$

whenever this sum is absolutely convergent. For a positive operator, the value of the trace is independent of the chosen orthonormal system. Hence we can define the "*trace norm*" of A by $\|A\|_1 \equiv \operatorname{tr} |A|$. The operators with finite trace norm are called "*trace class operators*". The set of all trace class operators with the trace norm is a Banach space, denoted by $\mathcal{B}_1(\mathfrak{H})$. For $A \in \mathcal{B}_1(\mathfrak{H})$ the definition (5.123) of $\operatorname{tr} A$ is again independent of the chosen orthonormal basis. Every trace class operator is compact. See [RS 72], Sect. VI.6 for further details.

Example 5.18. Let A be an integral operator in $L^2(\mathbb{R}^n)$,

$$A\psi = \int k(x,y)\, \psi(y)\, d^n y, \quad \text{all } \psi \in L^2(\mathbb{R}^n). \tag{5.124}$$

Assume that A is trace-class and that the kernel k is continuous in both variables x, y. Then

$$\operatorname{tr} A = \lim_{r \to \infty} \int_{|x| \le r} k(x,x)\, d^n x. \tag{5.125}$$

Note, however, that an integral operator with a continuous kernel, for which the right hand side of Eq. (5.125) exists does not necessarily belong to the trace class.

Now, let $\mathfrak{H}$ be a Hilbert space with a unitary involution τ and assume that $\mathfrak{H}_+ = \mathfrak{H}_- \equiv \mathfrak{H}$. Let A be a matrix operator in $\mathfrak{H} \oplus \mathfrak{H}$,

$$A = \begin{pmatrix} A_+ & A_{-+} \\ A_{+-} & A_- \end{pmatrix}. \tag{5.126}$$

We assume that $A_+ + A_-$ is trace class in $\mathfrak{H}$ and denote the "supertrace" by

$$\operatorname{str} A = \operatorname{tr}(A_+ + A_-). \tag{5.127}$$

If A is also trace class in $\mathfrak{H} \oplus \mathfrak{H}$, then $\operatorname{str} A = \operatorname{tr} A$, but A need not be trace class for (5.127) to exist. Occasionally, we denote the diagonal sum (the "matrix trace") of A by

$$\operatorname{mtr} A = A_+ + A_-. \tag{5.128}$$

An analogous definition can of course be used for higher dimensional matrices of operators. If A and B are bounded operators such that AB and BA belong to the trace class, then the relation $\operatorname{tr} AB = \operatorname{tr} BA$ holds[9], while usually $\operatorname{mtr} AB \neq \operatorname{mtr} BA$ (even for diagonal matrix operators), because the matrix elements are operators which need not commute.

Let Q be a supercharge in $\mathfrak{H} \oplus \mathfrak{H}$, defined with the help of a closed operator D as in Eq. (5.18). If $\operatorname{mtr} \tau (Q^2 - z)^{-1}$ is trace class for some $z \in \mathbb{C} \setminus [0, \infty)$, then we can define the "*resolvent regularized index*"

$$\operatorname{ind}_z Q = -z \operatorname{str} \tau (Q^2 - z)^{-1} = -z^{1/2} \operatorname{str} \tau (Q - z^{1/2})^{-1}. \tag{5.129}$$

Similarly, if $\operatorname{mtr} \tau e^{-Q^2 t}$ is trace class for some $t > 0$, we define the "*heat kernel regularization*"

$$\operatorname{ind}_t Q = \operatorname{str} \tau e^{-Q^2 t}. \tag{5.130}$$

Theorem 5.19. If $\exp(-Q^2 t)$ is trace class for some $t > 0$, then Q is Fredholm and

$$\operatorname{ind}_t Q = \operatorname{ind} Q \quad \text{(independent of } t\text{)}. \tag{5.131}$$

If $(Q^2 - z)^{-1}$ is trace class for some $z \in \mathbb{C} \setminus [0, \infty)$, then Q is Fredholm and

$$\operatorname{ind}_z Q = \operatorname{ind} Q \quad \text{(independent of } z\text{)}. \tag{5.132}$$

Proof. Since $\exp(-Q^2 t)$ is trace class, we obtain

$$\operatorname{ind}_t Q = \operatorname{tr} e^{-tD^* D} - \operatorname{tr} e^{-tDD^*}. \tag{5.133}$$

The self-adjoint trace class operators $\exp(-tD^* D)$ and $\exp(-tDD^*)$ have a purely discrete spectrum in $[0, 1]$. Hence (5.133) evaluates to

$$\operatorname{ind}_t Q = \sum_i (m_i \lambda_i - n_i \mu_i), \tag{5.134}$$

[9] see [Ka 80], Sect. X.1.4, or [Si 79].

where λ_i (resp. μ_i) are eigenvalues of multiplicity m_i (resp. n_i) of $\exp(-tD^*D)$ (resp. $\exp(-tDD^*)$). Since for trace class operators the eigenvalue 1 must be isolated and of finite multiplicity, we conclude that the same is true for the eigenvalue 0 of D^*D and DD^*. Hence 0 is not in the essential spectrum of these operators, which proves the Fredholm property for D^*D, DD^* and Q^2. By the spectral supersymmetry stated in Corollary 5.6, the contributions of all other eigenvalues cancel in Eq. (5.134). This proves the first statement. The proof of the second statement is similar. □

5.8 Spectral Shift and Witten Index

5.8.1 Krein's Spectral Shift Function

Let S and T be self-adjoint, such that $S - T$ is trace class. One sometimes wants to know if also $f(S) - f(T)$ is trace class, where f belongs to a suitable class of functions which we want to determine. Assuming that f is the inverse Fourier transform of an integrable function, we obtain by the spectral theorem

$$f(S) - f(T) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(p) \left(e^{\mathrm{i}pS} - e^{\mathrm{i}pT} \right) dp. \tag{5.135}$$

Using

$$e^{\mathrm{i}pS} - e^{\mathrm{i}qT} = \int_0^1 d\alpha \, \mathrm{i}p \, e^{\mathrm{i}\alpha pS} \, (S - T) \, e^{\mathrm{i}(1-\alpha)pT} \tag{5.136}$$

we obtain

$$\| e^{\mathrm{i}pS} - e^{\mathrm{i}qT} \|_1 \leq |p| \, \| S - T \|_1, \tag{5.137}$$

and hence the trace norm of $f(S) - f(T)$ can be estimated by

$$\| f(S) - f(T) \|_1 \leq \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} |p \, \hat{f}(p)| \, dp \, \| S - T \|_1. \tag{5.138}$$

Hence, a natural class of functions is

$$\mathcal{G} = \left\{ f : \mathbb{R} \to \mathbb{R} \;\middle|\; \int_{-\infty}^{\infty} |\hat{f}(p)| \, (1 + |p|) \, dp < \infty \right\}. \tag{5.139}$$

Clearly, $\mathcal{C}_0^\infty(\mathbb{R}) \subset \mathcal{G}$. Any $f \in \mathcal{G}$ is continuously differentiable and by the Riemann-Lebesgue lemma f and f' vanish as $|x| \to \infty$.

A useful technical tool for the calculation of traces (and hence of regularized indices) is Krein's spectral shift function ξ.

Theorem 5.20. Let T_1 and T_2 be bounded and self-adjoint and assume $T_1 - T_2$ to be trace class. Then there is an integrable function $\xi : \mathbb{R} \to \mathbb{R}$ such that

a) $\operatorname{tr}(T_1 - T_2) = \int_{-\infty}^{\infty} \xi(\lambda)\, d\lambda,$

b) $\operatorname{tr}\big(f(T_1) - f(T_2)\big) = \int_{-\infty}^{\infty} \xi(\lambda)\, f'(\lambda)\, d\lambda$, for all $f \in \mathcal{G}$.

c) $\xi(\lambda) = 0$, for λ to the left of $\sigma(T_1) \cup \sigma(T_2)$.

ξ is determined uniquely a.e. by b) and c).

Proof. We give the proof for the case that T_1 and T_2 have finite rank r. The general case is treated in [BW 83], Chapter 19. Let T be self-adjoint with finite rank r, i.e.,

$$T = \sum_{i=0}^{r} \lambda_i\, \phi_i\, (\phi_i, \cdot). \tag{5.140}$$

For any continuous function f we can write

$$\begin{aligned} \operatorname{tr} f(T) &= \sum_{i=0}^{r} f(\lambda_i) = \int_{-\infty}^{+\infty} \sum_{i=0}^{r} \delta(\lambda - \lambda_i)\, f(\lambda)\, d\lambda \\ &\equiv \int_{-\infty}^{+\infty} n'(\lambda)\, f(\lambda)\, d\lambda, \end{aligned} \tag{5.141}$$

where n' is the distributional derivative of the step function

$$n(\lambda) = \lim_{\epsilon \to 0} \int_{-\infty}^{\lambda+\epsilon} \sum_{i=0}^{r} \delta(\mu - \lambda_i)\, d\mu. \tag{5.142}$$

$n(\lambda)$ counts the number of eigenvalues of T which are less than or equal to λ. Clearly, n is continuous from above, with steps at λ_i of size m, if this eigenvalue occurs m times in the sum (5.140). In terms of the spectral family of T we can write

$$n(\lambda) = \operatorname{tr} E_T(\lambda). \tag{5.143}$$

Now, if T_1 and T_2 are of rank r, then

$$\begin{aligned} \operatorname{tr}\big(f(T_1) - f(T_2)\big) &= \int_{-\infty}^{+\infty} \big(n_1'(\lambda) - n_2'(\lambda)\big)\, f(\lambda)\, d\lambda \\ &= -\int_{-\infty}^{+\infty} \big(n_1(\lambda) - n_2(\lambda)\big)\, f'(\lambda)\, d \lesssim mbda. \end{aligned} \tag{5.144}$$

In the last step the boundary term from the partial integration vanishes, because $n_1(\lambda) - n_2(\lambda) = 0$ for $|\lambda|$ sufficiently large. Hence we can define

$$\xi(\lambda) = n_2(\lambda) - n_1(\lambda) = \operatorname{tr}\big(E_{T_2}(\lambda) - E_{T_1}(\lambda)\big). \tag{5.145}$$

ξ is continuous from above and vanishes for $|\lambda| > \max\{\|T_1\|, \|T_2\|\}$. □

Remark. The equality (5.145) is not true in general. There are examples where both sides in Eq. (5.145) are well defined but unequal (see Sect. 7.2.3).

Theorem 5.21. Let Q be a supercharge in $\mathfrak{H} \oplus \mathfrak{H}$ and assume that the operator $\operatorname{mtr} \tau (Q^2+1)^{-1}$ is trace class in $\mathfrak{H}$. Then there exists a function $\xi : [0, \infty) \to \mathbb{R}$ such that

$$\operatorname{str} \tau (Q^2 - z)^{-1} = -\int_0^\infty \xi(\lambda)\,(\lambda - z)^{-2}\, d\lambda, \quad \text{for } z \in \mathbb{C} \setminus [0, \infty), \tag{5.146}$$

and if f is a function on $[0, \infty)$ such that g defined as

$$g(\mu) = f(1/\mu - 1), \quad \mu \in (0, 1], \tag{5.147}$$

can be extended to a function in $\mathcal{G}$, then

$$\operatorname{str} \tau f(Q^2) = \int_0^\infty \xi(\lambda)\, f'(\lambda)\, d\lambda. \tag{5.148}$$

Proof. By Theorem 5.20 there exists a function η such that

$$\operatorname{str} \tau (Q^2+1)^{-1} = \operatorname{tr}\left((D^*D+1)^{-1} - (DD^*+1)^{-1}\right) = \int_0^1 \eta(\mu)\, d\mu, \tag{5.149}$$

and for $g \in \mathcal{G}$ we have

$$\operatorname{str} \tau g\big((Q^2+1)^{-1}\big) = \int_0^1 \eta(\mu)\, g'(\mu)\, d\mu. \tag{5.150}$$

Now the variable substitution $\lambda = -1 + 1/\mu$ converts these integrals into

$$\int_0^1 \eta(\mu)\, d\mu = \int_0^\infty \eta\big((\lambda+1)^{-1}\big)\,(\lambda+1)^{-2}\, d\lambda, \tag{5.151}$$

$$\int_0^1 \eta(\mu)\, g'(\mu)\, d\mu = -\int_0^\infty \eta\big((\lambda+1)^{-1}\big)\, f'(\lambda)\, d\lambda, \tag{5.152}$$

where we have set $f(\lambda) = g\big((\lambda+1)^{-1}\big)$. Hence we choose $\xi(\lambda) = -\eta\big((\lambda+1)^{-1}\big)$. Choosing $f(\lambda) = (\lambda - z)^{-1}$ we find that $g(\mu) = (\mu^{-1} - 1 - z)^{-1}$ can be extended to a $\mathcal{C}_0^\infty$-function, if $z \notin [0, \infty)$. □

We see that the regularized index $\operatorname{ind}_z Q$ of a supercharge can be expressed with the help of Krein's spectral shift function ξ,

$$\operatorname{ind}_z Q = \int_0^\infty \frac{z\,\xi(\lambda)\, d\lambda}{(\lambda - z)^2}. \tag{5.153}$$

Similarly, $\operatorname{ind}_t Q$ can be expressed by ξ as a consequence of the following theorem whose proof is analogous to that of Theorem 5.21.

Theorem 5.22. Let Q be a supercharge and assume that $\mathrm{mtr}\,\tau e^{-sQ^2}$ is trace class for some $s > 0$. Then there is a unique function $\xi : [0,\infty) \to \mathbb{R}$ such that

$$\mathrm{str}\,\tau e^{-tQ^2} = -t\int_0^\infty \xi(\lambda)\, e^{-\lambda t}\, d\lambda, \quad \text{for all } t \geq s. \tag{5.154}$$

If f is a function on $[0,\infty)$ such that g defined as

$$g(\mu) = f(-s^{-1}\ln\mu), \quad \mu \in (0,1], \tag{5.155}$$

can be extended to a function in $\mathcal{G}$, then

$$\mathrm{str}\,\tau f(Q^2) = \int_0^\infty \xi(\lambda)\, f'(\lambda)\, d\lambda. \tag{5.156}$$

Remark 1. For operators of finite rank, we obtain from the proof of Theorem 5.20

$$\mathrm{ind}\, Q \equiv \mathrm{tr}\,[E_{D^*D}(0) - E_{DD^*}(0)] = -\xi(0). \tag{5.157}$$

Again this is not generally true, because equality might fail if Q is not a Fredholm operator. The meaning of $\xi(0)$ in the general case will be described in Theorem 5.24.

Remark 2. If the assumptions of the Theorems 5.21 and 5.22 are both true, then the corresponding functions ξ coincide, because the integrals in (5.148) and (5.156) have the same value for all $\mathcal{C}_0^\infty$-functions.

Remark 3. By the same arguments as above a spectral shift function can be defined for arbitrary self-adjoint operators H_1 and H_2, for which the difference $[(H_1-z)^{-1}-(H_2-z)^{-1}]$ or $[\exp(-sH_1)-\exp(-sH_2)]$ is trace class. The spectral shift function can be interpreted as the determinant of the on-shell scattering operator for the scattering system (H_1, H_2), see Sect. 8.1.3. Consider, e.g., the operators

$$H_2 = -\frac{d^2}{dr^2}, \qquad H_1 = H_2 + V(r), \qquad \text{in } \mathfrak{H} = L^2(0,\infty). \tag{5.158}$$

Under suitable conditions on the potential V we can define the scattering phase shift $\eta(k)$ and find a finite number of eigenvalues λ_i of H_1. Krein's spectral shift function can be expressed as

$$\xi(\lambda) = \begin{cases} \eta(\sqrt{\lambda})/\pi, & \lambda > 0, \\ \int_{-\infty}^{\lambda} \sum_j \delta(\lambda - \lambda_j)\, d\lambda, & \lambda < 0. \end{cases} \tag{5.159}$$

5.8.2 The Witten Index and the Axial Anomaly

In the physically most important case where Q is not Fredholm one cannot expect the regularized indices $\mathrm{ind}_t\, Q$ and $\mathrm{ind}_z\, Q$ to be independent of t, resp. z. In this case one defines under the assumptions of Theorem 5.21 the "*Witten index*" as

$$W(Q) = \lim_{\substack{z\to 0 \\ |\arg z|>\epsilon>0}} \mathrm{ind}_z\, Q, \tag{5.160}$$

whenever this quantity exists. This definition reduces to the notion of the Fredholm index whenever Q is Fredholm

Theorem 5.23. Let Q be a Fredholm supercharge with $\mathrm{mtr}\,\tau(Q^2+1)^{-1}$ belonging to the trace class. Then $W(Q)$ exists and

$$W(Q) = \mathrm{ind}\, Q. \tag{5.161}$$

Proof. For a self-adjoint Fredholm operator H the resolvent has the Laurent expansion

$$(H-z)^{-1} = -\tfrac{1}{z}P + S(z), \tag{5.162}$$

where P is the projection onto the eigenspace belonging to the eigenvalue 0 of H (which is isolated and of finite degeneracy by the Fredholm property), and $S(z)$ is holomorphic[10]. Hence

$$-z\big((D^*D-z)^{-1} - (DD^*-z)^{-1}\big) = P_+ - P_- - z\big(S_+(z) - S_-(z)\big) \tag{5.163}$$

(where the index "+" belongs to D^*D and "−" to DD^*). By assumption, the operator $S_+(z)-S_-(z)$ is trace class for $z\in\mathbb{C}\setminus[0,\infty)$, in fact even holomorphic in z in the trace norm. Hence in the limit $z\to 0$ the trace of the expression (5.163) tends to $\mathrm{tr}\,(P_+ - P_-) = \mathrm{ind}\, Q$. □

If, instead, the assumptions of Theorem 5.22 are true, then one can try to define the Witten index alternatively as

$$W(Q) = \lim_{t\to\infty} \mathrm{ind}_t\, Q. \tag{5.164}$$

The two definitions are equivalent if Krein's spectral shift function is assumed to be continuous from above. This is a consequence of the next theorem and of Remark 2 in the previous section.

Theorem 5.24. a) Let ξ, defined under the assumptions of Theorem 5.21, be continuous from above at $\lambda = 0$. Then $W(Q)$, defined by (5.160), exists and

$$W(Q) = -\xi(0). \tag{5.165}$$

[10] The holomorphic part in the Laurent expansion of the resolvent is called the "reduced resolvent", [Ka 80], Sect. I.5.3.

b) If ξ is defined under the assumptions of Theorem 5.22 and if ξ is continuous from above at 0, then $W(Q)$, defined by (5.164), exists and (5.165) holds.

Proof. We have to show that

$$a \operatorname{str} \tau (Q^2 + a)^{-1} + \xi(0) = a \int_0^\infty \{\xi(0) - \xi(\lambda)\} (\lambda + a)^{-2} \, d\lambda \tag{5.166}$$

is less than ϵ for a sufficiently small. In (5.166) we have used (5.146) and

$$\int_0^\infty \frac{a \, d\lambda}{(\lambda + a)^2} = 1. \tag{5.167}$$

Next we split the integral in (5.166) into $\int_0^\delta + \int_\delta^\infty$. Choose δ small such that $|\xi(0) - \xi(\lambda)| < \epsilon/2$ for $\lambda < \delta$. Then the first integral is bounded by

$$a \int_0^\delta |\xi(0) - \xi(\lambda)| (\lambda + a)^{-2} \, d\lambda < \epsilon/2. \tag{5.168}$$

Given this δ, choose a so small, that the second integral, which is bounded by

$$a \int_\delta^\infty |\xi(0) - \xi(\lambda)| \lambda^{-2} \, d\lambda = a \operatorname{const.}(\delta), \tag{5.169}$$

is less than $\epsilon/2$. The proof for the second statement is similar. □

Finally, we define the "*axial anomaly*" by

$$A(Q) = - \lim_{\substack{z \to \infty \\ |\arg z| > \epsilon > 0}} \operatorname{ind}_z Q. \tag{5.170}$$

If $\xi(\infty) = \lim_{\lambda \to \infty} \xi(\lambda)$ exists, we obtain similarly as in Theorem 5.24a the result

$$A(Q) = \xi(\infty) \tag{5.171}$$

5.8.3 The Spectral Asymmetry

We consider a supersymmetric Dirac operator of the form

$$H = Q + m\tau, \qquad m > 0, \tag{5.172}$$

and define

$$\begin{aligned} \eta_t(H) &= \operatorname{str} \operatorname{sgn}(H) \, e^{-tH^2} = \operatorname{str} m (Q^2 + m^2)^{-1/2} \, e^{-t(Q^2 + m^2)} \\ &= m \int_0^\infty \xi(\lambda) \frac{d}{d\lambda} \frac{e^{-t(\lambda + m^2)}}{\sqrt{\lambda + m^2}} \, d\lambda. \end{aligned} \tag{5.173}$$

(We have used Eq. (5.155) to obtain the last expression). The "spectral asymmetry" can now be defined as

$$\begin{aligned} \eta(H) &= \lim_{t \to 0} \eta_t(H) \\ &= -\frac{m}{2} \int_0^\infty \xi(\lambda) (\lambda + m^2)^{-3/2} \, d\lambda. \end{aligned} \tag{5.174}$$

5.9 Topological Invariance of the Witten Index

5.9.1 Perturbations Preserving Supersymmetry

Let $H_{\rm ss} = Q + M\tau$ be a Dirac operator with supersymmetry. We can decompose $W = W_{\rm even} + W_{\rm odd}$ according to Sect. 5.1.2 and write $\tilde{Q} \equiv Q + W_{\rm odd}$, $\tilde{M} \equiv M + W_{\rm even}\tau$. If $\tilde{Q}$ and $\tilde{M}$ satisfy the assumptions of Sect. 5.4.1, then $H = H_{\rm ss} + W$ would again be a Dirac operator with supersymmetry. Among other things we have to verify on $\mathfrak{D}(\tilde{Q})$ the following condition.

$$\{\tilde{Q}, \tilde{M}\tau\} = \{W_{\rm odd}, M\tau\} + \{Q, W_{\rm even}\} + \{W_{\rm odd}, W_{\rm even}\} = 0, \tag{5.175}$$

which shows that supersymmetry is very sensitive against perturbations. Usually we assume the simplest case that a supersymmetry preserving perturbation is an odd operator $W = W_{\rm odd}$ so that the summands in (5.175) vanish separately:

Example 5.25. Let H_0 be the free Dirac operator and let $W = -c\boldsymbol{\alpha} \cdot \boldsymbol{A}(\boldsymbol{x}) = W_{\rm odd}$. If $H = H_0 + W$ is self-adjoint on some suitable domain (see, e.g., Theorem 4.2), then H is a Dirac operator with supersymmetry.

The following is a simple example for the fact that supersymmetry preserving perturbations need not be odd operators.

Example 5.26. Let P be an orthogonal projection in a Hilbert space $\mathfrak{H}_+ = \mathfrak{H}_-$, and let

$$H_0 = \begin{pmatrix} m & P \\ P & -m \end{pmatrix}, \quad m > 0. \tag{5.176}$$

For any real $a \neq -m$, and $b \neq m$, define

$$W = \begin{pmatrix} aP & -1 \\ -1 & bP \end{pmatrix}. \tag{5.177}$$

Then $H_0 + W$ is again a Dirac operator with supersymmetry.

5.9.2 Invariance of the Index under Perturbations

Concerning the behavior of the Fredholm index under supersymmetry preserving perturbations, we quote the following classical result which is known as the "topological invariance of the index".

Theorem 5.27. Let Q be a Fredholm supercharge, and C be symmetric, odd (Sect.5.2.2), and compact relative to Q. Then $Q + C$ is a Fredholm supercharge with

$$\operatorname{ind}(Q + C) = \operatorname{ind} Q. \tag{5.178}$$

Proof. See, e.g., [Ka 80], Sect. IV.5.3. □

Remark. For bounded Fredholm operators the topological invariance is usually stated in the following way: Two Fredholm operators have the same index if and only if they can be joined by a continuous path (i.e., a continuous map from $[0,1]$ into the set of Fredholm operators equipped with the operator-norm topology).

If Q is not a Fredholm operator, then the (regularized) index is not invariant under a relatively compact perturbation. Instead, one can prove the invariance under suitable relative trace class conditions.

Theorem 5.28. Let Q be a supercharge such that $\mathrm{mtr}\,\tau e^{-tQ^2}$ belongs to the trace class for all $t > 0$. Let W be a symmetric and odd operator which is infinitesimally bounded with respect to Q. Assume We^{-tQ^2} to be trace class in $\mathfrak{H} \oplus \mathfrak{H}$ such that for all $t > 0$

$$\|We^{-tQ^2}\| \leq \mathrm{const.}t^{-\alpha}, \qquad \text{for some } \alpha < 1/2, \tag{5.179}$$

$$\|We^{-tQ^2}\|_1 \leq \mathrm{const.}t^{-\beta}, \qquad \text{for some } \beta > 0. \tag{5.180}$$

Then $Q + W$ is a supercharge for which $\mathrm{mtr}\,\tau e^{-t(Q+W)^2}$ is trace class in $\mathfrak{H}$ for all $t > 0$, and

$$\mathrm{ind}_t\,(Q+W) = \mathrm{ind}_t\,Q \quad \text{for all } t > 0. \tag{5.181}$$

Proof. Let us denote $Q_\lambda = Q + \lambda W$. We give a proof of this theorem under the assumptions

$$e^{-tQ_\lambda^2} - e^{-tQ^2} \quad \text{is trace class for all } t > 0,\ \lambda \in \mathbb{R}, \tag{5.182}$$

$$We^{-tQ_\lambda^2} \quad \text{is trace class for all } t > 0,\ \lambda \in \mathbb{R}. \tag{5.183}$$

It has been shown in [171], Proposition 3.4, that the conditions (5.179) and (5.180) are sufficient to imply (5.182) and (5.183). In order to calculate the derivative of $\mathrm{tr}\,\tau(e^{-tQ_\lambda^2} - e^{-tQ^2})$ with respect to λ we consider

$$\tfrac{1}{h}\tau\big(e^{-tQ_{\lambda+h}^2} - e^{-tQ_\lambda^2}\big) = \tfrac{1}{h}\int_0^t ds\,\frac{d}{ds}\,\tau\, e^{-sQ_{\lambda+h}^2}\, e^{-(t-s)Q_\lambda^2}$$

$$= -\tfrac{1}{h}\int_0^t ds\,\tau\, e^{-sQ_{\lambda+h}^2}\big(hQ_\lambda W + hWQ_\lambda + h^2W^2\big)e^{-(t-s)Q_\lambda^2}. \tag{5.184}$$

Using (5.183) and the boundedness of operators of the form $Q_{\lambda_1}\, e^{-tQ_{\lambda_2}^2}$, we easily conclude that all summands of the integrand in (5.184) are trace class. In order to perform the limit $h \to 0$ we recall that for A trace class the map $B \to \mathrm{tr}\,BA$ is a continuous linear functional on the space of bounded linear operators. From this we conclude that

$$\frac{d}{d\lambda}\operatorname{tr}\tau\left(e^{-tQ_\lambda^2}-e^{-tQ^2}\right)$$

$$=-\int_0^t ds\operatorname{tr}\left[\tau e^{-sQ_\lambda^2}\left(Q_\lambda W+WQ_\lambda\right)e^{-(t-s)Q_\lambda^2}\right]. \tag{5.185}$$

Since the cyclicity of the trace holds for bounded operators, we regularize the operators Q_λ and W by replacing $Q\to Q_{\lambda,\varepsilon}=Q_\lambda(1+\varepsilon Q_\lambda^2)^{-1}$, and $W\to(1+\varepsilon Q_\lambda^2)^{-1}W$. Then all operators are bounded, and $Q_{\lambda,\varepsilon}$ anticommutes with τ, but commutes with $e^{-sQ_\lambda^2}$. Now we can use the commutation properties and the cyclicity of the trace to find

$$\operatorname{tr}\tau e^{-sQ_\lambda^2}\left(Q_{\lambda,\varepsilon}W+WQ_{\lambda,\varepsilon}\right)e^{-(t-s)Q_\lambda^2}=0, \tag{5.186}$$

and, by letting $\varepsilon\to 0$,

$$\frac{d}{d\lambda}\operatorname{tr}\tau\left(e^{-tQ_\lambda^2}-e^{-tQ^2}\right)=0, \tag{5.187}$$

hence

$$\operatorname{tr}\tau\left(e^{-tQ_\lambda^2}-e^{-tQ^2}\right)=0\quad\text{for all }\lambda. \tag{5.188}$$

Now, since $\operatorname{mtr}\tau e^{-tQ^2}$ is trace class by assumption, we conclude the same result for $\operatorname{mtr}\tau e^{-tQ_\lambda^2}$ and hence

$$\operatorname{ind}_t(Q+W)=\operatorname{tr}\operatorname{mtr}\tau e^{-tQ_1^2}=\operatorname{ind}_t Q. \tag{5.189}$$

□

The assumptions of the theorem are satisfied, e.g., if

$$W(Q^2+1)^{-\alpha}\quad\text{is bounded for some }\alpha<1/2, \tag{5.190}$$

$$W(Q^2+1)^{-\beta}\quad\text{is trace class for some }\beta>0, \tag{5.191}$$

because

$$\|We^{-tQ^2}\|=\|W(Q^2+1)^{-\alpha}\|\|e^{-tQ^2}(Q^2+1)^{\alpha}\|\le\text{const.}t^{-\alpha} \tag{5.192}$$

implies (5.179), and a similar argument applies to (5.191) and (5.180).

Remark. The theorem above is essentially a result on the invariance of the spectral shift function[11]. Hence there are analogous invariance results for the axial anomaly and the spectral asymmetry.

[11] see [56]

5.10 Fredholm Determinants

For practical calculations of the index in special situations, Fredholm determinants are a useful technical tool.

Definition 5.29. *Let A be a trace-class operator, $\{\phi_i\}$ an orthonormal base in $\mathfrak{H}$, and denote by $\mathbf{M}_n$ the $n \times n$-matrix*

$$(\mathbf{M}_n)_{j,k} = \big(\phi_j\,,\,(\mathbf{1}+A)\phi_k\big). \tag{5.193}$$

Then the determinant of $\mathbf{1}+A$ is defined by

$$\det(\mathbf{1}+A) = \lim_{n\to\infty} \det \mathbf{M}_n, \tag{5.194}$$

and this definition is independent of the chosen orthonormal base.

If λ_j are the eigenvalues of the trace-class operator A, then, by Lidskii's theorem

$$\det(\mathbf{1}+A) = \prod_{j=1}^{\infty}(1+\lambda_j), \qquad \operatorname{tr} A = \sum_{j=1}^{\infty}\lambda_j. \tag{5.195}$$

Hence the operator $(\mathbf{1}+A)^{-1}$ exists if and only if $\det(\mathbf{1}+A) \neq 0$. The determinant is related to the trace by

$$\det(\mathbf{1}+A) = e^{\operatorname{tr}\ln(\mathbf{1}+A)}. \tag{5.196}$$

This equation can also be used as a definition of the determinant[12]. For $\|A\| < 1$, the logarithm in Eq. (5.196) is given by the power series $\sum_{n=1}^{\infty}(-1)^{n-1}A^n/n$.

The importance of the determinant in the present context is due to a relation between $\operatorname{tr}\left[(H_2-z)^{-1}-(H_1-z)^{-1}\right]$ and the determinant of an operator to be defined below.

Let H_1 and H_2 be self-adjoint operators, $H_1 = H_2 + V$, and assume that $V = vu$, so that the resolvent difference can be written in the symmetric form

$$(H_2-z)^{-1} - (H_1-z)^{-1} = (H_2-z)^{-1}\,v\,[\mathbf{1}+A(z)]^{-1}\,u\,(H_2-z)^{-1}. \tag{5.197}$$

Here and in the following the operator $A(z)$ is defined as

$$A(z) \equiv u\,(H_2-z)^{-1}\,v. \tag{5.198}$$

Assuming that we can apply the cyclicity of the trace, we calculate

$$\operatorname{tr}\left\{(H_2-z)^{-1}-(H_1-z)^{-1}\right\} = \operatorname{tr}\left\{[\mathbf{1}+A(z)]^{-1}\,u\,(H_2-z)^{-2}\,v\right\} =$$

$$= \operatorname{tr}\left\{[\mathbf{1}+A(z)]^{-1}\,\frac{dA(z)}{dz}\right\} \tag{5.199}$$

[12] [Ka 80], p. 524

$$= \frac{d}{dz} \ln \det [\mathbf{1} + A(z)]. \tag{5.200}$$

We can verify the last step by the following formal calculation. If $\lambda_j(z)$ are the eigenvalues of $A(z)$, then (5.199) becomes

$$\sum [1+\lambda_j(z)]^{-1} \frac{d\lambda_j(z)}{dz} = \sum \frac{d}{dz} \ln[1+\lambda_j(z)] = \frac{d}{dz} \ln \prod [1+\lambda_j(z)], \tag{5.201}$$

and the last expression equals (5.200). In the following lemma we collect these results and the assumptions necessary to justify the calculation above.

Lemma 5.30. Let $H_1 = H_2 + vu$, such that $z \to A(z)$ defined as in Eq. (5.198) is analytic with respect to the trace-norm for $z \in \rho(H_2)$ and such that the operators $u(H_2 - z_0)^{-1}$, $(H_2 - z_0)^{-1}v$ are Hilbert-Schmidt for some $z_0 \in \rho(H_2)$. Then

$$\operatorname{tr} \left\{ (H_2 - z)^{-1} - (H_1 - z)^{-1} \right\} = \frac{d}{dz} \ln \det [\mathbf{1} + A(z)]. \tag{5.202}$$

Proof. See [GK 69], [274], [56]. □

The quantity $\det [\mathbf{1} + A(z)]$ is called "*perturbation determinant*" or "*Fredholm determinant*" for the operators H_1 and H_2. Let us compare this result with the formula

$$\operatorname{tr} \left\{ (H_2 - z)^{-1} - (H_1 - z)^{-1} \right\} = \int \frac{\xi(\lambda)\, d\lambda}{(\lambda - z)^2}, \tag{5.203}$$

where ξ is Krein's spectral shift function for the pair H_1, H_2 (see Eq. (5.145) and Remark 3 in Sect. 5.8.1). Assuming that $\xi(\lambda)/(\mathbf{1} + |\lambda|)$ is integrable, we obtain

$$\frac{d}{dz} \ln \det [\mathbf{1} + A(z)] = \frac{d}{dz} \int \frac{\xi(\lambda)\, d\lambda}{\lambda - z}, \tag{5.204}$$

and

$$\lim_{\substack{z \to \infty \\ |\operatorname{Im} z| > 0}} \int \frac{\xi(\lambda)\, d\lambda}{\lambda - z} = 0. \tag{5.205}$$

Hence, under the assumption

$$\lim_{\substack{z \to \infty \\ |\operatorname{Im} z| > 0}} \det [\mathbf{1} + A(z)] = \mathbf{1} \tag{5.206}$$

we conclude

$$\ln \det [\mathbf{1} + A(z)] = \int_{-\infty}^{\infty} \frac{\xi(\lambda)\, d\lambda}{\lambda - z}. \tag{5.207}$$

We can even obtain a representation of ξ itself in terms of Fredholm determinants. For this we assume that $\xi(\lambda)$ is a bounded, piecewise continuous function

of $\lambda \in \mathbb{R}$. Then ξ has a well known representation as the boundary value of a complex harmonic function, namely[13]

$$\tfrac{1}{2}[\xi(\lambda_+) + \xi(\lambda_-)] = \frac{1}{2\pi i} \lim_{\epsilon \to 0_+} \int_{-\infty}^{\infty} \frac{\xi(\mu)\, d\mu}{|\mu - \lambda - i\epsilon|^2} \tag{5.208}$$

Here $\xi(\lambda_\pm) = \lim_{\delta \to 0_+} \xi(\lambda \pm \delta)$. We can write

$$\frac{2i\epsilon}{|\lambda - \mu - i\epsilon|^2} = \frac{1}{\mu - \lambda - i\epsilon} - \frac{1}{\mu - \lambda + i\epsilon}, \tag{5.209}$$

and find, since $\xi(\mu)/(1 + |\mu|)$ is integrable,

$$\begin{aligned} &\tfrac{1}{2}[\xi(\lambda_+) + \xi(\lambda_-)] = \\ &= \frac{1}{2\pi i} \lim_{\epsilon \to 0_+} \left\{ \int_{-\infty}^{\infty} \frac{\xi(\mu)\, d\mu}{\mu - \lambda - i\epsilon} - \int_{-\infty}^{\infty} \frac{\xi(\mu)\, d\mu}{\mu - \lambda - i\epsilon} \right\} \\ &= \frac{1}{2\pi i} \lim_{\epsilon \to 0_+} \ln \frac{\det[\mathbf{1} + A(\lambda + i\epsilon)]}{\det[\mathbf{1} + A(\lambda - i\epsilon)]} \\ &= \frac{1}{\pi} \lim_{\epsilon \to 0_+} \arg \det[\mathbf{1} + A(\lambda + i\epsilon)]. \end{aligned} \tag{5.210}$$

Note that $\frac{1}{2}[\xi(\lambda_+) + \xi(\lambda_-)] = \xi(\lambda)$ if and only if ξ is continuous at λ. We collect these results in the following lemma.

Lemma 5.31. Assume the conditions of Lemma 5.30 and Eq. (5.206) and suppose the function $\xi(\lambda)/(1 + |\lambda|)$ to be integrable. Then

$$\ln \det[\mathbf{1} + A(z)] = \int_{-\infty}^{\infty} \frac{\xi(\lambda)\, d\lambda}{\lambda - z}. \tag{5.211}$$

If, in addition, ξ is bounded and piecewise continuous on $\mathbb{R}$, then

$$\tfrac{1}{2}[\xi(\lambda_+) + \xi(\lambda_-)] = \tfrac{1}{\pi} \lim_{\epsilon \to 0_+} \arg \det[\mathbf{1} + A(\lambda + i\epsilon)]. \tag{5.212}$$

Remark. Fredholm determinants turn out to be a useful tool for index-calculations especially of one-dimensional Dirac operators. However, the condition (5.206) is known to fail in higher-dimensional systems. In this case one can still reformulate the theory in terms of modified Fredholm determinants. This works well at least in two dimensions. See [56] for details.

Explicit examples of the index of Dirac operators in special situations will be presented in later sections. In Sect. 7.3 we consider the index of the Dirac operator in a two-dimensional magnetic field. In Sect. 9.4 the index of a one-dimensional Dirac operator with a "soliton"-potential is calculated using Fredholm determinants. Further examples can be found in the literature cited in the Notes.

[13] [Br 65], Sects. 5.3 and A.2.5.

5.11 Regularized Indices in Exactly Soluble Models

5.11.1 Scalar Potential in One Dimension

In the Hilbert space $\mathfrak{H} = L^2(\mathbb{R})^2$, consider the Dirac operator

$$Q = -\mathrm{i}\,\sigma_2 \partial_x + \sigma_1\,\phi(x), \tag{5.213}$$

where ϕ and $\partial_x \phi$ are bounded, real-valued functions satisfying

$$\lim_{x \to \pm\infty} \phi(x) = \phi_\pm, \tag{5.214}$$

$$\pm \int_0^{\pm\infty} (1+x^2)\,\{|\phi(x)-\phi_\pm| + |\phi_x(x)|\}\,dx < \infty. \tag{5.215}$$

Under these conditions it will be shown in Sect. 9.4.2 with the help of one-dimensional scattering theory, that

$$\mathrm{ind}_z\, Q = \frac{1}{2}\left[\frac{\phi_+}{\sqrt{\phi_+^2 - z}} - \frac{\phi_-}{\sqrt{\phi_-^2 - z}}\right] \tag{5.216}$$

Hence, using Eqs. (5.160) and (5.170) we obtain

$$W(Q) = (\mathrm{sgn}\,\phi_+ - \mathrm{sgn}\,\phi_-)/2, \qquad A(Q) = 0. \tag{5.217}$$

We summarize the zero energy properties of D^*D and DD^* in the following table [56]:

Asymptotics of ϕ	Behavior at E=0 of D^*D	DD^*	$W(Q)$	ind Q
$\phi_- < 0 < \phi_+$	eigenvalue	-	1	1
$\phi_- > 0 > \phi_+$	-	eigenvalue	-1	-1
$\phi_- = 0 < \phi_+$	resonance	-	1/2	0
$\phi_- = 0 > \phi_+$	-	resonance	-1/2	0
$\phi_- = 0 = \phi_+$	resonance	resonance	0	0
$\mathrm{sgn}\,\phi_- = \mathrm{sgn}\,\phi_+ \neq 0$	-	-	0	0

The zero energy results follow from the observation that $Af = 0$ is solved by

$$f(x) = f(0)\,\exp\Big\{-\int_0^x \phi(y)\,dy\Big\} = O(e^{-\phi_\pm x}), \quad \text{as } x \to \pm\infty, \tag{5.218}$$

and $A^*g = 0$ is solved by

$$g(x) = g(0)\,\exp\Big\{\int_0^x \phi(y)\,dy\Big\} = O(e^{\phi_\pm x}), \quad \text{as } x \to \pm\infty. \tag{5.219}$$

One can also evaluate Krein's spectral shift function using Eqs. (5.210), (9.113) and (9.115). We obtain for all $\lambda \in \mathbb{R}$

$$\xi(\lambda) = \frac{1}{\pi}\Big[\theta(\lambda-\phi_+^2)\,\arctan\Big(\tfrac{\sqrt{\lambda-\phi_+^2}}{\phi_+}\Big) - \theta(\lambda-\phi_-^2)\,\arctan\Big(\tfrac{\sqrt{\lambda-\phi_-^2}}{\phi_-}\Big)\Big]$$

$$- \frac{\theta(\lambda)}{2}\,[\operatorname{sgn}\phi_+ - \operatorname{sgn}\phi_-], \quad \text{if } \phi_- \neq 0 \text{ and } \phi_+ \neq 0, \tag{5.220}$$

$$\xi(\lambda) = \frac{1}{\pi}\,\theta(\lambda-\phi_+^2)\,\arctan\Big(\tfrac{\sqrt{\lambda-\phi_+^2}}{\phi_+}\Big) - \frac{\theta(\lambda)}{2}\operatorname{sgn}\phi_+, \quad (\phi_- = 0 \neq \phi_+). \tag{5.221}$$

This shows that also $\xi(\lambda)$ is independent of the local properties of the potential and depends only on the asymptotic values (topological invariance).

5.11.2 Magnetic Field in Two Dimensions

Let Q be the Dirac operator for an electron in a C_0^∞-magnetic field B with compact support in two dimensions. It is given by

$$Q = \sum_{k=1}^{2} c\sigma_k(-\mathrm{i}\partial_k - A_k(x)), \tag{5.222}$$

in the Hilbert space $L^2(\mathbb{R}^2)^2$, where $B = \partial_1 A_2 - \partial_2 A_1$. If we denote the flux of B by

$$F = \frac{1}{2\pi}\int_{\mathbb{R}^2} B(x)d^2x, \tag{5.223}$$

then (see Theorem 7.3 below)

$$\operatorname{ind} Q = (\operatorname{sgn} F)\cdot\begin{cases} n, & \text{if } F = n+\epsilon, \quad 0<\epsilon<1, \\ n-1, & \text{if } F = n, \quad n = 1,2,3,\ldots, \end{cases} \tag{5.224}$$

and (Theorem 7.4)

$$\operatorname{ind}_z Q = W(Q) = -A(Q) = F, \qquad \xi(\lambda) = \theta(\lambda)F. \tag{5.225}$$

5.11.3 Callias Index Formula

Let Q be the Dirac operator with a Higgs-field Φ in $\mathbb{R}^n$, n odd. The Hilbert space in this case is $\mathfrak{H} = L^2(\mathbb{R}^n)^{2pm}$, where $p = 2^{(n-1)/2}$ is the dimension of the spinor space over $\mathbb{R}^n$. We define the Dirac operator by

$$Q = \begin{pmatrix} 0 & D^* \\ D & 0 \end{pmatrix}, \qquad D = -\mathrm{i}\sum_{k=0}^{p}\tau_k\partial_k \otimes 1_m - \mathrm{i}1_p \otimes \Phi(x). \tag{5.226}$$

D is a $pm \times pm$ matrix differential operator, and Φ is a $m \times m$ Hermitian matrix of C^∞ functions. The constant $p \times p$ matrices τ_k, $k = 1,\ldots,n$ are the generalization of the Pauli matrices to the present case, they satisfy the algebra

$$\tau_j\tau_k + \tau_k\tau_j = 2\delta_{jk}1. \tag{5.227}$$

We assume that $|\Phi|$ is strictly positive for $|x| > R_0$ and asymptotically homogeneous of degree 0 as $x \to \infty$. We denote

$$U(x) = \Phi(x)/|\Phi(x)|, \quad x \in \mathbb{R}^n, \quad |x| > R_0. \tag{5.228}$$

Then Q is a Fredholm elliptic differential operator with index given by

$$\operatorname{ind} Q = \frac{1}{2\left(\frac{n-1}{2}\right)!}\left(\frac{\mathrm{i}}{8\pi}\right)^{\frac{n-1}{2}} \lim_{R\to\infty} \int_{S_R^{n-1}} \operatorname{tr}\left[U(x)(dU(x))^{n-1}\right]. \tag{5.229}$$

Here S_R^{n-1} is the sphere of radius R in $\mathbb{R}^n$, centered at the origin. $dU(x)$ is the matrix of differentials and $(dU(x))^{n-1}$ is the $(n-1)$th power, where the differentials are multiplied by exterior multiplication.

6 The Nonrelativistic Limit

In this chapter we analyze the behavior of the Dirac equation in the nonrelativistic limit and derive the explicit form of the first order relativistic correction. There are two main reasons for this investigation. The first is purely conceptual: It is important to see how the relativistic theory contains the successful nonrelativistic theory as a limiting case. The second reason is a practical one: In some cases it is useful to replace the Dirac theory by the much simpler Schrödinger theory together with some relativistic corrections. The first order corrections can sometimes be calculated explicitly, but it is not always necessary and is often impossible to calculate higher order corrections or the exact solution of the Dirac equation. Besides, for a higher accuracy we expect quantum electrodynamical effects to play a certain role (e.g., the Lamb shift). These effects cannot be described by the Dirac equation alone.

We achieve the nonrelativistic limit by letting c, the relativistic bound for the propagation speed of signals, tend to infinity. Unfortunately, the Dirac operator $H(\mathrm{c})$ itself, even after subtracting the rest mass, makes no sense for $c = \infty$. The correct way to analyze the parameter dependence of unbounded operators is to look at its resolvent. We shall prove norm-convergence as $\mathrm{c} \to \infty$ of $(H(\mathrm{c}) - m\mathrm{c}^2 - z)^{-1}$ for one (and hence all) z with $\operatorname{Im} z \neq 0$. The nonrelativistic limit of the Dirac resolvent is the resolvent of a Schrödinger or Pauli operator times a projection to the upper components of the Dirac wavefunction. The Dirac resolvent is even analytic in $1/\mathrm{c}$ (Sect. 6.1).

From the explicit expansion of the resolvent in powers of $1/\mathrm{c}$ we obtain complete information about the behavior of the relativistic energy spectrum in a neighborhood of $\mathrm{c} = \infty$ (Sect. 6.2). The necessary background from perturbation theory is quickly reviewed in Sect. (6.2.1). The Rayleigh-Schrödinger perturbation series for the eigenvalue $\lambda(c)$ of the resolvent determines its expansion into powers of $1/\mathrm{c}$. The corresponding expansion of the eigenvalue $E(\mathrm{c})$ of the Dirac operator is easily obtained from $\lambda(\mathrm{c}) = (E(c) - m\mathrm{c}^2 - z)^{-1}$. It turns out that the eigenvalues of the Dirac operator are analytic in the parameter $1/c^2$. We determine explicit formulas for the relativistic corrections to the nonrelativistic binding energies. For the corrections of order $1/c^2$ only the knowledge of the corresponding nonrelativistic solutions (Schrödinger or Pauli equation) is required. The result can be written as a sum of expectation values which have a nice physical interpretation (spin-orbit coupling, etc.).

We formulate the theory in terms of abstract Dirac operators in the supersymmetric framework of the previous chapter. In this way the calculations can be performed with the least amount of writing and the results are applicable to the widest range of concrete situations.

6.1 c-Dependence of Dirac Operators

6.1.1 General Setup

In nonrelativistic physics it is assumed that there is no principal bound for the propagation speed of signals. In the theory of relativity the constant parameter c (the velocity of light) represents such a bound. Nevertheless we expect that the relativistic theory is similar to the nonrelativistic one, if c is very large compared to all velocities of the system under consideration. In the nonrelativistic limit, c should be "infinitely large" compared to the other velocities. The only way to achieve this without restricting the consideration to motionless systems is to allow c to be a variable parameter. The nonrelativistic limit can then be mathematically described by letting c tend to infinity.

In this chapter we describe the dependence of the Dirac operator on c, especially in the region near $c = \infty$. The parameter c appears in various places in the Dirac equation. For example, in an electromagnetic field the Dirac operator reads

$$H(c) = c\boldsymbol{\alpha} \cdot \left(-\mathrm{i}\nabla - \frac{e}{c}\boldsymbol{A}(\boldsymbol{x})\right) + \beta mc^2 + e\,\phi_{\mathrm{el}}(\boldsymbol{x}). \tag{6.1}$$

Before defining a c-dependent abstract Dirac operator we want to make the following two remarks:

Remark 1. The Dirac operator describes the energy of the electron including its rest energy mc^2 ($-mc^2$ in the positron subspace). The rest energy is a purely relativistic object (it has no nonrelativistic limit) and has to be subtracted before letting c tend to infinity. Otherwise there is no possibility to get a nonrelativistic limit for the expression (6.1).

Remark 2. The factor $1/c$ in front of $\boldsymbol{A}(\boldsymbol{x})$ has nothing to do with relativistic quantum mechanics. It's origin is the replacement $\boldsymbol{p} \to \boldsymbol{p} - (e/c)\boldsymbol{A}$ (i.e., the "minimal coupling principle") hence it would also appear in the Schrödinger equation with an external magnetic field. So if we don't want to "turn the light off", we have to keep this factor constant in the nonrelativistic limit. For simplicity, we absorb the factor $1/c$ and the coupling constant e into $\boldsymbol{A}$ and write henceforth $H(c) = c\boldsymbol{\alpha} \cdot (-\mathrm{i}\nabla - \boldsymbol{A}) + \beta mc^2 + V$.

Motivated by these considerations we make the following definition of c-dependence for an abstract Dirac operator.

Let $\mathfrak{H}$ be a Hilbert space with a unitary involution τ, in which a supercharge Q and a strictly positive, self-adjoint operator M commuting with Q are defined as in Sect. 5.4.1. Define

$$H(c) \equiv cQ + Mc^2\tau + V, \qquad c > 0, \tag{6.2}$$

where V is symmetric on $\mathfrak{D}(Q)$ and bounded relative to Q, i.e.,

$$\|Vf\| < a\,\|Qf\| + b\,\|f\|, \qquad 0 < a, b < \infty. \tag{6.3}$$

Thus, if $c > a$, then $H(c)$ is self-adjoint on $\mathfrak{D}(Q)$ by the Kato-Rellich theorem. Moreover, we assume, that V is an even operator, i.e.,

$$\tau V = V\tau \quad \text{on } \mathfrak{D}(Q). \tag{6.4}$$

Hence we may conclude that $H(c)$ with $c > a$ is an abstract Dirac operator. In the standard representation we may write

$$H(c) = \begin{pmatrix} M_+c^2 + V_+ & cD^* \\ cD & -M_-c^2 + V_- \end{pmatrix}. \tag{6.5}$$

Our assumptions include in particular the Coulomb potential with an arbitrarily large coupling constant.

6.1.2 Supersymmetric Dirac Operators

The operator

$$H_0(c) \equiv cQ + \tau Mc^2, \qquad c > 0, \tag{6.6}$$

is a Dirac operator with supersymmetry. According to Remark 1 above we subtract the "rest energy" Mc^2 and investigate the convergence of $H_0(c) - Mc^2$ in the limit $c \to \infty$. It will turn out that only the positive energy part of this expression survives in the limit. Alternatively, in order to obtain a nontrivial limit in the negative energy subspace, we can *add* the term Mc^2 and consider the nonrelativistic limit of the operator $H_0(c) + Mc^2$.

The main mathematical tool for investigating the parameter dependence of unbounded operators (which need not have a common domain of definition for all values of the parameter) is the resolvent[1]. For any self-adjoint operator A and z with $\mathrm{Im}(z) \neq 0$, the resolvent is defined as the bounded operator $(A-z)^{-1}$. The next theorem gives an expression for the resolvent of the operator (6.6) from which the nonrelativistic limit can be read off immediately.

We use the following notation. As in Sect. 5.1.1 we define the projection operators

$$P_\pm \equiv \frac{1}{2}(1 \pm \tau). \tag{6.7}$$

M and M^{-1} are bounded and commute with Q (Sect. 5.4.1). Hence the operator

$$H_{0,\infty} \equiv \frac{1}{2M}Q^2 \tag{6.8}$$

is defined and self-adjoint on $\mathfrak{D}(Q^2)$. Moreover, $H_{0,\infty}$ is a Hamiltonian with supersymmetry (see Sect. 5.1.2). From the examples in Sect. 5.5 we see that in typical applications $H_{0,\infty}$ is a nonrelativistic Schrödinger or Pauli operator (a perturbation of the Laplacian).

[1] see, e.g., [Ka 80] or [RS 72]

Theorem 6.1. Let $H_0(c) = cQ + Mc^2\tau$ be a Dirac operator with supersymmetry. Then for each $z \in \mathbb{C} \setminus \mathbb{R}$

$$\left(H_0(c) \mp Mc^2 - z\right)^{-1} =$$

$$\left(P_\pm \pm \frac{1}{c^2}\frac{cQ \pm z}{2M}\right)\left(1 \mp \frac{1}{c^2}\frac{z^2}{2M}\left(\pm H_{0,\infty} - z\right)^{-1}\right)^{-1}\left(\pm H_{0,\infty} - z\right)^{-1}. \quad (6.9)$$

Proof. Denoting

$$A_\pm = H_0(c) \pm Mc^2 \pm z = cQ \pm 2Mc^2P_\pm \pm z, \quad (6.10)$$

we find

$$A_+A_- = A_-A_+ = c^2Q^2 - 2Mc^2z - z^2, \quad (6.11)$$

from which we obtain

$$A_\pm^{-1} = \frac{A_\mp}{2Mc^2}\left(\frac{Q^2}{2M} - z - \frac{z^2}{2Mc^2}\right)^{-1}. \quad (6.12)$$

Using

$$(A+B)^{-1} = (1 + A^{-1}B)^{-1}A^{-1} \quad (6.13)$$

with

$$A \equiv \frac{Q^2}{2M} - z, \qquad B \equiv -\frac{z^2}{2Mc^2} \quad (6.14)$$

the result (6.9) follows immediately. □

The operators

$$T_\pm(c) \equiv \frac{1}{c^2}\frac{z^2}{2M}\left(\pm H_{0,\infty} - z\right)^{-1} \quad (6.15)$$

which occur in Eq. (6.9) are bounded with norm less than 1 for c sufficiently large (depending on z). In this case we can expand

$$\left(1 \mp T_\pm(c)\right)^{-1} = \sum_{n=0}^{\infty}\left(\pm T_\pm(c)\right)^n, \quad \text{if } \|T_\pm(c)\| < 1, \quad (6.16)$$

where the sum is convergent in the operator norm. As $c \to \infty$, $\|T_\pm(c)\| \to 0$, and we obtain from (6.9) the following corollary.

Corollary 6.2. Let $H_0(c) = cQ + Mc^2\tau$ be a supersymmetric Dirac operator. Then

$$\lim_{c\to\infty}\left(H_0(c) \mp Mc^2 - z\right)^{-1} = P_\pm\left(\pm H_{0,\infty} - z\right)^{-1}. \quad (6.17)$$

The limit in (6.17) is a norm-limit of bounded operators. In the standard representation (6.17) can be written in the form

$$\lim_{c\to\infty}\begin{pmatrix} -z & cD^* \\ cD & -2M_-c^2 - z \end{pmatrix}^{-1} = \begin{pmatrix} \left((2M_+)^{-1}D^*D - z\right)^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \tag{6.18}$$

resp.

$$\lim_{c\to\infty}\begin{pmatrix} 2M_+c^2 - z & cD^* \\ cD & -z \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \left(-(2M_-)^{-1}DD^* - z\right)^{-1} \end{pmatrix}. \tag{6.19}$$

Inserting (6.16) into (6.9) gives an expansion of the resolvent of the operator $H_0(c) \mp Mc^2$ into powers of $1/c$. Thus the resolvent is holomorphic in $1/c$ in a z-dependent neighborhood of $1/c = 0$. We extend this result to arbitrary Dirac operators of the form (6.5) in the next section. We finally mention the following corollary, which is immediate from Eq. (6.12).

Corollary 6.3. Let $M = m\mathbf{1}$, $m > 0$. Then $z \in \mathbb{C}$ is in the resolvent set of the Dirac operator $H_0(c) - mc^2$ if and only if $z(1 + z/2mc^2)$ is in the resolvent set of $H_{0,\infty} = Q^2/2m$.

6.1.3 Analyticity of the Resolvent

From now on we consider only the Dirac operator with rest energy subtracted. The calculations are similar in the other case.

Theorem 6.4. Let $H(c) = H_0(c) + V$ be defined as in (6.2)-(6.5). Then, for $\mathrm{Im}\,(z) \neq 0$,

$$(H(c) - Mc^2 - z)^{-1} =$$

$$= \left(P_+ + \frac{1}{c^2}\frac{cQ+z}{2M}\right) K(c^{-2}) \left(\mathbf{1} + \frac{1}{c^2} V \frac{cQ+z}{2M} K(c^{-2})\right)^{-1}, \tag{6.20}$$

where

$$K(c^{-2}) = \left(H_\infty - z - \frac{1}{c^2}\frac{z^2}{2M}\right)^{-1} = \left(\mathbf{1} - \frac{1}{c^2}\frac{z^2}{2M} R_\infty\right)^{-1} R_\infty, \tag{6.21}$$

$$R_\infty \equiv (H_\infty - z)^{-1}, \qquad H_\infty = \frac{Q^2}{2M} + VP_+. \tag{6.22}$$

and where P_+ is defined as in (6.7).

Proof. We denote

$$K_0 = \left(\frac{Q^2}{2M} - z - \frac{1}{c^2}\frac{z}{2M}\right)^{-1}, \tag{6.23}$$

and A_- as in Eq. (6.10). Hence we obtain from (6.12)

$$\left(H(\mathrm{c}) - Mc^2 - z\right)^{-1} = (A_- + V)^{-1} = A_-^{-1}(1 + VA_-^{-1})^{-1}$$

$$= \left(P_+ + \frac{1}{c^2}\frac{cQ+z}{2M}\right) K_0 \left(\mathbf{1} + VP_+K_0 + \frac{1}{c^2} V \frac{cQ+z}{2M} K_0\right)^{-1}. \tag{6.24}$$

The last factor $(\ldots)^{-1}$ can be written as

$$(1 + VP_+K_0)^{-1} \left(\mathbf{1} + \frac{1}{c^2} V \frac{cQ+z}{2M} K_0 (1 + VP_+K_0)^{-1}\right)^{-1}. \tag{6.25}$$

Finally, we arrive at the result (6.20), by using the relation

$$K(\mathrm{c}^{-2}) = K_0(\mathbf{1} + VP_+K_0)^{-1}. \tag{6.26}$$

□

Corollary 6.5. Let $H(\mathrm{c}) = H_0(c) + V$ be as above. Then the resolvent $(H(\mathrm{c}) - Mc^2 - z)^{-1}$, $\mathrm{Im}\,(z) \neq 0$, is holomorphic in $1/c$ in a z-dependent neighborhood of $1/\mathrm{c} = 0$,

$$(H(\mathrm{c}) - Mc^2 - z)^{-1} = \sum_{n=0}^{\infty} \frac{1}{c^n} R_n(z). \tag{6.27}$$

The sum converges in the operator norm. We have

$$R_0(z) = R_\infty P_+ = (H_\infty - z)^{-1} P_+, \tag{6.28}$$

$$R_1(z) = P_+ R_\infty \frac{Q}{2M} + \frac{Q}{2M} R_\infty P_+, \tag{6.29}$$

$$R_2(z) = R_\infty \frac{Q}{2M} \cdot \left(z - \left(\frac{Q^2}{2M} - z\right) R_\infty V\right) \frac{Q}{2M} R_\infty, \tag{6.30}$$

etc.

Proof. Since R_∞ is bounded for z with $\mathrm{Im}\, z \neq 0$ the operator $K(1/\mathrm{c}^2)$ is analytic in $1/\mathrm{c}^2$ for c sufficiently large. For any fixed $z \in \mathbb{C} \setminus \mathbb{R}$ the norm of the operator

$$\frac{1}{\mathrm{c}^2} T(\mathrm{c}) \equiv \frac{1}{\mathrm{c}^2} V \frac{cQ+z}{2M} K(\mathrm{c}^{-2}) \tag{6.31}$$

is less than 1 for c sufficiently large. In this case the operator $1 + T(\mathrm{c})/\mathrm{c}^2$ occurring in the last factor of (6.20) is invertible and hence (6.20) is analytic in $1/\mathrm{c}$ around $1/\mathrm{c} = 0$. From (6.21) we obtain as in (6.16) explicitly the series expansion of the operator $K(1/c^2)$

$$K(\mathrm{c}^{-2}) = R_\infty + \frac{1}{\mathrm{c}^2}\frac{z^2}{2M} R_\infty^2 + \frac{1}{c^4}\frac{z^4}{4M^2} R_\infty^3 + \ldots \tag{6.32}$$

Inserting this in the Neumann series of the operator $(1+T(\mathrm{c})/\mathrm{c}^2)^{-1}$ we obtain finally the series expansion of the Dirac resolvent. We have used the relation

$$\mathbf{1} - R_\infty P_+ V = R_\infty \left(\frac{Q^2}{2M} - z \right) \tag{6.33}$$

in order to obtain the above expressions for R_1 and R_2. □

Remark. The operators R_0 and R_2 are even (they commute with the unitary involution τ), whereas R_1 is odd (i.e., anticommutes with τ). More generally, in the expansion (6.27) all operators R_{2n} are even operators, and all R_{2n+1} are odd. This can be seen as follows. The only odd operator occurring (6.20) is $Q/2M\mathrm{c}$. It is also the only operator coming with $1/\mathrm{c}$, all other terms in (6.20) either contain a factor $1/\mathrm{c}^2$, or they do not at all depend on c. Therefore the only odd terms in the expansion (6.27) are those terms which contain an odd number of factors $Q/2M\mathrm{c}$, and these are precisely the terms containing an odd power of $1/\mathrm{c}$.

6.1.4 Nonrelativistic Limit with Anomalous Moments

As an example we consider the Dirac operator with an anomalous electric and magnetic moment. This operator has been defined in Sects. 4.2.3 and 4.2.4. The potential terms describing the interaction due to the anomalous moments are given by Eqs. (4.21) and (4.25). In these expressions we substitute $\mu_a = \mu e/2mc$ and $\delta_a = \delta e/2mc$ (where μ and δ are real numbers) and absorb the constant e into ϕ_{el} and $\boldsymbol{E} = -\nabla\phi_{\mathrm{el}}$. As explained in Remark 2 of Sect. 6.1.1, we also substitute A for $(e/\mathrm{c})\boldsymbol{A}$ and correspondingly B for $(e/\mathrm{c})\boldsymbol{B}$. With these conventions, the Dirac operator becomes

$$H = \begin{pmatrix} mc^2 + V_+(\mathrm{c}) & \mathrm{c}D^*(\mathrm{c}) \\ \mathrm{c}D(\mathrm{c}) & -mc^2 + V_-(\mathrm{c}) \end{pmatrix}, \tag{6.34}$$

$$D(\mathrm{c}) = \boldsymbol{\sigma} \cdot (\boldsymbol{p} - \boldsymbol{A}) - \mathrm{i}\tfrac{1}{2mc}\boldsymbol{\sigma} \cdot (\tfrac{\mu}{c}\boldsymbol{E} + \delta\boldsymbol{B}), \tag{6.35}$$

$$V_\pm(\mathrm{c}) = \phi_{\mathrm{el}} \pm \tfrac{1}{2m}\boldsymbol{\sigma} \cdot (\tfrac{\delta}{c}\boldsymbol{E} - \mu\boldsymbol{B}). \tag{6.36}$$

Although the operators D and $V_\pm$ (and hence Q and V) now depend on c, we can repeat the calculation in the previous section without changes. The leading term R_∞ of the Dirac resolvent now also depends on c. We obtain the expression

$$R_\infty(\mathrm{c}) = \begin{pmatrix} (H_{\mathrm{P}}(c) - z)^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \tag{6.37}$$

$$H_{\mathrm{P}}(\mathrm{c}) = \tfrac{1}{2m}D^*(\mathrm{c})D(\mathrm{c}) + V_+(\mathrm{c}). \tag{6.38}$$

A calculation similar to Eq. (5.79) gives

$$H_{\mathrm{P}}(\mathrm{c}) = \tfrac{1}{2m}[(\boldsymbol{p} - \boldsymbol{A})^2 - \boldsymbol{\sigma} \cdot \boldsymbol{B}] + \tfrac{1}{2mc^2}X^2$$

$$- \tfrac{1}{2mc}[\mathrm{i}\boldsymbol{\sigma} \cdot \mathrm{rot}\, \boldsymbol{X} + 2\boldsymbol{\sigma} \cdot \boldsymbol{X} \wedge (\boldsymbol{p} - \boldsymbol{A}) + \mathrm{div}\, \boldsymbol{X}]$$
$$+ \tfrac{1}{2m}\boldsymbol{\sigma} \cdot (\tfrac{\delta}{c}\boldsymbol{E} - \mu\boldsymbol{B}) + \phi_{\mathrm{el}}, \tag{6.39}$$

where $\boldsymbol{X} = \frac{1}{2m}(\frac{\mu}{c}\boldsymbol{E} + \delta\boldsymbol{B})$. Assume that the c-dependent terms are bounded with respect to

$$H_{\mathrm{P}}(\infty) \equiv \tfrac{1}{2m}(\boldsymbol{p} - \boldsymbol{A})^2 - \tfrac{1+\mu}{2m}\boldsymbol{\sigma} \cdot \boldsymbol{B} + \phi_{\mathrm{el}}. \tag{6.40}$$

Then the resolvent equation shows convergence in the operator norm of

$$(H_{\mathrm{P}}(c) - z)^{-1} \to (H_{\mathrm{P}}(\infty) - z)^{-1}, \quad \text{as } c \to \infty. \tag{6.41}$$

Hence we consider (6.40) as the nonrelativistic limit of the Dirac operator with anomalous moments (6.34). Finally, we may reintroduce the factor e/c and obtain the "Pauli operator"

$$H_{\mathrm{P}} \equiv \tfrac{1}{2m}(\boldsymbol{p} - \tfrac{e}{c}\boldsymbol{A})^2 - (1+\mu)\tfrac{e}{2mc}\boldsymbol{\sigma} \cdot \boldsymbol{B} + e\phi_{\mathrm{el}}. \tag{6.42}$$

The operator H_{P} describes nonrelativistic particles interacting with an electromagnetic field $(\phi_{\mathrm{el}}, \boldsymbol{A})$. A term of the form $\boldsymbol{\mu} \cdot \boldsymbol{B}$ describes the interaction energy of a magnetic moment μ in a magnetic field. The magnetic moment μ, which is measured in units of Bohr magnetons $e/2mc$, is proportional to the spin $\frac{1}{2}\boldsymbol{\sigma}$ of the particle,

$$\boldsymbol{\mu} = g\tfrac{e}{2mc}\tfrac{1}{2}\boldsymbol{\sigma}. \tag{6.43}$$

The constant in Eq. (6.43) is called g-factor of the particle. For particles with small anomalous moments like electrons the g-factor is approximately two. This has been observed experimentally before the invention of the Dirac equation. A comparison of (6.43) with (6.42) shows that the Dirac equation gives the right prediction: The ordinary Dirac operator (4.15) describes particles with g-factor exactly equal to 2. If there is an additional interaction of the form (4.21) we obtain $g = 2(1+\mu)$. An anomalous electric moment gives no contribution in the nonrelativistic limit.

6.2 c-Dependence of Eigenvalues

6.2.1 Browsing Analytic Perturbation Theory

In this section we state some mathematical results which are needed later. The reader is referred to the literature for the proofs of the various results[2].

Let H be a self-adjoint operator in a Hilbert space $\mathfrak{H}$. The resolvent set $\rho(H)$ is given by those complex numbers z for which the resolvent $R(z) = (H - z)^{-1}$ exists and is a bounded operator. The complement $\sigma(H) = \mathbb{C} \setminus \rho(H)$ (the spectrum of H) is a closed subset of the real axis. The singularities of $R(z)$ are just the eigenvalues of H. Let E be an isolated eigenvalue of H and let Γ be

[2] [Ka 80], [RS 78]

a closed positively oriented curve which encloses λ but no other part of $\sigma(H)$. Then

$$P \equiv -\frac{1}{2\pi \mathrm{i}} \oint_\Gamma R(z)\, dz \tag{6.44}$$

is an orthogonal projector onto the eigenspace belonging to the eigenvalue E. The multiplicity $m \equiv \dim P\mathfrak{H}$ of the eigenvalue is assumed to be finite. Then we have the following representation[3], of H in $P\mathfrak{H}$

$$PHP = EP = -\frac{1}{2\pi \mathrm{i}} \oint_\Gamma z\, R(z)\, dz. \tag{6.45}$$

An eigenvalue E is called nondegenerate, if $m = 1$.

Now, let $H(\kappa)$ be an operator valued function of a (possibly complex) variable κ, such that the resolvent $R(\kappa, z)$ is analytic in κ, i.e.,

$$R(\kappa, z) = \sum_{n=0}^{\infty} \kappa^n R_n(z), \qquad z \in \mathbb{C} \setminus \mathbb{R}, \tag{6.46}$$

where all $R_n(z)$ are bounded operators and the sum converges in the operator norm, uniformly on compact subsets of $\rho(H(0))$. Assume that E_0 is an isolated eigenvalue of $H(0)$, and define the closed curve Γ as in (6.44). Then

$$P(\kappa) = -\frac{1}{2\pi \mathrm{i}} \oint_\Gamma R(\kappa, z)\, dz \tag{6.47}$$

is (for sufficiently small $|\kappa|$) a projection onto an m-dimensionsal subset of $\mathcal{H}$ (the orthogonal direct sum of the eigenspaces of all the eigenvalues of $H(\kappa)$ lying inside Γ). Obviously, $P(\kappa)$ is analytic around $\kappa = 0$,

$$P(\kappa) = \sum_{n=0}^{\infty} \kappa^n P_n, \qquad P_n = -\frac{1}{2\pi \mathrm{i}} \oint_\Gamma R_n\, dz. \tag{6.48}$$

With the help of the projection operators $P(\kappa)$ and $P_0 = P(0)$ we define the unitary operator[4]

$$U(\kappa) = \big(\mathbf{1} - (P(\kappa) - P_0)^2\big)^{-1/2} \big(P(\kappa)P_0 + (\mathbf{1} - P(\kappa))(\mathbf{1} - P_0)\big) \tag{6.49}$$

Note that $A \equiv (P(\kappa) - P_0)^2$ commutes with $P(\kappa)$ and P_0. We can define the inverse square root in Eq. (6.49) as

$$(\mathbf{1} - A)^{-1/2} = \sum_{n=0}^{\infty} \binom{-\frac{1}{2}}{n} (-A)^n = \mathbf{1} + \tfrac{1}{2} A + \tfrac{3}{8} A^2 + \ldots, \tag{6.50}$$

if $\|A\| < 1$ which is the case for sufficiently small $|\kappa|$, because $\lim_{\kappa \to 0} P(\kappa) = P_0$ in the operator norm.

[3] [Ka 80], Sect. I.5
[4] [Ka 80], Sects. I.4.6 and I.6.8.

The operator valued function $U(\kappa)$ is called transformation function for $P(\kappa)$, because

$$U(\kappa)\,P_0 = P(\kappa)\,U(\kappa), \tag{6.51}$$

i.e., $U(\kappa)$ intertwines between the projections $P(\kappa)$ and P_0. Clearly, $U(\kappa)$ is analytic in κ around $\kappa = 0$, from the expansion of $P(\kappa)$ and Eq. (6.50), we obtain

$$U(\kappa)\,P_0 = P_0 + \kappa P_1 P_0 + \kappa^2 (P_2 P_0 + \tfrac{1}{2}\,P_1^2 P_0) + \ldots \tag{6.52}$$

Similarly as in Eq. (6.45) we can define an analytic family of bounded self-adjoint operators

$$P(\kappa)H(\kappa)P(\kappa) = -\frac{1}{2\pi \mathrm{i}} \oint_\Gamma z\,R(\kappa, z)\,dz. \tag{6.53}$$

The range of the projection $P(\kappa)$ is generally different for each κ. But with the help of the transformation function we can define an analytic family of bounded self-adjoint operators which is unitarily equivalent to (6.53) and which acts on one fixed subspace $P_0\mathfrak{H}$.

$$\begin{aligned}\tilde{H}(\kappa) &= U(\kappa)^{-1} P(\kappa) H(\kappa) P(\kappa) U(\kappa) \\ &= -\frac{1}{2\pi \mathrm{i}}\,P_0 U(\kappa)^{-1} \oint_\Gamma z\,R(\kappa, z)\,dz\,U(\kappa)P_0 \\ &= E_0 P_0 - \frac{1}{2\pi \mathrm{i}}\,P_0 U(\kappa)^{-1} \oint_\Gamma (z - E_0)\,R(\kappa, z)\,dz\,U(\kappa)P_0. \end{aligned} \tag{6.54}$$

Hence the problem of finding the eigenvalues of $H(\kappa)$ near the eigenvalue E_0 of $H(0)$ is completely reduced to the diagonalization of a self-adjoint operator in a finite dimensional Hilbert space. Hence we can apply the following theorem of Rellich.

Theorem 6.6. Let $\tilde{H}(\kappa)$ be a family of operators in a finite dimensional Hilbert space, such that $\tilde{H}(\kappa)$ is analytic in a neighborhood of $\kappa = 0$. Suppose that $\tilde{H}(\kappa)$ is self-adjoint for real κ and let E_0 be an eigenvalue of $\tilde{H}(0)$ with multiplicity m. Then there are $k < m$ distinct functions, $E^1(\kappa), \ldots, E^k(\kappa)$, which are analytic in κ in a neighborhood of $\kappa = 0$, and which are all eigenvalues of $\tilde{H}(\kappa)$ with multiplicities m^j, such that $\sum_{j=1}^k m_j = m$.

We also note that the eigenvectors of $\tilde{H}(\kappa)$ are simply given by

$$\phi^l(\kappa) = U(\kappa)\phi_0^l, \quad l = 1, \ldots, m, \tag{6.55}$$

where the vectors ϕ_0^l, form a basis of the eigenspace of H_0 belonging to the eigenvalue E_0. This result follows immediately from the fact that the unitary operator $U(\kappa)$ maps $P_0\mathfrak{H}$ onto $P(\kappa)\mathfrak{H}$. Analyticity of $\tilde{H}$ and its eigenvalues implies that there is an expansion of the form

$$\tilde{H}(\kappa) = \sum_{n=0}^{\infty} \tilde{H}_n, \qquad E^j(\kappa) = \sum_{n=0}^{\infty} E_n^j. \tag{6.56}$$

If E_0 is nondegenerate, then the first order term in the expansion of $E(\kappa)$, is given by

$$E_1 = (\phi_0, \tilde{H}_1 \phi_0). \tag{6.57}$$

If E_0 has multiplicity m, then $E^j(\kappa)$, $j = 1, \ldots, k$, are the eigenvalues of the self-adjoint $m \times m$ matrix

$$A_{jk} = (\phi_0^j, \tilde{H}_1 \phi_0^k). \tag{6.58}$$

6.2.2 The Reduced Dirac Operator

We apply the general results of the previous section to the Dirac operator $H(c) - Mc^2$. From Sect. 6.1.3 we know that the resolvent of this operator is analytic in 1/c, and

$$\lim_{c \to \infty} (H(c) - Mc^2 - z)^{-1} = (H_\infty - z)^{-1} P_+. \tag{6.59}$$

We assume that E_0 is an isolated eigenvalue with multiplicity m of the operator $H_\infty P_+$. The corresponding eigenspace $P_0 \mathfrak{H}$ is contained in $P_+ \mathfrak{H}$. Let Γ be a circle in $\mathbb{C}$ which separates E_0 from the rest of $\sigma(H_0)$. The projection operator

$$P(\tfrac{1}{c}) = -\frac{1}{2\pi \mathrm{i}} \oint_\Gamma (H(c) - Mc^2 - z)^{-1} \, dz \tag{6.60}$$

is analytic in $1/c$. We can define the transformation operator

$$U(\tfrac{1}{c}) = \big(\mathbf{1} - (P(\tfrac{1}{c}) - P_0)^2\big)^{-1/2} \big(P(\tfrac{1}{c}) P_0 + (\mathbf{1} - P(\tfrac{1}{c}))(\mathbf{1} - P_0)\big), \tag{6.61}$$

which is analytic in 1/c. We shall need the first term in the series expansion of $U(1/c)P_0$. From Eq. (6.52) it is clear that

$$\lim_{c \to \infty} U(\tfrac{1}{c}) P_0 = P_0 = \lim_{c \to \infty} P_0 U(\tfrac{1}{c}). \tag{6.62}$$

We are interested in the reduced Dirac operator

$$\tilde{H}(\tfrac{1}{c}) = U(\tfrac{1}{c})^{-1} P(\tfrac{1}{c}) (H(c) - Mc^2) P(\tfrac{1}{c}) U(\tfrac{1}{c})$$

$$= E_0 P_0 - \frac{1}{2\pi \mathrm{i}} P_0 U(\tfrac{1}{c})^{-1} \oint_\Gamma (z - E_0) \, (H(c) - Mc^2 - z)^{-1} \, dz \, U(\tfrac{1}{c}) P_0 \tag{6.63}$$

which is bounded and self-adjoint and analytic in $1/c$ for sufficiently large c. In order to obtain the series expansion of $\tilde{H}$ in powers of $1/c$, we note that

$$\oint_\Gamma (z - E_0) \, R_0(z) \, dz = 0, \qquad \oint_\Gamma (z - E_0) \, R_1(z) \, dz = 0. \tag{6.64}$$

This can be seen from the explicit forms of R_0, R_1 given in Eqs. (6.28), (6.29) and Cauchy's integral formula, because

$$-\frac{1}{2\pi \mathrm{i}} \oint_\Gamma (z - E_0)\, R_\infty(z)\, P_0\, dz = -\frac{1}{2\pi \mathrm{i}} \oint_\Gamma \frac{z - E_0}{E_0 - z}\, dz = 0. \tag{6.65}$$

Therefore the first nontrivial term in the $1/c$-expansion of Eq. (6.63) is given by

$$-\frac{1}{2\pi \mathrm{i}}\, P_0 \oint_\Gamma (z - E_0)\, \tfrac{1}{c^2}\, R_2(z)\, dz\, P_0. \tag{6.66}$$

But from Eq. (6.30) we find

$$P_0 R_2(z) P_0 = P_0\, \frac{Q}{2M}\, \frac{z - V}{(E_0 - z)^2}\, \frac{Q}{2M}\, P_0. \tag{6.67}$$

Hence, with Cauchy's integral formula we obtain immediately

$$\tilde{H}(\tfrac{1}{c}) = E_0 P_0 + \frac{1}{c^2}\, P_0\, \frac{Q}{2M}\, (V - E_0)\, \frac{Q}{2M}\, P_0 + \dots \tag{6.68}$$

Remark. It is easy to see that the expansion (6.68) contains only even powers of $1/c$. As we know from the remark at the end of Sect. 6.1.3, the $1/c^{2n+1}$-terms in the expansion of the resolvent are all odd operators. Hence the same is true for the expansions of $P(1/c)$ and hence for the series of $U(1/c)P_0$ and $P_0 U(1/c)^*$. Therefore, also in the series expansion of $\tilde{H}(1/c)$ the odd powers of $1/c$ can only occur with odd operators. But $\tilde{H}(1/c) = P_+ \tilde{H}(1/c) P_+$ is an even operator and hence it is anlaytic in $1/c^2$. It follows immediately from this observation and from Theorem 6.6 that the eigenvalues of $\tilde{H}(1/c)$ are analytic in $1/c^2$. Using first order perturbation theory we obtain the following results.

6.2.3 Analyticity of Eigenvalues and Eigenfunctions

Theorem 6.7. Let $H(c) = cQ + \tau Mc^2 + V$ be a Dirac operator defined as in Eqs. (6.2)–(6.5). Let E_0 be an isolated eigenvalue with finite multiplicity m of the operator $H_\infty P_+$, which is the nonrelativistic limit of $H(c) - Mc^2$ (cf. Theorem 6.4). Then $H(c) - Mc^2$ has $k \leq m$ distinct eigenvalues $E^j(1/c^2)$, $j = 1, \dots, k$, with multiplicities m_j (with $\sum_j m_j = m$), such that each E^j is analytic in $1/c^2$ in a neighborhood of $c = \infty$. The corresponding eigenvectors ψ^{j,r_j}, $r_j = 1, \dots m_j$ can be chosen in the form

$$\psi^{j,r_j}(c) = \phi_+^{j,r_j}(\tfrac{1}{c^2}) + \tfrac{1}{c}\, \phi_-^{j,r_j}(\tfrac{1}{c^2}), \qquad \phi_\pm^{j,r_j}(\tfrac{1}{c^2}) \in P_\pm \mathfrak{H}, \tag{6.69}$$

where $\phi_\pm^{j,r_j}(\frac{1}{c^2})$ are analytic in $1/c^2$.

Proof. The result follows immediately from the analyticity of $\tilde{H}(\frac{1}{c})$ and Theorem 6.6. By the remark at the end of the preceding section, the series expansion of $U(\frac{1}{c})$ is of the form

$$U(\tfrac{1}{c}) = U_{\text{even}}(\tfrac{1}{c^2}) + \tfrac{1}{c} U_{\text{odd}}(\tfrac{1}{c^2}) \tag{6.70}$$

Eq. (6.69) follows, because the eigenvectors of $H_\infty P_+$ belonging to isolated (i.e., nonzero) eigenvalues are in $P_+ \mathfrak{H}$. □

6.2.4 First Order Corrections of Nonrelativistic Eigenvalues

Theorem 6.8. Under the assumptions of Theorem 6.7, the eigenvalues E^j of the Dirac operator $H(c) - Mc^2$ have the expansion

$$E^j(\tfrac{1}{c^2}) = E_0 + \tfrac{1}{c^2} E_1^j + O(\tfrac{1}{c^4}), \tag{6.71}$$

where the E_1^j, $j = 1, \ldots, k$, are the eigenvalues of the self-adjoint matrix

$$A_{ik} = \Big(\frac{Q}{2M} \phi_0^i \,,\, (V - E_0) \frac{Q}{2M} \phi_0^k \Big). \tag{6.72}$$

The vectors $\phi_0^1, \ldots, \phi_0^m$ form an orthonormal system of eigenvectors of $H_\infty P_+$ belonging to the eigenvalue E_0.

Proof. See the discussion after Theorem 6.6. □

Remark 1. Note that all eigenvectors ϕ_0^j are in $P_+ \mathfrak{H}$. The commutation relation $(Q/2M)P_+ = P_-(Q/2M)$ shows that only the part V_- of V in $P_- \mathfrak{H}$ is relevant for the calculation of the $1/c^2$-correction to the nonrelativistic eigenvalue.

Remark 2. For a nondegenerate eigenvalue E_0, i.e., $H_\infty \phi_0 = E_0 \phi_0$, with $\|\phi_0\| = 1$, there is only one eigenvalue $E(1/c^2) = E_0 + E_1/c^2 + \ldots$ of $H(c) - Mc^2$, and Eq. (6.72) simplifies to

$$E_1 = \Big(\frac{Q}{2M} \phi_0 \,,\, (V - E_0) \frac{Q}{2M} \phi_0 \Big). \tag{6.73}$$

6.2.5 Interpretation of the First Order Correction

In the standard representation, we denote the component of $\psi_0 \in P_+ \mathfrak{H}$ by ψ_0^+. Let E_0 be a nondegenerate eigenvalue of $H_\infty P_+$ with corresponding eigenvector ψ_0, i.e.,

$$\Big(\frac{1}{2M_+} D^* D + V_+ \Big) \psi_0^+ = E_0 \psi_0^+. \tag{6.74}$$

According to Eq. (6.73) the first relativistic correction E_1 can be written in the form

$$E_1 = \Big(\frac{1}{2M_-} D\psi_0^+ \,,\, (V_- - E_0)\frac{1}{2M_-} D\psi_0^+\Big). \tag{6.75}$$

The scalar product in (6.75) is the scalar product in $P_-\mathfrak{H}$.

Let us now consider a special case, namely the electron in an electrostatic potential. We have $\mathfrak{H} = L^2(\mathbb{R}^3)^4$, $\tau = \beta$,

$$V_+(\boldsymbol{x}) = V_-(\boldsymbol{x}) = \phi_{\mathrm{el}}(\boldsymbol{x})\mathbf{1}_2, \qquad \boldsymbol{x} \in \mathbb{R}^3, \tag{6.76}$$

$$D = D^* = \boldsymbol{\sigma}\cdot\boldsymbol{p} = -\mathrm{i}\,\boldsymbol{\sigma}\cdot\nabla, \qquad M_+ = M_- = m. \tag{6.77}$$

The nonrelativistic limit of the Dirac operator $H(c) - mc^2$ is given in $L^2(\mathbb{R}^3)^2$ by the following "Schrödinger operator with spin"

$$H_\infty = \Big(-\frac{1}{2m}\Delta + \phi_{\mathrm{el}}(\boldsymbol{x})\Big)\,\mathbf{1}_2. \tag{6.78}$$

Thus the Schrödinger operator H_∞ describes particles with spin (i.e., two-component wavefunctions) but the spin does not interact with the electrostatic field.

Theorem 6.9. Assume $\phi_{\mathrm{el}}(\boldsymbol{x})$ is a twice continuously differentiable function of $\boldsymbol{x}$. Let ψ_0^+ be a nondegenerate bound state of H_∞, i.e., $H_\infty\psi_0^+ = E_0\psi_0^+$, and $\|\psi_0\| = 1$. Then a first approximation to the corresponding eigenvalue of the Dirac operator $c\boldsymbol{\alpha}\cdot\boldsymbol{p} + (\beta - \mathbf{1})mc^2 + \phi_{\mathrm{el}}\mathbf{1}$ is given by $E_0 + E_1/c^2$, where

$$\begin{aligned} E_1 &= \frac{1}{4m^2}\,(\boldsymbol{\sigma}\cdot\boldsymbol{p}\,\psi_0^+, (\phi_{\mathrm{el}} - E_0)\boldsymbol{\sigma}\cdot\boldsymbol{p}\,\psi_0^+) \\ &= \frac{1}{4m^2}\Big(\psi_0^+ \,,\, \Big\{-\frac{1}{2m}\,\boldsymbol{p}^4 + \boldsymbol{\sigma}\cdot(\nabla\phi_{\mathrm{el}})\wedge\boldsymbol{p} + \frac{1}{2}\,(\Delta\phi_{\mathrm{el}})\Big\}\,\psi_0^+\Big). \end{aligned} \tag{6.79}$$

Proof. Inserting (6.77) into (6.75) gives

$$\begin{aligned} E_1 &= \frac{1}{4m^2}\,(\psi_0^+, \boldsymbol{\sigma}\cdot\boldsymbol{p}\,(\phi_{\mathrm{el}} - E_0)\,\boldsymbol{\sigma}\cdot\boldsymbol{p}\,\psi_0^+) \\ &= \frac{1}{4m^2}\,(\psi_0^+, \{\boldsymbol{\sigma}\cdot\boldsymbol{p}\,\phi_{\mathrm{el}}\,\boldsymbol{\sigma}\cdot\boldsymbol{p} - E_0(\boldsymbol{\sigma}\cdot\boldsymbol{p})^2\}\,\psi_0^+) \\ = \quad &= \frac{1}{4m^2}\,\big(\psi_0^+, \{\boldsymbol{\sigma}\cdot\boldsymbol{p}\,\phi_{\mathrm{el}}\,\boldsymbol{\sigma}\cdot\boldsymbol{p} - \big(\frac{1}{2m}\boldsymbol{p}^2 + \phi_{\mathrm{el}}\big)(\boldsymbol{\sigma}\cdot\boldsymbol{p})^2\}\psi_0^+\big) \\ &= \frac{1}{4m^2}(\psi_0^+, \{-\frac{1}{2m}\boldsymbol{p}^4 + [\boldsymbol{\sigma}\cdot\boldsymbol{p}, \phi_{\mathrm{el}}]\boldsymbol{\sigma}\cdot\boldsymbol{p}\}\,\psi_0^+). \end{aligned} \tag{6.80}$$

Using $\boldsymbol{p} = -\mathrm{i}\nabla$ we obtain

$$[\boldsymbol{\sigma}\cdot\boldsymbol{p}, \phi_{\mathrm{el}}]\,\boldsymbol{\sigma}\cdot\boldsymbol{p} = -\mathrm{i}\,(\boldsymbol{\sigma}\cdot\nabla\phi_{\mathrm{el}})\,\boldsymbol{\sigma}\cdot\boldsymbol{p}. \tag{6.81}$$

From the relation (1.212) we get

$$[\boldsymbol{\sigma}\cdot\boldsymbol{p},\phi_{\mathrm{el}}]\boldsymbol{\sigma}\cdot\boldsymbol{p} = -(\nabla\phi_{\mathrm{el}})\cdot\nabla + \boldsymbol{\sigma}\cdot(\nabla\phi_{\mathrm{el}})\wedge\boldsymbol{p}. \tag{6.82}$$

Next we calculate

$$\begin{aligned}&(\psi_0^+, \tfrac{1}{2}(\Delta\phi_{\mathrm{el}})\psi_0^+ + (\nabla\phi_{\mathrm{el}})(\nabla\psi_0^+))\\ &= \tfrac{1}{2}(\psi_0^+, [\Delta,\phi_{\mathrm{el}}]\psi_0^+) = \tfrac{1}{2}(\psi_0^+, 2m[\phi_{\mathrm{el}} - E_0, \phi_{\mathrm{el}}]\psi_0^+) = 0.\end{aligned} \tag{6.83}$$

This gives finally

$$(\psi_0^+, [\boldsymbol{\sigma}\cdot\boldsymbol{p}, \phi_{\mathrm{el}}]\boldsymbol{\sigma}\cdot\boldsymbol{p}\psi_0^+) = (\psi_0^+, \{\tfrac{1}{2}(\Delta\phi_{\mathrm{el}}) + \boldsymbol{\sigma}\cdot(\nabla\phi_{\mathrm{el}})\wedge\boldsymbol{p}\}\psi_0^+). \tag{6.84}$$

□

Remark. The various terms in Eq. (6.79) have a nice interpretation. The term $-(2m)^{-3}\boldsymbol{p}^4$ is the *kinetic energy correction* of order $1/c^2$ as expected from the correspondence principle: In classical mechanics, the relativistic kinetic energy as a function of the momentum is given by

$$\sqrt{c^2\boldsymbol{p}^2 - m^2c^4} - mc^2 = \frac{1}{2m}\boldsymbol{p}^2 - \frac{1}{8m^3c^2}\boldsymbol{p}^4 + \mathrm{O}\Big(\frac{1}{c^4}\Big). \tag{6.85}$$

The second summand in Eq. (6.79), $(2m)^{-2}\boldsymbol{\sigma}\cdot(\nabla\phi_{\mathrm{el}})\wedge\boldsymbol{p}$, is called *spin orbit coupling term.* It can be explained as follows. The electron has a magnetic moment $\boldsymbol{\mu} = -(eg/2mc)\boldsymbol{S} = -(e/2mc)\boldsymbol{\sigma}$ (the Dirac equation without modifications describes electrons with g=2). The magnetic moment interacts with an external magnetic field, the corresponding contribution to the energy is $-\boldsymbol{\mu}\cdot\boldsymbol{B}$. According to the special theory of relativity, an observer moving with velocity $\boldsymbol{v}$ in an electrostatic field of strength $\boldsymbol{E}$ feels a magnetic field of strength $\boldsymbol{B} = -\boldsymbol{E}\wedge\boldsymbol{v}/c$. Hence we expect that the interaction energy of order $1/c^2$ is given by

$$-\frac{e}{2m^2c^2}\boldsymbol{\sigma}\cdot\boldsymbol{E}\wedge\boldsymbol{p}. \tag{6.86}$$

This is twice the spin orbit term, if we set $-e\boldsymbol{E} = \nabla\phi_{\mathrm{el}}$. But there is still another contribution coming from the Thomas precession. This is a purely kinematical effect in the special theory of relativity. An accelerated frame of reference performs an additional precession with the frequency

$$\boldsymbol{\omega} = -\frac{1}{2c^2}\dot{\boldsymbol{v}}\wedge\boldsymbol{v}. \tag{6.87}$$

For the motion in an electric field, the acceleration is given by $\dot{\boldsymbol{v}} = -e\boldsymbol{E}/m$. The precession of the spin axis gives an additional interaction term

$$\boldsymbol{\omega}\cdot\boldsymbol{S} = \frac{e}{4m^2c^2}\boldsymbol{\sigma}\cdot\boldsymbol{E}\wedge\boldsymbol{p}, \tag{6.88}$$

which combines with (6.86) to give the spin orbit coupling term. The last contribution to Eq. (6.79), $\frac{1}{8m^2}(\Delta\phi_{\mathrm{el}})$, is known as the *Darwin term.* It can be heuristically explained as an effect related to Zitterbewegung.

6.2.6 Example: Separable Potential

We calculate the first-order relativistic correction for the bound state of the radial Schrödinger equation with a separable potential V. A separable potential is an operator of finite rank. Given some $v \in L^2([0,\infty); dr)$ and $\gamma > 0$ we assume that V is of the form

$$V\phi = -\gamma\,(v,\phi)\,v, \quad \text{all } \phi \in L^2([0,\infty); dr), \tag{6.89}$$

where $(v,\phi) = \int_0^\infty \overline{v(r)}\,\phi(r)\,dr$ is the scalar product in $L^2([0,\infty); dr)$. The radial Schrödinger equation with orbital angular momentum $l = 0$ and energy $E < 0$ becomes

$$-\phi''(r) - \mu\,(v,\phi)\,v(r) = -\epsilon^2\phi(r), \tag{6.90}$$

where we have used the abbreviations

$$\mu = \frac{2m\gamma}{\hbar^2} > 0, \qquad \epsilon^2 = -\frac{2mE}{\hbar^2} > 0. \tag{6.91}$$

A Fourier transformation $\phi \to \hat{\phi}$, where $\hat{\phi}(k) = \sqrt{2/\pi}\int_0^\infty \phi(r)\,\sin(kr)\,dr$, converts Eq. (6.90) into

$$k^2\,\hat{\phi}(k) - \mu\,(v,\phi)\,\hat{v}(k) = -\epsilon^2\hat{\phi}(k). \tag{6.92}$$

Hence the solution ϕ_ϵ must satisfy

$$\hat{\phi}_\epsilon(k) = \mu\,(v,\phi_\epsilon)\,\hat{u}_\epsilon(k), \qquad \text{where} \quad \hat{u}_\epsilon(k) = \frac{\hat{v}(k)}{\epsilon^2 + k^2}. \tag{6.93}$$

From $(v,\phi_\epsilon) = (\hat{v},\hat{\phi}_\epsilon) = \mu\,(v,\phi_\epsilon)\,(\hat{v},\hat{u}_\epsilon)$ we find

$$(\hat{v},\hat{u}_\epsilon) = (v,u_\epsilon) = 1/\mu. \tag{6.94}$$

This equation can be used to determine an energy ϵ for which a square-integrable u_ϵ exists.

For the explicit calculation we assume that V is a "Yamaguchi potential",

$$v(r) = e^{-ar}, \quad a > 0, \qquad \text{i.e.,} \quad \hat{v}(k) = \sqrt{\frac{2}{\pi}}\,\frac{k}{a^2 + k^2}. \tag{6.95}$$

Hence we find

$$u_\epsilon(r) = \frac{e^{-ar} - e^{-\epsilon r}}{\epsilon^2 - a^2}, \qquad (v,u_\epsilon) = \frac{1}{2a(\epsilon + a)^2}. \tag{6.96}$$

Therefore, with Eq. (6.94) we conclude that

$$\epsilon = (\mu/2a)^{1/2} - a, \tag{6.97}$$

which is only positive for $\mu > 2a^3$ (otherwise u_ϵ is not square-integrable). In this case the radial Schrödinger equation with the Yamaguchi potential supports precisely one bound state ϕ_0 with energy E_0,

$$\phi_0(r) = \sqrt{2\epsilon a\,(\epsilon + a)^3}\; u_\epsilon(r), \qquad E_0 = -\frac{\hbar^2}{2m}\,\epsilon^2. \tag{6.98}$$

The normalization factor has been chosen such that $\|\phi_0\| = 1$.

With our previous notation we have

$$D = \hbar\left(\frac{d}{dr} - \frac{1}{r}\right), \qquad H_\infty = \frac{\hbar^2}{2m}\,\frac{d^2}{dr^2} + V, \tag{6.99}$$

and we can use Eq. (6.73) to calculate E_1,

$$\begin{aligned} E_1 &= \frac{\hbar^2}{4m^2}\left\{-\gamma\left|(v\,,\,\phi_0' - \phi_0/r\,)\right|^2 + E_0\,(\phi_0\,,\phi_0'')\right\} \\ &= -\frac{\hbar^4}{8m^3}\,\epsilon\,a\left\{a\,(\epsilon + a)\left[1 - 2\,\frac{\epsilon + a}{\epsilon - a}\ln\frac{\epsilon + a}{2a}\right]^2 - \epsilon^2\right\}. \end{aligned} \tag{6.100}$$

The separable potential discussed here can be regarded as a very simple model of the nucleon-nucleon interaction. For a rough estimate we insert for m the reduced mass of the proton-neutron system, $mc^2 = 469,46$ MeV, and choose $a = 1$, $\gamma = 124,3$ MeV fm^{-1}. Then we have $E_0 = -2.08$ MeV and $E_1/c^2 = -0.13$ MeV. The constants have been chosen to fit the bound state energy of the proton-neutron system (the deuteron), $E \approx E_0 + E_1/c^2 = -2.22$ MeV. We see that the relativistic correction gives a contribution of about 6% of the nonrelativistic bound state energy.

7 Special Systems

In this chapter we consider Dirac operators with some special external field configurations. We have chosen problems which permit a very detailed discussion because of an underlying supersymmetric structure.

We know already that a spin-1/2 particle moving in a magnetic field provides a canonical example of a supersymmetric system. Supersymmetry essentially determines the eigenvalues of the Dirac equation in a homogeneous magnetic field. A further consequence of supersymmetry is the equivalence of the Dirac equation with the Pauli equation for a nonrelativistic spin-1/2 particle in a magnetic field, but it will turn out that there are some striking differences to the problem without spin. A very important effect specific to particles with spin is the existence of eigenvalues at threshold. In two dimensions a complete solution of this problem can be obtained, which relates the number of threshold eigenvalues with the flux of the magnetic field. Hence we obtain the index of the Dirac operator, which is not a Fredholm operator in this case. Hence the index differs from the Witten index, which is calculated in Sect. 7.2.3. In three dimensions the index always vanishes and only some specific examples of magnetic fields with threshold bound states are known so far (Sect. 7.2.2).

In Sect. 7.3 we calculate the essential spectrum for Dirac operators with magnetic fields. A special difficulty occurs since a magnetic field which decays at infinity might require the introduction of an increasing vector potential. In this case one can still use the local gauge freedom to conclude the invariance of the essential spectrum. This result is optimal in two dimensions, where the spectrum is shown to be discrete for magnetic fields which do not vanish at large distances. In three dimensions, however, the essential spectrum seems to be always the same as for the free Dirac operator, even if the field strength increases at infinity. Another curious effect is that in two dimensions, for magnetic fields which decay slowly at infinity, the spectrum consists of a dense set of eigenvalues. In this case no scattering can occur; there are only bound states. This can be seen most easily from calculating explicit examples with cylindrical symmetry (Sect. 7.3.3).

Supersymmetry also plays a role in the Dirac Coulomb problem (Sect. 7.4). We treat this problem with the help of the angular momentum decomposition obtained in Sect. 4.6. We show that the radial Dirac equation can be transformed to a supersymmetric form which enables us to give an almost algebraic derivation of the Coulomb eigenvalues and eigenfunctions. The solvability of the Dirac-Coulomb problem is related to the existence of a conserved quantity, the Biedenharn-Johnson-Lippmann operator, which is the relativistic analogue of the Pauli-Runge-Lenz vector (Sect. 7.4.4). We also discuss the dependence of the eigenvalues on the coupling constant and compare the behavior with and without an anomalous magnetic moment. Finally we describe the scattering phase shifts of the Coulomb problem and the supersymmetric relation between δ_κ and $\delta_{-\kappa}$.

7.1 Magnetic Fields

7.1.1 Introduction

In any space dimension $n \geq 2$ the magnetic field strength B is described by a 2-form

$$B(x) = \sum_{\substack{i,k=1 \\ i<k}}^{n} F_{ik}(x)\, dx_i \wedge dx_k \tag{7.1}$$

satisfying $dB = 0$ (exterior derivative). Hence we can write $B = dA$, or

$$F_{ik}(x) = \frac{\partial A_i(x)}{\partial x_k} - \frac{\partial A_k(x)}{\partial x_i} \tag{7.2}$$

with the magnetic "vector" potential (1-form)

$$A(x) = \sum_{i=1}^{n} A_i(x)\, dx_i. \tag{7.3}$$

We want to stress that the vector potential is not directly observable. Therefore, one should formulate all results under assumptions on the field strengths. Eventually, we shall use the gauge freedom (see Sect. 4.4.3) to make the description as simple as possible.

Throughout this chapter we assume that each component of B is a smooth function in $\mathcal{C}^\infty(\mathbb{R}^n)$. In connection with the Dirac equation we are interested in dimensions $n = 2, 3$. For $n = 3$, the differential forms B and A can be identified with vector fields

$$\boldsymbol{B}(\boldsymbol{x}) = \big(F_{23}(\boldsymbol{x}), F_{31}(\boldsymbol{x}), F_{12}(\boldsymbol{x})\big), \quad \boldsymbol{A}(\boldsymbol{x}) = \big(A_1(\boldsymbol{x}), A_2(\boldsymbol{x}), A_3(\boldsymbol{x})\big), \tag{7.4}$$

satisfying $\boldsymbol{B} = \mathrm{rot}\boldsymbol{A}$, i.e., $\mathrm{div}\boldsymbol{B} = 0$. In two dimensions, the magnetic field strength $B = \partial_1 A_2 - \partial_2 A_1$ is simply a scalar field. This corresponds to the three-dimensional situation $\boldsymbol{B}(\boldsymbol{x}) = \big(0, 0, B(x_1, x_2)\big)$.

7.1.2 Dirac and Pauli Operators

We recall the Dirac operator with a magnetic field

$$\boldsymbol{H}(A) \equiv \begin{cases} c\sum_{i=1}^{3} \alpha_i(p_i - A_i) + \beta mc^2 & \text{if } n = 3, \\ c\sum_{i=1}^{2} \sigma_i(p_i - A_i) + \sigma_3 mc^2 & \text{if } n = 2. \end{cases} \tag{7.5}$$

It is essentially self-adjoint on $\mathcal{C}_0^\infty(\mathbb{R}^3)^4$, resp. $\mathcal{C}_0^\infty(\mathbb{R}^2)^2$, even without restriction on the growth of B or A at infinity (Theorem 4.3).

In the standard representation $H(A)$ has the abstract supersymmetric form

$$H(A) = \begin{pmatrix} mc^2 & cD^* \\ cD & -mc^2 \end{pmatrix}, \tag{7.6}$$

where

$$D \equiv \begin{cases} \sum_{i=1}^{3} \sigma_i (p_i - A_i) & \text{if } n = 3, \\ (p_1 - A_1) + \mathrm{i}(p_2 - A_2) & \text{if } n = 2. \end{cases} \tag{7.7}$$

Note that $D \neq D^*$ in two dimensions. The Pauli operator

$$H_{\mathrm{P}}(A) \equiv \frac{1}{2m} D^* D = \begin{cases} H_{\mathrm{S}}(A)\mathbf{1} - (1/2m)\boldsymbol{\sigma} \cdot \boldsymbol{B}, & \text{if } \nu = 3, \\ H_{\mathrm{S}}(A) - (1/2m)B, & \text{if } \nu = 2, \end{cases} \tag{7.8}$$

can be obtained as the nonrelativistic limit of $H(A)$ (cf. Sect. 6.1.2). Here, $H_{\mathrm{S}}(A) = \frac{1}{2m}(-\mathrm{i}\nabla - A)^2$ denotes the Schrödinger operator for a nonrelativistic spinless particle in a magnetic field.

The supersymmetric structure (7.6) and Corollary 5.14 immediately imply the following result.

Theorem 7.1. The spectrum of $H(A)$ is symmetric with respect to 0 except possibly at $\pm mc^2$. The open interval $(-mc^2, +mc^2)$ does not belong to the spectrum. We have

$H(A)\Psi = mc^2\Psi$ if and only if

$$\Psi = \begin{pmatrix} \psi_1 \\ 0 \end{pmatrix} \quad \text{with} \quad D^* D\psi_1 = 0 \quad (\text{equivalently } D\psi_1 = 0). \tag{7.9}$$

On the other hand,

$H(A)\Psi = -mc^2\Psi$ if and only if

$$\Psi = \begin{pmatrix} 0 \\ \psi_2 \end{pmatrix} \quad \text{with} \quad DD^*\psi_2 = 0 \quad (\text{equivalently } D^*\psi_2 = 0). \tag{7.10}$$

Hence in three dimensions, where $D^* = D$, the spectrum is always symmetric, even at $\pm mc^2$.

Remark. The use of the vector potential in quantum mechanics is sometimes counterintuitive, because the vector potential is usually nonzero in regions where the magnetic field strength vanishes. Consider, e.g., a magnetic field $B(x)$ in two dimensions with compact support and nonvanishing flux $\int B(x) d^2x$. Clearly in this case we expect the particle to move freely once it has left the support of B. But using Stokes law $\oint A\, ds = \int B\, d^2x$, where the circulation of A is taken along a large circle outside the support of B, we see that $A(x)$ cannot decay faster than $|x|^{-1}$, as $|x| \to \infty$. Hence the vector potential keeps influencing the wavefunction of the particle also at large distances from the support of B.

7.1.3 Homogeneous Magnetic Field

Supersymmetry essentially determines the spectrum of $H(A)$ in case of a homogeneous magnetic field $\boldsymbol{B}(\boldsymbol{x}) = (0, 0, B_0)$, where we assume $B_0 > 0$. For this situation it is sufficient to consider the two-dimensional Dirac operator $H(A)$ with the vector potential

$$A(x) = \frac{B_0}{2}(-x_2, x_1). \tag{7.11}$$

With $D = (-\mathrm{i}\,\partial_1 - A_1) + (\partial_2 - \mathrm{i}A_2)$ we find

$$DD^* = D^*D + 2B_0. \tag{7.12}$$

Hence the spectrum of DD^* equals the spectrum of D^*D shifted by $2B_0$. Since $D^*D \geq 0$, we have $DD^* \geq 2B_0$, i.e., DD^* has no spectrum in $[0, 2B_0)$. But supersymmetry implies $\sigma(D^*D) = \sigma(DD^*)$ except at 0, and therefore $\sigma(D^*D) \cap (0, 2B_0) = \emptyset$. Hence the first nonzero eigenvalue of D^*D can only occur at $2B_0$. The same chain of arguments works for the next interval $(2B_0, 4B_0)$. We conclude that

$$\sigma(D^*D) \subset \{0, 2B_0, 4B_0, \ldots\}, \tag{7.13}$$

$$\sigma(DD^*) \subset \{2B_0, 4B_0, \ldots\}. \tag{7.14}$$

Hence we find

$$\sigma(H(A)) \subset \left\{\sqrt{2nB_0 + mc^2}, -\sqrt{2(n+1)B_0 + mc^2} \;\middle|\; n = 0, 1, 2, \ldots\right\}. \tag{7.15}$$

In order to obtain "$\supset$" and the eigenfunctions we proceed as follows: Assume $D^*D\psi_0 = 0$ or equivalently $D\psi_0 = 0$ for some $\psi_0 \in L^2(\mathbb{R}^2)$. At the same time ψ_0 is an eigenvector of DD^*, because from (7.12) we obtain $DD^*\psi_0 = 2B_0\psi_0$. This shows that $2B_0 \in \sigma(DD^*)$ provided $0 \in \sigma(D^*D)$. Supersymmetry implies that $\psi_1 \equiv D^*\psi_0$ is an eigenvector of D^*D belonging to the same eigenvalue $2B_0$. Applying (7.12) again we find $DD^*\psi_1 = 4B_0\psi_1$. If we proceed in this way we obtain a sequence of eigenvectors $\psi_n \equiv (D^*)^n\psi_0$, $n = 0, 1, 2, \ldots$ satisfying

$$\begin{aligned} D^*D\psi_n &= 2nB_0\psi_n, \\ DD^*\psi_n &= 2(n+1)B_0\psi_n, \quad n = 0, 1, 2, \ldots \end{aligned} \tag{7.16}$$

The corresponding eigenvectors of the Dirac equation can be found by an inverse Foldy-Wouthuysen transformation (Sect. 5.6.1):

$$H(A)\,U_{\mathrm{FW}}^{-1}\begin{pmatrix}\psi_n\\0\end{pmatrix} = \sqrt{2nB_0 + mc^2}\,U^{-1}\begin{pmatrix}\psi_n\\0\end{pmatrix}, \tag{7.17}$$

$$H(A)\,U_{\mathrm{FW}}^{-1}\begin{pmatrix}0\\\psi_n\end{pmatrix} = -\sqrt{2(n+1)B_0 + mc^2}\;U^{-1}\begin{pmatrix}0\\\psi_n\end{pmatrix}. \tag{7.18}$$

Hence everything depends on whether we can find a ψ_0 with $D\psi_0 = 0$ or equivalently a solution of the Dirac equation with energy mc^2. This will be done next.

We define an auxiliary scalar field

$$\phi(x) \equiv \frac{B_0}{4}(x_1^2 + x_2^2), \tag{7.19}$$

such that

$$A(x) = \nabla \wedge \phi = (-\partial_2\phi, \partial_1\phi), \quad \text{i.e.,} \quad \triangle\phi(x) = B(x). \tag{7.20}$$

Then it is easy to verify that if $D\psi_0 = 0$ the function

$$\omega \equiv e^{\phi}\psi_0 \tag{7.21}$$

satisfies

$$0 = De^{-\phi}\omega = -\mathrm{i}\,e^{-\phi}(\partial_1 + \mathrm{i}\,\partial_2)\omega \tag{7.22}$$

The equation

$$\frac{\partial\omega}{\partial x_1} + \mathrm{i}\,\frac{\partial\omega}{\partial x_2} = 0 \tag{7.23}$$

is equivalent to the Cauchy-Riemann equations. Hence ω must be an entire analytic function of $x_1 + \mathrm{i}\,x_2$. There is one further restriction, namely that $e^{-\phi}\omega = e^{-B_0x^2/4}\omega = \psi_0$ must be square integrable. Hence any polynomial in $x_1 + \mathrm{i}\,x_2$ gives a solution $\psi_0^{m_j}$ of $D\psi_0^{m_j} = 0$, if we set

$$\psi_0^{m_j} = e^{-\frac{B_0}{4}(x_1^2+x_2^2)}\,(x_1 + \mathrm{i}\,x_2)^{m_j - \frac{1}{2}}, \tag{7.24}$$

where $m_j \in \{\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots\}$. Moreover,

$$J_3\begin{pmatrix}\psi_0^{m_j}\\ 0\end{pmatrix} = m_j\begin{pmatrix}\psi_0^{m_j}\\ 0\end{pmatrix}, \tag{7.25}$$

where $J_3 = -\mathrm{i}\,x_1\partial_2 + \mathrm{i}\,x_2\partial_1 + \sigma_3/2$ is the angular momentum of the particle. We collect our results in the following theorem.

Theorem 7.2. The Dirac operator in two dimensions with a constant magnetic field B_0 has the eigenvalues

$$\sqrt{2nB_0 + mc^2}, \quad -\sqrt{2(n+1)B_0 + mc^2}, \quad n = 0, 1, 2, \ldots. \tag{7.26}$$

Each eigenvalue is infinitely degenerate.

If we start with $B_0 < 0$ the reasoning is analogous, but we obtain an eigenvalue $-mc^2$ instead of $+mc^2$ of $H(A)$. The missing supersymmetry at $\pm mc^2$ is quite typical in two dimensions as we shall learn in the following section.

7.2 The Ground State in a Magnetic Field

7.2.1 Two Dimensions

The method of finding the ground state of the Dirac operator which we applied in the last section can be used to obtain the following result

Theorem 7.3. In two dimensions, let $B(x)$ be a magnetic field with compact support, and denote

$$F = \frac{1}{2\pi}\int_{\mathbb{R}^2} B(x)d^2x. \tag{7.27}$$

a) If $F = n+\epsilon$ (where n is a positive integer, and $0 \le \epsilon < 1$), then $+mc^2$ (but not $-mc^2$) is an eigenvalue of the Dirac operator $H(A)$ defined in (7.5).
b) If $F = -n-\epsilon$, then $-mc^2$ (but not $+mc^2$) is an eigenvalue of $H(A)$.

In both cases the multiplicity of the eigenvalue is n, if $\epsilon > 0$, and $n-1$, if $\epsilon = 0$.

Proof. The Green function of $\triangle$ in two dimensions is $\frac{1}{2\pi}\ln|x-y|$, therefore

$$\phi(x) = \frac{1}{2\pi}\int_{\mathbb{R}^2} \ln|x-y|B(y)d^2y \tag{7.28}$$

satisfies $\triangle\phi(x) = B(x)$, and

$$\phi(x) - F\ln|x| = O\Big(\frac{1}{|x|}\Big), \quad \text{as } |x| \to \infty. \tag{7.29}$$

We choose the vector potential $A = (-\partial_2\phi, \partial_1\phi)$, and look for a solution of

$$c\boldsymbol{\sigma}\cdot(p-A)\psi = 0, \quad \boldsymbol{\sigma} = (\sigma_1, \sigma_2). \tag{7.30}$$

Writing

$$\omega = \mathrm{e}^{\sigma_3\phi}\psi \tag{7.31}$$

we find that (7.30) is equivalent to

$$\boldsymbol{\sigma}\cdot p\,\omega = 0 \quad \text{or} \quad \begin{cases} \Big(\dfrac{\partial}{\partial x_1} + \mathrm{i}\dfrac{\partial}{\partial x_2}\Big)\omega_1(x) = 0, \\ \Big(\dfrac{\partial}{\partial x_1} - \mathrm{i}\dfrac{\partial}{\partial x_2}\Big)\omega_2(x) = 0. \end{cases} \tag{7.32}$$

These equations are equivalent to the Cauchy-Riemann equations. Hence ω_1 (resp. ω_2) has to be an entire analytic function in the variable $z = x_1 + \mathrm{i}x_2$ (resp. $\overline{z} = x_1 - \mathrm{i}x_2$). For large $|z| = |x|$ these functions behave as

$$\omega_1(x) \approx e^{+F\ln|x|}\psi_1(x) = |x|^{+F}\psi_1(x), \tag{7.33}$$

$$\omega_2(x) \approx e^{-F\ln|x|}\psi_2(x) = |x|^{-F}\psi_2(x). \tag{7.34}$$

If $F > 0$ then ω_2 is square integrable at infinity and hence zero, because an analytic function cannot vanish in all directions, as $|z| \to \infty$. This shows that $\psi_2 = 0$ and therefore only $+mc^2$ can be an eigenvalue of $H(A)$. But for this we have to fulfill the condition

$$\psi_1 = e^{-\phi}\omega_1 \in L^2(\mathbb{R}^2), \tag{7.35}$$

which requires that ω_1 should not increase faster than $|x|^{F-1-\delta}$, for some $\delta > 0$. Since ω_1 is an entire function, it must be a polynomial in $x_1 + \mathrm{i}\,x_2$ of degree $\leq n-1$ (resp. $n-2$, if $\epsilon = 0$). Hence there are n linearly independent solutions ψ_1 of $D\psi_1 = 0$, namely (for $\epsilon \neq 0$)

$$\mathrm{e}^{-\phi},\ \mathrm{e}^{-\phi}(x_1 + \mathrm{i}\,x_2),\ e^{-\phi}(x_1 + \mathrm{i}\,x_2)^2,\ \ldots\ ,\ e^{-\phi}(x_1 + \mathrm{i}\,x_2)^{n-1}. \tag{7.36}$$

An analogous reasoning applies to the case $F < 0$. □

7.2.2 Three Dimensions

There is no analogue of Theorem 7.3 in three dimensions. Concerning the existence of eigenvalues at $\pm mc^2$, only some examples are known so far.

Example 7.4. If we had a solution of

$$\boldsymbol{\sigma} \cdot \boldsymbol{p}\, \Psi(\boldsymbol{x}) = \lambda(\boldsymbol{x})\Psi(\boldsymbol{x}) \tag{7.37}$$

for some real-valued λ, which satisfies

$$\big(\Psi, \Psi\big)_2(\boldsymbol{x}) \equiv \sum_{i=1}^{2} \overline{\psi_i(\boldsymbol{x})}\, \psi_i(\boldsymbol{x}) \neq 0, \tag{7.38}$$

then we could find a vector potential $\boldsymbol{A}$ and a solution of $\boldsymbol{\sigma} \cdot (\boldsymbol{p} - \boldsymbol{A})\, \Psi = 0$. First note that it follows from

$$\big(\Psi, \boldsymbol{\sigma}\Psi\big)_2^2 = \sum_{i=1}^{3} \big(\Psi, \sigma_i \Psi\big)_2^2 = \big(\Psi, \Psi\big)_2^2, \tag{7.39}$$

that Ψ satisfies

$$\sum_{i=1}^{3} \frac{\sigma_i\, (\Psi, \sigma_i \Psi)_2}{(\Psi, \Psi)_2}\, \Psi = \Psi, \tag{7.40}$$

and hence

$$\boldsymbol{\sigma} \cdot \boldsymbol{A}(\boldsymbol{x})\, \Psi(\boldsymbol{x}) = \lambda(\boldsymbol{x})\, \Psi(\boldsymbol{x}), \tag{7.41}$$

if we choose

$$\boldsymbol{A}(\boldsymbol{x}) = \lambda(\boldsymbol{x})\, \frac{(\Psi, \boldsymbol{\sigma}\Psi)_2}{(\Psi, \Psi)_2}. \tag{7.42}$$

But a solution of (7.37) is easy to find. Choose, for example,

$$\Psi(\boldsymbol{x}) = \frac{1 + \mathrm{i}\,\boldsymbol{\sigma}\cdot\boldsymbol{x}}{(1+x^2)^{3/2}}\,\Phi_0, \tag{7.43}$$

where $\Phi_0 \in \mathbb{C}^2$, with $(\Phi_0, \Phi_0)_2 = 1$. Note that

$$0 \neq \big(\Psi, \boldsymbol{\sigma}\Psi\big)_2(\boldsymbol{x}) = \frac{1}{(1+x^2)^3}\,\{(1-x^2)\boldsymbol{w} + 2(\boldsymbol{w}\cdot\boldsymbol{x})\boldsymbol{x} + 2\boldsymbol{w}\wedge\boldsymbol{x}\}, \tag{7.44}$$

where $w = (\Phi_0, \boldsymbol{\sigma}\Phi_0)_2$ is a unit vector in $\mathbb{R}^3$. We obtain

$$\boldsymbol{\sigma}\cdot\boldsymbol{p}\;\Psi(\boldsymbol{x}) = \frac{3}{1+x^2}\,\Psi(\boldsymbol{x}), \tag{7.45}$$

and finally

$$\boldsymbol{A}(\boldsymbol{x}) = 3(1+x^2)\,(\Psi, \boldsymbol{\sigma}\Psi)_2, \qquad \boldsymbol{B}(\boldsymbol{x}) = 12\,(\Psi, \boldsymbol{\sigma}\Psi)_2. \tag{7.46}$$

The vector field A can be obtained by stereographic projection from a parallel basis vector field on the three-dimensional sphere. Hence the flow lines are circles on the Hopf tori.

7.2.3 Index Calculations

Theorem 7.3 shows that for a magnetic field with compact support in two dimensions the index of the operator

$$Q = c\boldsymbol{\sigma}\cdot(\boldsymbol{p} - \boldsymbol{A}) \quad \text{in } L^2(\mathbb{R}^3)^2 \tag{7.47}$$

is given by

$$\operatorname{ind} Q = (\operatorname{sgn} F)\cdot\begin{cases} n, & \text{if } F = n + \epsilon, \\ n-1, & \text{if } F = n. \end{cases} \tag{7.48}$$

Here F is the flux of the magnetic field, n a positive integer, and $0 < \epsilon < 1$. In three dimensions, since $D = D^*$, the index vanishes. The operator Q is not Fredholm, because under the assumptions of Theorem 7.3 we have (see Remark 2 in Sect. 5.7.1 and Theorem 7.7 below)

$$\sigma_{\mathrm{ess}}(Q^2) = \sigma_{\mathrm{ess}}(H(\boldsymbol{A})^2 - m^2c^4) = [0, \infty). \tag{7.49}$$

It is interesting to compare (7.48) with the result for the Witten index.

Theorem 7.5. Under the assumptions of Theorem 7.3, we have

$$\operatorname{ind}_z Q = F. \tag{7.50}$$

Proof. Here we only give a sketch of the proof, see the Notes for references. One considers a suitable class of magnetic fields with a fixed value of the flux $F = \frac{1}{2\pi}\int B(\boldsymbol{x})\,d^2\boldsymbol{x}$ and defines the Hamiltonians

$$H_1 = D^*D, \qquad H_2 = DD^* = H_1 + 2B(x). \tag{7.51}$$

One first shows that the interaction satisfies suitable trace class conditions, which imply that Krein's spectral shift function $\xi(\lambda)$ is independent of the magnetic field in the class and depends only on the flux F (see Theorem 5.28). Next one considers as an example the family $\{B^R \mid R > 0\}$ of magnetic fields with flux F, where $B^R(x) = \triangle\phi^R(x)$, and

$$\phi^R(x) = F \begin{cases} \frac{|x|^2}{2R^2} + \frac{1}{2} - \ln R, & |x| \le R, \\ \ln|x|, & |x| \ge R, \end{cases} \qquad R > 0. \tag{7.52}$$

We have $\phi^R \in \mathcal{C}^2(\mathbb{R}^2)$ and the corresponding Hamiltonians H_j^R, $j = 1, 2$, satisfy the following scaling properties,

$$U_\epsilon H_j^R U_\epsilon^{-1} = \epsilon H_j^{\epsilon R}, \qquad \epsilon, R > 0, \quad j = 1, 2, \tag{7.53}$$

where

$$U_\epsilon \psi(x) = \psi(x/\epsilon)/\epsilon, \qquad \text{all } \psi \in L^2(\mathbb{R}^2). \tag{7.54}$$

Let $S^R(\lambda)$ be the on-shell scattering operator in $L^2(S^1)$ which is associated with the scattering system (H_1^R, H_2^R) (see Sect. 8.1). Eq. (7.54) implies

$$S^R(\lambda) = S^{R/\epsilon}(\epsilon^2\lambda), \qquad \epsilon, R, \lambda > 0, \tag{7.55}$$

and for Krein's function $\xi^R(\lambda)$, which is related to the S matrix by (see also Theorem 8.4)

$$S^R(\lambda) = e^{-2\pi i \xi^R(\lambda)}, \qquad \text{for almost every } \lambda \in \sigma_{\text{a.c.}}(H_2^R) = [0, \infty), \tag{7.56}$$

we obtain the same scaling properties,

$$\xi^R(\lambda) = \xi^{R/\epsilon}(\epsilon^2\lambda), \qquad \epsilon, R, \lambda > 0. \tag{7.57}$$

But since the magnetic fields B^R all have the same flux F, we find that $\xi^R(\lambda)$ cannot depend on R, hence Eq. (7.57) implies that Krein's spectral shift function for $\lambda > 0$ cannot depend on λ either. From Eq. (5.153) we obtain

$$\operatorname{ind}_z Q = \xi_0, \tag{7.58}$$

where ξ_0 is the constant value of the spectral shift function for $\lambda > 0$. Hence the regularized index $\operatorname{ind}_z Q$ does not depend on z. It is most easily calculated in the limit $z \to \infty$. Iterating the resolvent equation and using appropriate Bessel function estimates one obtains, with $H_0 = -\triangle$,

$$\begin{aligned} \operatorname{ind}_z Q &= \lim_{\substack{z\to\infty \\ |\arg z| > \epsilon > 0}} z \operatorname{tr}\left[(H_2 - z)^{-1}(-2B)(H_2 - z)^{-1}\right] \\ &= \lim_{\substack{z\to\infty \\ |\arg z| > \epsilon > 0}} z \operatorname{tr}\left[(H_0 - z)^{-1}(-2B)(H_0 - z)^{-1}\right] \\ &= \frac{1}{2\pi}\int_{\mathbb{R}^2} B(x)\, d^2x = F. \end{aligned} \tag{7.59}$$

□

7.3 Magnetic Fields and the Essential Spectrum

7.3.1 Infinitely Degenerate Threshold Eigenvalues

The proof of the Theorem 7.3 shows that if one can find a solution ϕ of $\triangle\phi(x) = B(x)$, such that $e^{-\phi}$ (or $e^{+\phi}$) is a rapidly decreasing function in $\mathcal{S}(\mathbb{R}^3)$, then the eigenvalue $+mc^2$ (or $-mc^2$) is infinitely degenerate and hence in $\sigma_{\text{ess}}(H(A))$. As we have seen, this is indeed the case for a homogeneous magnetic field.

In case of a cylindrically symmetric magnetic field in two dimensions ($B(x) = B(r)$, $r = |x|$) a solution of $\triangle\phi(r) = \big(\partial^2/\partial r^2 + (1/r)\partial/\partial r\big)\phi(r) = B(r)$ is given by

$$\phi(r) = \int_0^r ds\, \frac{1}{s} \int_0^s dt\, B(t)\, t. \tag{7.60}$$

Hence for a magnetic field with infinite flux like

$$B(r) \sim r^{\delta-2}, \quad \text{for some } \delta > 0,\ r \text{ large}, \tag{7.61}$$

we find

$$\phi(r) \sim \delta^{-2}\, r^{\delta}, \quad \text{for } r \text{ large}, \tag{7.62}$$

i.e., $e^{-\phi}$ decreases faster than any polynomial in $|x|$. Therefore $+mc^2$ is infinitely degenerate in this case. If even $B(r) \to \infty$, as $r \to \infty$, then the next theorem shows, that $+mc^2$ is the only possible point in the essential spectrum of the Dirac operator.

Theorem 7.6. If in two dimensions $B(x) \to \infty$ (resp. $B(x) \to -\infty$), as $|x| \to \infty$, then λ with $\lambda \neq +mc^2$ (resp. $\lambda \neq -mc^2$) is not in the essential spectrum of the Dirac operator.

Proof. We assume $B(x) \to +\infty$, the other case can be treated analogously. We show that λ with $\lambda \neq mc^2$ is not in $\sigma_{\text{ess}}(H(A))$, because for all $\Psi = \binom{\psi_1}{\psi_2}$ in $C_0^\infty(\mathbb{R}^2)^2$ with support outside a ball with sufficiently large radius R there is a constant $C(\lambda)$ such that

$$\big\|\big(H(A) - \lambda\big)\Psi\big\| \geq C(\lambda)\, \|\Psi\|. \tag{7.63}$$

In order to prove this, we choose R so large, that

$$B(x) \geq \frac{1}{c^2}|\lambda - mc^2|(3 + 2|\lambda + mc^2|), \quad \text{for all } |x| \geq R. \tag{7.64}$$

Denoting $\Phi = \binom{\phi_1}{\phi_2} = \big(H(A) - \lambda\big)\Psi$, i.e.,

$$\begin{aligned} \phi_1 &= cD^*\psi_2 - (\lambda - mc^2)\psi_1, \\ \phi_2 &= cD\psi_1 - (\lambda + mc^2)\psi_2, \end{aligned} \tag{7.65}$$

we find

$$\|D^*\psi_2\|^2 = (\psi_2, D^*D\psi_2) = \|(p-A)^2\psi_2\|^2 + (\psi_2, B(x)\psi_2)$$
$$\geq \frac{1}{c^2}\,|\lambda - mc^2|\,(3 + 2|\lambda + mc^2|)\,\|\psi_2\|^2, \tag{7.66}$$

provided $\operatorname{supp}\psi_2$ is outside the ball with radius R. Hence

$$(3 + 2|\lambda + mc^2|)\|\psi_2\|^2 \leq \frac{1}{|\lambda - mc^2|}\,\|\phi_1 + (\lambda - mc^2)\psi_1\|^2$$
$$= \frac{1}{|\lambda - mc^2|}\,\|\phi_1\|^2 + 2(\operatorname{sgn}\lambda)\operatorname{Re}(\phi_1, \psi_1) + |\lambda - mc^2|\,\|\psi_1\|^2. \tag{7.67}$$

Since

$$(\operatorname{sgn}\lambda)\operatorname{Re}(\phi_1, \psi_1) = (\operatorname{sgn}\lambda)\operatorname{Re}(cD^*\psi_2, \psi_1) - |\lambda - mc^2|\,\|\psi_1\|^2$$
$$\leq \|\psi_2\|\,\|cD\psi_1\| - |\lambda - mc^2|\,\|\psi_1\|^2$$
$$\leq \|\psi_2\|\,\|\phi_2\| + |\lambda + mc^2|\,\|\psi_2\|^2 - |\lambda - mc^2|\,\|\psi_1\|^2 \tag{7.68}$$

we find

$$3\,\|\psi_2\|^2 + |\lambda - mc^2|\,\|\psi_1\|^2 \leq \frac{1}{|\lambda - mc^2|}\,\|\phi_1\|^2 + 2\|\psi_2\|\,\|\phi_2\|. \tag{7.69}$$

Now we have either $\|\psi_2\| \leq \|\phi_2\|$ or $\|\psi_2\| \geq \|\phi_2\|$. In each case

$$\|\Psi\|^2 = \|\psi_1\|^2 + \|\psi_2\|^2 \leq 2\max\left\{1, \frac{1}{(\lambda - mc^2)^2}\right\}\,\|\Phi\|^2, \tag{7.70}$$

which proves the theorem. □

7.3.2 A Characterization of the Essential Spectrum

We want to determine the essential spectrum of the Dirac operator with a magnetic field $B(x)$ which tends to 0, as $|x| \to \infty$. Our results of Sect. 4.3.4 cannot be applied, because the potential matrix need not decay at infinity. For example, the vector potential of a two-dimensional magnetic field with infinite flux might even increase (see the remark at the end of Sect. 7.1.2).

Theorem 7.7. In two or three dimensions, if $|B(x)| \to 0$, as $|x| \to \infty$, then

$$\sigma_{\text{ess}}(H(A)) = (-\infty, -mc^2] \cup [mc^2, \infty). \tag{7.71}$$

Proof. It is sufficient to consider the essential spectrum of the operator

$$D_\nu = c\sum_{i=1}^{\nu} \sigma_i(p_i - A_i) \equiv c\boldsymbol{\sigma}\cdot(p - A) \tag{7.72}$$

in dimensions $\nu = 2, 3$, because $H(A)$ is unitarily equivalent to

$$\sigma_3\sqrt{(D_2)^2 + m^2c^4} \quad \text{for } \nu = 2, \tag{7.73}$$

and

$$\begin{pmatrix} \sqrt{(D_3)^2 + m^2c^4}\,\mathbf{1} & 0 \\ 0 & -\sqrt{(D_3)^2 + m^2c^4}\,\mathbf{1} \end{pmatrix} \quad \text{for } \nu = 3. \tag{7.74}$$

In order to prove $k \in \sigma_{\text{ess}}(D_\nu)$ it is sufficient to find an orthonormal sequence of vectors $\Psi^{(n)}$ in the domain of D_ν, such that

$$\lim_{n\to\infty} \|(D_\nu - k)\Psi^{(n)}\| = 0 \tag{7.75}$$

(Weyl's criterion). Moreover, the distance between k and $\sigma_{\text{ess}}(D_\nu)$ is less than d, if for a suitable orthonormal sequence $\Psi^{(n)}$

$$\|(D_\nu - k)\Psi^{(n)}\| \leq d. \tag{7.76}$$

We are going to construct suitable vectors $\Psi^{(n)}$ as follows. Let $B_n = B_{\rho_n}(x^{(n)})$ be a sequence of disjoint balls with centers $x^{(n)}$ and radii ρ_n. Any two L^2-functions with support in different balls are orthogonal. We use the gauge freedom to define within these balls vector potentials $A^{(n)}$ which are determined by the local properties of B in that region (unlike the original A-field). For each n we define

$$A^{(n)}(x) = \int_0^1 B\big(x^{(n)} + (x - x^{(n)})s\big) \wedge (x - x^{(n)})\, s\, ds, \tag{7.77}$$

or, written in components $(i = 1, \ldots, \nu)$

$$A_i^{(n)}(x) = \int_0^1 \sum_{i=1}^{\nu} F_{ki}\big(x^{(n)} + (x - x^{(n)})s\big)(x_k - x_k^{(n)})\, s\, ds. \tag{7.78}$$

It is easy to see that

$$\sup_{x\in B_n} |A^{(n)}(x)| \leq \rho_n \sup_{x\in B_n} |B(x)|. \tag{7.79}$$

Furthermore, if A is the vector potential we started with, then

$$A - A^{(n)} = \nabla g^{(n)}, \quad \text{with } g^{(n)} \in \mathcal{C}^\infty(\mathbb{R}^\nu). \tag{7.80}$$

Finally, we choose

$$\Psi^{(n)}(x) = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \frac{1}{\rho_n^{\nu/2}}\; j\big(\tfrac{x - x^{(n)}}{\rho_n}\big) \exp\big(\mathrm{i}\, g^{(n)}(x) - \mathrm{i}\, k x_1\big), \tag{7.81}$$

where j is a localization function with the following properties:

$$j \in \mathcal{C}_0^\infty(\mathbb{R}^\nu), \quad \operatorname{supp} j \subset \{x \mid |x| \leq 1\}, \quad \int |j(x)|^2 d^\nu x = 1. \tag{7.82}$$

It is easily verified that $\operatorname{supp}\Psi^{(n)} \subset B_n$, and $\|\Psi^{(n)}\| = 1$. A little calculation gives for all $k \in \mathbb{R}$

$$\{\boldsymbol{\sigma}\cdot(p-A(x))-k\}\Psi^{(n)}(x)=$$

$$=-\mathrm{i}\frac{1}{\rho_n}\boldsymbol{\sigma}\cdot\nabla j\left(\tfrac{x-x^{(n)}}{\rho_n}\right)\ \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}\frac{1}{\rho_n^{\nu/2}}\exp\left(\mathrm{i}\,g^{(n)}(x)-\mathrm{i}\,kx_1\right)$$

$$-\boldsymbol{\sigma}\cdot A^{(n)}(x)\Psi^{(n)}(x). \tag{7.83}$$

Using (7.79) we obtain the estimate

$$\|\{\boldsymbol{\sigma}\cdot(p-A)-k\}\Psi^{(n)}\|\leq\frac{1}{\rho_n}\int|\nabla j(x)|^2d^\nu x+\rho_n\sup_{x\in B_n}|B(x)|. \tag{7.84}$$

If $|B(x)|\to 0$, as $|x|\to\infty$, then there is a sequence of disjoint balls B_n with increasing radius ρ_n, such that

$$\sup_{x\in B_n}|B(x)|\leq\frac{1}{\rho_n^2}. \tag{7.85}$$

But then (7.84) is bounded by constant$/\rho_n\to 0$, as $n\to\infty$. Hence any $k\in\mathbb{R}$ is in the essential spectrum of D_ν. □

Remark. If $B(x)$ is bounded, then the distance from an arbitrary point $\lambda\notin(-mc^2,mc^2)$ to $\sigma_{\mathrm{ess}}(H(A))$ is less than $4\sqrt{3}\sup\sqrt{|B(x)|}$. This can be seen as follows. Assume $|B(x)|\leq M$ for all x. In the proof of the theorem above, choose $\rho_n=\rho$, all n, to find that (7.84) is bounded. Let $j(x)$ satisfy (7.82) and choose $j(x)=\text{const.}\cos^2(\pi|x|/2)$ for $|x|\leq 1$. Then it is easy to see that $\int|\nabla j(x)|^2d^3x\approx 11.62$. Setting $\rho=(12/M)^{1/2}$ we obtain the bound $4(3M)^{1/2}$ for (7.84). Hence the distance of an arbitrary $k\in\mathbb{R}$ to $\sigma_{\mathrm{ess}}(D_\nu)$ is less than this constant. The distance from an arbitrary $\lambda\notin(-mc^2,mc^2)$ to the next point in $\sigma_{\mathrm{ess}}(H(A))$ is bounded by the same constant.

It is immediately clear from the proof of Theorem 7.7 that the condition $|B(x)|\to 0$ can be weakened considerably. It is sufficient to require that there is a sequence of balls with increasing radius on which B tends to zero. These balls can be widely separated and it does not matter how B behaves elsewhere. This result is not so typical for Dirac operators, because similar statements are true for the nonrelativistic Schrödinger operator without spin. For Dirac operators in three dimensions, however, the result is true under much more general conditions. More, precisely, one defines functions

$$\epsilon_r(x)=\frac{\sum_{|\alpha|=r}|D^\alpha B|}{1+\sum_{|\alpha|<r}|D^\alpha B|},\quad\text{if } r\geq 1,\text{ and } \epsilon_0(x)=|B(x)|. \tag{7.86}$$

and introduces the assumption

A_r: There exist a sequence of disjoint balls B_n of radii r_n with $r_n\to\infty$ such that the function $\epsilon_r(x)$ restricted to the union of these balls tends to zero at infinity.

It can be seen that if (A_r) holds for some $r \geq 2$, then one of the assumptions (A_0) or (A_1) is true. If the components of B are polynomials of degree r, then (A_{r+1}) holds. The following theorem applies to this case.

Theorem 7.8. In three dimensions, if (A_r) holds for some $r \geq 0$, then

$$\sigma_{\text{ess}}(H(A)) = (-\infty, -mc^2] \cup [mc^2, \infty). \tag{7.87}$$

It should be clear from Theorem 7.6 that this result is very specific to three dimensions. Theorem 7.8 is very remarkable, because magnetic fields increasing like polynomials are known to yield Schrödinger operators with compact resolvent.

Finally we quote a theorem which gives criteria for the absence of eigenvalues in the region $(-\infty, -mc^2] \cup [mc^2, \infty)$.

Theorem 7.9. If $B(x) \to 0$ and $x \wedge B(x) \to 0$, as $|x| \to \infty$, then the Dirac operator has no eigenvalues λ with $|\lambda| > mc^2$.

7.3.3 Cylindrical Symmetry

In case of electric or scalar potentials which decay at infinity, the essential spectrum mainly consists of a continuous spectrum associated with scattering states. This is not necessarily the case for magnetic fields as can be seen most clearly by looking at cylindrically symmetric examples.

In two dimensions, if the magnetic field strength is cylindrically symmetric, we can pass to coordinates

$$r = |x|, \quad \phi = \arctan \frac{x_2}{x_1}. \tag{7.88}$$

in $\mathbb{R}^2 \setminus \{\mathbf{O}\}$. We denote the coordinate unit vectors by

$$\boldsymbol{e}_r = \frac{1}{r}(x_1, x_2), \quad \boldsymbol{e}_\phi = \frac{1}{r}(-x_2, x_1), \tag{7.89}$$

write $B(x) \equiv B(r)$, and choose $A(x) = A_\phi(r)\boldsymbol{e}_\phi$, where

$$A_\phi(r) = \frac{1}{r}\int_0^r B(s)\, s\, ds, \tag{7.90}$$

$$B(r) = \Big(\frac{d}{dr} + \frac{1}{r}\Big) A_\phi(r) = \frac{1}{r}\frac{d}{dr}\big(A_\phi(r)\, r\big). \tag{7.91}$$

In this notation the flux of B is given by

$$F = 2\pi \int_0^\infty B(s)\, s\, ds = \lim_{r\to\infty} \big(A_\phi(r)\, r\big) \tag{7.92}$$

In order to obtain the Dirac operator in cylindrical coordinates we write

$$\boldsymbol{\sigma}\cdot(p-A)\equiv(\boldsymbol{\sigma}\cdot\boldsymbol{e}_r)\,\boldsymbol{e}_r\cdot(p-A)+(\boldsymbol{\sigma}\cdot\boldsymbol{e}_\phi)\,\boldsymbol{e}_\phi\cdot(p-A). \tag{7.93}$$

Using the formulas

$$\boldsymbol{e}_r\cdot p=-\mathrm{i}\,\frac{\partial}{\partial r},\qquad \boldsymbol{e}_\phi\cdot p=\frac{-\mathrm{i}}{r}\frac{\partial}{\partial\phi}\equiv\frac{1}{r}L_3 \tag{7.94}$$

and

$$\boldsymbol{\sigma}\cdot\boldsymbol{e}_\phi=\mathrm{i}\,(\boldsymbol{\sigma}\cdot\boldsymbol{e}_r)\sigma_3,\qquad (\boldsymbol{\sigma}\cdot\boldsymbol{e}_r)=\begin{pmatrix}0 & e^{-\mathrm{i}\,\phi}\\ e^{\mathrm{i}\,\phi} & 0\end{pmatrix}, \tag{7.95}$$

we obtain

$$\begin{aligned}H(A)&\equiv c\boldsymbol{\sigma}\cdot(p-A)+\sigma_3mc^2\\ &=c(\boldsymbol{\sigma}\cdot\boldsymbol{e}_r)\Big\{-\mathrm{i}\left(\frac{\partial}{\partial r}+\frac{1}{2r}\right)+\mathrm{i}\,\frac{1}{r}\sigma_3J_3-\mathrm{i}\,\sigma_3A_\phi(r)\Big\}+\sigma_3mc^2.\end{aligned} \tag{7.96}$$

The angular momentum operator $J_3=L_3+\sigma_3/2$ commutes with $H(A)$ and the spinors

$$\chi_{m_j}=\begin{pmatrix}a\,e^{\mathrm{i}\,(m_j-1/2)\phi}\\ b\,e^{\mathrm{i}\,(m_j+1/2)\phi}\end{pmatrix},\quad a,b\in\mathbb{C},\quad m_j=\pm\frac{1}{2},\pm\frac{3}{2},\pm\frac{5}{2},\ldots \tag{7.97}$$

form a complete set of orthogonal eigenvectors of J_3 in $L^2(S^1)^2$ with the properties

$$J_3\chi_{m_j}=m_j\chi_{m_j}, \tag{7.98}$$

$$(\boldsymbol{\sigma}\cdot\boldsymbol{e}_r)\chi_{m_j}=\begin{pmatrix}b\,e^{\mathrm{i}\,(m_j-1/2)\phi}\\ a\,e^{\mathrm{i}\,(m_j+1/2)\phi}\end{pmatrix}. \tag{7.99}$$

Any function $\Psi(r,\phi)$ in $L^2(\mathbb{R}^2)^2$ can be written as a sum

$$\Psi(r,\phi)=\sum_{m_j}\begin{pmatrix}\dfrac{1}{\sqrt{r}}\,f_{m_j}(r)\,e^{\mathrm{i}\,(m_j-1/2)\phi}\\ -\mathrm{i}\,\dfrac{1}{\sqrt{r}}\,g_{m_j}(r)\,e^{\mathrm{i}\,(m_j+1/2)\phi}\end{pmatrix}, \tag{7.100}$$

with suitable functions f_{m_j} and g_{m_j} satisfying

$$\int_0^\infty\left\{|f_{m_j}(r)|^2+|g_{m_j}(r)|^2\right\}dr<\infty. \tag{7.101}$$

The action of $H(A)$ on Ψ can be described on each angular momentum subspace as the action of a "radial Dirac operator" h_{m_j} defined in $L^2([0,\infty),dr)$

$$h_{m_j}\begin{pmatrix}f_{m_j}\\ g_{m_j}\end{pmatrix}=\begin{pmatrix}mc^2 & cD^*\\ cD & -mc^2\end{pmatrix}\begin{pmatrix}f_{m_j}\\ g_{m_j}\end{pmatrix} \tag{7.102}$$

with

$$D = \frac{d}{dr} - \frac{m_j}{r} + A_\phi(r), \tag{7.103}$$

and $H(A)$ is unitarily equivalent to a direct sum of the operators h_{m_j}. A little calculation shows

$$\left.\begin{matrix} D^*D \\ DD^* \end{matrix}\right\} = -\frac{d^2}{dr^2} + \frac{\left(m_j \mp \frac{1}{2}\right)^2 - \frac{1}{4}}{r^2} - 2\frac{m_j \mp \frac{1}{2}}{r} A_\phi(r) + A_\phi^2(r) \mp B(r). \tag{7.104}$$

From (7.91) we see that if $B(r)r \to \infty$ then also $A_\phi(r) \to \infty$, as $r \to \infty$. In this case the term A_ϕ^2 dominates in (7.104) the interaction at large values of r and clearly the Schrödinger operator D^*D (resp. DD^*) has a pure point spectrum. By Corollary 5.14 the same is true for the Dirac operator h_{m_j} on each angular momentum subspace and hence for $H(A)$. Let us summarize these observations in the following theorem.

Theorem 7.10. In two dimensions, if B is cylindrically symmetric and $B(r)r \to \infty$, as $r \to \infty$, then the Dirac operator $H(A)$ has a pure point spectrum. In addition, if $B(r) \to 0$, then $B(r)r \to \infty$ implies that there is a complete set of orthonormal eigenvectors of $H(A)$ belonging to eigenvalues which are dense in $(-\infty, -mc^2] \cup [mc^2, \infty)$.

7.4 The Coulomb Problem

The Dirac equation with the Coulomb potential $\phi_{\rm el}(\boldsymbol{x}) = \gamma/|\boldsymbol{x}|$ describes the motion of an electron in the field of an atomic nucleus. This problem can be solved exactly and the solutions almost perfectly agree with the experiments. Since the hydrogen atom is fundamental to relativistic atomic physics, this success of the Dirac equation has been one of the main historical reasons for its quick acceptance. The exact solvability of the Coulomb problem can be explained with the help of supersymmetric quantum mechanics.

7.4.1 The Hidden Supersymmetry

In this section we show that the Dirac operator for an electron (without anomalous moment) has a hidden supersymmetric structure. We start with the radial Dirac operator (cf. Eq. (4.129))

$$h_\kappa = \begin{pmatrix} mc^2 + \frac{\gamma}{r} & c\left\{-\frac{d}{dr} + \frac{\kappa}{r}\right\} \\ c\left\{\frac{d}{dr} + \frac{\kappa}{r}\right\} & -mc^2 + \frac{\gamma}{r} \end{pmatrix}, \quad \kappa = \pm 1, \pm 2, \ldots. \tag{7.105}$$

and assume $-c < \gamma < 0$. The negative sign of γ corresponds to an attractive Coulomb potential. By our results in Sect. 4.6.6, h_κ is essentially self-adjoint on $C_0^\infty(0,\infty)$ for all values of κ, if $|\gamma| < c\sqrt{3}/2$. For γ not in this range we shall have to specify a boundary condition at zero for the wavefunctions in the domain of h_κ.

We are interested in the eigenvalues and square integrable eigenfunctions in $L^2((0,\infty),dr)^2$; i.e.,

$$(h_\kappa - E)\begin{pmatrix} f \\ g \end{pmatrix} = 0, \qquad \int_0^\infty \{|f(r)|^2 + |g(r)|^2\}\, dr < \infty. \tag{7.106}$$

It is useful to rearrange this system of differential equations such that the derivatives appear in the main diagonal:

$$\begin{aligned} &\mathrm{i}\sigma_2 (h_\kappa - E) \\ &\quad = c\,\mathbf{1}\frac{d}{dr} + \begin{pmatrix} c\kappa & \gamma \\ -\gamma & -c\kappa \end{pmatrix}\frac{1}{r} + \begin{pmatrix} 0 & -E - mc^2 \\ E - mc^2 & 0 \end{pmatrix}. \end{aligned} \tag{7.107}$$

We can even diagonalize the matrix in front of $1/r$.

$$\mathbf{A}^{-1}\begin{pmatrix} c\kappa & \gamma \\ -\gamma & -c\kappa \end{pmatrix}\mathbf{A} = c\begin{pmatrix} s & 0 \\ 0 & -s \end{pmatrix}, \quad s = \sqrt{\kappa^2 - \gamma^2/c^2}, \tag{7.108}$$

$$\mathbf{A} = \begin{pmatrix} -c(\kappa + s) & \gamma \\ \gamma & -c(\kappa + s) \end{pmatrix}. \tag{7.109}$$

Therefore, with

$$\begin{pmatrix} u \\ v \end{pmatrix} \equiv \mathbf{A}^{-1}\begin{pmatrix} f \\ g \end{pmatrix} \tag{7.110}$$

we can rewrite the eigenvalue equation (7.106) in the following form

$$\mathrm{i}\sigma_2\mathbf{A}^{-1}\mathrm{i}\sigma_2(h_\kappa - E)\mathbf{A}\begin{pmatrix} u \\ v \end{pmatrix} = 0, \tag{7.111}$$

which is the same as

$$\begin{pmatrix} mc^2 & c\left\{-\frac{d}{dr} + \frac{s}{r}\right\} + \frac{\gamma E}{cs} \\ c\left\{\frac{d}{dr} + \frac{s}{r}\right\} + \frac{\gamma E}{cs} & -mc^2 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = \frac{\kappa E}{s}\begin{pmatrix} u \\ v \end{pmatrix}. \tag{7.112}$$

For each E the matrix operator in (7.112) is a Dirac operator with supersymmetry. We denote

$$D_0 \equiv D_0(E) \equiv \frac{d}{dr} + \frac{s}{r} + \frac{\gamma E}{c^2 s}. \tag{7.113}$$

By a Foldy-Wouthuysen transformation U_{FW} (cf. Sect. 5.6.1) we can transform equation (7.112) into

$$\sqrt{c^2 D_0^* D_0 + m^2c^4}\,\phi = \frac{\kappa E}{s}\phi, \tag{7.114a}$$

$$\sqrt{c^2 D_0 D_0^* + m^2c^4}\,\psi = -\frac{\kappa E}{s}\psi, \tag{7.114b}$$

where

$$\begin{pmatrix} \phi \\ \psi \end{pmatrix} = U_{\mathrm{FW}}\begin{pmatrix} u \\ v \end{pmatrix}. \tag{7.115}$$

We want to stress that the pair of equations (7.114) is completely equivalent to the stationary Dirac equation (7.106).

7.4.2 The Ground State

It is surprisingly simple to determine a solution of (7.114). Just remember (5.25) and (5.26): If we could find (for arbitrary E) a vector ϕ in $\operatorname{Ker} D_0 = \operatorname{Ker} D_0^* D_0$, then we could automatically solve (7.114a) by choosing E appropriately. Similarly, ψ in $\operatorname{Ker} D_0^*$ would give a solution of (7.114b). Indeed,

$$D_0^* \psi \equiv \left\{ -\frac{d}{dr} + \frac{s}{r} + \frac{\gamma E_0}{c^2 s} \right\} \psi = 0 \tag{7.116}$$

is a very simple differential equation which is solved by

$$\psi_0(r) = r^s e^{(\gamma E_0 / c^2 s) r}. \tag{7.117}$$

This solution is square integrable if and only if $\gamma E_0 < 0$. Since we have chosen $\gamma < 0$ we find that we must have $E_0 > 0$. From (7.114b) and $D_0 D_0^* \psi_0 = 0$ we obtain immediately

$$E_0 = -\frac{mc^2 s}{\kappa} = mc^2 \left\{ 1 + \frac{\gamma^2}{c^2 \kappa^2 - \gamma^2} \right\}^{-\frac{1}{2}}. \tag{7.118}$$

From $E_0 > 0$ we conclude that κ has to be negative for this solution. Obviously, $-\kappa E_0 / s$ is the smallest positive eigenvalue which can occur in (7.114b). Thus E_0 is the ground state energy of the Dirac-Coulomb problem. The corresponding solution of the radial Dirac equation (7.106) (with $\kappa < 0$ and $E = E_0$) is given by

$$\begin{pmatrix} f_0 \\ g_0 \end{pmatrix} = n_0 \mathbf{A} U_{\mathrm{FW}}^{-1} \begin{pmatrix} 0 \\ \psi_0 \end{pmatrix} = n_0 \begin{pmatrix} \gamma \psi_0 \\ -c(\kappa + s)\psi_0 \end{pmatrix}, \tag{7.119}$$

n_0 being an appropriate normalization constant. We have used Eq. (7.109) and $U_{\mathrm{FW}} = \mathbf{1}$ on $\operatorname{Ker} Q$ (Sect. 5.6.1).

On the other hand, a solution of the differential equation $D_0 \phi = 0$ is given by

$$\phi(r) = r^{-s} e^{-(\gamma E / c^2 s) r}. \tag{7.120}$$

Because of the singularity at the origin this solution is not square integrable for $s > 1/2$, or $|\gamma| < c\sqrt{\kappa^2 - 1/4}$, and has to be excluded. Hence $\operatorname{Ker} D_0 = \{0\}$ and Eq. (7.114a) has no L^2-solution for $E = E_0$, i.e., E_0 is not an eigenvalue of h_κ with $\kappa > 0$.

For $s < 1/2$, (7.120) is square integrable if $\gamma E > 0$. In this case the solution (7.120) can only be excluded by specifying a boundary condition of the form

$$\lim_{r \to 0} \phi(r) = 0. \tag{7.121}$$

This procedure amounts to choosing a distinguished self-adjoint extension of the operator h_κ for values of γ for which h_κ is not essentially self-adjoint.

Remark. The system of differential equations $(h_\kappa - E_0)\psi = 0$ has two independent solutions which need not be square integrable. The preceding discussion shows that for $|\gamma| < c\sqrt{\kappa^2 - 1/4}$ only one of these solutions is in $L^2(0,\epsilon)$, whereas for $|\gamma| > c\sqrt{\kappa^2 - 1/4}$ both solutions are square integrable at 0. At $r = \infty$ there is always only one square integrable solution. Thus we are in the limit point case[1] at both 0 and ∞, only if $|\gamma|$ is sufficiently small. In this case the Dirac operator h_κ, defined on the set of locally absolutely continuous functions with compact support in $(0,\infty)$ has defect indices $(0,0)$ and hence is essentially self-adjoint there. For $|\gamma| > c\sqrt{\kappa^2 - 1/4}$ we are in the limit circle case at 0 and hence the defect indices of h_κ are (1,1). Our choice of the boundary condition (7.121) corresponds to choosing the particular self-adjoint realization of h_κ on the domain

$$\mathfrak{D}(h_\kappa) = \{\Psi \in L^2(0,\infty)^2 \mid \text{each component of } \Psi \text{ is locally absolutely continuous, and } h_\kappa\Psi \in L^2(0,\infty)^2,\ \Psi(r=0) = (0,0)\}. \quad (7.122)$$

7.4.3 Exited States

Iterating Eqs. (7.114) gives the following second order equations

$$(c^2 D_0^* D_0 + m^2c^4)\phi = \left\{E^2 + \frac{\gamma^2 E^2}{c^2 s^2}\right\}\phi, \quad (7.123a)$$

$$(c^2 D_0 D_0^* + m^2c^4)\psi = \left\{E^2 + \frac{\gamma^2 E^2}{c^2 s^2}\right\}\psi. \quad (7.123b)$$

We have used $\kappa^2 = s^2 + \gamma^2/c^2$. With D_0 given as in (7.113)

$$c^2 D_0^* D_0 = c^2\left\{-\frac{d^2}{dr^2} + \frac{s(s+1)}{r^2}\right\} + \frac{2\gamma E}{r} + \frac{\gamma^2 E^2}{c^2 s^2}, \quad (7.124a)$$

$$c^2 D_0 D_0^* = c^2\left\{-\frac{d^2}{dr^2} + \frac{s(s-1)}{r^2}\right\} + \frac{2\gamma E}{r} + \frac{\gamma^2 E^2}{c^2 s^2}. \quad (7.124b)$$

Inserting (7.124) into (7.123) we obtain

$$\left\{c^2\left(-\frac{d^2}{dr^2} + \frac{s(s+1)}{r^2}\right) + \frac{2\gamma E}{r} + m^2c^4\right\}\psi = E^2\psi. \quad (7.125a)$$

$$\left\{c^2\left(-\frac{d^2}{dr^2} + \frac{s(s-1)}{r^2}\right) + \frac{2\gamma E}{r} + m^2c^4\right\}\psi = E^2\psi. \quad (7.125b)$$

This shows that Eq. (7.123a) can be obtained from Eq. (7.123b) by replacing the parameter s with $s+1$. Hence Eq. (7.123a) is the same as

[1] See, e.g., [RS 75], Appendix to X.1. For systems of differential equations the assertions on limit point/circle case, defect indices, and self-adjoint realizations are proven in [467]. See Sect. 4.6.6 for related results.

$$(c^2 D_1 D_1^* + m^2 c^4)\phi = \left\{ E^2 + \frac{\gamma^2 E^2}{c^2(s+1)^2} \right\} \phi, \tag{7.126}$$

with

$$D_1 \equiv \frac{d}{dr} + \frac{s+1}{r} + \frac{\gamma E}{c^2(s+1)}. \tag{7.127}$$

Again, it is easy to obtain a solution of (7.126). For $E = E_1$, which still has to be determined, the equation $D_1^* \phi = 0$ is solved by

$$\phi_1(r) = r^{s+1} \exp\left(\frac{\gamma E_1}{c^2(s+1)} r \right), \tag{7.128}$$

which is square integrable for $E_1 > 0$ (since $\gamma < 0$). ϕ_1 is a solution of (7.126) if we choose

$$E_1 = mc^2 \left\{ 1 + \frac{\gamma^2}{c^2(s+1)^2} \right\}^{-\frac{1}{2}}. \tag{7.129}$$

At the same time, ϕ_1 is a solution of equation (7.123a) which is identical to (7.126). The relation between (7.123a) and the Dirac equation (7.106) is given by the following lemma.

Lemma 7.11. Let $E > E_0$, $\gamma < 0$, $s = (\kappa^2 - \gamma^2/c^2)^{1/2}$. Then ϕ is a square integrable solution of (7.123a) if and only if E is an eigenvalue of the Dirac operators h_κ, $\kappa = \pm(s^2 + \gamma^2/c^2)^{1/2}$, with corresponding eigenvectors given by

$$\begin{pmatrix} f^+ \\ g^+ \end{pmatrix} = \mathbf{A} U_{\mathrm{FW}}^{-1} \begin{pmatrix} \phi \\ 0 \end{pmatrix}, \qquad \text{for } \kappa > 0, \tag{7.130}$$

$$\begin{pmatrix} f^- \\ g^- \end{pmatrix} = \mathbf{A} U_{\mathrm{FW}}^{-1} \begin{pmatrix} 0 \\ D_0 \phi \end{pmatrix}, \qquad \text{for } \kappa < 0. \tag{7.131}$$

Proof. Any square integrable solution ϕ of (7.123a) is an eigenvector of $D_0^* D_0$ and hence of the square root operator in (7.114a). However, (7.114a) can only be satisfied, if $\kappa E/s > 0$. Since $E > 0$ we must have $\kappa > 0$. We have seen in Sect. 7.4.2 that ϕ is not in $\mathrm{Ker}\, D_0$, because this set contains only the zero vector. Supersymmetry implies that $D_0\phi$ is an eigenvector of $D_0 D_0^*$ and hence a solution of (7.123b) with the same E (cf. Sect. 5.2.3, in particular Eq. (5.29)). (7.114b) is solved by $D_0\phi$ if and only if $\kappa < 0$. It is clear from (7.110) and (7.115) that $\mathbf{A} U_{\mathrm{FW}}^{-1}$ turns the solutions $(\phi, 0)^\top$ resp. $(0, D_0\phi)^\top$ of (7.123) into solutions of the original Dirac equation with $\kappa > 0$ resp. $\kappa < 0$. □

We conclude that E_1 is an eigenvalue of the Dirac operator. E_1 is the smallest parameter for which (7.126) resp. (7.123a) has a L^2-solution (just note that $D_1 D_1^*$ is nonnegative). Since the solutions of the Dirac equation with $E > E_0$ are in one-to-one correspondence to the solutions of (7.123a), we find that there is no further eigenvalue between E_0 and E_1.

The key for a complete solution of the Dirac Coulomb problem lies in the following lemma.

Lemma 7.12. For $n = 0, 1, 2, \ldots$, define the operators

$$D_n \equiv \frac{d}{dr} + \frac{s+n}{r} + \frac{\gamma E}{c^2(s+n)}. \tag{7.132}$$

If, for some $n \geq 1$, ϕ is a L^2-solution of

$$(c^2 D_n D_n^* + m^2 c^4)\phi = \left\{ E^2 + \frac{\gamma^2 E^2}{c^2(s+n)^2} \right\} \phi, \tag{7.133}_n$$

then $D_{n-1}\phi$ is a solution of $(7.133)_{n-1}$.

Proof. For $n = 1$ the result follows from the considerations above. In this case $(7.133)_1$ is identical to (7.126) and $(7.133)_0$ equals (7.123b). In the general case we introduce a supersymmetric partner of Eq. $(7.133)_{n-1}$ by reversing the order of D_{n-1} and D_{n-1}^*, namely

$$(c^2 D_{n-1}^* D_{n-1} + m^2 c^4)\phi = \left\{ E^2 + \frac{\gamma^2 E^2}{c^2(s+n-1)^2} \right\} \phi. \tag{7.134}$$

The operators D_n have the following crucial property

$$c^2 D_{n-1}^* D_{n-1} - \frac{\gamma^2 E^2}{c^2(s+n-1)^2} = c^2 D_n D_n^* - \frac{\gamma^2 E^2}{c^2(s+n)^2}, \tag{7.135}$$

which shows that (7.134) is equivalent to $(7.133)_n$. Moreover,

$$c^2 D_{n-1}^* D_{n-1} \geq \frac{\gamma^2 E^2}{c^2(s+n-1)^2} - \frac{\gamma^2 E^2}{c^2(s+n)^2} > 0, \tag{7.136}$$

and hence $\operatorname{Ker} D_{n-1} = \{0\}$. This shows that any square integrable solution ϕ of (7.134) is an eigenvector of $D_{n-1}^* D_{n-1}$ belonging to a nonzero eigenvalue. Hence, by Corollary 5.6 and Eq. (5.29), the operator $D_{n-1} D_{n-1}^*$ (which occurs in $(7.133)_{n-1}$) has the same eigenvalue, and the corresponding eigenvector is given by $\psi = D_{n-1}\phi$. This is true for any nonzero eigenvalues of $D_{n-1} D_{n-1}^*$ and all corresponding solutions of $(7.133)_{n-1}$ can be obtained in this way from solutions of $(7.133)_n$. □

This lemma tells us how to obtain solutions of Eq. (7.123a): Obviously, if ϕ is a solution of $(7.133)_n$ with $n \geq 2$, then

$$\psi = D_1 D_2 \ldots D_{n-1}\phi \tag{7.137}$$

is a solution of (7.126) and hence of (7.123a). In fact, we can determine successively all solutions of (7.123a) by considering only the ground state solutions for the fictitious problems $(7.133)_n$. This can be seen as follows. Among all solutions of $(7.133)_n$ the ground state has the lowest value of E. Any excited

state (i.e., a solution belonging to larger values of E) belongs to a nonzero eigenvalue of $D_n D_n^*$. Hence, by the same procedure as in the proof above, we can obtain the excited state as a solution of $(7.133)_{n+1}$. Moreover, the first excited state of $(7.133)_n$ is obviously the ground state of $(7.133)_{n+1}$.

Using Eq. (5.26), we find the ground state solution of $(7.133)_n$ from

$$(D_n)^* \psi = \left\{ -\frac{d}{dr} + \frac{s+n}{r} + \frac{\gamma E_n}{c^2(s+n)} \right\} \psi = 0, \tag{7.138}$$

which gives

$$\psi_n(r) = r^{s+n} \exp\left(\frac{\gamma E_n}{c^2(s+n)} r \right). \tag{7.139}$$

Again, for $\gamma < 0$, ψ_n is square integrable if and only if $E_n > 0$. Inserting ψ_n into $(7.133)_n$ gives immediately

$$E_n = mc^2 \left\{ 1 + \frac{\gamma^2/c^2}{\left(n + \sqrt{\kappa^2 - \gamma^2/c^2}\right)^2} \right\}^{-\frac{1}{2}}. \tag{7.140}$$

Finally, from Lemma 7.11 above, we find the solutions of the Dirac equation (7.106). For $\kappa > 0$,

$$\begin{pmatrix} f_n^+(r) \\ g_n^+(r) \end{pmatrix} = \mathbf{A} U_{\mathrm{FW}}^{-1} \begin{pmatrix} D_1 D_2 \ldots D_{n-1} \psi_n(r) \\ 0 \end{pmatrix}, \quad n = 2, 3, \ldots, \tag{7.141}$$

is the unique solution of (7.106) with eigenvalue E_n. For $\kappa < 0$ the solution of (7.106) is given by

$$\begin{pmatrix} f_n^-(r) \\ g_n^-(r) \end{pmatrix} = \mathbf{A} U_{\mathrm{FW}}^{-1} \begin{pmatrix} 0 \\ D_0 D_1 D_2 \ldots D_{n-1} \psi_n(r) \end{pmatrix}, \quad n = 1, 2, \ldots. \tag{7.142}$$

Of course these solutions are not normalized.

7.4.4 The BJL Operator

The explicit solvability of the relativistic Coulomb problem is related to the existence of an additional conserved quantity. A little calculation shows that the Dirac-Coulomb operator

$$H = c\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta mc^2 + \frac{\gamma}{|\boldsymbol{x}|} \tag{7.143}$$

commutes with the Biedenharn-Johnson-Lippmann (BJL) operator

$$B \equiv \tfrac{\mathrm{i}}{mc^2} K \gamma_5 (H - \beta mc^2) + \tfrac{2\gamma}{c} \boldsymbol{S} \cdot \boldsymbol{e}_r. \tag{7.144}$$

Here we have used the usual definitions

$$K = \beta(2\boldsymbol{S} \cdot \boldsymbol{L} + \mathbf{1}), \qquad \boldsymbol{S} = \tfrac{\mathrm{i}}{4} \boldsymbol{\alpha} \wedge \boldsymbol{\alpha}, \qquad \boldsymbol{L} = \boldsymbol{x} \wedge \boldsymbol{p},$$

$$\gamma_5 = -\mathrm{i}\alpha_1\alpha_2\alpha_3, \qquad e_r = \frac{x}{|x|}. \tag{7.145}$$

The operator $\mathrm{i}K\gamma_5$ is symmetric and commutes with $H - \beta mc^2$ on the domain $\mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{\mathrm{O}\})^4$, hence B is symmetric. Using Temple's operator

$$\Gamma \equiv \beta K - \mathrm{i}\tfrac{\gamma}{c}\boldsymbol{\alpha}\cdot\boldsymbol{e}_r, \tag{7.146}$$

we can rewrite B as

$$B = \mathrm{i}\gamma_5\big(\Gamma - \tfrac{1}{mc^2}KH\big). \tag{7.147}$$

The operator Γ appears if we write the Coulomb-Dirac operator H with the help of Eq. (4.104) as

$$H = -\mathrm{i}\,c(\boldsymbol{\alpha}\cdot\boldsymbol{e}_r)\left(\tfrac{\partial}{\partial r} + \tfrac{1}{r} - \tfrac{1}{r}\Gamma\right) + \beta mc^2. \tag{7.148}$$

Temple's operator Γ is not symmetric, but $\mathrm{i}\gamma_5\Gamma$ is self-adjoint on $\mathfrak{D}(K)$. Eliminating $H - \beta mc^2$ from (7.144) with the help of (7.148) we obtain the expression

$$B = \tfrac{2}{mc^2}\beta\boldsymbol{S}\cdot\boldsymbol{e}_r\left(\tfrac{\gamma}{c}H - c\Gamma\left(\tfrac{\partial}{\partial r} + \tfrac{1}{r} - \tfrac{1}{r}\Gamma\right)\right). \tag{7.149}$$

Another form of B can be obtained if we insert K from Eq. (7.145) into (7.144) and use

$$(2\boldsymbol{S}\cdot\boldsymbol{L} + \mathbf{1})(\boldsymbol{S}\cdot\boldsymbol{p}) = \tfrac{\mathrm{i}}{2}\boldsymbol{S}\cdot(\boldsymbol{L}\wedge\boldsymbol{p} - \boldsymbol{p}\wedge\boldsymbol{L}). \tag{7.150}$$

Then we get

$$B = 2\boldsymbol{S}\cdot\left(\tfrac{\gamma}{c}\boldsymbol{e}_r - \tfrac{\beta}{2mc}(\boldsymbol{L}\wedge\boldsymbol{p} - \boldsymbol{p}\wedge\boldsymbol{L})\right) + \mathrm{i}\tfrac{\gamma}{mc^2}\tfrac{1}{|x|}K\gamma_5. \tag{7.151}$$

This shows that B is the relativistic counterpart of the Pauli-Runge-Lenz vector

$$\boldsymbol{R} = \gamma\boldsymbol{e}_r - \tfrac{1}{2m}(\boldsymbol{L}\wedge\boldsymbol{p} - \boldsymbol{p}\wedge\boldsymbol{L}), \tag{7.152}$$

which is a conserved quantity for the nonrelativistic Coulomb problem. But in contrast to the nonrelativistic case, the operator B is not reduced by the angular momentum subspaces (Sect. 4.6.4), because B does not commute with K. Instead we have

$$\{B, K\} = BK + KB = 0, \quad \text{on } \mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{\mathrm{O}\})^4. \tag{7.153}$$

If Ψ is an angular momentum eigenfunction as described in Eqs. (4.124) and (4.125), with energy E and spin-orbit quantum number κ_j, then $B\Psi$ is an eigenfunction of H and K with eigenvalues E and $-\kappa_j$. This explains the degeneracy of the Dirac-Coulomb eigenvalues with respect to the sign of κ.

Finally, we investigate the action of B on the angular momentum eigenfunctions

$$\Psi_{m_j,\kappa_j}(r,\vartheta,\varphi) = \tfrac{1}{r}f(r)\,\Phi^+_{m_j,\kappa_j}(\vartheta,\varphi) + \tfrac{1}{r}g(r)\,\Phi^-_{m_j,\kappa_j}(\vartheta,\varphi), \tag{7.154}$$

where the functions $\Phi^{\pm}_{m_j,\kappa_j}$ are defined in Sect. 4.6.4. The operator B has a "radial part" which acts as a 2×2 matrix operator on the radial wavefunctions and an "angular part" acting only on $\Phi^{\pm}_{m_j,\kappa_j}$. This is best seen in the expression (7.147). The angular part is completely contained in the factor $i\gamma_5$. Using the standard representation of γ_5, Eq. (2.203), and the explicit form of the angular momentum eigenfunctions, Eq. (4.111), we easily obtain

$$\gamma_5 \Phi^{\pm}_{m_j,\kappa_j} = \Phi^{\mp}_{m_j,-\kappa_j}, \quad \gamma_5 \Psi_{m_j,\kappa_j} = -\tfrac{1}{r} \mathrm{i} g \Phi^{+}_{m_j,-\kappa_j} + \tfrac{1}{r} \mathrm{i} f \Phi^{-}_{m_j,-\kappa_j}. \tag{7.155}$$

with Ψ_{m_j,κ_j} defined as in Eq. (7.154). Hence the operator γ_5 replaces the angular momentum eigenfunctions $\Phi^{\pm}_{m_j,\kappa_j}$ with $\Phi^{\pm}_{m_j,-\kappa_j}$ and the action on the radial part of Ψ_{m_j,κ_j} is given by

$$\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} -\mathrm{i}g \\ \mathrm{i}f \end{pmatrix}. \tag{7.156}$$

The second factor $\Gamma - \frac{1}{mc^2} KH$ of B has only a radial part. From Eq. (7.146) and the properties of the angular momentum eigenfunctions we easily conclude that Temple's operator in the radial Hilbert space $L^2(0,\infty)$ is given by the matrix

$$\Gamma = \begin{pmatrix} -\kappa & -\gamma/c \\ \gamma/c & \kappa \end{pmatrix}. \tag{7.157}$$

We conclude that the action of B on radial wavefunctions $\begin{pmatrix} f \\ g \end{pmatrix}$ is described by the matrix operator

$$b_\kappa = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \left[\begin{pmatrix} -\kappa & -\gamma/c \\ \gamma/c & \kappa \end{pmatrix} + \frac{\kappa}{mc^2} h_{\kappa_j} \right]. \tag{7.158}$$

Hence, denoting $\begin{pmatrix} h \\ k \end{pmatrix} \equiv b_{\kappa_j} \begin{pmatrix} f \\ g \end{pmatrix}$, we find with Ψ_{m_j,κ_j} as in Eq. (7.154)

$$B\Psi_{m_j,\kappa_j} = \tfrac{1}{r} h(r) \Phi^{+}_{m_j,-\kappa_j} + \tfrac{1}{r} g(r) \Phi^{-}_{m_j,-\kappa_j}. \tag{7.159}$$

If, moreover, $f(E,r)$ and $g(E,r)$ define a solution of $(h_\kappa - E)\begin{pmatrix} f \\ g \end{pmatrix} = 0$, then

$$b_{\kappa_j} \begin{pmatrix} f(E,r) \\ g(E,r) \end{pmatrix} = \begin{pmatrix} \gamma/\mathrm{c} & \kappa + \frac{\kappa E}{mc^2} \\ \kappa - \frac{\kappa E}{mc^2} & \gamma/c \end{pmatrix} \begin{pmatrix} f(E,r) \\ g(E,r) \end{pmatrix} \equiv \begin{pmatrix} h(E,r) \\ k(E,r) \end{pmatrix} \tag{7.160}$$

is a solution of $(h_{-\kappa} - E)\begin{pmatrix} h \\ k \end{pmatrix} = 0$.

7.4.5 Discussion

The eigenstates of the Dirac Coulomb operator H are clearly labelled by the eigenvalues $\kappa = \pm 1, \pm 2, \ldots$ of the operator $-K$, and the quantum number $n = 0, 1, 2, \ldots$ counting the (nondegenerate) eigenvalues of the partial wave operator h_κ. Note that the angular momentum quantum number j is uniquely determined by κ,

$$j = \begin{cases} -\kappa - 1/2 & \text{if } \kappa < 0, \\ \kappa - 1/2 & \text{if } \kappa > 0. \end{cases} \tag{7.161}$$

We know from Sect. 4.6.5 that h_κ does not depend on the angular momentum quantum number m_j, the eigenvalue of J_3. Hence each eigenvalue has the multiplicity $2j+1$ as a consequence of the spherical symmetry. For the Coulomb problem, Eq. (7.140) shows that the energies also do not depend on the sign of κ. This doubles the multiplicity of each eigenvalue except of those with $n = 0$, for which we must have $\kappa < 0$. This additional degeneracy occurs because the BJL operator commutes with H and anticommutes with K.

In the nonrelativistic limit we find from (7.140)

$$E_n - mc^2 \to E_{\text{n.r.}} = -\frac{m\gamma^2}{2(n+|\kappa|)^2}, \tag{7.162}$$

which shows that for the Schrödinger-Coulomb problem the energy-eigenvalues depend only on the "principal quantum number"

$$N \equiv n + |\kappa|, \tag{7.163}$$

which implies a much higher degeneracy than in the relativistic case. In the nonrelativistic limit, the angular momentum operators $\boldsymbol{S}$ and $\boldsymbol{L}$ commute and are conserved separately. Furthermore, as $c \to \infty$, we have $\beta \to \mathbf{1}$ on eigenstates. Hence, if the operator $K = \beta(2\boldsymbol{S}\cdot\boldsymbol{L} + \mathbf{1})$ is positive on some eigenstate (i.e., $\kappa < 0$), this means that the spin is parallel to the orbital angular momentum in the nonrelativistic limit, i.e., $j = l + 1/2$. On the other hand, $\kappa > 0$ implies $j = l - 1/2$ (here l is the quantum number for the orbital angular momentum, cf. Eq. (4.117)). The nonrelativistic quantum numbers N, l, and j are used to label the Coulomb eigenstates in the "spectroscopic notation" Nx_j, where x is a letter characterizing the orbital angular momentum:

$$\begin{aligned} &l = 0, 1, 2, 3, 4, \ldots \quad \text{corresponds to} \\ &x = s, p, d, f, g, \ldots . \end{aligned} \tag{7.164}$$

Since by Theorem 6.7 there is a one to one correspondence between the relativistic eigenstates and their nonrelativistic limit, the spectroscopic notation can also be used to formally label the relativistic states. Hence the eigenstates of h_κ can be denoted as follows:

$$\begin{aligned} &1s_{1/2} \\ &2s_{1/2} \quad 2p_{1/2} \quad 2p_{3/2} \\ &3s_{1/2} \quad 3p_{1/2} \quad 3p_{3/2} \quad 3d_{3/2} \quad 3d_{5/2} \\ &\text{etc.} \end{aligned} \tag{7.165}$$

Note that j and l differ at most by $\pm 1/2$. Clearly, the spectroscopic notation does not distinguish between states that belong to different eigenvalues m_j of J_3. Hence all states in (7.165) have multiplicity $2j+1$, moreover, the additional

degeneracy of the Coulomb problem implies, that the following states have, respectively, the same energy:

$Np_{1/2}$ ($\kappa = +1$) and $Ns_{1/2}$ ($\kappa = -1$), $N \geq 2$,

$Nd_{3/2}$ ($\kappa = +2$) and $Np_{3/2}$, ($\kappa = -2$) $N \geq 3$, etc.

The states $1s_{1/2}$, $2p_{3/2}$, $3d_{5/2}$, etc., corresponding to $n = 0$ are nondegenerate. All states with the same N have the same energy in the nonrelativistic limit. κ is obtained from j and l as follows,

$$\kappa = \begin{cases} l & \text{if } j = l - 1/2, \\ -l - 1 & \text{if } j = l + 1/2. \end{cases} \tag{7.166}$$

We also note that the relativistic electron bound state energies are below the corresponding nonrelativistic eigenvalues.

Next we consider the curves $E_{n,\kappa}(\gamma)$ which describe the coupling constant dependence of the energies belonging to the quantum numbers n and κ. It is typical for long-range nature of the Coulomb problem, that if the coupling strength $|\gamma|$ is increased, the eigenvalues do not emerge one after another from the upper continuum at $+mc^2$. Instead, as soon as $|\gamma| > 0$, all eigenvalues are present and strictly below the threshold mc^2. If the coupling strength is increased, the eigenvalues move through the gap towards $E = -mc^2$, but as soon as the ground state reaches $E = 0$ at $|\gamma| = c$, the partial wave Dirac operator with $|\kappa| = 1$ ceases to be well defined (Sect. 4.3.3). According to Eq. (7.140) the eigenvalues become complex for $|\kappa| = 1$ and $|\gamma| > c$ which corresponds to the choice of a non-self-adjoint extension of h_κ. The ground state approaches 0, as $\gamma \to -1$, with $dE_0(\gamma)/d\gamma \to \infty$. No eigenvalue dives below $E = 0$.

There are several possibilities of defining self-adjoint extensions for $|\gamma| > c$. Each choice amounts to some regularization of the Coulomb singularity at the origin. The singularity is of course a mathematical idealization which does not take into account the finite size of the nucleus. One can avoid all problems with the self-adjointness by considering an extended nuclear charge distribution. This amounts to cutting off the Coulomb singularity. For large nuclear charges, however, the results depend significantly on the manner in which the potential is cut off.

As we know from Sect. 5.3.2 an additional term in the Dirac operator describing a small anomalous magnetic moment also has a regularizing influence. Hence it is interesting to look at the curves $E_{n,\kappa}(\gamma)$ if a small anomalous magnetic moment is turned on, because then the Dirac operator is well defined for all values of γ. Since no exact solution is known for this case, we present the results of a numerical solution in Fig. 7.1. This figure displays the eigenvalues of the operator

$$h_\kappa = \begin{pmatrix} 1 + \frac{\gamma}{r} & -\frac{d}{dr} + \frac{\kappa}{r} + \mu_a \frac{\gamma}{r^2} \\ \frac{d}{dr} + \frac{\kappa}{r} + \mu_a \frac{\gamma}{r^2} & -1 + \frac{\gamma}{r} \end{pmatrix}, \tag{7.167}$$

for $\mu_a = 0.00058$, $\gamma < 0$ and $\kappa = \pm 1$.

As expected, the anomalous moment gives only a little contribution to the energies for small values of $|\gamma|$. However, the degeneracy of the states with $\pm\kappa$

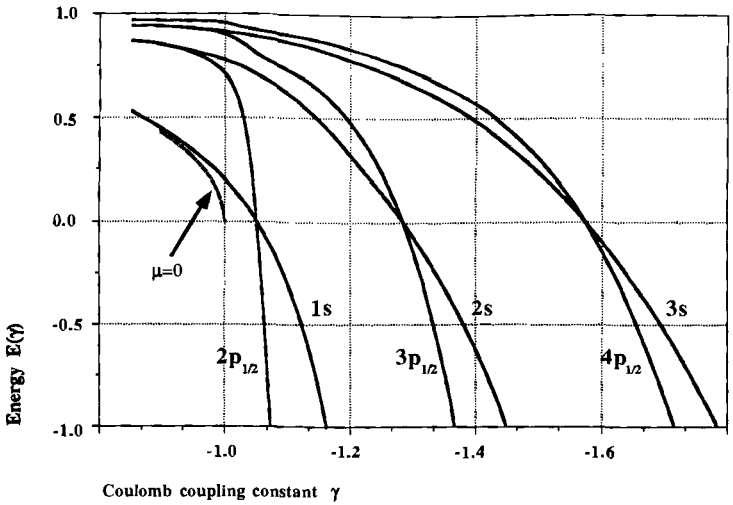

Fig. 7.1. Coupling constant dependence of the bound state energies of electrons with an anomalous magnetic moment in a Coulomb potential

is removed. As the coupling strength is increased, the eigenvalues now move continuously through the gap and finally dive into the lower continuum. As $|\gamma|$ is increased, the electron becomes more and more localized in the vicinity of the origin and the anomalous moment becomes the dominating interaction. The most interesting phenomenon is the level crossing at energy 0 which happens in a quite similar way also for $\kappa = \pm 2, \pm 3$, etc. The numerical calculation leads to the following conjecture: If γ_0 is a zero of $E_{n,\kappa}(\gamma)$ with $\kappa < 0$, then this curve is crossed at γ_0 by the curve $E_{n+1,-\kappa}(\gamma)$. Hence $E_{n,\kappa}(\gamma_0) = E_{n+1,-\kappa}(\gamma_0) = 0$. For example, at $E = 0$, $1s_{1/2}$ is crossed by $2p_{1/2}$, $2s_{1/2}$ is crossed by $3p_{1/2}$, $2p_{3/2}$ is crossed by $3d_{3/2}$, etc.

7.4.6 Stationary Coulomb Scattering

Here we give a very brief description of the partial wave scattering theory for the Dirac-Coulomb equation. Stationary scattering theory is based on the asymptotic analysis of certain "continuum eigenfunctions" of h_κ with energies $|E| > mc^2$. Physical states in the domain of h_κ are wavepackets formed with the help of the regular solution. The regular solution $\Psi_\kappa^{\mathrm{reg}}(E,r)$ is a distributional eigenfunction of h_κ, which is defined by its limiting behavior for small r,

$$\Psi_\kappa^{\mathrm{reg}}(E,r) \approx \begin{pmatrix} \gamma/c \\ -\kappa - s \end{pmatrix} r^s, \quad \text{as } r \to 0, \quad s = \sqrt{\kappa^2 - \gamma^2/c^2}. \tag{7.168}$$

The regular solution is real, because it is a solution of a real differential equation with a real boundary condition. For each $E \in \mathbb{R}$ the system of differential

equations $(h_\kappa - E)\Psi = 0$ has two linearly independent solutions (in a distributional sense, not necessarily square integrable). The Jost solutions $W_\kappa^\pm(E,r)$ are the unique solutions satisfying the asymptotic condition

$$W_\kappa^\pm(E,r) \approx \begin{pmatrix} \sqrt{E+mc^2} \\ \pm \mathrm{i}\sqrt{E-mc^2} \end{pmatrix} \exp\{\pm \mathrm{i}(kr + \nu \ln 2kr)\}, \tag{7.169}$$

We have used the abbreviations

$$k = \tfrac{1}{c}\sqrt{E^2 - m^2c^4}, \qquad \nu = -\frac{\gamma E}{c^2 k}. \tag{7.170}$$

The possible asymptotic forms of the solutions for $r \to 0$ or ∞ are easily obtained from an asymptotic analysis of the Dirac equation. The logarithmic phase in Eq. (7.169) is a consequence of the long-range nature of the Coulomb potential. This is a situation quite similar to the nonrelativistic Coulomb problem. The Coulomb potential keeps influencing the particles at large distances such that the asymptotic behavior is not comparable to the free motion. This will be discussed further in Sect. 8.3.2.

The two Jost solutions are linearly independent and hence the regular solution must be a linear combination

$$\Psi_\kappa^{\mathrm{reg}}(E,r) = A_\kappa^+(E)\, W_\kappa^+(E,r) + A_\kappa^+(E)\, W_\kappa^-(E,r). \tag{7.171}$$

Since the regular solution is real, and the Jost solutions are the complex conjugate of each other, we must have

$$A_\kappa^-(E) = \overline{A_\kappa^+(E)}, \qquad \text{or} \qquad \frac{A_\kappa^+(E)}{A_\kappa^-(E)} = e^{2\mathrm{i}\delta_\kappa(E)}. \tag{7.172}$$

The quantity $\delta_\kappa(E)$ is called the scattering phase shift at energy E. The asymptotic behavior of the regular solution for large r is now given by

$$\Psi_\kappa^{\mathrm{reg}}(E,r) \approx 2|A_\kappa^+(E)| \begin{pmatrix} \sqrt{E+mc^2}\, \cos\big(kr+\nu \ln 2kr+\delta_\kappa(E)\big) \\ -\sqrt{E-mc^2}\, \sin\big(kr+\nu \ln 2kr+\delta_\kappa(E)\big) \end{pmatrix}. \tag{7.173}$$

Since the relativistic Coulomb problem has been solved exactly, the phase shifts can be calculated by determining explicitly the asymptotic behavior of the Coulomb eigenfunctions. One obtains

$$e^{2\mathrm{i}\delta_\kappa(E)} = \frac{\kappa + \mathrm{i}(\gamma m/k)}{s - \mathrm{i}\nu} \frac{\Gamma(s+1-\mathrm{i}\nu)}{\Gamma(s+1+\mathrm{i}\nu)}\, e^{-\mathrm{i}\pi s} \tag{7.174}$$

We finally show that the difference $\delta_\kappa(E) - \delta_{-\kappa}(E)$ is completely determined by supersymmetry in a straightforward way. We only need to know that for any eigensolution Ψ_κ of the Dirac operator with energy E in the angular momentum eigenspace labelled by κ, the corresponding eigensolution with $-\kappa$ is given by $B\Psi$, where B is the BJL operator defined in Sect. 7.4.4. This remains true for the distributional eigenfunctions belonging to the continuous energy spectrum. The action of B on the radial eigenfunctions is given by the matrix operator b_κ,

cf. Eq. (7.160). Comparing the asymptotic behavior as $r \to 0$ of $b_\kappa \Psi_\kappa^{\mathrm{reg}}(E,r)$ with that required for any regular solution, Eq. (7.168), we find

$$\left(b_\kappa \Psi_\kappa^{\mathrm{reg}}\right)(E,r) = \frac{\gamma}{c(s-\kappa)}\left(s + \frac{\kappa E}{mc^2}\right) \Psi_{-\kappa}^{\mathrm{reg}}(E,r), \tag{7.175}$$

where $\Psi_{-\kappa}^{\mathrm{reg}}(E,r)$ is the regular eigenfunction of $h_{-\kappa}$. On the other hand, the action of b_κ on the Jost solutions is easily determined asymptotically. Inserting Eq. (7.148) into the expression (7.147) for B and omitting all terms of order $1/r$ we easily derive

$$b_\kappa W_\kappa^{+}(E,r) \approx \left(\frac{\gamma}{c} \pm \mathrm{i}\frac{\kappa k}{mc}\right) \begin{pmatrix} \sqrt{E+mc^2} \\ \pm \mathrm{i}\sqrt{E-mc^2} \end{pmatrix} \exp\{\pm \mathrm{i}(kr + \nu \ln 2kr)\}, \tag{7.176}$$

as $r \to \infty$. Inserting this asymptotic relation into

$$\begin{aligned} b_\kappa \Psi_\kappa^{\mathrm{reg}} &= A_\kappa^{+} b_\kappa W_\kappa^{+} + A_\kappa^{-} b_\kappa W_\kappa^{-} \\ &= \tfrac{\gamma}{c(s-\kappa)}(A_{-\kappa}^{+} W_{-\kappa}^{+} + A_{-\kappa}^{-} W_{-\kappa}^{-}) \end{aligned} \tag{7.177}$$

and using (7.172) we obtain

$$e^{2\mathrm{i}\delta_{-\kappa}(E)} = \frac{\gamma + \mathrm{i}(\kappa k/mc)}{\gamma - \mathrm{i}(\kappa k/mc)}\, e^{2\mathrm{i}\delta_\kappa(E)} = \frac{\kappa - \mathrm{i}(\gamma m/k)}{\kappa + \mathrm{i}(\gamma m/k)}\, e^{2\mathrm{i}\delta_\kappa(E)}. \tag{7.178}$$

8 Scattering States

One of the basic problems in a mathematical formulation of scattering theory is the proof of asymptotic completeness. In this chapter we solve this problem for the Dirac equation in a number of quite general situations. Asymptotic completeness is a statement on the approximation of scattering states by freely evolving states and implies, e.g., the existence of a unitary scattering operator (Sect. 8.1). We are going to prove asymptotic completeness by time dependent methods due to V. Enss. A basic ingredient is the theory of asymptotic observables which describes the large-time behavior of observables like position, velocity, and the projections to positive/negative kinetic energy.

For scattering states obeying the Dirac equation the "average velocity" $\boldsymbol{x}(t)/t$ asymptotically approaches the classical velocity $c^2 \boldsymbol{p} H_0^{-1}$ (without Zitterbewegung!), as $|t| \to \infty$. This fact is related to the observation that each of the parts of a wavefunction with positive or negative kinetic energies is conserved asymptotically. From this one can derive a quasiclassical asymptotic localization of scattering states in phase space, which is important for proving asymptotic completeness. All these results are true essentially whenever the external potential decreases sufficiently fast, as $|\boldsymbol{x}| \to \infty$. In Sect. 8.3 the existence and completeness of wave operators and the scattering operator is proven for short-range potentials. Coulomb-type potentials require an asymptotic modification of the approximating time evolution (corresponding to the logarithmic phase shift in stationary scattering theory, Sect. 7.4.6). The form of the modifications for long-range electrostatic and scalar potentials is given in Sect. 8.3.2.

Long-range magnetic fields are an exceptional case because of the supersymmetric structure and the gauge freedom. By supersymmetry, the scattering operators for Dirac particles in magnetic fields are related to the corresponding nonrelativistic operators. The gauge freedom can be used to make the description as simple as possible. This is useful because in general long-range potentials cannot be avoided even for magnetic fields with compact support. We show that in these cases asymptotic completeness holds without modifications in a suitably chosen gauge and remains true for magnetic fields with a much weaker decay than one would normally expect (Sect. 8.4). In Sect. 8.4.2 we prove the existence of an unmodified asymptotic free time evolution for a situation where the corresponding classical trajectories do not even have asymptotes.

Finally, we investigate time-dependent potentials in Sect. 8.5. Since we consider only bounded potentials vanishing for large times, the scattering operator can be defined by a Dyson series. We describe some results which will be needed in Chapter 10.

8.1 Preliminaries

8.1.1 Scattering Theory

In the following H and H_0 are self-adjoint operators. In the applications, H is the Dirac operator with a static external field and H_0 is the free Dirac operator. Time dependent fields are discussed in Sect. 8.5. We denote by $\mathfrak{H}^{\mathrm{pp}}$ the closure of the linear span of eigenvectors of H and by $\mathfrak{H}^{\mathrm{cont}}$ the continuous spectral subspace of H,

$$\mathfrak{H}^{\mathrm{cont}} \equiv \mathfrak{H}^{\mathrm{cont}}(H) = \{\, \psi \in \mathfrak{H} \mid (\psi, E_H(\lambda)\psi) \text{ is continuous } \}. \tag{8.1}$$

Here $E_H(\lambda)$ denotes the spectral family of H. If $\mu(\lambda) = (\psi, E_H(\lambda)\psi)$ is even absolutely continuous, then we write $\psi \in \mathfrak{H}^{\mathrm{a.c.}}$, and if $\mu(\lambda)$ is singularly continuous (like a Cantor function with a Cantor set of measure zero), then $\psi \in \mathfrak{H}^{\mathrm{s.c.}}$. We shall assume that H_0 satisfies $\mathfrak{H}^{\mathrm{cont}}(H_0) = \mathfrak{H}^{\mathrm{a.c.}}(H_0) = \mathfrak{H}$.

It is possible to distinguish geometrically between bound states and scattering states as soon as H has the local compactness property (see Sect. 4.3.4).

Theorem 8.1. Assume that H has the local compactness property. Then the vector $\psi \in \mathfrak{H}$ is in $\mathfrak{H}^{\mathrm{pp}}$ if and only if for all ϵ there exists a constant $R > 0$ such that

$$\sup_{t \in \mathbb{R}} \| \chi(|\boldsymbol{x}| > R)\, e^{-\mathrm{i}Ht}\, \psi \| < \epsilon. \tag{8.2}$$

(Here χ denotes the characteristic function of the indicated region). On the other hand, $\psi \in \mathfrak{H}^{\mathrm{cont}}$ if and only if for all $R \in (0, \infty)$

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T \left\| \chi(|\boldsymbol{x}| < R)\, e^{-\mathrm{i}Ht}\, \psi \right\|^2 dt = 0. \tag{8.3}$$

Proof. [Pe 83], Thm.2.1. □

A state with the property (8.2) is called a bound state. It remains within a sufficiently large ball for all times. Eq. (8.3) says that the probability of finding the particle in a ball of radius R vanishes in the time mean in the limit of large time intervals. Such a state is called scattering state. By the theorem above these geometric properties can be equivalently characterized as spectral properties.

Scattering states can only occur if the strength of the external field tends to zero, as $|\boldsymbol{x}| \to \infty$. In this section we are interested in the asymptotic behavior of scattering states under certain conditions on the decay of V at infinity. The following problems are of basic interest in any scattering theory. The first question is whether there exist sufficiently many states $\psi(t) = \exp(-\mathrm{i}Ht)\psi$, which for large $|t|$ can be approximated by solutions $\phi(t)$ of the free Dirac equation. In fact, we want to have a solution of the Dirac equation for *every*

incoming asymptotic configuration[1] $\phi(t)$, i.e., for every "initial condition at $t \to -\infty$". Hence we ask for conditions on the external field such that the following statement is true.

Existence. For every asymptotic configuration $\exp(-\mathrm{i}H_0 t)\phi$, with $\phi \in \mathfrak{H}$, there exist scattering states ψ_+ and ψ_- such that

$$\lim_{t\to\pm\infty} \| e^{-\mathrm{i}Ht}\psi_\pm - e^{-\mathrm{i}H_0 t}\phi \| = 0. \tag{8.4}$$

The states $\psi_\pm$ are called "asymptotically free scattering states".

The next question is whether the scattering solutions of the Dirac equation are completely characterized by their asymptotic behavior at $t \to \pm\infty$.

Completeness. For every scattering state $\psi \in \mathfrak{H}^{\mathrm{cont}}$ there are "asymptotic configurations" $\phi_\pm$ such that

$$\lim_{t\to\pm\infty} \| e^{-\mathrm{i}Ht}\psi - e^{-\mathrm{i}H_0 t}\phi_\pm \| = 0. \tag{8.5}$$

8.1.2 Wave Operators

It is useful to introduce the "Møller wave operators"

$$\Omega_\pm \psi \equiv \Omega_\pm(H, H_0)\,\psi \equiv \lim_{t\to\pm\infty} e^{\mathrm{i}Ht} e^{-\mathrm{i}H_0 t}\psi, \quad \text{for all } \psi \in \mathfrak{H}, \tag{8.6}$$

which can be defined if and only if the scattering system has the existence property (8.4). The completeness property is easily seen to be equivalent to

$$\operatorname{Ran}\Omega_+ = \operatorname{Ran}\Omega_- = \mathfrak{H}^{\mathrm{cont}}. \tag{8.7}$$

A scattering system (H, H_0) for which the wave operators exist and are complete is called "asymptotically complete".

Theorem 8.2. If the wave operators $\Omega_\pm = \Omega_\pm(H, H_0)$ exist, then $\Omega_\pm$ are isometric operators from $\mathfrak{H}$ to $\operatorname{Ran}\Omega_\pm \subset \mathfrak{H}^{\mathrm{cont}}$ (i.e., $\Omega_\pm^*\Omega_\pm = 1$ on $\mathfrak{H}$ and the operators $\Omega_\pm\Omega_\pm^*$ are projectors onto $\operatorname{Ran}\Omega_\pm$). We have the following relations:

$$e^{-\mathrm{i}Ht}\,\Omega_\pm = \Omega_\pm\, e^{-\mathrm{i}H_0 t}, \tag{8.8}$$

$$\Omega_\pm\, \mathfrak{D}(H_0) \subset \mathfrak{D}(H), \qquad H\Omega_\pm = \Omega_\pm H_0 \quad \text{on } \mathfrak{D}(H_0). \tag{8.9}$$

Proof. See [RS 79], Sect. XI.3, or any book on mathematical scattering theory. □

[1] We prefer to call the approximating vectors $\phi(t)$ "asymptotic configurations" rather than "states", because they are auxiliary quantities and not states of the scattering system.

Remark 1. Eqs. (8.8) and (8.9) are called intertwining relations. They imply for any function f with integrable Fourier transform $\hat{f} \in L^1(\mathbb{R})$

$$f(H)\,\Omega_\pm = \frac{1}{\sqrt{2\pi}} \int dt\, \hat{f}(t)\, e^{\mathrm{i}Ht}\, \Omega_\pm$$

$$= \Omega_\pm \frac{1}{\sqrt{2\pi}} \int dt\, \hat{f}(t)\, e^{\mathrm{i}H_0 t} = \Omega_\pm\, f(H_0). \tag{8.10}$$

Remark 2. If asymptotic completeness holds, then the adjoint wave operators are given by

$$\Omega_\pm^*\, \psi = \lim_{t \to \pm\infty} e^{\mathrm{i}H_0 t}\, e^{-\mathrm{i}Ht}\, P^{\mathrm{cont}}\, \psi \quad \text{for all } \psi \in \mathfrak{H}. \tag{8.11}$$

They map $\mathfrak{H}^{\mathrm{cont}}$ onto $\mathfrak{H}$. From (8.10) we infer

$$f(H_0)\, \Omega_\pm^* = \Omega_\pm^*\, f(H). \tag{8.12}$$

Remark 3. If (H, H_0) is asymptotically complete and if H_0 has a purely absolutely continuous spectrum (like the free Dirac operator), then the singularly continuous spectrum of H is absent, i.e.,

$$\mathfrak{H}^{\mathrm{cont}} = \mathfrak{H}^{\mathrm{a.c.}}. \tag{8.13}$$

8.1.3 The Scattering Operator

Theorem 8.3. For an asymptotically complete scattering system (H, H_0) (or if $\mathrm{Ran}\,\Omega_+ = \mathrm{Ran}\,\Omega_-$) the scattering operator

$$S\,\psi \equiv \Omega_+^*\, \Omega_-\, \psi = \lim_{t \to \infty} e^{\mathrm{i}H_0 t}\, e^{-2\mathrm{i}Ht}\, e^{\mathrm{i}H_0 t}\, \psi \tag{8.14}$$

is defined for all $\psi \in \mathfrak{H}$ and unitary. Moreover, S commutes with H_0.

Proof. Because of $\mathrm{Ran}\,\Omega_+ = \mathrm{Ran}\,\Omega_-$ we obtain

$$S^* = \Omega_-^*\, \Omega_+ = \Omega_-^{-1} \Omega_+ = (\Omega_+^{-1} \Omega_-)^{-1} = S^{-1}, \tag{8.15}$$

i.e., S is unitary. Combining (8.10) and (8.12) we find

$$S f(H_0) = f(H_0) S. \tag{8.16}$$

Similarly, Eq. (8.9) and its adjoint imply

$$S\,\mathfrak{D}(H_0) \subset \mathfrak{D}(H_0), \qquad SH_0 = H_0 S \quad \text{on } \mathfrak{D}(H_0). \tag{8.17}$$

□

The scattering operator maps asymptotic configurations for $t \to -\infty$ onto asymptotic configurations for $t \to +\infty$. Hence it describes the connection between the free configurations before and after the scattering process. In a scattering experiment only the asymptotic configurations can be observed. Eq. (8.17) expresses the conservation of energy.

Since S commutes with H_0, it is decomposable in the spectral representation of H_0, i.e.,

$$[U_{\mathrm{sp}} S\psi](\lambda) = S(\lambda)[U_{\mathrm{sp}}\psi](\lambda), \tag{8.18}$$

where each $S(\lambda)$, $\lambda \in \sigma(H_0)$, is a unitary operator in the Hilbert space $\mathfrak{K}$ of the spectral representation. For the Dirac operator, the Hilbert space $\mathfrak{K}$ and the unitary transformation $U_{\mathrm{sp}} : \mathfrak{H} \to \mathfrak{K}$ is given in Sect. 1.4.5. $S(\lambda)$ is called the on-shell scattering operator. We quote the following theorem in order to round off our discussion of Krein's spectral shift function in Chapter 5.

Theorem 8.4. Let $(H - z)^{-1} - (H_0 - z)^{-1}$ be trace-class and let $\xi(\lambda)$ denote Krein's spectral shift function for the pair (H, H_0), i.e.,

$$\mathrm{tr}\,\{(H - z)^{-1} - (H_0 - z)^{-1}\} = -\int \xi(\lambda)\,(\lambda - z)^{-2}\,d\lambda. \tag{8.19}$$

Then the scattering system (H, H_0) is asymptotically complete, and the on-shell scattering operator can be written as

$$S(\lambda) = e^{-2i\pi K(\lambda)}, \tag{8.20}$$

where the "phase shift operator" $K(\lambda)$ is a self-adjoint trace class operator satisfying

$$\mathrm{tr}\,K(\lambda) = \xi(\lambda), \quad \text{for almost every } \lambda \in \sigma(H_0). \tag{8.21}$$

Proof. See, e.g., [BW 83], Sect. 19.1.5. □

8.2 Asymptotic Observables

We want to describe the asymptotic behavior of selected observables under the interacting time evolution. With the help of these results we will be able to give a short proof of asymptotic completeness in Sect. 8.3.1.

8.2.1 Introduction

Let Q be self-adjoint, $H = H_0 + V$ be the Dirac operator in an external field, and denote

$$Q(t) = e^{\mathrm{i}Ht}\, Q\, e^{-\mathrm{i}Ht}. \tag{8.22}$$

We are mainly interested in the asymptotic behavior, as $t \to \pm\infty$ of the Zitterbewegung $\boldsymbol{F}$ (Sect. 1.6), the position operator $\boldsymbol{x}$ and the operator

$$A \equiv \tfrac{1}{2}\left(H_0^{-1}\boldsymbol{p}\cdot\boldsymbol{x} + \boldsymbol{x}\cdot\boldsymbol{p}H_0^{-1}\right) = H_0^{-1}\boldsymbol{p}\cdot\boldsymbol{x} + \tfrac{\mathrm{i}}{2c}\, H_0^{-1}\boldsymbol{\alpha}\cdot\boldsymbol{F}, \tag{8.23}$$

which is defined and essentially self-adjoint on $\mathfrak{D}(|\boldsymbol{x}|)$ and on $C_0^\infty(\mathbb{R}^3)^4$. The operator A is (up to a factor c^2) the symmetrized inner product of the classical velocity $c^2\boldsymbol{p}H_0^{-1}$ with the position of the particle. The sign of A determines whether the averaged motion of the particle is towards the origin or away from it, and it takes into account that wave packets with negative energy move in a direction opposite to their momentum. Therefore the spectral projections of A characterize incoming and outgoing states just as the spectral projections of the dilation generator D do in the nonrelativistic situation.

We have chosen the standard position operator $\boldsymbol{x}$ for a description of the asymptotic localization of particles. We want to stress, however, that the operators $\boldsymbol{x}_{\mathrm{NW}}$ and $\tilde{\boldsymbol{x}}$ which were discussed in Sect. 1.7 differ from $\boldsymbol{x}$ only by bounded operators so that for large times $\boldsymbol{x}(t)/t \sim \boldsymbol{x}_{\mathrm{NW}}(t)/t \sim \tilde{\boldsymbol{x}}(t)/t$. Therefore our main results (e.g., Theorem 8.17) remain true also with the other position operators.

We shall prove the results on asymptotic observables under the convenient assumption that (each component of) the potential matrix $V(\boldsymbol{x})$ is continuously differentiable and

$$V(\boldsymbol{x}) \to 0, \quad \text{and} \quad \boldsymbol{x}\cdot(\nabla V)(\boldsymbol{x}) \to 0, \quad \text{as } |\boldsymbol{x}| \to \infty. \tag{8.24}$$

This implies that V is infinitesimally H_0-bounded and H_0-compact, i.e., the operator $V(H_0 - z)^{-1}$ is compact for all $z \in \rho(H_0)$. Hence (Sect. 4.3.4)

$$\mathfrak{D}(H) = \mathfrak{D}(H_0), \quad \sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(H_0) = (-\infty, -mc^2] \cup [mc^2, \infty). \tag{8.25}$$

Occasionally we shall use further assumptions in order to simplify the proofs. The results remain true if one includes local singularities of Coulomb type. More precisely, we can add a singular short-range potential V_{sr} which satisfies

$$(H_0 - z)^{-1}\,(1 + |\boldsymbol{x}|)\, V_{\mathrm{sr}}\, (H_0 + V_{\mathrm{sr}} - z)^{-1} \quad \text{is compact.} \tag{8.26}$$

This is essentially a condition on the decay of $(1 + |\boldsymbol{x}|)\, V_{\mathrm{sr}}(\boldsymbol{x})$ at infinity (see Sect. 4.3.4).

8.2.2 Invariant Domains

The change in time of a self adjoint operator Q is given by $\mathrm{i}[H, Q(t)]$. The commutator can be defined properly, if there is a dense domain $\mathfrak{D} \subset \mathfrak{D}(Q)$ which is invariant with respect to the time evolution. As in Sect. 1.6.2 we find that the domain of $\boldsymbol{x}$ is invariant under the time evolution in the external field. The proof is the same as for Theorem 1.3, because the position operator $\boldsymbol{x}$ commutes with the potential V.

Theorem 8.5. Let $\mathfrak{D} = \mathfrak{D}(H_0) \cap \mathfrak{D}(V) \subset \mathfrak{D}(H)$ be a dense subset of $\mathfrak{H}$, where V is a 4×4 matrix multiplication operator[2]. Then

$$e^{-\mathrm{i}Ht}\, \mathfrak{D}(|\boldsymbol{x}|^n) \subset \mathfrak{D}(|\boldsymbol{x}|^n), \quad n = 0, 1, 2, \ldots \tag{8.27}$$

and there are constants $k_n(\psi)$ depending only on n and ψ such that

$$\| \, |\boldsymbol{x}|^n \, e^{-\mathrm{i}Ht} \psi \, \| \leq k_n(\psi)\, (1 + c|t|)^n, \quad \text{for all } \psi \in \mathfrak{D}(|\boldsymbol{x}|^n). \tag{8.28}$$

Proof. Clearly, $\mathfrak{D}(|\boldsymbol{x}|^0) = \mathfrak{D}(\mathbf{1}) = \mathfrak{H}$ is invariant under the time evolution in the external field. We proceed inductively and assume that the result is true for $n-1$. The operator

$$B_\lambda(x) = \frac{x^n}{1 + \lambda x^n}, \qquad \text{where } x \equiv |\boldsymbol{x}|, \tag{8.29}$$

is bounded and has a bounded derivative. Hence it leaves $\mathfrak{D}$ invariant and on this domain we can calculate

$$\frac{d}{dt} B_\lambda\big(x(t)\big) = \mathrm{i}[H, B_\lambda\big(x(t)\big)] = e^{\mathrm{i}Ht} \frac{\boldsymbol{\alpha} \cdot \boldsymbol{x}}{x} \frac{nc\, x^{n-1}}{(1 + \lambda x^n)^2} \, e^{-\mathrm{i}Ht}. \tag{8.30}$$

We see that the commutator defines a bounded operator which can be extended by linearity to all of $\mathfrak{H}$. Hence for $\psi \in \mathfrak{H}$ we find

$$\| \, B_\lambda(x)\, e^{-\mathrm{i}Ht} \psi \, \| = \| \, B_\lambda(x)\, \psi \, \| + \int_0^{|t|} nc \left\| \frac{x^{n-1}}{(1 + \lambda x^n)^2} \, e^{-\mathrm{i}Hs} \psi \right\| ds. \tag{8.31}$$

By assumption, $\mathfrak{D}(x^{n-1})$ is invariant under $e^{-\mathrm{i}Hs}$. For $\psi \in \mathfrak{D}(x^n) \subset \mathfrak{D}(x^{n-1})$ this implies that all expressions on the right hand side of Eq. (8.31) are bounded uniformly in λ, as $\lambda \to 0$. Hence we find $e^{-\mathrm{i}Ht} \psi \in \mathfrak{D}(x^n)$ and

$$\begin{aligned} \| \, x^n \, e^{-\mathrm{i}Ht} \psi \, \| &\leq \| \, x^n \, \psi \, \| + \int_0^{|t|} nc \, \| \, x^{n-1} \, e^{-\mathrm{i}Hs} \psi \, \| \, ds \\ &\leq \| \, x^n \, \psi \, \| + \int_0^{|t|} nc \, k_{n-1}(\psi)\, (1 + c|s|)^{n-1} \, ds \end{aligned}$$

[2] This is a condition on the local singularities and can be further relaxed, see [129]. It is remarkable that this theorem needs no condition restricting the behavior of V at infinity. The conclusion of this theorem is false in nonrelativistic quantum mechanics [371].

$$\leq \| x^n \psi \| + \tilde{k}_n(\psi)\,(1 + c|t|)^n \leq k_n(\psi)\,(1 + c|t|)^n. \tag{8.32}$$

□

Remark. The estimate (8.28) for $n = 1$ shows that irrespective of the external field the particle cannot escape faster than with the velocity of light. Another consequence of the finite propagation speed is that the essential self-adjointness of H is insensitive to the large $\boldsymbol{x}$ behavior of the potential (Sect. 4.3.2). This also shows up in the following corollary.

Corollary 8.6. Let H be as above, $\operatorname{Im} z \neq 0$, and let n, k be integers with $n \geq 0$, and $k \geq 1$. Then H is essentially self-adjoint on

$$\mathfrak{D} \equiv (H - z)^{-k}\,\mathfrak{D}(|\boldsymbol{x}|^n) \subset \mathfrak{D}(|\boldsymbol{x}|^n). \tag{8.33}$$

Proof. $\mathfrak{D}$ is dense for all $k \geq 0$, because $\mathfrak{D}(|\boldsymbol{x}|^n)$ is dense and $(H - z)^{-k}$ is a bounded operator with injective adjoint. For $\psi \in \mathfrak{D}(|\boldsymbol{x}|^n)$, $\operatorname{Im} z > 0$, (8.28) implies

$$\begin{aligned} \| \,|\boldsymbol{x}|^n\,(H - z)^{-k}\,\psi \,\| &= \text{const.} \left\| \int_0^\infty dt\, e^{\mathrm{i}zt}\, t^{k-1}\, |\boldsymbol{x}|^n\, e^{-\mathrm{i}Ht}\,\psi \right\| \\ &\leq \int_0^\infty dt\, e^{-(\operatorname{Im} z)t}\, t^{k-1}\, k_n(\psi)\,(1 + ct)^n < \infty, \end{aligned} \tag{8.34}$$

which shows that $\mathfrak{D} \subset \mathfrak{D}(|\boldsymbol{x}|^n)$. Since for $k \geq 1$

$$(H - z)\mathfrak{D} = (H - z)^{-k+1}\,\mathfrak{D}(|\boldsymbol{x}|^n) \tag{8.35}$$

is a dense set, H is essentially self-adjoint on $\mathfrak{D}$ by the basic criterion ([RS 72], corollary to Thm. VIII.3). □

Corollary 8.7. Let H be as above. Then the operator $\frac{1}{t}|\boldsymbol{x}|\, e^{-\mathrm{i}Ht}$ converges weakly to zero, i.e.,

$$\lim_{|t| \to \infty} \left| \left(\phi,\, \tfrac{1}{t}|\boldsymbol{x}|\, e^{-\mathrm{i}Ht}\,\psi\right) \right| = 0, \quad \text{for all } \phi \in \mathfrak{H}, \text{ and } \psi \in \mathfrak{D}(|\boldsymbol{x}|). \tag{8.36}$$

Hence, if C is any compact operator, we have

$$\lim_{|t| \to \infty} C\, \tfrac{1}{t}|\boldsymbol{x}|\, e^{-\mathrm{i}Ht}\,\psi = 0, \quad \text{for all } \psi \in \mathfrak{D}(|\boldsymbol{x}|). \tag{8.37}$$

Proof. We approximate ϕ by $\phi' \in \mathfrak{D}(|\boldsymbol{x}|)$ and apply the Cauchy Schwarz inequality to obtain

$$\left| \left(\phi,\, \tfrac{1}{t}|\boldsymbol{x}|\, e^{-\mathrm{i}Ht}\,\psi\right) \right| \leq \|\phi - \phi'\| \cdot \left\| \tfrac{1}{t}|\boldsymbol{x}|\, e^{-\mathrm{i}Ht}\,\psi \right\| + \tfrac{1}{|t|} \left\| \,|\boldsymbol{x}|\phi' \right\| \cdot \|\psi\|. \tag{8.38}$$

The first summand can be made smaller than $\epsilon/2$ by choosing ϕ' appropriately. With this ϕ' the second summand is smaller than $\epsilon/2$ for $|t|$ large enough. This proves the weak convergence. The result (8.37) follows, because a compact operator maps a weakly convergent sequence into a strongly convergent sequence ([RS 72], Thm. VI.11). □

8.2.3 RAGE

Our results on asymptotic observables are based on the following lemma which together with Theorem 8.1 is known as the RAGE theorem.

Lemma 8.8. Let C be compact and H be self-adjoint. Then

$$\lim_{T\to\infty} \left\| \frac{1}{T} \int_0^T e^{\mathrm{i}Ht}\, C\, e^{-\mathrm{i}Ht}\, P^{\mathrm{cont}}\, dt \right\| = 0, \tag{8.39}$$

where P^{cont} is the projector onto $\mathfrak{H}^{\mathrm{cont}}(H)$.

Proof. See, e.g., [CFKS 87], Thm 5.8. □

8.2.4 Asymptotics of Zitterbewegung

Our results in Sect. 8.2.2 show that the operators $x^2(t)/t^2$ and $A(t)/t$ are asymptotically bounded. In order to calculate the limit $t \to \infty$ explicitly we need some information about Zitterbewegung in the presence of external fields. The time evolution of $x^2(t)$ is described by

$$\frac{dx^2(t)}{dt} = \mathrm{i}[H, x^2(t)] = 2c^2 A(t) + \big(\boldsymbol{F}\cdot\boldsymbol{x} + \boldsymbol{x}\cdot\boldsymbol{F}\big)(t) \tag{8.40}$$

on the dense invariant domain $\mathfrak{D} = (H-z)^{-1}\mathfrak{D}(x^2)$. The operator $\boldsymbol{F}$ describing the Zitterbewegung has been investigated in Sect. 1.6. We are now going to describe the time evolution of $\boldsymbol{F}$ and of $\boldsymbol{F}\cdot\boldsymbol{x} + \boldsymbol{x}\cdot\boldsymbol{F}$ in the presence of external fields. The results are given in the form needed for a proof of the Theorems 8.12 and 8.13 under the simplifying assumption (8.24).

Lemma 8.9. Let $H = H_0 + V$, where V is H_0-compact. Then the operators $\boldsymbol{F} = c\,\boldsymbol{\alpha} - c^2 \boldsymbol{p} H_0^{-1}$ and $G = \beta - mc^2 H_0^{-1}$ (cf. Sect. 1.6) fulfil

$$\lim_{T\to\infty} \left\| \frac{1}{T} \int_0^T \boldsymbol{F}(t)\, P^{\mathrm{cont}}\, dt \right\| = 0, \quad \lim_{T\to\infty} \left\| \frac{1}{T} \int_0^T G(t)\, P^{\mathrm{cont}}\, dt \right\| = 0. \tag{8.41}$$

Proof. On $\mathfrak{D}(H_0) = \mathfrak{D}(H)$ we calculate

$$\frac{d}{dt}\boldsymbol{F}(t) = \mathrm{i}[H, \boldsymbol{F}(t)] = -2\mathrm{i}\,\boldsymbol{F}(t)\,H_0(t) + \mathrm{i}[V, \boldsymbol{F}](t)$$

$$= -2\mathrm{i}\,\boldsymbol{F}(t)\,H + \mathrm{i}\{V, \boldsymbol{F}\}(t). \tag{8.42}$$

We multiply (8.42) from the right by the bounded operator $H^{-1}P^{\mathrm{cont}}$, integrate from 0 to T, and divide by T. This gives

$$\frac{1}{T}\big(\boldsymbol{F}(T) - \boldsymbol{F}(0)\big)\, H^{-1} P^{\mathrm{cont}}$$

$$= \frac{-2\mathrm{i}}{T} \int_0^T dt\, \boldsymbol{F}(t)\, P^{\mathrm{cont}} + \frac{1}{T} \int_0^T dt\, \{V, \boldsymbol{F}\}\, H^{-1}\, P^{\mathrm{cont}}. \tag{8.43}$$

The operator $\{V, \boldsymbol{F}\}\, H^{-1}\, P^{\mathrm{cont}}$ is easily seen to be compact. By Lemma 8.8 the last summand vanishes in norm, as $T \to \infty$. Finally,

$$\frac{1}{T} \left\| \left(\boldsymbol{F}(T) - \boldsymbol{F}(0) \right) H^{-1} P^{\mathrm{cont}} \right\| \leq \frac{2}{T} \frac{\|\boldsymbol{F}\|}{mc^2} \to 0, \quad \text{as } T \to \infty, \tag{8.44}$$

proves the result for $\boldsymbol{F}$. The proof for G is completely analogous. □

Lemma 8.10. Let $\psi \in \mathfrak{D}(\boldsymbol{x})$. Then

$$\lim_{|T| \to \infty} \frac{1}{T^2} \int_0^T e^{\mathrm{i}Ht} (\boldsymbol{F} \cdot \boldsymbol{x} + \boldsymbol{x} \cdot \boldsymbol{F}) e^{-\mathrm{i}Ht}\, \psi\, dt = 0. \tag{8.45}$$

Proof. Since

$$\boldsymbol{F} \cdot \boldsymbol{x} - \boldsymbol{x} \cdot \boldsymbol{F} = c^2 (H_0^{-1} c\boldsymbol{\alpha} \cdot \boldsymbol{p} + c\boldsymbol{\alpha} \cdot \boldsymbol{p} H_0^{-1}) = \mathrm{i}c H_0^{-1} \boldsymbol{\alpha} \cdot \boldsymbol{F} \tag{8.46}$$

is bounded it is sufficient to estimate the expression with $\boldsymbol{F} \cdot \boldsymbol{x}$. We prove (8.45) under the assumption that $(1/t) \|(1 - P^{\mathrm{cont}})\, \boldsymbol{x}(t)\, \psi\| \to 0$, as $t \to \infty$. This is reasonable, because bound states are expected to stay essentially within a bounded region. For the general case we refer to the literature cited in the Notes. We obtain

$$\left\| \frac{1}{T^2} \int_0^T \boldsymbol{F}(t)(1 - P^{\mathrm{cont}}) \cdot \boldsymbol{x}(t)\, \psi\, dt \right\|$$

$$\leq \frac{1}{T^2} \int_0^T t\, dt\, \|\boldsymbol{F}\| \cdot \left\| (1 - P^{\mathrm{cont}}) \boldsymbol{x}(t)\, \psi \right\|. \tag{8.47}$$

Using our assumption this is easily seen to vanish as $|T| \to \infty$. It remains to estimate

$$\left\| \frac{1}{T^2} \int_0^T \boldsymbol{F}(t) P^{\mathrm{cont}} \cdot \boldsymbol{x}(t)\, \psi\, dt \right\|. \tag{8.48}$$

With the help of a partial integration we find that (8.48) is equal to

$$\frac{1}{T^2} \left\| \int_0^T dt\, \boldsymbol{F}(t) P^{\mathrm{cont}} \cdot \boldsymbol{x}(T)\, \psi - \int_0^T dt \int_0^t ds\, \boldsymbol{F}(s) P^{\mathrm{cont}} \cdot c\boldsymbol{\alpha}(t)\, \psi \right\|$$

$$\leq \left\| \frac{1}{T} \int_0^T dt\, \boldsymbol{F}(t) P^{\mathrm{cont}} \right\| \cdot \frac{1}{T} \|\boldsymbol{x}(T)\psi\|$$

$$+ \frac{1}{T^2} \int_0^T t\, dt \left\| \frac{1}{t} \int_0^t dt\, \boldsymbol{F}(t) P^{\mathrm{cont}} \right\| \cdot \|c\boldsymbol{\alpha}\| \cdot \|\psi\|. \tag{8.49}$$

By Lemma 8.9 and the fact that $(1/T)\|\boldsymbol{x}(T)\psi\|$ is bounded uniformly in T for $\psi \in \mathfrak{D}(\boldsymbol{x})$ we easily conclude that (8.49) vanishes, as $T \to \infty$. □

8.2.5 Asymptotic Observables

We shall need the following technical results on strong resolvent convergence.

Lemma 8.11. Let T_n and T be self-adjoint in $\mathfrak{H}$.
a) If there is a core $\mathfrak{D}_0$ of T (i.e., a domain where T is essentially self-adjoint), such that $\mathfrak{D}_0 \subset \mathfrak{D}(T_n)$ and $\lim_{n\to\infty} T_n\phi = T\phi$ for all $\phi \in \mathfrak{D}_0$, then T_n converges to T in the strong resolvent sense, i.e., for some $z \in \mathbb{C} \setminus \mathbb{R}$

$$\lim_{n\to\infty} (T_n - z)^{-1}\phi = (T - z)^{-1}\phi, \quad \text{all } \phi \in \mathfrak{H}. \tag{8.50}$$

b) If $T_n \to T$ in the strong resolvent sense, then

$$\lim_{n\to\infty} f(T_n)\phi = f(T)\phi, \quad \text{all } \phi \in \mathfrak{H}, \tag{8.51}$$

for every bounded, continuous function f.
c) If $T_n \to T$ in the strong resolvent sense, then

$$\lim_{n\to\infty} E_{T_n}(\lambda)\phi = E_T(\lambda)\phi, \quad \text{all } \phi \in \mathfrak{H}, \tag{8.52}$$

where λ is not an eigenvalue of T.

Proof. [We 80], Thms.9.16(i), 9.17, and 9.19 or [RS 72], Thms. VIII.20 and VIII.24. □

The following result on the asymptotic behavior of the operator $A(t)$ corresponds to classical kinematics which gives

$$A/t = \frac{\boldsymbol{v}}{c^2} \cdot \frac{\boldsymbol{x}}{t} \approx \frac{\boldsymbol{v}^2}{c^2} = \left(1 - \frac{m^2c^4}{E^2}\right). \tag{8.53}$$

Theorem 8.12. Let $H = H_0 + V$, and $V = V_{\mathrm{lr}} + V_{\mathrm{sr}}$, where V_{lr} satisfies Eq. (8.24) and V_{sr} satisfies Eq. (8.26). Then

$$\lim_{|t|\to\infty} \frac{A(t)}{t} = \left(1 - \frac{m^2c^4}{H^2}\right) P^{\mathrm{cont}} \tag{8.54}$$

in the strong resolvent sense.

Proof. We give the proof for $V = V_{\mathrm{lr}}$. Let $H\psi = E\psi$, f bounded and continuous. Then

$$\lim_{|t|\to\infty} f(A(t)/t)\,\psi = \lim_{|t|\to\infty} e^{\mathrm{i}(H-E)t} f(A/t)\,\psi = f(0)\,\psi \tag{8.55}$$

proves that

$$\lim_{|t|\to\infty} A(t)/t = 0 \quad \text{on } (1 - P^{\mathrm{cont}})\mathfrak{H} \tag{8.56}$$

in the strong resolvent sense. It remains to prove (8.54) on $\mathfrak{H}^{\mathrm{cont}}$. Using Eq. (1.242), the time dependence of $A(t)$ is given by

$$\frac{dA(t)}{dt} = \mathrm{i}[H, A](t) = (c^2 p^2 H_0^{-1})(t) + \mathrm{i}[V, A](t)$$

$$= (\mathbf{1} - m^2 c^4 H^{-2}) + m^2 c^4 (H^{-2} - H_0^{-2})(t) + \mathrm{i}[V, A](t). \tag{8.57}$$

The commutator is well defined on the domain $\mathfrak{D} = (H - z)^{-1}\mathfrak{D}(|\boldsymbol{x}|)$, which is invariant by Corollary 8.6. The second summand in (8.57) is compact. If $\mathrm{i}[V, A]$ is also compact, then we integrate (8.57) and obtain for $\psi \in \mathfrak{D}$

$$\frac{A(T) - A(0)}{T} P^{\mathrm{cont}} \psi$$

$$= (\mathbf{1} - m^2 c^4 H^{-2}) P^{\mathrm{cont}} \psi + \frac{1}{T} \int_0^T K_1(t)\, dt\, P^{\mathrm{cont}} \psi, \tag{8.58}$$

where K_1 is compact and $A(0) = A$. Next we apply Lemma 8.8 to find that the last expression vanishes, as $T \to \infty$. Clearly $(A/T)P^{\mathrm{cont}}\psi$ vanishes as well. This implies convergence of $A(T)/T$ on the dense set $\mathfrak{D}$. Since the limit $(\mathbf{1} - m^2 c^4 H^{-2})\, P^{\mathrm{cont}}$ is bounded, $\mathfrak{D}$ is a core, and strong resolvent convergence follows by Lemma 8.11. However, there remains a little problem. We have

$$\mathrm{i}[V, A] = \mathrm{i} H_0^{-1} \boldsymbol{p} \cdot \boldsymbol{x}[H_0, V] H_0^{-1} + K_2 \tag{8.59}$$

where K_2 is compact. The first summand is compact whenever $\boldsymbol{x}[H_0, V]$ decays for $|\boldsymbol{x}| \to \infty$. This is the case for electrostatic potentials, but if V is an arbitrary 4×4 matrix, then

$$\boldsymbol{x}\,[H_0, V] = \boldsymbol{x}\,[c\boldsymbol{\alpha}, V] \cdot \boldsymbol{p} + \boldsymbol{x}\, mc^2 [\beta, V] - \mathrm{i}\boldsymbol{x}\, c\boldsymbol{\alpha} \cdot (\nabla V) \tag{8.60}$$

might even increase at infinity so that (8.59) is not even bounded. In this case we define the auxiliary operator

$$\tilde{A} \equiv \tfrac{1}{2} \left(H^{-1} \boldsymbol{p} \cdot \boldsymbol{x} + \boldsymbol{x} \cdot \boldsymbol{p} H^{-1} \right) \tag{8.61}$$

which is well defined on $\mathfrak{D}(|\boldsymbol{x}|)$ and for which one can show that

$$\mathrm{i}[H, \tilde{A}] = \mathbf{1} - \frac{m^2 c^4}{H^2} + K_3, \quad \text{on } \mathfrak{D}, \tag{8.62}$$

where K_3 is compact. Hence we have the result

$$\frac{\tilde{A}(t)}{t} \psi \to \left(\mathbf{1} - \frac{m^2 c^4}{H^2} \right) P^{\mathrm{cont}} \psi, \quad \text{as } |t| \to \infty, \tag{8.63}$$

for ψ in an invariant dense set. By the following argument this would be sufficient to prove Theorem 1.2. The difference of $\tilde{A}$ and A is given by

$$A - \tilde{A} = (\boldsymbol{p} H_0^{-1} - \boldsymbol{p} H^{-1}) \cdot \boldsymbol{x} + B \tag{8.64}$$

where B is bounded. Hence

$$\tfrac{1}{t}\| \left(A(t) - \tilde{A}(t) \right) \psi \|$$

$$\leq \| (\boldsymbol{p}H_0^{-1} - \boldsymbol{p}H^{-1}) \cdot \tfrac{1}{t}\boldsymbol{x}\, e^{-\mathrm{i}Ht}\psi \| + \tfrac{1}{t}\| B\, e^{-\mathrm{i}Ht}\psi \|. \tag{8.65}$$

The last summand tends to zero as $|t| \to \infty$. Since VH^{-1} is compact, the difference

$$\boldsymbol{p}H_0^{-1} - \boldsymbol{p}H^{-1} = \boldsymbol{p}H_0^{-1}VH^{-1} \tag{8.66}$$

is again compact and by Corollary 8.7 the first summand in (8.65) vanishes asymptotically. Hence (8.63) implies the same result for $A(t)$. □

Theorem 8.13. Let $H = H_0 + V$, and $V = V_{\mathrm{lr}} + V_{\mathrm{sr}}$, where V_{lr} satisfies Eq. (8.24) and V_{sr} satisfies Eq. (8.26). Then

$$\lim_{|t|\to\infty} \frac{x^2(t)}{t^2} = c^2\Big(1 - \frac{m^2c^4}{H^2}\Big)P^{\mathrm{cont}} \tag{8.67}$$

in the strong resolvent sense.

Proof. The proof for bound states is the same as in the preceding theorem. It remains to prove (8.67) on $\mathfrak{H}^{\mathrm{cont}}$. From Eq. (8.40) we obtain for $\psi \in (H - z)^{-1}\mathfrak{D}(x^2)$

$$\frac{x^2(t)}{t^2}\psi = \frac{x^2}{t^2}\psi + \frac{2c^2}{t^2}\int_0^t ds\, A(s)\psi$$

$$+ \frac{1}{t^2}\int_0^t ds\, e^{\mathrm{i}Hs}(\boldsymbol{F}\cdot\boldsymbol{x} + \boldsymbol{x}\cdot\boldsymbol{F})e^{-\mathrm{i}Hs}\psi. \tag{8.68}$$

The last term in (8.68) vanishes as $|t| \to \infty$ by Lemma 8.10, and $\|(x^2/t^2)\psi\|$ decays as well. Next we estimate

$$\Big\| \Big(\frac{2}{t^2}\int_0^t ds\, A(s)\psi\Big) - \Big(1 - \frac{m^2c^4}{H^2}\Big)P^{\mathrm{cont}}\psi \Big\|$$

$$\leq \frac{2}{t^2}\int_0^t s\, ds \Big\| \Big\{\tfrac{1}{s}A(s) - \Big(1 - \frac{m^2c^4}{H^2}\Big)P^{\mathrm{cont}}\Big\}\psi \Big\|. \tag{8.69}$$

The expression (8.69) vanishes, as $|t| \to \infty$, by Theorem 8.12. Therefore $x^2(t)/t^2$ converges on a dense set which is a core of the bounded limit operator. This implies strong resolvent convergence by Lemma 8.11. □

This result can be used to describe the behavior of states $\psi \in \mathfrak{H}^{\mathrm{cont}}$ more detailed than in Theorem 8.1.

Corollary 8.14. Let H be as above and $\psi \in \mathfrak{H}^{\mathrm{cont}}$. Then

$$\lim_{|t|\to\infty} \left\| \chi(|\boldsymbol{x}| < R)\, e^{-\mathrm{i}Ht}\, \psi \right\| = 0, \quad \text{for all } R, \tag{8.70}$$

where χ is the characteristic function of the indicated region.

Proof. Lemma 8.11c and the strong resolvent convergence of $x^2(t)/t$ imply for $\psi \in \mathfrak{H}^{\mathrm{cont}}$

$$\chi(\boldsymbol{x}^2(t)/t^2 < v^2)\, \psi \to \chi(\mathbf{1} - m^2c^4\, H^{-2} < v^2/c^2)\, \psi. \tag{8.71}$$

The characteristic function of H can be defined with the spectral theorem,

$$\chi(\mathbf{1} - m^2c^4\, H^{-2} < v^2/c^2) = \int_B dE_H(\lambda), \tag{8.72}$$

where $B = \{\lambda \in \mathbb{R} \mid 1 - m^2c^4/\lambda^2 < v^2/c^2\}$. In the expression

$$\begin{aligned} &\| \chi(|\boldsymbol{x}| < R)\, e^{-\mathrm{i}Ht}\, \psi \| \\ &\quad \le \| \chi(|\boldsymbol{x}| < R)\, e^{-\mathrm{i}Ht}\, \chi(|H| < mc^2/\sqrt{1 - v^2/c^2})\, \psi \| \\ &\quad + \| \chi(|\boldsymbol{x}| < R)\, e^{-\mathrm{i}Ht}\, \chi(|H| > mc^2/\sqrt{1 - v^2/c^2})\, \psi \| \end{aligned} \tag{8.73}$$

the first summand is $< \epsilon/2$ for some small v. With this v we can choose $|t|$ so large that the second summand is $< \epsilon/2$ by (8.71). Hence $\chi(|\boldsymbol{x}| < R)\, e^{-\mathrm{i}Ht}\, \psi$ is small for large $|t|$ which proves the corollary. □

In the next corollary a scattering state with positive energy is asymptotically approximated by a configuration with positive "kinetic" energy. We denote by $P^{\mathrm{cont}}_{\mathrm{pos,neg}}$ the projectors on the positive and negative energy subspaces of $\mathfrak{H}^{\mathrm{cont}}$. The projectors P^0_{pos} and P^0_{neg} are associated with the free Dirac operator H_0, cf. Sect. 1.4.2.

Corollary 8.15. Let H be as above and $\psi \in \mathfrak{H}^{\mathrm{cont}}(H)$. Then

$$\lim_{|t|\to\infty} \| (P^0_{\mathrm{pos}} - P^{\mathrm{cont}}_{\mathrm{pos}})\, e^{-\mathrm{i}Ht}\, \psi \| = \lim_{|t|\to\infty} \| (P^0_{\mathrm{neg}} - P^{\mathrm{cont}}_{\mathrm{neg}})\, e^{-\mathrm{i}Ht}\, \psi \| = 0. \tag{8.74}$$

Moreover, for all $g \in C_0^\infty(\mathbb{R})$

$$\lim_{|t|\to\infty} \| \big(g(H) - g(H_0) \big)\, e^{-\mathrm{i}Ht}\, \psi \| = 0. \tag{8.75}$$

Proof. Let $\phi \in \mathfrak{H}$, $\psi \in \mathfrak{H}^{\mathrm{cont}}$, with $\|\phi\| = \|\psi\| = 1$. Then

$$|(\phi, e^{-\mathrm{i}Ht}\, \psi)| \le \| \chi(|\boldsymbol{x}| > R)\, \phi \| + \| \chi(|\boldsymbol{x}| < R)\, e^{-\mathrm{i}Ht}\, \phi \| < \epsilon, \tag{8.76}$$

if one chooses R large enough to have the first summand $< \epsilon/2$ and then takes $|t|$ large enough to get the second term $< \epsilon/2$ by Corollary 8.14. Hence $\exp(-\mathrm{i}Ht)\psi$ converges weakly to zero for $\psi \in \mathfrak{H}^{\mathrm{cont}}$, and if C is any compact operator, we have

$$\lim_{|t|\to\infty} C\, e^{-\mathrm{i}Ht}\,\psi = 0, \quad \text{for all } \psi \in \mathfrak{H}^{\mathrm{cont}}. \tag{8.77}$$

Since the operator $H^{-1} - H_0^{-1}$ is compact on $\mathfrak{H}^{\mathrm{cont}}$ we obtain

$$\| (H^{-1} - H_0^{-1}) e^{-\mathrm{i}Ht}\,\psi \| \to 0, \tag{8.78}$$

i.e., $H_0(t)$ converges in the strong resolvent sense to H. This implies $P_{\mathrm{pos}}(t)\,\psi \to P_{\mathrm{pos}}^{\mathrm{cont}}\,\psi$ and $g(H_0(t))\psi \to g(H)\psi$ for all $g \in \mathcal{C}_0^\infty$, and all $\psi \in \mathfrak{H}^{\mathrm{cont}}$ by Lemma 8.11 (see also the proof of Theorem 8.17 in Sect. 8.2.6). □

Theorem 8.16. Let H be as above. Then

$$\lim_{|t|\to\infty} \Big(\frac{c^2\boldsymbol{p}}{H_0}\Big)^2(t)\,\psi = c^2\Big(\mathbf{1} - \frac{m^2c^4}{H^2}\Big)\,\psi, \quad \text{for all } \psi \in \mathfrak{H}^{\mathrm{cont}}. \tag{8.79}$$

Proof. Since $H_0^2 = c^2p^2 + m^2c^4$ we have

$$\mathbf{1} - m^2c^4H^{-2} - c^2p^2H_0^{-2} = m^2c^4(H_0^{-2} - H^{-2}), \tag{8.80}$$

which is compact by our assumptions on V. By the weak convergence (8.76) of $\exp(-\mathrm{i}Ht)\psi$ we conclude as in Corollary 8.7

$$\lim_{|t|\to\infty} \| \left(\mathbf{1} - m^2c^4H^{-2} - c^2p^2H_0^{-2}\right) e^{-\mathrm{i}Ht}\,\psi \| = 0. \tag{8.81}$$

□

8.2.6 Propagation in Phase Space

Theorem 8.17. Let $H = H_0 + V$, and $V = V_{\mathrm{lr}} + V_{\mathrm{sr}}$, where V_{lr} satisfies Eq. (8.24) and V_{sr} satisfies Eq. (8.26). Assume that f or $1 - f$ is a function in $\mathcal{C}_0^\infty(\mathbb{R}^3)$. Then for all $\psi \in \mathfrak{H}^{\mathrm{cont}}$

$$\lim_{|t|\to\infty} \| \{ f(\boldsymbol{x}/t) - f(c^2\boldsymbol{p}H_0^{-1}) \}\, e^{-\mathrm{i}Ht}\,\psi \| = 0. \tag{8.82}$$

Denoting $\boldsymbol{u}(\boldsymbol{p}) = c^2\boldsymbol{p}/\sqrt{c^2p^2 + m^2c^4}$ we have

$$\lim_{|t|\to\infty} \| \{ f(\boldsymbol{x}/t) - f(\boldsymbol{u}(\boldsymbol{p})) \}\, e^{-\mathrm{i}Ht}\, P_{\mathrm{pos}}^{\mathrm{cont}}\,\psi \| = 0, \tag{8.83}$$

$$\lim_{|t|\to\infty} \| \{ f(\boldsymbol{x}/t) - f(-\boldsymbol{u}(\boldsymbol{p})) \}\, e^{-\mathrm{i}Ht}\, P_{\mathrm{neg}}^{\mathrm{cont}}\,\psi \| = 0. \tag{8.84}$$

Proof. By (8.74), Eqs. (8.83) and (8.84) are equivalent to Eq. (8.82). We shall prove this theorem for ψ in the domain

$$\mathfrak{D} \equiv (H - z)^{-2}\mathfrak{D}(x^2) \cap P_{\mathrm{pos}}^{\mathrm{cont}}\mathfrak{H}, \tag{8.85}$$

under the assumption that $\mathfrak{D}$ is dense in the subspace $P_{\mathrm{pos}}^{\mathrm{cont}}\mathfrak{H}$ of positive energy scattering states (without this assumption the theorem is proved with the help

of an additional approximation argument). The proof for $P_{\text{neg}}^{\text{cont}}\mathfrak{H}$ is completely analogous. Now, let $\psi \in \mathfrak{D}$, $\|\psi\| = 1$,

$$\begin{aligned}
&\| \{ f(\boldsymbol{x}/t) - f(c^2 \boldsymbol{p} H_0^{-1}) \} e^{-\mathrm{i}Ht} \psi \| \\
&\quad = \| \{ f(\boldsymbol{x}/t) - f(\boldsymbol{u}(\boldsymbol{p})) \} e^{-\mathrm{i}Ht} \psi \| \\
&\quad \leq \frac{1}{(2\pi)^{3/2}} \int d^3q \, |\hat{f}(\boldsymbol{q})| \, \| \{ e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}/t} - e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{u}(\boldsymbol{p})} \} e^{-\mathrm{i}Ht} \psi \|. \qquad (8.86)
\end{aligned}$$

By the Lebesgue dominated convergence theorem the integral vanishes if the norm vanishes as $|t| \to \infty$ for any fixed $\boldsymbol{q}$.

$$\begin{aligned}
&\| \{ e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}/t} - e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{u}(\boldsymbol{p})} \} e^{-\mathrm{i}Ht} \psi \| \\
&\leq \| \{ e^{\mathrm{i}\boldsymbol{q}\cdot[\boldsymbol{x}/t - \boldsymbol{u}(\boldsymbol{p})]} - \mathbf{1} \} e^{-\mathrm{i}Ht} \psi \| + \| e^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{u}(\boldsymbol{p})} e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}/t} - e^{\mathrm{i}\boldsymbol{q}\cdot[\boldsymbol{x}/t - \boldsymbol{u}(\boldsymbol{p})]} \|. \qquad (8.87)
\end{aligned}$$

By the canonical commutation relations,

$$e^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{u}(\boldsymbol{p})} e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}/t} = e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}/t} e^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{u}(\boldsymbol{p}+\boldsymbol{q}/t)}, \qquad (8.88)$$

$$e^{\mathrm{i}\boldsymbol{q}\cdot[\boldsymbol{x}/t - \boldsymbol{u}(\boldsymbol{p})]} = e^{-\mathrm{i}\lambda(p)t} e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}/t} e^{\mathrm{i}\lambda(p)t} = e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}/t} e^{\mathrm{i}t[\lambda(p) - \lambda(|\boldsymbol{p}+\boldsymbol{q}/t|)]}, \qquad (8.89)$$

where $\lambda(p) = (c^2p^2 + m^2c^4)^{1/2}$. Since

$$\begin{aligned}
&\left| -t[\lambda(p) - \lambda(|\boldsymbol{p} + \boldsymbol{q}/t|)] - \boldsymbol{q} \cdot \boldsymbol{u}(\boldsymbol{p} + \boldsymbol{q}/t) \right| \\
&\quad = \left| \int_0^1 ds \, \boldsymbol{q} \cdot [\boldsymbol{u}(\boldsymbol{p} + s\boldsymbol{q}/t) - \boldsymbol{u}(\boldsymbol{p} + \boldsymbol{q}/t)] \right| \leq \frac{q^2}{t} \|\nabla \boldsymbol{u}\| \to 0, \qquad (8.90)
\end{aligned}$$

as $|t| \to \infty$ for bounded $\boldsymbol{q}$, we find that (8.88) and (8.89) are asymptotically equal and hence the second summand in (8.87) vanishes asymptotically. It remains to estimate

$$\begin{aligned}
&\frac{1}{q^2} \| \{ e^{\mathrm{i}\boldsymbol{q}\cdot[\boldsymbol{x}/t - \boldsymbol{u}(\boldsymbol{p})]} - \mathbf{1} \} e^{-\mathrm{i}Ht} \psi \|^2 \\
&\quad = \frac{1}{q^2} \left\| \int_0^1 ds \, e^{\mathrm{i}s\boldsymbol{q}\cdot[\boldsymbol{x}/t - \boldsymbol{u}(\boldsymbol{p})]} \, \boldsymbol{q} \cdot [\, \boldsymbol{x}/t - \boldsymbol{u}(\boldsymbol{p}) \,] \, e^{-\mathrm{i}Ht} \psi \right\|^2 \\
&\quad \leq \| [\, \boldsymbol{x}/t - \boldsymbol{u}(\boldsymbol{p}) \,] \, e^{-\mathrm{i}Ht} \psi \|^2 = (\psi, [\, \boldsymbol{x}/t - c^2 \boldsymbol{p} H_0^{-1} \,]^2(t) \, \psi) \\
&\quad \leq \left\| \left\{ \frac{x^2(t)}{t^2} - 2c^2 \frac{A(t)}{t} + \left(\frac{c^2 \boldsymbol{p}}{H_0} \right)^2 (t) \right\} \psi \right\|. \qquad (8.91)
\end{aligned}$$

From Theorems 8.12, 8.13, and 8.16, we conclude that this expression vanishes as $|t| \to \infty$ for all $\psi \in \mathfrak{D}$. This proves the theorem. It is immediately clear that the same proof works for any function f for which $\mathcal{F}f$ or $\mathcal{F}(1-f)$ is integrable, but we shall not need this generalization. □

Remark. This theorem expresses an asymptotic correlation between the localization of a scattering state and its velocity. If f is a smooth function with a small support around some average velocity v_0, then $f(c^2 \boldsymbol{p} H_0^{-1})\psi$ is the component of the state ψ with velocities near v_0. The theorem states that this

component is localized near $v_0 t$ at large times (where the localization region spreads linearly in time: $f(x/t)$ describes localization in a narrow cone of space-time). Hence the scattering states asymptotically behave in a quasiclassical way. Note that we have obtained these results for arbitrary matrix-valued potentials and with very few assumptions on the decay of the potential at infinity.

Corollary 8.18. Under the assumptions of Theorem 8.17,

$$\lim_{|t|\to\infty} \| \{ f(\boldsymbol{x}/t - c^2 \boldsymbol{p} H_0^{-1}) - f(0) \} e^{-\mathrm{i}Ht} \psi \| = 0. \tag{8.92}$$

Proof. Eq. (8.92) is proven on the positive energy subspace by observing that the first summand in (8.87) vanishes, as $|t| \to \infty$. □

Corollary 8.19. Let ψ be a positive energy scattering state with energies in the interval (a, b), i.e.,

$$\psi = \chi(a < H < b)\psi \in \mathfrak{H}_{\mathrm{pos}}^{\mathrm{cont}}, \quad mc^2 < a < b < \infty. \tag{8.93}$$

Define $u_a \equiv c(1 - m^2c^4/a^2)^{1/2}$, and similarly u_b. These are the classical velocities corresponding to the energies a and b, respectively. Choose a function $g \in \mathcal{C}_0^\infty(\mathbb{R})$ such that $g = 1$ on the interval $[u_a^2, u_b^2]$. Define

$$\phi(t) \equiv e^{-\mathrm{i}H_0 t} P_{\mathrm{pos}}^0 \, g\big(\boldsymbol{u}^2(\boldsymbol{p})\big) \, \chi(|\boldsymbol{x}| < \delta|t|) \, e^{\mathrm{i}H_0 t} e^{-\mathrm{i}Ht} \psi. \tag{8.94}$$

Then

$$\lim_{|t|\to\infty} \| \phi(t) - e^{-\mathrm{i}Ht} \psi \| = 0. \tag{8.95}$$

Proof. For any $\delta > 0$,

$$\begin{aligned} &\| \chi(|\boldsymbol{x}| > \delta|t|) \, e^{\mathrm{i}H_0 t} e^{-\mathrm{i}Ht} \psi \| \\ &\quad = \| \chi(|\boldsymbol{x}/t - c^2 \boldsymbol{p} H_0^{-1} + \boldsymbol{B}/t| > \delta) \, e^{-\mathrm{i}Ht} \psi \| \\ &\quad \le \| f(\boldsymbol{x}/t - c^2 \boldsymbol{p} H_0^{-1} + \boldsymbol{B}/t) \, e^{-\mathrm{i}Ht} \psi \|, \end{aligned} \tag{8.96}$$

where f has been chosen such that $1 - f \in \mathcal{C}_0^\infty(\mathbb{R}^3)$, $f(0) = 0$, and $f(\boldsymbol{x}) = 1$ for $|\boldsymbol{x}| \ge \delta$. The operator B is bounded, as can be seen from Eq. (1.119). Now Eq. (8.92) implies

$$\lim_{|t|\to\infty} \| \chi(|\boldsymbol{x}| > \delta|t|) \, e^{\mathrm{i}H_0 t} e^{-\mathrm{i}Ht} \psi \| = 0. \tag{8.97}$$

Next we estimate

$$\| \phi(t) - e^{-\mathrm{i}Ht} \psi \| \tag{8.98}$$

$$= \| \{ \mathbf{1} - P_{\mathrm{pos}}^0 \, g\big(\boldsymbol{u}^2(\boldsymbol{p})\big) \, \chi(|\boldsymbol{x}| < \delta|t|) \} \, e^{\mathrm{i}H_0 t} e^{-\mathrm{i}Ht} \psi \| \tag{8.99}$$

$$\le \| P_{\mathrm{pos}}^0 \, g\big(\boldsymbol{u}^2(\boldsymbol{p})\big) \| \cdot \| \chi(|\boldsymbol{x}| > \delta|t|) \, e^{\mathrm{i}H_0 t} e^{-\mathrm{i}Ht} \psi \| \tag{8.100}$$

$$+ \| \{1 - P^0_{\text{pos}}\, g(u^2(p))\}\, e^{-iHt}\psi \|. \tag{8.101}$$

According to (8.97), the expression (8.100) vanishes, as $|t| \to \infty$. The summand (8.101) vanishes, because by Eq. (8.74),

$$\lim \| P^0_{\text{neg}}\, e^{-iHt}\psi \| = 0, \tag{8.102}$$

and by Eq. (8.79),

$$\lim_{|t|\to\infty} \| \{ g(u^2(p)) - g(c^2(1 - m^2c^4H^{-2}))\}\, e^{-iHt}\psi \| = 0. \tag{8.103}$$

□

Corollary 8.19 can be interpreted as follows. For large times $|t|$, the state $\psi(t)$ can be replaced by an asymptotic configuration with positive energy, which has the same velocity distribution as $\psi(t)$ and is initially localized in the region $|x| < \delta|t|$ (where $\delta > 0$ arbitrarily small).

8.3 Asymptotic Completeness

8.3.1 Short-Range Potentials

Theorem 8.20. Let $H = H_0 + V$ be a Dirac operator with a short-range potential, i.e., V is a Hermitian 4×4 matrix-valued matrix multiplication operator satisfying

$$\int_0^\infty \| V\,(H_0 - z)^{-1}\, \chi(|x| > R) \|\, dR < \infty. \tag{8.104}$$

Then the scattering system (H, H_0) is asymptotically complete.

Proof. We prove that

$$\sup_{t\geq 0} \| \{ e^{-iHt} - e^{-iH_0t} \}\, e^{-iHs}\psi \| \to 0, \quad \text{as } s \to +\infty, \tag{8.105}$$

which (together with an analogous statement for negative times) is equivalent to the completeness property: (8.105) is just the Cauchy criterion for the existence of the limit (8.5). It is sufficient to prove (8.105) for positive and negative energy states separately. We give the proof for a dense set $\mathfrak{D}$ of states in $\mathfrak{H}^{\text{cont}}_{\text{pos}}$. This proves (8.105) for all $\psi \in \mathfrak{H}^{\text{cont}}_{\text{pos}}$, because the operators in (8.105) are bounded. We choose $\mathfrak{D}$ to be the set of states with compact energy support away from threshold. According to Corollary 8.19 any $\psi \in \mathfrak{D}$ can be approximated at late times s by a "well behaved" state $\phi(s)$. We choose g in (8.94) with $|g| \leq 1$, $\operatorname{supp} g \subset (4u^2, c^2)$, $u = u_a/4 > 0$. We can choose s so large that

$$\sup_{t\geq 0} \| \{ e^{-iHt} - e^{-iH_0t} \} \{ e^{-iHs}\psi - \phi(s) \} \| < \epsilon/2. \tag{8.106}$$

It remains to estimate

$$\sup_{t\geq 0} \| \{ e^{-\mathrm{i}Ht} - e^{-\mathrm{i}H_0 t} \} \phi(s) \| \tag{8.107}$$

$$\leq \sup_{t\geq 0} \Big\| \int_0^t e^{\mathrm{i}Ht'} V(\boldsymbol{x}) e^{-\mathrm{i}H_0 t'} \phi(s)\, dt' \Big\|$$

$$\leq \int_0^\infty \| V(\boldsymbol{x}) e^{-\mathrm{i}H_0(t'+s)} P^0_{\mathrm{pos}} g\big(\boldsymbol{u}^2(\boldsymbol{p})\big) \chi(|\boldsymbol{x}| < \delta|t|) \| \, dt'$$

$$\leq \int_0^\infty \|V(\boldsymbol{x})(H_0 - z)^{-1}\| \, \| P^0_{\mathrm{pos}} \chi(|\boldsymbol{x}| < (t'+s)u) \times$$

$$\times e^{-\mathrm{i}\lambda(p)(t'+s)} (H_0 - z) g\big(\boldsymbol{u}^2(\boldsymbol{p})\big) \chi(|\boldsymbol{x}| < \delta s) \| \, dt' \tag{8.108}$$

$$+ \int_0^\infty \big\| V(\boldsymbol{x})\, P^0_{\mathrm{pos}}\, g\big(\boldsymbol{u}^2(\boldsymbol{p})\big) \chi(|\boldsymbol{x}| > (t'+s)u) \big\| \, dt' \tag{8.109}$$

By assumption, (8.109) vanishes, as $s \to \infty$. Choose $\delta = u/2$. Then by the non-stationary phase method one can prove exactly as in Corollary 1.9,

$$\big\| \chi(|\boldsymbol{x}| < (t'+s)u)\, e^{-\mathrm{i}\lambda(p)(t'+s)}\, g\big(\boldsymbol{u}^2(\boldsymbol{p})\big) \chi(|\boldsymbol{x}| < \delta s) \big\|$$

$$\leq C_n (1 + t' + s)^{-n}, \tag{8.110}$$

for any function g with the chosen support properties. In particular, each component of the matrix $(H_0 - z) g\big(\boldsymbol{u}^2(\boldsymbol{p})\big)$ satisfies the required properties. Hence also (8.108) vanishes, as $s \to \infty$, and it is possible to choose s so large that (8.107) is less than $\epsilon/2$. Together with (8.106) this proves the completeness property. The same estimates also apply a fortiori, if we replace $\exp(-\mathrm{i}Hs)$ in (8.105) by $\exp(-\mathrm{i}H_0 s)$. Hence the existence property (8.4) is proven at the same time. □

8.3.2 Coulomb Potentials

The result of the previous section is wrong for long-range potentials like the Coulomb potential $\gamma/|\boldsymbol{x}|$. Even in classical mechanics the Coulomb force is known to distort the asymptotic motion of a scattered particle, so that it cannot be approximated at large times by the motion of a free particle. It is, nevertheless, possible to describe the asymptotic motion in a simple way with the help of a time evolution which depends only on the momentum operator. This "modified free time evolution" is in case of an electrostatic long-range potential given by

$$U(t,0) = U^+(t,0) P_{\mathrm{pos}} + U^-(t,0) P_{\mathrm{neg}}, \tag{8.111}$$

$$U^\pm(t,0) = e^{\mp \mathrm{i}\lambda(p)t} \exp\Big\{ -\mathrm{i} \int_0^t \phi_{\mathrm{el}}\big(\pm \boldsymbol{u}(\boldsymbol{p}) s\big)\, ds \Big\}. \tag{8.112}$$

Here P_{pos}, P_{neg} are the projectors on positive and negative free energy, respectively, as defined in Sect. 1.4.2, $\lambda(p) = (\mathrm{c}^2 p^2 + m^2 \mathrm{c}^4)^{1/2}$, $\boldsymbol{u} = \nabla\lambda$. In case of a long-range scalar potential we may choose

$$U^{\pm}(t,0) = e^{\mp i\lambda(p)t} \exp\Big\{\mp i \frac{mc^2}{\lambda(p)} \int_0^t \phi_{sc}\big(\pm \boldsymbol{u}(\boldsymbol{p})s\big)\, ds\Big\}. \tag{8.113}$$

Remark. The form of the modified free time evolution can be understood with the help of classical mechanics. For large times quantum mechanical wavepackets behave in a quasiclassical way. This means that the time evolution can be approximated by an expression of the form $\exp\{-iW(t,\boldsymbol{p})\}$. Here $W(t,\boldsymbol{p})$ is the classical action as a function of the momentum, which is given by

$$W(t,\boldsymbol{p}) = \boldsymbol{x}(t)\cdot\boldsymbol{p} + \int_0^t \big\{\, H\big(\boldsymbol{p}(s),\boldsymbol{x}(s)\big) - \dot{\boldsymbol{x}}(s)\cdot\boldsymbol{p}(s)\,\big\}\, ds. \tag{8.114}$$

$H(\boldsymbol{p},\boldsymbol{x})$ is the classical Hamilton function and $\big(\boldsymbol{p}(s),\boldsymbol{x}(s)\big)$ is the solution of the canonical equations with boundary conditions $\boldsymbol{p}(t) = \boldsymbol{p}$, $\boldsymbol{x}(0) = \boldsymbol{x}_0$. If the Hamilton function is of the form

$$H(\boldsymbol{p},\boldsymbol{x}) = \sqrt{c^2p^2 + m^2c^4} + \phi_{el}(\boldsymbol{x}), \tag{8.115}$$

or in case of a scalar potential,

$$H(\boldsymbol{p},\boldsymbol{x}) = \sqrt{c^2p^2 + (mc^2 + \phi_{sc}(\boldsymbol{x}))^2}, \tag{8.116}$$

where the potential functions decay like $\gamma/|\boldsymbol{x}|$, then it is easy to see from the canonical equations that $\dot{\boldsymbol{x}}(s)$ and $\boldsymbol{p}(s)$ are asymptotically constant and therefore $\boldsymbol{x}(s) = \boldsymbol{u}(\boldsymbol{p})s + O(\ln s)$ (independent of the initial condition in space). Inserting this into (8.114) and keeping only the terms which diverge as $t \to \infty$ gives a function $\tilde{W}(t,\boldsymbol{p})$ which approximates the classical action for large times:

$$\tilde{W}(t,\boldsymbol{p}) = \lambda(p)t + \int_0^t \phi_{el}\big(\boldsymbol{u}(\boldsymbol{p})s\big)\, ds, \tag{8.117}$$

resp.

$$\tilde{W}(t,\boldsymbol{p}) = \lambda(p)t + \frac{mc^2}{\lambda(p)} \int_0^t \phi_{sc}\big(\boldsymbol{u}(\boldsymbol{p})s\big)\, ds. \tag{8.118}$$

Of course this consideration neglects the spin and the negative energy states. Nevertheless, the following theorem is true.

Theorem 8.21. Let ϕ_{el} (resp. ϕ_{sc}) be a long-range potential satisfying

$$\phi_{el}(\boldsymbol{x}) = \gamma/|\boldsymbol{x}|, \quad \text{for } \gamma \in \mathbb{R} \text{ and } |\boldsymbol{x}| \geq R_0 > 0. \tag{8.119}$$

Then the modified wave operators, defined by

$$\Omega_{\pm}\,\psi = \lim_{t\to\pm\infty} e^{iHt}\, U(t,0)\,\psi, \quad \text{for all } \psi \in \mathfrak{H}, \tag{8.120}$$

exist and are complete, where $U(t,0)$ is given by Eqs. (8.111) and (8.112) (resp. (8.113)).

For a proof of this theorem see the references in the Notes.

8.4 Supersymmetric Scattering and Magnetic Fields

8.4.1 Existence of Wave Operators

We assume that H is a supersymmetric Dirac operator of the form

$$H = Q + m\tau, \quad m \in \mathbb{R}. \tag{8.121}$$

The spectral properties of this operator are closely related to the spectral properties of a "nonrelativistic" operator Q^2. We expect that a similar relationship is true for scattering theory. The following theorem is an application of the invariance principle of wave operators.

Theorem 8.22. Let $H = Q + m\tau$, $H_0 = Q_0 + m\tau$ be two Dirac operators with supersymmetry. Assume that for all $0 < a < b < \infty$ and for ψ in some dense subset of $\chi(a<Q_0^2<b)\,\mathfrak{H}^{\text{a.c.}}(Q_0^2)$ the following condition is satisfied for $k = 1, 2$.

$$\|(Q^k - Q_0^k)\, e^{-\mathrm{i}Q_0^2 t}\,\psi\| \le \text{const.}(1+|t|)^{1-k-\delta}, \quad \delta > 0. \tag{8.122}_k$$

Then the wave operators $\Omega_\pm(H, H_0)$ exist, and

$$\Omega_\pm(H, H_0) = \Omega_\pm(Q^2, Q_0^2)\,\chi(H_0 > 0) + \Omega_\mp(Q^2, Q_0^2)\,\chi(H_0 < 0). \tag{8.123}$$

Proof. The assumption $(8.122)_2$ implies existence of the "nonrelativistic" wave operators $\Omega_\pm^{\text{nr}} \equiv \Omega_\pm(Q^2, Q_0^2)$ by the following argument. First note that the set of states $\psi \in \mathfrak{H}^{\text{a.c.}}(Q_0^2)$ for which there exist constants a and b such that $\psi = \chi(a < Q_0^2 < b)\psi$ is a dense subset of $\mathfrak{H}^{\text{a.c.}}(Q_0^2)$. For ψ in this subset we have

$$\begin{aligned}
&\lim_{s\to\infty} \sup_{t\ge 0} \|(e^{\mathrm{i}Q^2 t}\, e^{-\mathrm{i}Q_0^2 t} - e^{\mathrm{i}Q^2 s}\, e^{-\mathrm{i}Q_0^2 s})\,\psi\| \\
&\quad = \lim_{s\to\infty} \sup_{t\ge 0} \left\| \int_s^t e^{\mathrm{i}Q^2 t'}\,(Q^2 - Q_0^2)\, e^{-\mathrm{i}Q_0^2 t'}\,\psi\, dt' \right\| \\
&\quad \le \lim_{s\to\infty} \int_s^\infty \|(Q^2 - Q_0^2) e^{-\mathrm{i}Q_0^2 t'}\,\psi\|\, dt' = 0.
\end{aligned} \tag{8.124}$$

We have used that by $(8.122)_2$, the integrand in the last expression decays integrably in time. But (8.124) is just the Cauchy criterion for the existence of Ω_+^{nr}. A similar argument proves existence of Ω_-^{nr}.

According to Theorem 5.13 there are unitary operators

$$U = a_+ + \tau(\operatorname{sgn} Q)a_-, \qquad U_0 = a_+^0 + \tau(\operatorname{sgn} Q)a_-^0, \tag{8.125}$$

such that $UHU^* = \tau|H|$, and $U_0 H U_0^* = \tau|H_0|$. The operators $|H|$ and $|H_0|$ are functions of Q^2 and Q_0^2, respectively, and by the invariance principle the existence of the wave operators $\Omega_\pm(|H|, |H_0|)$ follows from the existence of $\Omega_\pm^{\text{nr}}$. Moreover,

$$\Omega_{\pm}(|H|,|H_0|) = \Omega_{\pm}^{\mathrm{nr}}. \tag{8.126}$$

Hence we conclude the existence of

$$\Omega_{\pm}^{\mathrm{rel}} \equiv \Omega_{\pm}(\tau|H|,\tau|H_0|) = \Omega_{\pm}^{\mathrm{nr}} \tfrac{1}{2}(1+\tau) + \Omega_{\mp}^{\mathrm{nr}} \tfrac{1}{2}(1-\tau). \tag{8.127}$$

It remains to show that for all $\psi \in \mathfrak{H}^{\mathrm{a.c.}}(H_0)$ we can find $\phi_{\pm} \in \mathfrak{H}$ such that

$$0 = \lim_{t\to\pm\infty} \|e^{\mathrm{i}Ht} e^{-\mathrm{i}H_0 t}\psi - \phi_{\pm}\| \tag{8.128}$$

$$\leq \lim_{t\to\pm\infty} \|e^{\mathrm{i}\tau|H|t} e^{-\mathrm{i}\tau|H_0|t} U_0\psi - U\phi_{\pm}\| \tag{8.129}$$

$$+ \lim_{t\to\pm\infty} \|(UU_0^* - 1)e^{-\mathrm{i}\tau|H_0|t} U_0\psi\|. \tag{8.130}$$

From the existence of (8.127) we conclude that (8.129) vanishes, if we choose

$$\phi_{\pm} = U^* \Omega_{\pm}^{\mathrm{rel}} U_0 \psi. \tag{8.131}$$

Using the explicit forms of U and U_0 we can estimate the term (8.130)

$$\|(U-U_0)\, e^{-\mathrm{i}\tau|H_0|t}\psi\| \tag{8.132}$$

$$\leq \|(a_+ - a_+^0)\, e^{-\mathrm{i}\tau|H_0|t}\psi\| + \|(a_- - a_-^0)\, e^{-\mathrm{i}\tau|H_0|t}\psi\| \tag{8.133}$$

$$+ \|(\operatorname{sgn} Q - \operatorname{sgn} Q_0)\, e^{-\mathrm{i}\tau|H_0|t}\, a_-^0\, \psi\|. \tag{8.134}$$

The operators $a_{\pm}$ are bounded functions of $|H| = |UHU^{-1}|$, and $a_{\pm}^0$ are defined in the same way with $|H_0|$. Hence we can apply the intertwining relation Eq. (8.10),

$$a_{\pm}\, \Omega^{\mathrm{rel}} = \Omega^{\mathrm{rel}}\, a_{\pm}^0, \tag{8.135}$$

where Ω^{rel} is either Ω_+^{rel} or Ω_-^{rel} to conclude that (8.133) vanishes, as $|t| \to \infty$. Since in (8.134) the operator $\operatorname{sgn} Q$ is not simply a bounded function of $\tau|H|$, we have to be a little bit more careful. First we note that for $\eta = |Q_0|\psi$

$$\|(\operatorname{sgn} Q - \operatorname{sgn} Q_0)\, e^{-\mathrm{i}Q_0^2 t}\, \eta\| \tag{8.136}$$

$$\leq \|(Q-Q_0)\, e^{-\mathrm{i}Q_0^2 t}\, \psi\| + \|(|Q| - |Q_0|)\, e^{-\mathrm{i}Q_0^2 t}\, \psi\|. \tag{8.137}$$

Here the last summand of (8.137) vanishes for $\psi \in \mathfrak{D}(|Q_0|)$ in the limit $|t| \to \infty$ because of the intertwining relations for $\Omega_{\pm}^{\mathrm{nr}}$. The first summand vanishes by assumption $(8.122)_1$ for $\psi \in \chi(a < Q_0^2 < b)\mathfrak{H}^{\mathrm{a.c.}}$. The set of all vectors of the form $\eta = |Q_0|\psi$, $\psi \in \chi(a < Q_0^2 < b)\mathfrak{H}^{\mathrm{a.c.}}$ with arbitrary $0 < a < b < \infty$ is dense in $\mathfrak{H}^{\mathrm{a.c.}}$, hence we have shown for all $\psi \in \mathfrak{H}^{\mathrm{a.c.}}$

$$0 = \lim_{|t|\to\infty} \|(\operatorname{sgn} Q - \operatorname{sgn} Q_0)\, e^{-\mathrm{i}Q_0^2 t}\, \psi\|$$

$$= \|\big((\operatorname{sgn} Q)\Omega_{\pm}^{\mathrm{nr}} - \Omega_{\pm}^{\mathrm{nr}}(\operatorname{sgn} Q_0)\big)\psi\|, \tag{8.138}$$

or

$$(\operatorname{sgn} Q)\, \Omega_{\pm}^{\mathrm{nr}} = \Omega_{\pm}^{\mathrm{nr}}\, (\operatorname{sgn} Q_0). \tag{8.139}$$

With the help of (8.127) we can express $\Omega_{\pm}^{\mathrm{nr}}$ in terms of $\Omega_{\pm}^{\mathrm{rel}}$. Taking into account

$$(\operatorname{sgn} Q)\, \tfrac{1}{2}(1 \pm \tau) = \tfrac{1}{2}(1 \mp \tau)\, (\operatorname{sgn} Q) \tag{8.140}$$

and the same result with Q_0, we obtain from (8.139)

$$(\operatorname{sgn} Q)\, \Omega_{\pm}^{\mathrm{rel}} = \Omega_{\mp}^{\mathrm{rel}}\, (\operatorname{sgn} Q_0). \tag{8.141}$$

But this implies almost immediately for all $\chi \in \mathfrak{H}^{\mathrm{a.c.}}$

$$\lim_{|t| \to \infty} \| (\operatorname{sgn} Q - \operatorname{sgn} Q_0)\, e^{-\mathrm{i}\tau |H_0| t} a_-^0 \chi \| = 0. \tag{8.142}$$

This completes the proof of existence of $\Omega_{\pm}(H, H_0)$. In order to show (8.123) we note that by (8.135) and (8.139)

$$U^* \Omega_{\pm}^{\mathrm{nr}} = \Omega_{\pm}^{\mathrm{nr}} U_0^*. \tag{8.143}$$

Now we calculate, using (8.131)

$$\begin{aligned} \Omega_{\pm}(H, H_0) &= U^*\, \Omega_{\pm}^{\mathrm{rel}} U_0 \\ &= \Omega_{\pm}^{\mathrm{nr}}\, U_0^*\, \tfrac{1}{2}(1 + \tau)\, U_0 + \Omega_{\mp}^{\mathrm{nr}}\, U_0^*\, \tfrac{1}{2}(1 - \tau)\, U_0. \end{aligned} \tag{8.144}$$

Finally, the relation

$$U_0^*\, \tfrac{1}{2}(1 \pm \tau)\, U_0 = \tfrac{1}{2}(1 \pm H/|H|) = \chi(H \gtrless 0) \tag{8.145}$$

completes the proof of the theorem. □

Remark. Instead of assuming $(8.122)_1$, it would have been sufficient to require vanishing of (8.136) in the limit of large times. In the applications, however, it is usually easier to verify $(8.122)_1$.

8.4.2 Scattering in Magnetic Fields

We know already that long-range magnetic vector potentials can occur even in short-range situations (see the remark at the end of Sect. 7.1.2). If the potential matrix $c\boldsymbol{\alpha} \cdot \boldsymbol{A}(\boldsymbol{x})$ decays like $|\boldsymbol{x}|^{-1}$, a similar consideration as in Sect. 8.3.2 shows asymptotic completeness with the modified free time evolution

$$U^{\pm}(t, 0) = e^{\mp \mathrm{i}\lambda(p)t}\, \exp\Big\{ \mp \mathrm{i} \int_0^t \boldsymbol{A}\big(\pm \boldsymbol{u}(\boldsymbol{p}) s\big) \cdot \boldsymbol{u}(\boldsymbol{p})\, ds \Big\}. \tag{8.146}$$

The form of this approximating time evolution has been obtained by replacing the matrix $c\boldsymbol{\alpha} \cdot \boldsymbol{A}(\boldsymbol{x})$ by $\pm \boldsymbol{A}\big(\pm \boldsymbol{u}(\boldsymbol{p}) s\big) \cdot \boldsymbol{u}(\boldsymbol{p})$ on positive (or negative) energy states. Since it is not easy to justify the asymptotic vanishing of the Zitterbewegung in (8.146), we proceed as follows. We first consider the nonrelativistic

problem (the Pauli equation) and then use the supersymmetric structure of the problem (Theorem 8.22) in order to circumvent the problems with Zitterbewegung. From Sect. 8.3.2 one expects that the modified asymptotic time evolution (8.146) has to be used, whenever $\boldsymbol{A}(\boldsymbol{x})$ vanishes like $1/|\boldsymbol{x}|$, as $|\boldsymbol{x}| \to \infty$, which might be even the case for magnetic fields with compact support (see the remark in Sect. 7.1.2). Clearly, it is not satisfying to use a modified time evolution in situations where particles move freely. Fortunately, asymptotic modifications of the free time evolution can be avoided by choosing a special gauge.

In order to apply Theorem 8.22 to the Dirac operator in an external magnetic field we have to verify the two conditions $(8.122)_k$. The condition $(8.122)_1$ is not very restrictive. It just says that we have to choose a gauge in which the vector potential decays at infinity like $|x|^{-\delta}$, $\delta > 0$. Since $Q - Q_0 = -c\boldsymbol{\alpha} \cdot A$, Eq. $(8.122)_1$ simply becomes

$$\|\boldsymbol{A}(\boldsymbol{x})\, e^{-\mathrm{i}p^2 t}\, \psi\| \leq \text{const.}(1 + |t|)^{-\delta} \tag{8.147}$$

for suitable ψ. If $|\boldsymbol{A}(\boldsymbol{x})| \leq \text{const.}(1 + |\boldsymbol{x}|)^{-\delta}$, then Eq. (8.147) follows immediately from

$$\| \chi(|\boldsymbol{x}| \leq u_0|t|)\, e^{-\mathrm{i}\boldsymbol{p}^2 t}\, \psi \| \leq C_N\, (1 + |t|)^{-N}. \tag{8.148}$$

The inequality (8.148) holds for all ψ with Fourier transform $\hat{\psi} \in \mathcal{C}_0^\infty(\mathbb{R}^3)^4$ having support outside the sphere with radius u_0 and can be obtained exactly as in Corollary 1.9 by a non-stationary phase argument.

The condition $(8.122)_2$ is more restrictive. With

$$\tfrac{1}{c}Q^2 = p^2 - 2\boldsymbol{A} \cdot \boldsymbol{p} + \mathrm{i}\,\mathrm{div}\,\boldsymbol{A} + A^2 - \boldsymbol{\sigma} \cdot \boldsymbol{B}, \qquad \tfrac{1}{c}Q_0^2 = p^2. \tag{8.149}$$

Eq. $(8.122)_2$ becomes

$$\| \left(-2\boldsymbol{A} \cdot \boldsymbol{p} + \mathrm{i}\,\mathrm{div}\,\boldsymbol{A} + A^2 - \boldsymbol{\sigma} \cdot \boldsymbol{B} \right) e^{-\mathrm{i}\boldsymbol{p}^2 t}\, \psi \| \leq \text{const.}(1 + |t|)^{-1-\delta}. \tag{8.150}$$

It is sufficient to show this condition for ψ with Fourier transform $\hat{\psi} \in \mathcal{C}_0^\infty(\mathbb{R}^3)^4$ having support in $|\boldsymbol{p}| > u_0 > 0$. Eq. (8.150) can be satisfied by choosing a suitable gauge under the following assumption on the magnetic field strength.

Assumption: Let the magnetic field strength B decay at infinity, such that for some $\delta > 0$

$$|\boldsymbol{B}(\boldsymbol{x})| \leq \text{const.}(1 + |\boldsymbol{x}|)^{-3/2-\delta}. \tag{8.151}$$

From the form of the modification in (8.146) we see that a simplification can be achieved, if we require

$$\boldsymbol{A}(\boldsymbol{x}) \cdot \boldsymbol{x} = 0. \tag{8.152}$$

Indeed, we can always find a vector potential with this property. Eq. (8.152) uniquely characterizes the transversal (or Poincaré) gauge which in terms of the field strength $\boldsymbol{B}$ is given by

$$\boldsymbol{A}(\boldsymbol{x}) = \int_0^1 s\, \boldsymbol{B}(\boldsymbol{x}s) \wedge \boldsymbol{x}\, ds, \quad \text{(in three dimensions)} \tag{8.153}$$

or, more generally, by

$$A_i(x) = \int_0^1 s \sum_k F_{ki}(xs)\, x_k\, ds. \tag{8.154}$$

In the transversal gauge we conclude from (8.151)

$$|\boldsymbol{A}(\boldsymbol{x})| \leq \text{const.}(1 + |\boldsymbol{x}|)^{-1/2-\delta}. \tag{8.155}$$

Hence the expressions $\operatorname{div} \boldsymbol{A}$, A^2, and $\boldsymbol{\sigma} \cdot \boldsymbol{B}$ occurring in $Q^2 - Q_0^2$ are all of short-range. The crucial long-range term is $\boldsymbol{A}(\boldsymbol{x}) \cdot \boldsymbol{p}$. It can be written as

$$\boldsymbol{A}(\boldsymbol{x}) \cdot \boldsymbol{p} = \boldsymbol{G}(\boldsymbol{x}) \cdot (\boldsymbol{x} \wedge \boldsymbol{p}) = \boldsymbol{G}(\boldsymbol{x}) \cdot \boldsymbol{L}, \tag{8.156}$$

where $\boldsymbol{L}$ is the orbital angular momentum, and

$$\boldsymbol{G}(\boldsymbol{x}) = \int_0^1 s\, \boldsymbol{B}(\boldsymbol{x}s)\, ds \tag{8.157}$$

satisfies,

$$|\boldsymbol{G}(\boldsymbol{x})| \leq \text{const.}(1 + |\boldsymbol{x}|)^{-3/2-\delta}. \tag{8.158}$$

Using the fact that $\boldsymbol{L}$ commutes with the nonrelativistic free time evolution $\exp(-\mathrm{i}p^2 t)$ we find

$$\begin{aligned} &\| \left(-2\boldsymbol{G} \cdot \boldsymbol{L} + \mathrm{i} \operatorname{div} \boldsymbol{A} + A^2 - \boldsymbol{\sigma} \cdot \boldsymbol{B} \right) e^{-\mathrm{i}p^2 t}\, \psi \| \\ &\leq 2\|\boldsymbol{G}\chi(|\boldsymbol{x}| > u_0 t)\| \cdot \|\boldsymbol{L}\| + 2\|\boldsymbol{G}\|\, \|\chi(|\boldsymbol{x}| \leq u_0 t)\, e^{-\mathrm{i}p^2 t}\, \boldsymbol{L}\, \psi \| \\ &\quad + \| \left(\mathrm{i} \operatorname{div} \boldsymbol{A} + A^2 - \boldsymbol{\sigma} \cdot \boldsymbol{B} \right) \chi(|\boldsymbol{x}| > u_0 t) \| \\ &\quad + \| \mathrm{i} \operatorname{div} \boldsymbol{A} + A^2 - \boldsymbol{\sigma} \cdot \boldsymbol{B} \|\, \|\chi(|\boldsymbol{x}| \leq u_0 t)\, e^{-\mathrm{i}p^2 t}\, \psi \|. \end{aligned} \tag{8.159}$$

For ψ with $\hat{\psi} \in \mathcal{C}_0^\infty(\mathbb{R}^3)^4$, $\operatorname{supp} \psi \subset \{\boldsymbol{p} \mid |\boldsymbol{p}| > u_0 > 0\}$ (the Fourier transform of $\boldsymbol{L}\psi$ has the same support properties) we can use a non-stationary phase argument to show rapid decay of $\|\chi(|\boldsymbol{x}| \leq u_0 t)\, e^{-\mathrm{i}p^2 t}\, \psi \|$ and the same expression with $\boldsymbol{L}\psi$ (cf. Eq. (8.148)). These estimates together with (8.151), (8.155), and (8.158) prove $(8.122)_2$. Since all assumptions of Theorem 8.22 are satisfied, we have proven the following theorem.

Theorem 8.23. Let $H = H(A)$ be defined as in (7.5) and $H_0 = H(0)$ be the free Dirac operator. Assume that the magnetic field strength B satisfies (8.151). Then both the relativistic and the nonrelativistic wave operators exist in the transversal gauge, and are related by (8.123).

Asymptotic completeness is equivalent to the existence of the adjoint wave operators $\Omega_\pm(H(0), H(A))$. Hence we simply have to exchange the roles of H

and H_0 in Theorem 2 in order to get conditions for the completeness of the relativistic system, which are formulated entirely in terms of the nonrelativistic time evolution. The proof, however, is more complicated in this case, because the time dependence of the angular momentum has to be estimated under the full time evolution $\exp(-\mathrm{i}Q^2t)$. Since magnetic fields are usually not spherically symmetric (in three dimensions, a singularity free magnetic field is never spherically symmetric), $\boldsymbol{L}$ is not a conserved quantity (i.e., it does not commute with $\exp(-\mathrm{i}Q^2t)$). Nevertheless, asymptotic completeness is true under the same decay conditions on the magnetic field strength. We only quote the corresponding result, see the Notes for a reference to the proof.

Theorem 8.24. Let $H(A)$ and H_0 be as above and assume that the magnetic field strength B satisfies

$$D^\gamma B(x) \leq \text{const.}(1+|x|)^{-3/2-\delta-\gamma}, \tag{8.160}$$

for some $\delta > 0$ and multiindices γ with $|\gamma| = 0, 1, 2$. Then the scattering system $(H(A), H_0)$ is asymptotically complete in the transversal gauge (8.154).

Remark. It is quite remarkable that asymptotic completeness holds without modifications under the extremely weak decay condition (8.160). These magnetic fields and the corresponding potential matrix $\boldsymbol{\alpha} \cdot \boldsymbol{A}$ have, respectively, a much slower decay than the electric field and its potential in the Coulomb case (where modifications have to be introduced, see Sect. 8.3.2). Even classically long-range situations are included by our assumptions. From special examples we know that classical paths of particles in magnetic fields satisfying our requirements do not even have asymptotes. In Fig. 8.1 this situation is explained qualitatively. For $\boldsymbol{B}$ satisfying (8.160) the classical velocity of the particles is asymptotically constant, $\boldsymbol{v} = \lim \dot{\boldsymbol{x}}(t)$ exists. But if we compare the asymptotic motion of a particle in a magnetic field with a free motion, one would have to add a correction $\boldsymbol{a}(t) \equiv \boldsymbol{x}(t) - \boldsymbol{v}t$ which is transversal to the asymptotic velocity $\boldsymbol{v}$ and diverges for $\delta < 1/2$ like $t^{1/2-\delta}$. Thus $\boldsymbol{B}$ is classically long-range for $\delta < 1/2$ since the time evolution is not asymptotically free. The classical paths – like parabolas – have an asymptotic direction but no asymptote. The situation seems to be even worse than in the Coulomb problem. There the interacting particles also cannot be asymptotically approximated by free particles, but at least the classical paths do have asymptotes. (The correction in the Coulomb problem increases like $\ln|t|$ and is parallel to the asymptotic velocity). Nevertheless, the classical wave operators exist for our magnetic fields and are asymptotically complete (see [294] for details). Existence follows from the convergence of $\boldsymbol{b}(t) \equiv \boldsymbol{x}(t) - \boldsymbol{p}(t)t$, as $t \to \infty$, which is indicated in Fig. 8.1. Here $\boldsymbol{p}(t) = \dot{\boldsymbol{x}}(t) + \boldsymbol{A}(\boldsymbol{x}(t))$ is the (gauge-dependent) canonical momentum.

Why is it, that the quantum time evolution has free asymptotes while the classical time evolution has not? Note that the classical path finally enters any cone with arbitrary small opening angle around the asymptotic direction. The correction $a(t)$ is thus asymptotically dominated by the effect of linear spreading of wave packets in quantum mechanics.

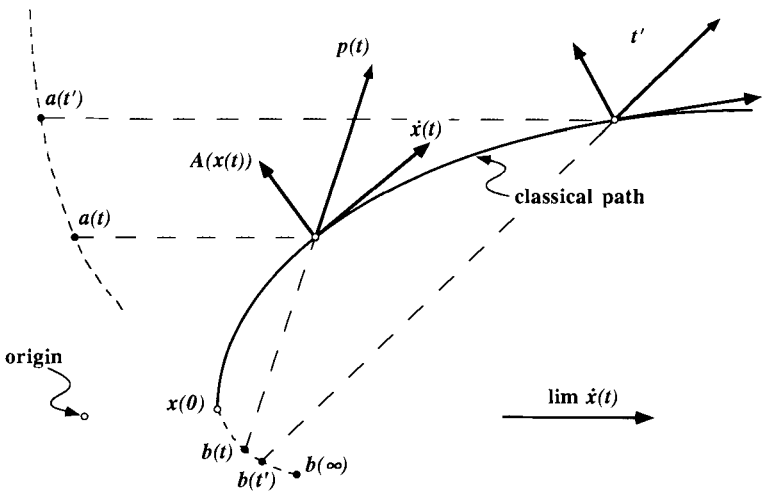

Fig. 8.1. Classical motion of charged particles in a long-range magnetic field. The convergence of $b(t)$ explains the existence of classical (unmodified) wave operators.

Asymptotic completeness in the magnetic field case is obviously due to the transversality of A. In another gauge (e.g., if ∇g is long-range), the unmodified wave operators possibly do not exist. Instead, we conclude from Theorem 8.24 that the wave operators $\Omega_{\pm}(H(A), H(\nabla g))$ exist and are asymptotically complete. Note that although the wave and scattering operators depend on the chosen gauge, the physically observable quantities like scattering cross sections are gauge independent.

Under weaker decay conditions on the magnetic field strength the wave operators would not exist in that form, because then the term A^2 occurring in $Q^2 - Q_0^2$ would become long-range. In this case one needs modified wave operators even in the transversal gauge.

8.5 Time-Dependent Fields

Here we give a brief discussion of scattering theory for the Dirac operator with time-dependent fields

$$H(t) = H_0 + \lambda V(t). \tag{8.161}$$

We assume that $V(t)$ is bounded for each t, the mapping $t \to V(t)\Psi$ is continuous for all Ψ, and that $\|V(t)\|$ is integrable with respect to time. Then the time evolution $U(t,s)$ is given by the Dyson series (4.63), and we can define the scattering operator for all $\Psi \in \mathfrak{H}$ as

$$S\Psi = \lim_{\substack{t\to\infty \\ s\to-\infty}} e^{iH_0 t}\, U(t,s)\, e^{-iH_0 s}\Psi \tag{8.162}$$

We obtain from (4.63)

$$S = \sum_{n=0}^{\infty} (-i\lambda)^n S_n,$$

$$S_n = \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_{n-1}} dt_n\, \tilde{V}(t_1)\cdots\tilde{V}(t_n) \tag{8.163}$$

The series for S converges in norm for all $\lambda \in \mathbb{C}$, because

$$\|S_n\| \le \frac{1}{n!}\left(\int_{-\infty}^{\infty} \|V(t)\|\, dt\right)^n \tag{8.164}$$

The scattering operator is unitary for real λ, and by analytic continuation we obtain

$$S(\lambda)\, S(\bar{\lambda})^* = S(\bar{\lambda})^*\, S(\lambda) = \mathbf{1}, \qquad \text{for all } \lambda \in \mathbb{C}. \tag{8.165}$$

If τ is a unitary involution in $\mathfrak{H}$, then we can write S as a matrix (cf. Sect. 5.2.1)

$$S = \begin{pmatrix} S_+ & S_{+-} \\ S_{-+} & S_- \end{pmatrix} \tag{8.166}$$

The case $\tau = \operatorname{sgn} H_0$, where H_0 is the free Dirac operator, is of particular interest. We note that in case of static external fields, S commutes with $\operatorname{sgn} H_0$ by Theorem 8.3, hence in this case $S_{+-} = S_{-+} = 0$. But for time-dependent fields, S will not commute with H_0 or $\operatorname{sgn} H_0$. In this case $|(\Psi_{\text{out}}, S_{+-}\Psi_{\text{in}})|$ is the probability that an incoming free particle $\Psi_{\text{in}} \in \mathfrak{H}_{\text{pos}}$ with positive energy finally leaves the scattering region in a state Ψ_{out} with negative energy. Similarly, S_{-+} describes a transition from negative to positive energies. These scattering events cannot be explained in a satisfactory way within the framework of one-particle quantum mechanics. In Chapter 10 we are going to describe these phenomena within quantum field theory as particle creation or annihilation processes in an external field. But this is only possible, if the scattering operator can be implemented as a unitary operator in the free particle Fock space. It will turn out that this is the case if and only if S_{+-} and S_{-+} are Hilbert-Schmidt operators. This requirement means a severe restriction on the class of allowed external fields. Let us quote the following result.

Theorem 8.25. We assume that the external field is an operator of multiplication with a matrix $V(t,\boldsymbol{x})$ and denote by $W_n(t)$ the strong derivatives $d^n V(t)/dt^n$, $n = 0,1,2$. Let the family $W_n(t)$ of matrix-multiplication operators on $\mathfrak{H} = L^2(\mathbb{R}^3)^4$ be strongly continuous in t. Assume that each component of the Fourier transform $\hat{W}_n(\boldsymbol{p},t)$ is integrable and square integrable with respect to $\boldsymbol{p}$, such that $\int_{-\infty}^{\infty} \|\hat{W}_n(.,t)\|^k\, dt$ is finite for $k = 1,2$, $n = 0,1,2$.

Then the operators S_{+-} and S_{-+} are Hilbert-Schmidt.

9 Solitons

This chapter is an introduction to the theory of solitons of the modified Korteweg-deVries (mKdV) equation, which is closely related to the Dirac equation with a time-dependent scalar potential. The mKdV equation is a nonlinear evolution equation in one spatial dimension. If $\phi(t,x)$ is a solution of the mKdV equation, then the spectrum of the (time-dependent) Dirac operator with the scalar potential $\phi(t,x)$ is time independent. The Dirac operators at different times are unitarily equivalent if the potential evolves according to the mKdV equation (Sects. 9.1 and 9.2).

Under suitable assumptions the potential ϕ can be described in terms of the "scattering parameters", i.e., the eigenvalues E_n, the bound state normalization constants c_n, and the reflection coefficient $R(E)$. The unique connection of the scattering parameters and the potential is given by the "inverse scattering transformation". The scattering parameters $R(E)$ and c_n also have a simple and explicitly known time evolution if the potential obeys the mKdV equation. Hence under appropriate restrictions the mKdV equation is an integrable system and the scattering parameters provide a "canonical coordinate system" in which every initial value problem can be solved explicitly, at least in principle.

Of particular importance are the reflectionless potentials (which remain reflectionless for all times), because in this case the inverse scattering transformation is particularly simple. The potentials obtained in this way are called soliton solutions of the mKdV equation.

This method of solving the mKdV equation is just a special example of a much more general method valid for a large class of nonlinear equations. Historically, the first equation treated in this way was the Korteweg-deVries (KdV) equation, originally designed for the description of shallow water waves. It is related to a one-dimensional Schrödinger operator which is just the square of the Dirac operator related to the mKdV equation. Hence we expect some relationship between the solutions of the mKdV and KdV equations. Indeed, the well known "Miura transformation" gives two KdV solutions for every mKdV solution. In Sects. 9.1 and 9.2 we describe the connection between mKdV and KdV with Dirac and Schrödinger operators using the Lax approach. In this framework the supersymmetric background of the Miura transformation becomes especially clear.

In Sect. 9.3 we are going to exploit supersymmetry in order to describe the solutions of the mKdV equation in terms of the KdV solutions (i.e., by "inverting" the Miura transformation — at least in some sense). This is possible because the underlying Dirac and Schrödinger problems are essentially equivalent. Starting with a KdV solution $V(t,x)$ one usually obtains a whole family of mKdV solutions which are related to V by Miura's transformation. We illustrate this method by constructing the soliton solutions of the mKdV equation from the well known KdV solitons. We also indicate how to obtain the KdV solitons by the inverse scattering method for the Schrödinger equation (Sect. 9.5). There exist mKdV solitons which are kink-like scalar potentials for the Dirac equation with different spatial asymptotics to the right and left ("critical case"). In Sect. 9.4.1 we give a short introduction to the stationary scattering theory of the Dirac equation for this situation and describe its supersymmetric relation to the corresponding Schrödinger scattering problem. In Sect. 9.4.2 we combine the Jost-function techniques of Sect. 9.4.1 with the results of Sect. 5.10 on Fredholm determinants in order to calculate the regularized index $\mathrm{ind}_z Q$ of a Dirac operator with a soliton-like potential.

9.1 Time Dependent Scalar Potential

9.1.1 Scalar Potentials in One Dimension

The Dirac operator with a time-dependent scalar potential ϕ in one space dimension, $H(t) = -\mathrm{i}\,\sigma_1\partial_x + \sigma_3\,\phi(t,x)$, is a supercharge in $L^2(\mathbb{R}, dx)^2$ with respect to the unitary involution $\tau = \mathrm{i}\sigma_1\sigma_3$ (cf. Sect. 5.5.1). Here σ_k, $k = 1,\ldots,3$, denote the Pauli matrices defined in Appendix 1A. After a transformation to the representation where τ is diagonal, we obtain the operator

$$\begin{aligned} Q(t) &= -\mathrm{i}\,\sigma_2\partial_x + \sigma_1\,\phi(t,x) \\ &= \begin{pmatrix} 0 & -\partial_x + \phi(t,x) \\ \partial_x + \phi(t,x) & 0 \end{pmatrix} \equiv \begin{pmatrix} 0 & D^* \\ D & 0 \end{pmatrix}. \end{aligned} \tag{9.1}$$

This operator is of particular importance because of its striking relation to some nonlinear partial differential equations. We assume the scalar potential ϕ to be infinitely differentiable with respect to both variables (t,x) such that ϕ, $\partial_x\phi \equiv \phi_x$, and $\partial_x^2\phi \equiv \phi_{xx}$ are bounded, i.e.,

$$\phi \in C^\infty(\mathbb{R}^2), \quad \partial_x^n\phi \in L^\infty(\mathbb{R}^2), \quad n = 0,1,2. \tag{9.2}$$

In this case the operator $Q(t)$ is well defined and self-adjoint for all t. The domain of $Q(t)$ is time invariant by the Kato-Rellich Theorem,

$$\mathfrak{D}(Q(t)) = \mathfrak{D}(Q(0)) = \mathfrak{D}(-\mathrm{i}\,\sigma_2\partial_x) = H^1(\mathbb{R})^2. \tag{9.3}$$

Under the above conditions the existence and uniqueness of solutions of the Dirac (or Schrödinger) equation is obtained as a consequence of Theorem 4.10.

Theorem 9.1. Let $Q(t)$ be the one-parameter family of Dirac operators defined above. Then there is a "unitary evolution operator" $U(t,s)$, and if $\psi \in \mathfrak{D} \equiv \mathfrak{D}\big(Q(t)\big)$, then $U(s,t)\psi$ is in $\mathfrak{D}$ for all t and

$$\mathrm{i}\,\frac{\partial}{\partial t}\,U(t,s)\,\psi = Q(t)\,U(t,s)\,\psi, \tag{9.4}$$

$$\mathrm{i}\,\frac{\partial}{\partial s}\,U(t,s)\,\psi = -U(t,s)\,Q(s)\,\psi. \tag{9.5}$$

We define the derivative of the parameter dependent operator $Q(t)$ by

$$\frac{dQ(t)}{dt}\,f = \lim_{\delta\to 0}\frac{Q(t+\delta) - Q(t)}{\delta}\,f \tag{9.6}$$

on the domain consisting of all f for which the above limit exists. In case of our Dirac operator we simply have

$$\frac{dQ(t)}{dt} = \sigma_1\,\phi_t(t,x). \tag{9.7}$$

9.1.2 Generation of Time Dependence

The time dependence of Q takes the simplest form if

$$Q(t) = W(t,s)\,Q(s)\,W(s,t), \tag{9.8}$$

where $W(t,s)$ is a unitary evolution operator. In this case the Dirac operators at different times are unitarily equivalent, hence the spectra of $Q(t)$ do not depend on t.

We assume that $W(t,s)$ is generated by a family of self-adjoint operators $B(t)$, such that

$$\mathrm{i}\,\partial_t W(t,s) = B(t)\,W(t,s), \tag{9.9}$$

and such that the commutator $[B(t), Q(t)]$ is densely defined. Then, (9.8) and (9.9) imply

$$\frac{dQ(t)}{dt} = -\mathrm{i}\,[B(t), Q(t)]. \tag{9.10}$$

In view of Eq. (9.7) it would be interesting to find an operator $B(t)$ such that the commutator with $Q(t)$ is simply a matrix multiplication operator,

$$-\mathrm{i}\,[B(t), Q(t)] = \sigma_1\, m(t,x), \tag{9.11}$$

where m is a suitable function which may depend of course on ϕ. From (9.7) it is then clear that any time-dependent scalar potential ϕ satisfying

$$\phi_t(t,x) = m(t,x) \tag{9.12}$$

produces a family of Dirac operators $Q(t)$, $t \in \mathbb{R}$, with a time dependence of the form (9.8).

From Eq. (9.11) it is clear that in our standard representation — where both $Q(t)$ and σ_1 are off-diagonal matrices — the operator B must be of the form

$$B(t) = \begin{pmatrix} B_+(t) & 0 \\ 0 & B_-(t) \end{pmatrix}. \tag{9.13}$$

Comparing

$$-\mathrm{i}[B,Q] = \begin{pmatrix} 0 & \mathrm{i}\,(D^* B_- - B_+ D^*) \\ \mathrm{i}\,(DB_+ - B_- D) & 0 \end{pmatrix} \tag{9.14}$$

with Eq. (9.11) we find that the operators $B_\pm$ should satisfy

$$\mathrm{i}\,(DB_+ - B_- D) = \mathrm{i}\,(D^* B_- - B_+ D^*) = m(t,x). \tag{9.15}$$

9.1.3 The Miura Transformation

Simultaneously with $Q(t)$ we may consider the "Schrödinger operator"

$$Q^2(t) = \begin{pmatrix} -\partial_x^2 + V_+(t,x) & 0 \\ 0 & -\partial_x^2 + V_-(t,x) \end{pmatrix}, \quad V_\pm \equiv \phi^2 \mp \phi_x. \tag{9.16}$$

Theorem 9.1 also applies to this case. If the time evolution of $Q(t)$ is governed by Eq. (9.8), then also the time evolution of the corresponding time-dependent Schrödinger operator (9.16) is determined by $W(t,s)$,

$$Q^2(t) = W(t,s)\,Q^2(s)\,W(s,t), \tag{9.17}$$

and

$$\frac{dQ^2(t)}{dt} = -\mathrm{i}\,[B(t), Q^2(t)] = -\mathrm{i}\,\{\,Q(t)\,,\,[B(t), Q(t)]\,\}, \tag{9.18}$$

where $\{\cdot,\cdot\}$ denotes the anticommutator. If $B(t)$ satisfies (9.11) then

$$-\mathrm{i}\,\{\,Q(t)\,,\,[B(t), Q(t)]\,\} = \begin{pmatrix} -m_x + 2\phi m & 0 \\ 0 & m_x + 2\phi m \end{pmatrix}. \tag{9.19}$$

The transition

$$m(t,x) \longrightarrow \pm m_x(t,x) + 2\phi(t,x)m(t,x) \tag{9.20}$$

is usually called the "Miura transformation". The Miura transformation links (9.12) with the corresponding equation for the potentials $V_\pm$ defined in (9.16),

$$(V_\pm)_t = \mp\phi_{t,x} + 2\phi\phi_t = \mp m_x + 2\phi m. \tag{9.21}$$

9.2 The Korteweg-deVries Equation

9.2.1 Construction of an Operator B

Next we are going to construct a particular example for the operator $B(t)$ which we described in Sect. 9.1.2. We assume that $B_\pm$ are differential operators of the general form

$$B_\pm(t) = \frac{1}{2}\sum_{k=0}^{n}\left(b_k^\pm(t,x)\,p^k + p^k\,b_k^\pm(t,x)\right), \tag{9.22}$$

where $p = -\mathrm{i}\,\partial_x$ is the momentum operator and $b_k^\pm$ are real functions which have to be determined. But since $m(t,x)$ and the expressions for D and D^* are real it is sufficient to look for real operators $\mathrm{i}\,B_\pm$. All summands in $\mathrm{i}\,B_\pm$ are real if the derivatives in Eq. (9.22) are of odd order. Hence we choose $b_k^\pm = 0$, for all even k.

Next we determine $b_1^\pm$ for $n = 1$, i.e., we make the ansatz

$$\mathrm{i}\,B_\pm = \frac{1}{2}\big(b_1^\pm \partial_x + \partial_x b_1^\pm\big). \tag{9.23}$$

If we insert this into (9.15) we see that the terms containing second derivatives cancel if and only if $b_1^+(t,x) = b_1^-(t,x) \equiv c(t,x)$. In this case

$$\mathrm{i}\,(DB_+ - B_-D) = \mathrm{c}_x\partial_x - \mathrm{c}\phi_x + c_{xx}/2, \tag{9.24}$$

which is a multiplication operator if $\mathrm{c}(t,x)$ is constant with respect to x. Hence we arrive at

$$B_+ = B_- = c(t)\,p, \qquad W(t,s) = e^{-\mathrm{i}\,p\int_s^t \mathrm{c}(\tau)\,d\tau}, \tag{9.25}$$

and Eq. (9.12) becomes

$$\phi_t(t,x) = -\mathrm{c}(t)\,\phi_x(t,x) \tag{9.26}$$

which is solved by

$$\phi(t,x) = \phi\big(x - \int_0^t \mathrm{c}(\tau)\,d\tau\big). \tag{9.27}$$

If the time dependence of the scalar potential is as given by (9.27), then the Dirac operators at different times are unitarily equivalent. However, we could have known this in advance, because the time-dependent translation $x \to x - \int_0^t \mathrm{c}(\tau)\,d\tau$ is clearly a unitary transformation in $L^2(\mathbb{R})^2$.

Hoping for a more interesting result we turn to the case where B is of third order:

$$\mathrm{i}B_\pm = \tfrac{1}{2}\big(b_3^\pm\partial_x^3 + \partial_x^3 b_3^\pm + b_1^\pm\partial_x + \partial_x b_1^\pm\big). \tag{9.28}$$

Again we calculate $\mathrm{i}DB_+ - \mathrm{i}B_-D$ and require this to be a multiplication operator. We see immediately that the coefficients of the fourth order derivatives can only vanish if $b_3^+ = b_3^- \equiv b$. But then the coefficient of ∂_x^3 simply becomes $b_x/2$. We conclude that b should not depend on x, hence $b = b(t)$. Under this condition we obtain

$$\begin{aligned}\mathrm{i}(DB_+ - B_-D) &= (b_1^+ - b_1^- - 3b\phi_x)\,\partial_x^2\\ &+\big(b_{1,x}^+ + \tfrac{1}{2}(b_{1,x}^+ - b_{1,x}^-) + (b_1^+ - b_1^-)\phi - 3b\phi_{xx}\big)\,\partial_x\\ &+\tfrac{1}{2}b_{11,xx} + \tfrac{1}{2}(b_{1,x}^+ - b_{1,x}^-)\phi - b_1^-\phi_x - b\phi_{xxx}.\end{aligned} \tag{9.29}$$

The coefficients of the differential operators ∂_x^2 and ∂_x vanish, if

$$b_{1,x}^+ = -\tfrac{3}{2}b\,(2\phi\phi_x - \phi_{xx}) = -\tfrac{3}{2}b\,(\phi^2 - \phi_x)_x \tag{9.30}$$

and hence

$$b_1^+(t,x) = -\tfrac{3}{2}b(t)\big(\phi^2(t,x) - \phi_x(t,x)\big) + c(t), \tag{9.31}$$

$$b_1^-(t,x) = -\tfrac{3}{2}b(t)\big(\phi^2(t,x) + \phi_x(t,x)\big) + c(t). \tag{9.32}$$

Finally, using $V_\pm$ defined in Eq. (9.16), we arrive at

$$B_\pm = -b(t)\,p^3 - \tfrac{3}{4}b(t)\,\{V_\pm\,,\,p\} + c(t)\,p. \tag{9.33}$$

Remark. The operators $B_\pm$ are known explicitly for arbitrary positive odd integers n in Eq. (9.22). We refer to the literature for details.

9.2.2 Differential Equations for the Potentials

We insert the expression obtained for B into Eq. (9.29) and obtain with Eqs. (9.15) and (9.12)

$$\phi_t = \tfrac{1}{4}b(t)(-\phi_{xxx} + 6\phi^2\phi_x) - c(t)\,\phi_x. \tag{9.34}$$

The corresponding equation (9.21) for the potentials $V_\pm$ of the Schrödinger equation is easily determined with the Miura transformation (9.20). We collect our results in the following theorems.

Theorem 9.2. Assume that $\phi(t,x)$ is infinitely differentiable such that ϕ and $\partial_x\phi \equiv \phi_x$ are bounded. Assume further that ϕ is a solution of

$$\phi_t + \tfrac{1}{4}b(t)(-6\phi^2\phi_x + \phi_{xxx}) + c(t)\,\phi_x = 0, \tag{9.35}$$

where b and c are some infinitely differentiable functions. Then the Dirac operator $Q(t) = -\mathrm{i}\,\sigma_2\partial_x + \sigma_1\phi(t,x)$ satisfies

$$Q(t) = W(t,s)\,Q(s)\,W(s,t), \quad \text{for all } s,t \in \mathbb{R}, \tag{9.36}$$

where W is a unitary evolution operator.

Theorem 9.3. Assume that $V(t,x)$ is infinitely differentiable such that V and $\partial_x V \equiv V_x$ are bounded. Assume further that V is a solution of

$$V_t + \tfrac{1}{4}b(t)\,(-6VV_x + V_{xxx}) + \mathrm{c}(t)\,V_x = 0, \tag{9.37}$$

with $b, \mathrm{c} \in C^\infty(\mathbb{R})$. Then the Schrödinger operator $H_\mathrm{s}(t) = -\partial_x^2 + V(t,x)$ satisfies

$$H_\mathrm{s}(t) = W(t,s)\,H_\mathrm{s}(s)\,W(s,t), \quad \text{for all } s,t \in \mathbb{R}, \tag{9.38}$$

where W is a unitary evolution operator.

Remark 1. If we choose $b(t) = 4$ and $c(t) = 0$ we obtain from (9.35) the "modified Korteweg-deVries equation" (mKdV)

$$\phi_t - 6\phi^2\phi_x + \phi_{xxx} = 0. \tag{9.39}$$

and from (9.37) the "Korteweg-de Vries equation" (KdV)

$$V_{\pm,t} - 6V_{\pm}V_{\pm,x} + V_{\pm,xxx} = 0. \tag{9.40}$$

This equation describes the time evolution of waves which are influenced by two antagonizing effects. The nonlinear term causes a steepening of the wave which can be compensated by a dispersion due to the third order term. Indeed, the equation has solutions which preserve their shape. These solutions are known as "solitons" or "solitary waves". (Strictly speaking, only the one-soliton solution is shape-preserving. A more precise definition of solitons is given in Sect. 9.5).

Eq. (9.40) was originally derived to describe the behavior of shallow water waves. There are many other physical applications, e.g., in hydrodynamics, plasma physics, acoustics, solid state physics, and elementary particle theory.

Remark 2. If ϕ satisfies the mKdV equation then

$$\tilde{\phi}(t,x) = \phi\Big(\int^t \frac{b(s)}{4}\,ds\,,\; x - \int^t c(s)\,ds\Big) \tag{9.41}$$

is a solution of (9.35). A similar statement holds for the KdV equation and Eq. (9.37). In the following we restrict our attention without loss of generality to the simpler equations (9.39) and (9.40).

Remark 3. The Miura transformation $V_{\pm} = \phi^2 \mp \phi_x$ gives two solutions $V_{\pm}$ of (9.37) for each solution ϕ of (9.35). In that case the operators W in (9.36) and (9.38) coincide. But since the nonlinearity of (9.37) is weaker than that of (9.35) it would be more desirable to construct solutions of the modified equation starting with a solution of (9.37). We shall describe this procedure in the next section.

Remark 4. The operators B and Q are called a "*Lax pair*" for the mKdV equation. Since there is a Lax pair B_n, Q for every positive odd integer n (see the remark at the end of Sect. 9.2.1), one obtains a whole set of nonlinear equations, the "mKdV hierarchy". The methods of this chapter can be extended to all equations of this hierarchy.

9.3 Inversion of the Miura Transformation

We assume that we have a solution V of the KdV equation (9.40) and want to find a solution ϕ of the mKdV equation (9.39), such that

$$V(t,x) = \phi^2(t,x) - \phi_x(t,x). \tag{9.42}$$

This will give simultaneously a second solution $\phi^2 + \phi_x$ of the KdV equation. For each t and given V, (9.42) is a Riccati differential equation for ϕ. Usually, it is solved by the substitution

$$\psi(x) = k \exp\{-\int^x \phi(y)\,dy\}, \qquad \phi = -\frac{\psi_x}{\psi}, \tag{9.43}$$

where k is some constant, which in our case may depend on the parameter t. Inserting (9.43) into (9.42) gives for ψ the equation

$$-\psi_{xx} + V\psi = 0, \tag{9.44}$$

which is just the Schrödinger equation for zero energy. Hence everything depends on whether we can choose for each time t a positive solution of (9.44) in such a way, that $-\psi_x/\psi$ satisfies the mKdV equation. The main problem here is to choose the correct time dependence. For this we recall that the time dependence of the Schrödinger operator $-\partial_x^2 + V(t,x)$ is generated by the operator

$$B_+(t) = -4p^3 - 3\{V,p\}. \tag{9.45}$$

Hence it seems reasonable to assume

$$\psi_t = -\mathrm{i}B_+\psi = -4\psi_{xxx} + 6V\psi_x + 3V_x\psi. \tag{9.46}$$

With (9.44) this is equivalent to the first order equation

$$\psi_t = 2V\psi_x - V_x\psi. \tag{9.47}$$

Indeed, a little calculation with $\phi = -\psi_x/\psi$ gives

$$\begin{aligned}\phi_t &- 6\phi^2\phi_x + \phi_{xxx} \\ &= \psi^{-2}\,(\psi_t\psi_x - 6V\psi_x^2 - \psi\psi_{xt} + 3\psi_{xx}^2 + 4\psi_x\psi_{xxx} - \psi\psi_{xxxx}).\end{aligned} \tag{9.48}$$

This expression can be shown to vanish identically if one takes into account Eq. (9.46). Hence, at least formally, ϕ defined in this way indeed satisfies the mKdV equation. We still have to verify that the function $\psi(t,x)$ determined by Eq. (9.46) is a positive zero energy solution of the Schrödinger equation for all t, and that ϕ has all of the required properties (9.2). The following theorem states that all smooth solutions of the mKdV equation can be obtained in this way.

Theorem 9.4. Suppose $V \in \mathcal{C}^\infty(\mathbb{R}^2)$ is a solution of the KdV equation (9.40) such that V and V_x are bounded and such that the Schrödinger operator $-\partial_x^2 + V(0,x)$ is nonnegative. Then

$$-\frac{\partial^2\psi(x)}{\partial x^2} + V(0,x)\,\psi(x) = 0 \tag{9.49}$$

has at least one weak solution $\psi_0(x) > 0$, all x, which is in $\mathcal{C}^\infty(\mathbb{R})$ (but which need not be square integrable). Define $\psi \in \mathcal{C}^\infty(\mathbb{R}^2)$ as the unique solution of (9.47) with initial condition $\psi(0,x) = \psi_0(x)$, all $x \in \mathbb{R}$.

a) If ψ_0 is unique (up to multiplication with a constant), then $\phi(t,x) = -\psi_x(t,x)/\psi(t,x)$ is the unique solution of the mKdV equation (9.39) satisfying (9.2) and $V = \phi^2 - \phi_x$.

b) If (9.49) has two linearly independent positive solutions $\psi_{\pm,0}$ then the solutions of the mKdV equation satisfying (9.2) and $V = \phi^2 - \phi_x$ form a one-parameter family given by

$$\phi_\sigma(t,x) = -\frac{\psi_{\sigma,x}(t,x)}{\psi_\sigma(t,x)}, \quad \psi_\sigma(t,x) = \frac{1-\sigma}{2}\psi_-(t,x) + \frac{1+\sigma}{2}\psi_+(t,x), \quad (9.50)$$

with $\sigma \in [-1,1]$.

Remark. A nonnegative Schrödinger operator $H_s = -\partial_x^2 + V(x)$ is called "critical" iff $H_s\psi = 0$ has a unique positive solution. (This is case a in the theorem above. It occurs, e.g., if 0 is an eigenvalue of H_s). Otherwise, H_s is called "subcritical". In this case there are two linearly independent solutions of $H_s\psi = 0$ which are not square integrable. See [174] for details.

Proof. 1) In a first step we note that the nonnegativity of the Schrödinger operator at time $t = 0$ implies nonnegativity for all times, because Schrödinger operators at different times are unitarily equivalent if the potential evolves according to the KdV equation. (See Theorem 9.3). Nonnegativity of the Schrödinger operator further implies existence of a positive zero energy solution by well-known Sturm-(non)oscillation-type results[1].

2) In the second step we prove that the function ψ determined with (9.46) or (9.47) is for any t a unique solution of the zero energy Schrödinger equation. The zero energy Schrödinger equation at time t is equivalent to the Volterra equation

$$\psi(t,x) = c(t) + d(t)x + \int_0^x (x-y)\, V(t,y)\, \psi(t,y)\, dy, \quad (9.51)$$

where $c(t) + d(t)x$ with $c, d \in \mathcal{C}^\infty(\mathbb{R})$ is a solution of the homogeneous equation $\phi_{xx} = 0$. For each $c(t)$ and $d(t)$ there is a unique solution of

$$-\frac{\partial^2\psi(t,x)}{\partial x^2} + V(t,x)\psi(t,x) = 0 \quad (9.52)$$

which is obtained by iterating (9.51). In particular $c(0)$ and $d(0)$ are fixed by ψ_0. We have to show that there are unique functions c and d such that the $\psi(t,x)$ also satisfies (9.47). From (9.52) we obtain $-\psi_{txx} + V\psi_t = -V_t\psi$. But the function

$$\Psi(t,x) \equiv 2V(t,x)\psi_x(t,x) - V_x(t,x)\psi(t,x) \quad (9.53)$$

also satisfies $-\Psi_{xx} + V\Psi = -V_t\psi$. Hence $(\Psi - \psi_t)$ is a solution of (9.52). It is the zero solution iff

$$0 = (\Psi - \psi_t)(t,0) = 2V(t,0)d(t) - V_x(t,0)c(t) - \dot{c}(t), \quad (9.54)$$

$$0 = (\Psi - \psi_t)_x(t,0) = V_x(t,0)d(t) + \big(2V(t,0)^2 - V_{xx}(t,0)\big)c(t) - \dot{d}(t), \quad (9.55)$$

[1] See [174].

from which $c(t)$ and $d(t)$ are uniquely determined given c(0) and $d(0)$. Hence we obtain a unique ψ which satisfies $\psi_t = \Psi$, i.e., Eq.(9.47).

3) We show that $\psi(t,x) > 0$ for all $(t,x) \in \mathbb{R}^2$ if $\psi_0(x) > 0$. Assume that $\psi(t,x(t)) = 0$, for all $t \in \mathbb{R}$. Differentiating this and using (9.47) gives

$$\dot{x}(t) = -2V(t,x(t)). \tag{9.56}$$

Now, assume $\psi(t_0,x_0) = 0$ for some (t_0,x_0). Then (9.56) has a unique solution $x(t)$ with $x(t_0) = x_0$. The function $\psi(t,x(t))$ fulfills the differential equation

$$\begin{aligned}\frac{d}{dt}\psi(t,x(t)) &= \psi_t(t,x(t)) + \dot{x}(t)\,\psi_x(t,x(t)) \\ &= \{2V(t,x(t)) + \dot{x}(t)\}\,\psi_x(t,x(t)) - V_x(t,x(t))\,\psi(t,x(t)) \\ &= -V_x(t,x(t))\,\psi(t,x(t))\end{aligned} \tag{9.57}$$

which has the unique solution

$$\psi(t,x(t)) = \psi(t_0,x_0)\exp\Big\{\int_{t_0}^{t} V_x(t',x(t'))\,dt'\Big\} = 0. \tag{9.58}$$

Hence $\psi(t,\cdot)$ has a zero for all t if it has a zero for some t_0. Conversely, if $\psi(t,\cdot) > 0$ for $t = 0$, then the same must be true for all t.

4) Since $\psi(t,x)$ is positive we can form the logarithmic derivative $\phi(t,x) = -\psi_x(t,x)/\psi(t,x)$. Using [Ha 82], Corollary XI.6.5 on p. 358, we find that ϕ is bounded, provided V is bounded. Since $V = \phi^2 - \phi_x$ and V_x are bounded we obtain boundedness of ϕ_x and ϕ_{xx}. Hence ϕ satisfies (9.2).

5) Now, assume that we have two solutions $\psi_\pm$ of (9.49) from which we obtain two solutions of (9.52) according to steps 1) to 4). We can form the following general linear combination

$$\psi_\sigma(t,x) = \tfrac{1}{2}[1-\sigma(t)]\,\psi_-(t,x) + \tfrac{1}{2}[1+\sigma(t)]\,\psi_+(t,x), \tag{9.59}$$

where $\sigma : \mathbb{R} \to [-1,1]$ is in $C^\infty(\mathbb{R})$. Since ψ_σ is positive, our results above apply to ψ_σ as well and we can define $\phi_\sigma = -\psi_{\sigma,x}(t,x)/\psi_\sigma(t,x)$. Then Eq. (9.48) becomes

$$\phi_{\sigma,t} - 6\phi_\sigma^2\phi_{\sigma,x} + \phi_{\sigma,xxx} = \frac{2k^2}{\psi_\sigma^2}\,W(\psi_-,\psi_+)\,\dot{\sigma}, \tag{9.60}$$

where $W(\psi_-,\psi_+) = \psi_-(\partial_x\psi_+) - (\partial_x\psi_-)\psi_+$ is the Wronskian of the two solutions. Using Eqs. (9.47) and (9.52) it can be shown that the Wronskian is time independent. Hence (9.60) vanishes for all $t \in \mathbb{R}$ either if $\sigma = $ const. or if the Wronskian $W(\psi_{-,0},\psi_{+,0})$ vanishes i.e., if the two solutions are linearly dependent. In the second case the solution of (9.49) is unique up to multiplication with a constant and ϕ_σ indeed does not depend on σ. Since ψ_σ is the general solution of the zero energy Schrödinger equation, the corresponding function ϕ_σ is the general solution of the Riccati equation (9.42). Hence this construction gives all smooth solutions of the mKdV equation related to V via a Miura transformation. This completes the proof of the theorem. □

9.4 Scattering in One Dimension

9.4.1 The Scattering Matrix

It is useful to have a closer look on the spectral and scattering theory for the Dirac operator

$$Q = \begin{pmatrix} 0 & D^* \\ D & 0 \end{pmatrix}, \qquad D = \partial_x + \phi(x). \tag{9.61}$$

We shall assume that the potential ϕ satisfies

$$\lim_{x \to \pm\infty} \phi(x) = \phi_\pm, \qquad 0 < \phi_-^2 \leq \phi_+^2, \tag{9.62}$$

and that the limit is approached sufficiently rapidly. For example, the following condition would be sufficient,

$$\pm \int_0^{\pm\infty} (1+x^2) \left\{ |\phi(x) - \phi_\pm| + |\phi_x(x)| \right\} dx < \infty. \tag{9.63}$$

Potential functions with these properties arise as soliton solutions of the mKdV equation, cf. Sect. 9.5 below. Supersymmetry allows us to relate the Dirac operator Q to the following pair of Schrödinger operators

$$H_j \equiv -\partial_x^2 + V_j, \qquad V_j \equiv \phi^2 + (-1)^j \phi_x, \qquad j = 1, 2. \tag{9.64}$$

Hence we can derive the spectral properties of Q from well known results about one-dimensional Schrödinger operators with bounded potentials $\phi^2 \mp \phi_x$ which are asymptotically equal to the constants $\phi_\pm^2$.

We find that Q has finitely many nondegenerate eigenvalues in the interval $(-|\phi_-|, |\phi_-|)$ and a purely absolutely continuous spectrum

$$\sigma_{\text{a.c.}}(Q) = (-\infty, -|\phi_-|] \cup [|\phi_-|, \infty). \tag{9.65}$$

Moreover, Q has simple spectrum in $(-|\phi_+|, |\phi_-|) \cup (|\phi_-|, |\phi_+|)$ iff this set is non-empty. This situation corresponds to total reflection, it does not occur if $|\phi_-| = |\phi_+|$. The spectral multiplicity in $(-\infty, -|\phi_+|] \cup [|\phi_+|, \infty)$ is two, corresponding to the fact that we can form two orthogonal scattering solutions with same energies, one moving to the right and one to the left (see also Sect. 4.5). For simplicity, we restrict ourselves to the energy range $E^2 > \phi_+^2$ for the rest of this section.

Let us first consider the solutions of the Dirac equation $Q\psi = E\psi$ with a constant potential $\phi(x) = \phi_0$. The two linearly independent solutions are given by

$$\underset{\rightarrow}{\omega}(E, \phi_0, x) = C(E) \begin{cases} \begin{pmatrix} 1 \\ E^{-1}(\mathrm{i}k + \phi_0) \end{pmatrix} e^{\mathrm{i}kx}, & E > 0, \\ \begin{pmatrix} E^{-1}(\mathrm{i}k + \phi_0) \\ 1 \end{pmatrix} e^{-\mathrm{i}kx}, & E < 0, \end{cases} \tag{9.66}$$

$$\underset{\leftarrow}{\omega}(E,\phi_0,x) = \overline{\underset{\rightarrow}{\omega}(E,\phi_0,x)}, \tag{9.67}$$

where $k = (E^2 - \phi_0^2)^{1/2}$, and $C(E) = \sqrt{|E|/4\pi k}$. These solutions are oscillatory and bounded for $E^2 > \phi_0^2$. In this case $\underset{\rightarrow}{\omega}(E,\phi_0,x)e^{-iEt}$ is a plane-wave solution of the Dirac equation which moves to the right. Similarly, $\underset{\leftarrow}{\omega}$ is related to solutions moving to the left.

Remark. A calculation similar to Sect. 1.6 leads to the mean velocity operator $v_{\mathrm{cl}} = pQ^{-1} = \sigma_2 - i\phi_0 Q^{-1}\sigma_3$. With the solutions (9.66) and (9.67) we find for the $\mathbb{C}^2$-scalar product

$$\big(\underset{\rightleftarrows}{\omega}(E,\phi_0,x)\,,\, v_{\mathrm{cl}}\,\underset{\rightleftarrows}{\omega}(E,\phi_0,x)\big)_{\mathbb{C}^2} = \pm 2\frac{k}{|E|} \gtrless 0. \tag{9.68}$$

Hence the expectation value of v_{cl} in a state given as a (square integrable) superposition of functions $\underset{\rightarrow}{\omega}$ (or $\underset{\leftarrow}{\omega}$) is always positive (or negative).

One defines the "*Jost solutions*" of the Dirac equation with potential $\phi(x)$ by the following boundary conditions.

1) Outgoing Jost solutions:

$$\underset{\rightarrow}{\Psi}(E,x) \overset{x\to\infty}{\longrightarrow} \underset{\rightarrow}{\omega}(E,\phi^+,x), \qquad \underset{\leftarrow}{\Psi}(E,x) \overset{x\to-\infty}{\longrightarrow} \underset{\leftarrow}{\omega}(E,\phi^-,x). \tag{9.69}$$

2) Incoming Jost solutions:

$$\underset{\rightarrow}{\Phi}(E,x) \overset{x\to-\infty}{\longrightarrow} \underset{\rightarrow}{\omega}(E,\phi^-,x), \qquad \underset{\leftarrow}{\Phi}(E,x) \overset{x\to\infty}{\longrightarrow} \underset{\leftarrow}{\omega}(E,\phi^+,x). \tag{9.70}$$

Any (distributional) eigenfunction $\Psi = \binom{\psi_1}{\psi_2}$ of Q satisfies

$$\psi_2 = E^{-1}D\psi_1, \qquad \psi_1 = E^{-1}D^*\psi_2, \tag{9.71}$$

$$D^*D\psi_1 = E^2\psi_1, \qquad DD^*\psi_2 = E^2\psi_2. \tag{9.72}$$

Hence we can relate the Dirac-Jost solutions with the Schrödinger-Jost solutions. These can be defined as the unique solutions of the following Volterra integral equations (for later use we give these equations for complex energies z)

$$f_j^{\pm}(z,x) = e^{\pm ik^{\pm}x} - \frac{1}{k^{\pm}}\int_x^{\pm\infty} \sin[k^{\pm}(x-y)]\,[V_j(y)-\phi_{\pm}^2]\,f_j^{\pm}(z,y)\,dy \tag{9.73}$$

$$g_j^{\pm}(z,x) = e^{\mp ik^{\pm}x} - \frac{1}{k^{\pm}}\int_x^{\pm\infty} \sin[k^{\pm}(x-y)]\,[V_j(y)-\phi_{\pm}^2]\,g_j^{\pm}(z,y)\,dy, \tag{9.74}$$

where $z \in \mathbb{C}$, $x \in \mathbb{R}$, $k^{\pm} \equiv k^{\pm}(z) \equiv \sqrt{z-\phi_{\pm}^2}$. The square root is defined with the branch-cut on the positive real axis, so that $\mathrm{Im}\,k^{\pm} \geq 0$. Iterating these equations and applying standard techniques we find that the Jost solutions $f_j^{\pm}$ are analytic with respect to $z \in \mathbb{C} \setminus [\phi_{\pm}^2, \infty)$. The functions $f_j^{\pm}$ and $g_j^{\pm}$ are solutions of the differential equation

$$\{-\partial_x^2 + V_j(x)\}\, f(z,x) = z f(z,x). \tag{9.75}$$

For real $z = \lambda > \phi_+^2$ the Jost solutions $f_j^\pm$ and $g_j^\pm$ are respectively the outgoing and incoming generalized eigenfunctions of H_j with energy λ which satisfy the boundary conditions

$$f_j^\pm(\lambda,x) \overset{x\to\pm\infty}{\longrightarrow} e^{\pm ik^\pm x}, \quad g_j^\pm(\lambda,x) \overset{x\to\pm\infty}{\longrightarrow} e^{\mp ik^\pm x}, \quad k^\pm = \sqrt{\lambda - \phi_\pm^2}. \tag{9.76}$$

Comparing the asymptotic behavior of $f_j^\pm(\lambda,x)$, $E^{-1}Df_j^\pm(\lambda,x)$, etc., where $\lambda = E^2$, with the asymptotic behavior of the Dirac Jost solutions (9.69) and (9.70) we find

$$\left(\underset{\rightarrow}{\Psi}\right)_{\text{pos}} = \begin{pmatrix} f_1^\mp \\ E^{-1}Df_1^\mp \end{pmatrix}, \qquad \left(\underset{\rightarrow}{\Psi}\right)_{\text{neg}} = \begin{pmatrix} E^{-1}D^* g_2^\mp \\ g_2^\mp \end{pmatrix}, \tag{9.77}$$

$$\left(\underset{\leftarrow}{\Phi}\right)_{\text{pos}} = \begin{pmatrix} g_1^\pm \\ E^{-1}Dg_1^\pm \end{pmatrix}, \qquad \left(\underset{\leftarrow}{\Phi}\right)_{\text{neg}} = \begin{pmatrix} E^{-1}D^* f_2^\pm \\ f_2^\pm \end{pmatrix}. \tag{9.78}$$

We can use the Jost solutions to describe a scattering process. Obviously, for $|E| > |\phi_+|$, the outgoing solution to the left, $\underset{\leftarrow}{\Psi}$, must be a linear combination of the linearly independent solutions $\underset{\leftarrow}{\Phi}$ and $\underset{\rightarrow}{\Psi}$, i.e.,

$$T(E)\underset{\leftarrow}{\Psi}(E,x) = \underset{\leftarrow}{\Phi}(E,x) + R^r(E)\underset{\rightarrow}{\Psi}(E,x). \tag{9.79}$$

This describes a situation, where a particle beam coming in from the right is split into a transmitted part escaping to the left and into a reflected part moving back to the right. Hence $T(E)$ is called transmission coefficient, and $R^r(E)$ is called reflection coefficient to the right. A similar consideration is valid for particles scattered to the left, with a reflection coefficient $R^l(E)$. Using the Wronski determinant

$$W(\Phi,\Psi) = \phi_1(x)\psi_2(x) - \psi_1(x)\phi_2(x) \tag{9.80}$$

and the well known facts that $W(\Phi,\Psi)$ does not depend on x and vanishes, whenever Φ and Ψ are linearly dependent, we obtain from Eq. (9.79)

$$R^r(E) = -W(\underset{\leftarrow}{\Psi},\underset{\leftarrow}{\Phi})/W(\underset{\leftarrow}{\Psi},\underset{\rightarrow}{\Psi}), \tag{9.81}$$

and similarly

$$R^l(E) = W(\underset{\rightarrow}{\Psi},\underset{\rightarrow}{\Phi})/W(\underset{\leftarrow}{\Psi},\underset{\rightarrow}{\Psi}), \qquad T(E) = 2i\sqrt{k^+k^-}|E|^{-1}/W(\underset{\leftarrow}{\Psi},\underset{\rightarrow}{\Psi}). \tag{9.82}$$

This representation has the advantage that the Wronski determinants can be evaluated by inserting the asymptotic forms of the solutions. The on-shell scattering operator can be represented by the matrix

$$S(E) = \begin{pmatrix} T(E) & R^r(E) \\ R^l(E) & T(E) \end{pmatrix}, \qquad |E| > |\phi_+|. \tag{9.83}$$

Of course, similar considerations hold for the Jost solutions $f_j^\pm$ and $g_j^\pm$ associated with the Schrödinger operators H_j. One obtains, e.g.

$$T_j(\lambda)\, f_j^-(\lambda,x) = g_j^+(\lambda,x) + R_j^r(\lambda)\, f_j^+(\lambda,x)$$

$$\overset{x\to+\infty}{\longrightarrow} e^{-\mathrm{i}k^+x} + R_j^r(\lambda)\, e^{+\mathrm{i}k^+x}, \qquad \lambda > 0. \tag{9.84}$$

Here $R_j^r(\lambda)$ is the nonrelativistic reflection coefficient, and $T_j(\lambda)$ the transmission coefficient corresponding to H_j, and (with $W(f,g) = f\partial_x g - g\partial_x f$) we obtain

$$R_j^r = \frac{-W(f_j^-, g_j^+)}{W(f_j^-, f_j^+)}, \quad R_j^l = \frac{W(f_j^+, g_j^-)}{W(f_j^-, f_j^+)}, \quad T_j = \frac{2\mathrm{i}\sqrt{k^+k^-}}{W(f_j^-, f_j^+)}, \tag{9.85}$$

where $k^\pm = \sqrt{\lambda - \phi_\pm^2}$. Because of (9.71) and (9.72) we can even relate the two Schrödinger problems with $j = 1, 2$ and the Dirac problem. If $f_1^\pm$ and $g_1^\pm$ are the Jost solutions of the Schrödinger problem with V_1, then the correctly normalized Jost solutions of the problem with V_2 are given by

$$f_2^\pm = (\pm\mathrm{i}k^\pm + \phi_\pm)^{-1} D f_1^\pm \qquad g_2^\pm = (\mp\mathrm{i}k^\pm + \phi_\pm)^{-1} D g_1^\pm. \tag{9.86}$$

Conversely,

$$f_1^\pm = (\mp\mathrm{i}k^\pm + \phi_\pm)^{-1} D^* f_2^\pm, \qquad g_1^\pm = (\pm\mathrm{i}k^\pm + \phi_\pm)^{-1} D^* g_2^\pm. \tag{9.87}$$

For two (distributional) solutions $f_j(z,x)$ and $g_j(z,x)$ of $(-\partial_x^2 - V_j)\psi = z\psi$, $z \in \mathbb{C}$, we find

$$W(Df_1(z), Dg_1(z)) = zW(f_1(z), g_1(z)), \tag{9.88}$$

$$W(D^*f_2(z), D^*g_2(z)) = zW(f_2(z), g_2(z)). \tag{9.89}$$

Hence we obtain

$$R_1^r(\lambda) = \frac{-\mathrm{i}k^+ + \phi_+}{\mathrm{i}k^+ + \phi_+} R_2^r(\lambda), \qquad T_1(\lambda) = \frac{(\mathrm{i}k^- + \phi_-)(-\mathrm{i}k^+ + \phi_+)}{\lambda} T_2(\lambda). \tag{9.90}$$

$$R_1^l(\lambda) = \frac{\mathrm{i}k^- + \phi_-}{-\mathrm{i}k^- + \phi_-} R_2^l(\lambda),$$

Using (9.77) and (9.78) we obtain relations between the Wronskians of the Dirac solutions and the Wronski determinants of the Schrödinger Jost solutions. We shall need in particular the following result, which shows that if one of the potentials ϕ, $\phi^2 \mp \phi_x$ is a reflectionless potential, then all three are reflectionless potentials:

$$R^r(E) = \begin{cases} R_1^r(E^2), & \text{if } E > |\phi_+|, \\ \overline{R_2^r(E^2)}, & \text{if } E < -|\phi_+|. \end{cases} \tag{9.91}$$

In order to prove, e.g., Eq. (9.91) with $E < -|\phi_+|$, we insert the negative-energy parts of Eqs. (9.77) and (9.78) into (9.81). This leads to

$$R^r(E) = -\frac{f_2^+ D^* g_2^- - g_2^- D^* f_2^+}{g_2^+ D^* g_2^- - g_2^- D^* g_2^+} = -\frac{W(g_2^-, f_2^+)}{W(g_2^-, g_2^+)}. \tag{9.92}$$

Using the relation $\overline{f_j^{\pm}(\lambda, x)} = g_j^{\pm}(\lambda, x)$, which holds for $\lambda \in \mathbb{R}$, we arrive at $R^r(E) = \overline{R_2^r(E^2)}$ (E negative) by comparison with Eq. (9.85). Similar calculations show that Eq. (9.91) also holds with R^r replaced by R^l or T. Hence we can represent the relativistic scattering operator in terms of the nonrelativistic scattering operators $S_j(\lambda)$ (which are defined as in Eq. (9.83) with the help of the nonrelativistic reflection and transmission coefficients)

$$S(E) = \begin{cases} S_1(E^2), & \text{if } E > |\phi_+|, \\ \overline{S_2(E^2)}, & \text{if } E < -|\phi_+|. \end{cases} \tag{9.93}$$

9.4.2 Relative Scattering and the Regularized Index

In this section we calculate the index of the Dirac operator with soliton-like potentials. This serves as an illustration of the techniques developed in Chapter 5. We use the Jost solutions $f_j^{\pm}$, $j = 1, 2$, given by the Volterra equations (9.73) and the relation between Fredholm determinants and the index described in Sect. 5.10. We assume Q to be of the form (9.61), with a scalar potential ϕ satisfying the conditions (9.62) and (9.63).

Since we are interested in relative scattering, we write

$$H_1 = H_2 + V, \qquad V = -2\phi_x, \tag{9.94}$$

and express the solutions $f_1^{\pm}$ with the help of Green-functions associated with H_2. We obtain, as usual, the Volterra equations

$$f_1^{\pm}(z, x) = f_2^{\pm}(z, x) - \int_x^{\pm\infty} \tilde{g}(z, x, y)\, V(y)\, f_1^{\pm}(z, y)\, dy, \tag{9.95}$$

for all $z \in \mathbb{C} \setminus \{\sigma_p(H_2) \cup \{\phi_-^2\}\}$. The integral kernel $\tilde{g}$ is given by

$$\tilde{g}(z, x, y) = \frac{1}{W(f_2^-(z), f_2^+(z))} [f_2^+(z, x) f_2^-(z, y) - f_2^-(z, x) f_2^+(z, y)]. \tag{9.96}$$

Another fundamental solution of the equation $(H_2 - z)f = 0$ is

$$g(z, x, y) = \frac{-1}{W(f_2^-(z), f_2^+(z))} \begin{cases} f_2^-(z, x) f_2^+(z, y), & x \le y, \\ f_2^+(z, x) f_2^-(z, y), & x \ge y. \end{cases} \tag{9.97}$$

The Jost solutions $f_1^{\pm}$ obey the Fredholm integral equations

$$f_1^{\pm}(z, x) = \frac{1}{T(z)} f_2^{\pm}(z, x) - \int_{-\infty}^{+\infty} g(z, x, y)\, V(y)\, f_1^{\pm}(z, y)\, dy. \tag{9.98}$$

The coefficient $T(z)$ is a "relative transmission coefficient" and can be written as

$$T(z) = \frac{W(f_2^-(z), f_2^+(z))}{W(f_1^-(z), f_1^+(z))} =$$

$$= \left\{ 1 - \frac{1}{W(f_2^-(z), f_2^+(z))} \int f_2^-(z,x)\, V(x)\, f_1^+(z,x)\, dx \right\}^{-1} \tag{9.99}$$

Similar formulas and expressions are familiar from the one-dimensional scattering theory with $H_2 = H_0 = -\partial_x^2$, and the generalization to the present case is straightforward.

Our aim is to calculate the regularized index $\mathrm{ind}_z\,(Q)$ with the help of the Fredholm determinant $\det(\mathbf{1} + u(H_2 - z)^{-1}v)$, where

$$v(x) \equiv |V(x)|^{1/2}, \qquad u(x) \equiv |V(x)|^{1/2} \mathrm{sgn}\, V(x). \tag{9.100}$$

We omit the technical proof that $(H_1 - z)^{-1} - (H_2 - z)^{-1}$ belongs to the trace class under the assumptions (9.62) and (9.63) (see [159], Thm. 2.8 for details). One can also show that $u(H_j - z)^{-1}v$ is trace class. The trace of this operator is explicitly given by (cf. Eqs. (9.97) and (5.125))

$$\mathrm{tr}\, u(H_j - z)^{-1}v = \frac{-1}{W(f_j^-(z), f_j^+(z))} \int_{-\infty}^{+\infty} f_j^-(z,x)\, V(x)\, f_j^+(z,x)\, dx. \tag{9.101}$$

Next we replace V by γV and calculate, using Eqs. (5.199), (5.200)

$$\frac{d}{d\gamma} \ln \det\left[1 + \gamma u(H_2 - z)^{-1}v\right] = \mathrm{tr}\left[1 + \gamma u(H_2 - z)^{-1}v\right]^{-1} u(H_2 - z)^{-1}v =$$

$$= \mathrm{tr}\, u(H_1 - z)^{-1}v. \tag{9.102}$$

Now, from Eq. (9.99) we find

$$\frac{d}{d\gamma} \ln T(z) = -T(z) \frac{dT^{-1}(z)}{d\gamma} =$$

$$= T(z) \frac{1}{W(f_2^-(z), f_2^+(z))} \int f_2^-\, V \left\{ f_1^+ + \gamma \frac{d}{d\gamma} f_1^+ \right\} dx$$

$$= \frac{1}{W(f_1^-(z), f_1^+(z))} \int f_2^-\, V \left\{ f_1^+ + \gamma \frac{d}{d\gamma} f_1^+ \right\} dx. \tag{9.103}$$

We can use the Volterra equation (9.95) to calculate $df_1^+/d\gamma$. If $\tilde{G}^+$ denotes the integral operator with kernel given by $\tilde{g}$ (Eq. (9.96)) for $y \geq x$, and 0 for $y \leq x$, then we can write Eq. (9.95) as

$$f_1^+ = f_2^+ - \gamma \tilde{G}^+ V f_1^+, \tag{9.104}$$

hence

$$\tfrac{d}{d\gamma} f_1^+ = -\tilde{G}^+ V f_1^+ - \gamma \tilde{G}^+ V \tfrac{d}{d\gamma} f_1^+ \tag{9.105}$$

or

$$\gamma \tfrac{d}{d\gamma} f_1^+ = -(1+\gamma\tilde{G}^+V)^{-1}\gamma\tilde{G}^+Vf_1^+ = (1+\gamma\tilde{G}^+V)^{-1}f_1^+ - f_1^+. \tag{9.106}$$

Inserting this result into Eq. (9.103) we obtain

$$\frac{d}{d\gamma}\ln T = \frac{-1}{W(f_1^-(z), f_1^+(z))}\int f_2^-\, V\,(1+\gamma\tilde{G}^+V)^{-1}f_1^+\, dx =$$

$$= \frac{-1}{W(f_1^-(z), f_1^+(z))}\int f_2^-\,(1+\gamma V\tilde{G}^+)^{-1}V\, f_1^+\, dx \tag{9.107}$$

In order to evaluate the last integral, we consider first the expression

$$-\gamma\int_{-\infty}^{+\infty} dx \int_{-\infty}^{x} dy\, \tilde{g}(z,x,y)\, V(y)\, f_1^-(z,y)\, h(z,x)$$

$$= \gamma\int_{-\infty}^{+\infty} dy\, f_1^-(z,y)\, V(y)\int_{y}^{+\infty} dx\, \tilde{g}(z,y,x)\, h(z,x)$$

$$= \int_{-\infty}^{+\infty} dy\, f_1^-(z,y)[\gamma V\tilde{G}^+h](z,y), \tag{9.108}$$

with some suitable function h. Hence, using (9.95), we calculate

$$\int_{-\infty}^{+\infty} dx\, f_2^-(z,x)\, h(z,x)$$

$$= \int_{-\infty}^{+\infty} dx \left\{ f_1^-(z,x) - \gamma\int_{-\infty}^{x} dy\, \tilde{g}(z,x,y)\, V(y)\, f_1^-(z,y)\right\} h(z,x)$$

$$= \int_{-\infty}^{+\infty} dy\, f_1^-(z,y)\,[(1+\gamma V\tilde{G}^+)h](z,y). \tag{9.109}$$

Inserting $h = (1+\gamma V\tilde{G}^+)Vf_1^+$ into (9.109), we obtain from Eqs. (9.107) and (9.101)

$$\frac{d}{d\gamma}\ln T = \frac{1}{W(f_1^-(z), f_1^+(z))}\int f_1^-(z,x)\, V(x)\, f_1^+(z,x)\, dx$$

$$= -\operatorname{tr} u(H_1 - z)^{-1}v. \tag{9.110}$$

Combining this result with Eq. (9.102) we find

$$\frac{d}{d\gamma}\ln\{T\det[\mathbf{1}+\gamma u(H_2-z)^{-1}v]\} = 0, \tag{9.111}$$

Since $\gamma = 0$ implies $H_1 = H_2$ and

$$\det[\mathbf{1}+\gamma u(H_2-z)^{-1}v] = \det\mathbf{1} = 1 = T(z), \qquad (\gamma = 0) \tag{9.112}$$

we arrive at

$$\det\left[1 + u(H_2 - z)^{-1}v\right] = \frac{1}{T(z)} = \frac{W(f_1^-(z), f_1^+(z))}{W(f_2^-(z), f_2^+(z))}. \tag{9.113}$$

Finally, we employ the supersymmetric relation between f_1 and f_2, namely

$$f_2^\pm(z, x) = (\pm ik^\pm + \phi_\pm)\, Df_1^\pm(z, x), \tag{9.114}$$

and the identity $W(Df_1^-(z), Df_1^+(z)) = zW(f_1^-(z), f_1^+(z))$, cf. (9.88), to calculate

$$\begin{aligned}\frac{W(f_1^-(z), f_1^+(z))}{W(f_2^-(z), f_2^+(z))} &= (-ik^- + \phi_-)\,(ik^+ + \phi_+)\,\frac{W(f_1^-(z), f_1^+(z))}{W(Df_1^-(z), Df_1^+(z))} \\ &= \tfrac{1}{z}\,(-ik^- + \phi_-)\,(ik^+ + \phi_+).\end{aligned} \tag{9.115}$$

We can now use the results of Sect. 5.10 to obtain the regularized index

$$\begin{aligned}\mathrm{ind}_z\, Q &= -z\,\frac{d}{dz}\,\ln\det\left[\mathbf{1} + u(H_2 - z)^{-1}v\right] \\ &= \frac{1}{2}\left[\frac{\phi_+}{\sqrt{\phi_+^2 - z}} - \frac{\phi_-}{\sqrt{\phi_-^2 - z}}\right]\end{aligned} \tag{9.116}$$

and the other formulas of Sect. 5.11.1.

9.5 Soliton Solutions

As an illustration of the methods described in Sect. 9.3 we are going to construct the soliton solutions of the mKdV equation from the well known solitons of the KdV equation. In the next section we briefly describe the KdV solitons and indicate how to find them. See the notes for references to the literature on that subject.

9.5.1 Solitons of the KdV Equation

The KdV solitons are usually obtained by the inverse scattering method. The idea is to use the connection between solutions of the KdV equation and potentials for Schrödinger operators (see Theorem 9.3). Instead of solving the (nonlinear) KdV equation with initial condition $V(0, x) = V(x)$, one first solves the (linear) Schrödinger equation

$$H_s\psi(x) = -\partial_x^2\psi(x) + V(x)\psi(x) = \lambda\psi(x). \tag{9.117}$$

Here and in the following the potential V is assumed to satisfy certain regularity conditions, e.g,

$$\int_{-\infty}^{\infty}(1 + |x|^2)|V(x)|dx < \infty. \tag{9.118}$$

In this case the solutions ψ of Eq. (9.117) in turn uniquely determine the potential $V(x)$. The reconstruction of the potential from a certain set of "scattering data" is the aim of inverse scattering theory. If the time dependence of the Schrödinger operator is given by (9.38), then the data needed to determine the potential have a simple, explicitly known time dependence. Hence we can obtain $V(t,x)$ (i.e., the KdV solution) at any t from the scattering data at time t.

For the following we assume $\lim_{x\to\pm\infty} V(x) = m^2$, $m \geq 0$ (the limit being approached sufficiently fast). We denote by $f^{\pm}(\lambda, x)$ the Jost solutions of (9.117) which satisfy the boundary conditions

$$f^{\pm}(\lambda,x) \overset{x\to\pm\infty}{\longrightarrow} e^{\pm ikx}, \qquad k = \sqrt{\lambda - m^2}. \tag{9.119}$$

If $\lambda < m^2$, then f^+ decays exponentially for $x \to +\infty$ and f^- for $x \to -\infty$. Therefore, λ is an eigenvalue of H_s if and only if the f^+ and f^- are linearly dependent. In this case there is a square integrable eigenfunction which decays exponentially for $x \to +\infty$ and $x \to -\infty$, and which is unique up to normalization. The normalized eigensolution $f \equiv c^{\pm} f^{\pm}$, where

$$c^{\pm} = \|f^{\pm}\|^{-1}, \tag{9.120}$$

behaves asymptotically like

$$f(x) \overset{x\to\pm\infty}{\longrightarrow} c^{\pm} e^{\mp\kappa x}, \qquad \kappa = \sqrt{m^2 - \lambda}. \tag{9.121}$$

We assume that there are N bound states with energies λ_n, $n = 1,\ldots,N$, and denote the corresponding norming constants by $c_n^{\pm}$. It turns out that the knowledge of the "scattering data" $\{R^r(\lambda), \lambda_n, c_n^+\}$, $\lambda > m^2$, $n = 1,\ldots,N$, is sufficient to determine the potential $V(x)$ uniquely. In order to obtain the potentials for some given scattering data, we have to solve the Marchenko integral equation

$$K(x,y) + G(x,y) + \int_0^{\infty} K(x,z)\, G(z,y)\, dz = 0, \tag{9.122}$$

with

$$G(x,y) = \int_{-\infty}^{\infty} R^r(\lambda)\, e^{ik(x+y)}\, dk + \sum_{n=1}^{N} (c_n^+)^2\, e^{-\kappa_n (x+y)}, \tag{9.123}$$

where $\lambda > m^2$, $k = \sqrt{\lambda - m^2}$, and

$$\kappa_n = \sqrt{m^2 - \lambda_n}, \quad 0 < \kappa_N < \kappa_{N-1} < \cdots < \kappa_1. \tag{9.124}$$

Finally, the potential is given by

$$V(x) = m^2 - 2\partial_x K(x,x). \tag{9.125}$$

Now we assume that the potential depends on time, such that it is a solution $V(t,x)$ of the KdV equation. Then the time dependence of the scattering data

is easily calculated. We know already that the eigenvalues λ_n do not depend on time by Theorem 9.3. Furthermore, the time dependence of a bound state f with energy λ is given by

$$f_t = (2V + 4\lambda)f_x - V_x f \tag{9.126}$$

as can be seen easily by repeating the steps leading to (9.47). Asymptotically for $x \to \infty$, (9.126) becomes $f_t = (2m^2 + 4\lambda)f_x$ and if we insert the asymptotic form $f(t,x) \approx c^+(t)\exp(-\kappa x)$ we obtain an equation for $c^+(t)$ which is easily solved. In a similar way one can determine the time dependence of the reflection coefficient. We obtain for the time dependence of $\{R^r(t,\lambda), \lambda_n, c_n^+(t)\}$, if $V(t,x)$ is assumed to obey the KdV equation, the relations

$$R^r(t,\lambda) = R^r(0,\lambda)\, e^{8ik^3 t}, \tag{9.127}$$

$$\lambda_n(t) = \lambda_n(0), \quad \text{hence } \kappa_n(t) = \kappa_n(0), \tag{9.128}$$

$$c_n^+(t) = c_n^+(0)\, e^{(4\kappa_n^3 - 6m^2\kappa_n)t}. \tag{9.129}$$

The procedure above allows us to construct solutions $V(t,x)$ of the KdV equation in a systematic way by simply assuming certain initial values $R^r(0,\lambda)$, κ_n, $c_n^+(0)$. The scattering data may be considered a set of "canonical coordinates" for the KdV equation, similar to the action-angle variables of an integrable Hamiltonian system. One can solve the initial value problem for the KdV equation by the following procedure

1. Consider the given function $V(0,x)$ as a potential for the one-dimensional Schrödinger equation and evaluate the scattering data $R^r(0,\lambda)$, κ_n, $c_n^+(0)$.
2. Use the time evolution of the scattering data given by Eqs. (9.127)-(9.129) to determine the scattering data at some later time t.
3. Finally, perform an inverse scattering transformation (Eqs. (9.122)-(9.125)) to determine $V(t,x)$.

Essentially the same procedure works with the mKdV equation and the Dirac equation[2]. In the next section we determine mKdV solutions using a different method, which is based on the results of Sects. 9.3 and 9.4 and takes the KdV solutions as a starting point.

By definition, a "*N-soliton solution*" is a solution of the mKdV equation which corresponds to a *reflectionless* potential of the Dirac equation which has precisely N bound states. All N-soliton solutions can be obtained by an inverse scattering transformation from N arbitrary values λ_n, $c_n^+(0)$, assuming

$$R^r(0,\lambda) = 0, \quad \text{all } \lambda > m^2. \tag{9.130}$$

The resulting potentials $V(t,x)$ are reflectionless for all times by Eq. (9.127).

Assuming (9.130) the Marchenko equation greatly simplifies and can be solved by the separation ansatz

[2] See [347], [187], [188].

$$K(t,x,y) = -\sum_{n=1}^{N} c_n^+(t)\,\chi_n(t,x)\,e^{-\kappa_n y}, \tag{9.131}$$

which allows to determine χ_n. We obtain

$$K(t,x,x) = \partial_x \ln\det\left(\mathbf{1}_N + \mathbf{C}(t,x)\right), \tag{9.132}$$

where $\mathbf{1}_N$ is the $N \times N$ unit matrix, and $\mathbf{C}(t,x) = \big(c_{kn}(t,x)\big)_{k,n=1\ldots N}$ with

$$c_{kn}(t,x) = \frac{c_k^+(t)c_n^+(t)}{\kappa_k + \kappa_n} e^{-(\kappa_k+\kappa_n)x}. \tag{9.133}$$

Hence, using (9.125), the N-soliton solution of the KdV equation reads

$$V(t,x) = m^2 - 2\partial_x^2 \ln\det\big(\mathbf{1}_N + \mathbf{C}(t,x)\big). \tag{9.134}$$

Example (The one soliton solution). For $N = 1$, $c_1^+ \equiv c$, $\kappa_1 \equiv \kappa$, we obtain from (9.134)

$$V(t,x) = m^2 - \frac{2\kappa^2}{\cosh^2\big((4\kappa^3 - 6m^2\kappa)t - \kappa x + \frac{1}{2}\ln\frac{c^2}{2\kappa}\big)}. \tag{9.135}$$

9.5.2 mKdV Solitons in the Critical Case

Next we are going to determine the soliton solutions of the mKdV equation, which correspond to the KdV solitons (9.134) by Theorem 9.4. We construct the mKdV solitons from the given numbers m^2, κ_n, $c_n^+(0)$, where $n = 1,\ldots,N$, $m^2 \geq \kappa_1^2$, $\kappa_1 > \kappa_2 > \cdots > \kappa_N$. According to Theorem 9.4, we have to distinguish between two cases. In this section we treat the critical case, which occurs if $H_s = -\partial_x^2 + V(0,x)$ has a zero eigenvalue $\lambda_1 = m^2 - \kappa_1^2 = 0$. Hence we assume $\kappa_1 = m$.

We denote the zero energy eigensolution by $f(t,x)$, i.e.,

$$H_s(t)\,f(t,x) = -f_{xx}(t,x) + V(t,x)\,f(t,x) = 0. \tag{9.136}$$

The potential $V(t,x)$ is connected to $\{\kappa_n, c_n(t)\}$ by Eq. (9.134). We write

$$H_s(t) = -\partial_x^2 + V(t,x) = D^*(t)D(t), \qquad D(t) = \partial_x + \phi(t,x), \tag{9.137}$$

where according to Theorem 9.4 ϕ is given by

$$\phi(t,x) = -f_x(t,x)/f(t,x). \tag{9.138}$$

In order to calculate ϕ we need not actually solve Eq. (9.136). Instead we use the relation

$$\phi = (\lim_{x\to\infty}\phi) - \int_x^\infty \phi_x\,dx = (\lim_{x\to\infty}\phi) - \frac{1}{2}\int_x^\infty (V_- - V_+)\,dx, \tag{9.139}$$

where $V_+ = V = \phi^2 - \phi_x$, and $V_- = \phi^2 + \phi_x$. Now it is our main task to determine the supersymmetric partner potential $V_-(t,x)$. It will turn out, that V_- corresponds to a $N-1$ soliton solution of the KdV equation.

From (9.121) and (9.138) we easily find

$$\lim_{x\to\pm\infty} \phi(t,x) = \pm\kappa_1 = \pm m. \tag{9.140}$$

Using Eq. (9.90), we find that V_- is reflectionless, because its supersymmetric partner V_+ is reflectionless. We conclude, that $V_-(t,x)$ is a soliton solution of the KdV equation. It can be expressed by a formula like (9.134), if we succeed to determine the bound state energies belonging to V_- and the norming constants of the corresponding eigenfunctions.

Eq. (9.140) implies that the solution of $D^*(t)\psi = -\partial_x\psi + \phi(t,x)\psi = 0$, which is proportional to $\exp\left(\int^x \phi(t,y)\,dy\right)$ behaves asymptotically, as $x \to \pm\infty$, like const. $\exp(\pm\kappa_1 x)$ and hence is not square integrable. This implies that $D(t)D^*(t)$ has no zero eigenvalue. But since DD^* and D^*D are unitarily equivalent on $(\mathrm{Ker}\, D)^\perp$, we find that the operator $DD^* = -\partial_x^2 + V_-$ has exactly $N-1$ bound states. If f_n^+ is the eigenstate of D^*D with $f_n^+(t,x) \to \exp(-\kappa_n x)$, as $x \to +\infty$, then

$$g_n^+ \equiv \frac{1}{m-\kappa_n} Df_n^+ \overset{x\to+\infty}{\longrightarrow} \frac{1}{m-\kappa_n}(\partial_x + m)e^{-\kappa_n x} = e^{-\kappa_n x} \tag{9.141}$$

and g_n^+ is a solution of

$$D(t)D^*(t)g = \lambda_n g, \qquad \lambda_n = m^2 - \kappa_n^2. \tag{9.142}$$

The norming constants $d_n^+(0)$ of the solutions g_n^+ can be obtained by a very straightforward calculation:

$$(d_n^+)^2 = \|g_n\|^{-2} = (m-\kappa_n)^2\|Df_n^+\|^{-2} = (m-\kappa_n)^2(f_n^+, D^*Df_n^+)^{-2}$$

$$(m-\kappa_n)^2\lambda_n^{-2}(c_n^+)^2 = \frac{m-\kappa_n}{m+\kappa_n}(c_n^+)^2. \tag{9.143}$$

We have shown that $V_-(t,x)$ is a $N-1$ soliton solution of the KdV equation, which is determined by inverse scattering theory from the $N-1$ eigenvalues λ_n and the corresponding constants

$$d_n^+(0) = \left(\frac{m-\kappa_n}{m+\kappa_n}\right)^{1/2} c_n^+(0), \qquad n = 2,\ldots,N. \tag{9.144}$$

Define

$$d_n^+(t) \equiv d_n^+(0)\, e^{(4\kappa_n^3 - 6m^2)t}. \tag{9.145}$$

$$d_{kn}(t,x) \equiv \frac{d_k^+(t)d_n^+(t)}{\kappa_k+\kappa_n} e^{-(\kappa_k+\kappa_n)x}, \tag{9.146}$$

$$\mathbf{D}(t,x) = \big(d_{kn}(t,x)\big)_{k,n=2,\ldots,N}. \tag{9.147}$$

Then, as in Sect. 9.3.1, the $N-1$ soliton solution $V_-(t,x)$ is given by

$$V_-(t,x) = m^2 - 2\partial_x^2 \ln\det\big(\mathbf{1}_{N-1} + \mathbf{D}(t,x)\big). \tag{9.148}$$

If we insert (9.148) and (9.134) into (9.139) we obtain the mKdV solution $\phi(t,x)$, which according to Theorem 9.4 is uniquely determined.

$$\phi(t,x) = m + \partial_x \ln\Big\{\frac{\det\big(\mathbf{1}_N + \mathbf{C}(t,x)\big)}{\det\big(\mathbf{1}_{N-1} + \mathbf{D}(t,x)\big)}\Big\}. \tag{9.149}$$

From Eq. (9.91) it is clear that $\phi(t,x)$ is a reflectionless potential for the Dirac equation, hence ϕ is a soliton solution of the mKdV equation. If we start from a critical Schrödinger operator D^*D with N bound states, then the corresponding Dirac operator has $2N-1$ bound states. Hence we call $\phi(t,x)$ a $2N-1$ soliton solution of the mKdV equation.

Example (One soliton mKdV solution). We start with the KdV soliton $V = V_+$ given by Eq. (9.135) and assume that we are in the critical case, i.e., $m = \kappa_1 = \kappa$. With $(c_1^+)^2 = 2\kappa$ we obtain $V_- = \phi^2 + \phi_x = \kappa^2$, and

$$\phi(t,x) = -\kappa\tanh(\kappa x + 2\kappa^3 t). \tag{9.150}$$

9.5.3 mKdV Solitons in the Subcritical Case

Again we start from an N-soliton solution $V(t,x)$ of the KdV equation, given by the numbers m^2, κ_n, $c_n^+(0)$, where $n = 1,\dots,N$. But now we assume that the lowest eigenvalue of the operator $H_s = -\partial_x^2 + V(0,x)$ is strictly positive, $\lambda_1 > 0$. Hence there are two linearly independent not square integrable solutions of $H_s\psi = 0$, which are given by the Jost solutions $f^\pm(im,x)$. These solutions are characterized by the boundary conditions $f^\pm(im,x) \to e^{\mp mx}$, as $x \to \pm\infty$. Since they are not square integrable, they must diverge, as $x \to \mp\infty$, respectively. Hence we find, with some suitable constants $c^\pm$,

$$f^\pm(im,x) \overset{x\to\mp\infty}{\longrightarrow} c^\pm e^{\mp\kappa x}. \tag{9.151}$$

If we now define the functions $\psi_\pm(t,x)$ to be solutions of the differential equation (9.47) with initial condition $\psi_\pm(0,x) = f^\pm(im,x)$, we find the asymptotic behavior

$$\psi_\pm(t,x) \overset{x\to\pm\infty}{\longrightarrow} e^{\mp m(x+2m^2t)}, \quad \psi_\pm(t,x) \overset{x\to\mp\infty}{\longrightarrow} c^\pm e^{\mp m(x+2m^2t)}, \tag{9.152}$$

from which we conclude the asymptotic behavior of the functions ϕ_σ, which are defined according to (9.50):

$$\phi_\sigma^\pm = \lim_{x\to\pm\infty}\phi_\sigma(t,x) = \begin{cases} -\sigma m & \text{for } \sigma = \pm 1\,, \\ \pm m & \text{for } \sigma \in (-1,1)\,. \end{cases} \tag{9.153}$$

With the help of ϕ_σ we can define a potential $V_\sigma = \phi_\sigma^2 + (\phi_\sigma)_x$. The Dirac operator Q with the scalar potential ϕ_σ is related to the two Schrödinger operators with the potentials $V_1 = V$ and $V_2 = V_\sigma$ via supersymmetry. A little

consideration of the asymptotic behavior of solutions of the zero energy Dirac equation shows that it has no square integrable eigensolution if ϕ_σ^+ and ϕ_σ^- have the same sign. On the other hand $Q\Psi = 0$ always has a square integrable solution if $\phi_\sigma^+ = -\phi_\sigma^-$. This is obviously the case for $\sigma \in (-1,1)$. From $\operatorname{Ker} Q = \operatorname{Ker} H_s \oplus \operatorname{Ker} H_s^\sigma$ we conclude that in this case either H_s or H_s^σ has a zero energy eigenstate. Since, by assumption, H_s is strictly positive, we find that the equation $H_s^\sigma \psi = -\psi_{xx} + V_\sigma(0,x)\psi = 0$ has a square integrable solution. Hence, for each $\sigma \in (-1,1)$ we can use the $N+1$ soliton potential V_σ to construct mKdV soliton solutions as in the previous section in the critical case. Since the mKdV equation is symmetric with respect to the exchange of V_1 and V_2 (this exchange corresponds to the replacement $\phi \to -\phi$), we conclude, that (up to a sign) all these solitons have already been obtained in the last section.

From now on, it is sufficient to consider the cases $\sigma = \pm 1$. In this case $\phi^+ = \phi^-$ and hence H_s^σ has no zero energy eigenstate. The eigenvalues of H_s^σ are given by $\lambda_n = m^2 - \kappa_n^2$, $n = 1, \dots, N$, and hence $V_\sigma(t,x)$ is a N-soliton solution of the KdV equation. (It is reflectionless by Eq. (9.90)). As in the previous section we find

$$V_\sigma(t,x) = m^2 - 2\partial_x^2 \ln \det\big(\mathbf{1}_N + \mathbf{D}(t,x)\big), \tag{9.154}$$

$$\mathbf{D}(t,x) = \big(d_{kn}(t,x)\big)_{k,n=1,\dots,N}, \tag{9.155}$$

$$d_{kn}(t,x) = \Big(\frac{\sigma m - \kappa_k}{\sigma m + \kappa_k} \cdot \frac{\sigma m - \kappa_n}{\sigma m + \kappa_n}\Big)^{1/2} c_{kn}(t,x). \tag{9.156}$$

The functions $c_{kn}(t,x)$ are obtained by (9.129) and (9.133) from the given norming constants $c_n^+(0)$. The mKdV solutions are now given, as in the previous section, by Eq. (9.139),

$$\phi(t,x) = \sigma m + \partial_x \ln\left\{\frac{\det\big(\mathbf{1}_N + \mathbf{C}(t,x)\big)}{\det\big(\mathbf{1}_N + \mathbf{D}(t,x)\big)}\right\}. \tag{9.157}$$

Example (Two soliton mKdV solution). Again we start with the KdV soliton $V = V_+$ given by Eq. (9.135) and $(c_1^+)^2 = c^2 = 2\kappa$, now assuming the subcritical case, i.e., $m > \kappa$. We obtain with $\sigma = \pm 1$

$$V(t,x) \equiv V_+(t,x) = m^2 - \frac{2\kappa^2}{\cosh^2\big((4\kappa^3 - 6m^2\kappa)t - \kappa x\big)}, \tag{9.158}$$

$$V_\sigma(t,x) = m^2 - \frac{2\kappa^2}{\cosh^2\big[(4\kappa^3 - 6m^2\kappa)t - \kappa x + \frac{1}{2}\ln b\big]}, \tag{9.159}$$

$$\begin{aligned}\phi_\sigma(t,x) &= \sigma m + \kappa \tanh\big[(4\kappa^3 - 6m^2\kappa)t - \kappa x\big] \\ &\quad - \kappa \tanh\big[(4\kappa^3 - 6m^2\kappa)t - \kappa x + \tfrac{1}{2}\ln b\big],\end{aligned} \tag{9.160}$$

where $b = (\sigma m - \kappa)/(\sigma m + \kappa)$.

10 Quantum Electrodynamics in External Fields

This chapter is a short introduction to the theory of the "second quantized" electron–positron field interacting with an external classical electromagnetic field. Our discussion neglects the existence of photons, but provides us with a simple model of quantum field theory without divergences or ill defined expressions.

First we need a Hilbert space suitable for the description of a system consisting of an arbitrary number of particles. The appropriate framework is given by the fermionic Fock space. Its construction is based on the one-particle Hilbert space, which is split into an electron subspace and a positron subspace. The Fock space is obtained as a direct sum of tensor products of the one-particle space. It contains vectors corresponding to states with n electrons and m positrons. There is even a vacuum state Ω describing the possibility that there is no particle at all. The basic quantities of the theory are the field operators (the electron–positron field) which can be understood in terms of (anti-) particle creation and annihilation operators, see Sect. 10.1.

The one-particle positron subspace is obtained via a charge conjugation from the negative energy subspace of the Dirac operator. The many-particle theory can be formulated in such a way that the generator of the time evolution in the Fock space has a positive spectrum. Hence the Fock space formalism solves the problem with negative energies occurring in the one-particle theory.

For the external field problem a nonperturbative treatment is possible, because the whole theory is essentially determined by the corresponding one-particle problem for the Dirac equation. All results of the second quantized theory are obtained from the corresponding results for the Dirac equation with the help of some Fock space machinery. In the case of weak and time independent external fields quantum field theory essentially reproduces the one-particle theory. Everything depends on how the Dirac scattering operator (or even the whole time evolution generated by the Dirac equation) can be implemented in the Fock space of free particles. This restricts the class of external fields admitted for our consideration. The crucial condition for the Fock space implementation of unitary transformations is that the parts which mix the electron and positron subspaces are Hilbert-Schmidt operators (Sect. 10.2).

The number of particles need not be constant during the time evolution of a quantum system in Fock space. Hence the theory is designed to describe particle creation and annihilation. This phenomenon may happen whenever transitions from positive to negative energies (or vice versa) occur in the one-particle theory. It can be shown, however, that static fields vanishing at infinity are unable to create particle/antiparticle pairs. In this case, the quantized theory is essentially equivalent to the one-particle theory.

In the case of time dependent fields, the implementation of the time evolution in Fock space has no covariant meaning, and hence a consistent particle interpretation can only be maintained asymptotically. The scattering operator is unitarily implementable for a sufficiently large class of physically interesting external fields. The possibility of pair creation is described by the vacuum expectation value of the scattering operator, see Sect. 10.4.

Finally, we briefly discuss the difficulties with defining the "spontaneous pair creation", i.e., a sudden change of the pair creation probability which one expects if the coupling constant is increased beyond a critical threshold.

10.1 Quantization of the Dirac Field

10.1.1 The Fock Space

We give a mathematically rigorous version of what is commonly known as the procedure of second quantization. We first need a Hilbert space which is capable of describing states with an arbitrary number of particles and antiparticles. It is convenient to choose the antisymmetrized Fock space $\mathfrak{F}$ which we are going to describe in this section.

1. The one-particle subspaces. Let $\mathfrak{H}$ be the Hilbert space of the Dirac equation. We assume that $\mathfrak{H}$ can be split into two orthogonal spectral subspaces of the Dirac operator H,

$$\mathfrak{H} = \mathfrak{H}_+ \oplus \mathfrak{H}_-, \tag{10.1}$$

such that $\mathfrak{H}_+$ can be interpreted as the Hilbert space for a particle. In particular we assume that the Dirac operator H is semibounded from below if restricted to $\mathfrak{H}_+$. For example, in case of free particles, we choose $\mathfrak{H}_+$ to be the Hilbert space $\mathfrak{H}_{\text{pos}}$ of positive energy solutions of the free Dirac equation, cf. Sect. 1.4.2. Similarly, let H be semibounded from above on $\mathfrak{H}_-$.

In view of our considerations on the interpretation of negative energies in Sect. 1.4.6, we assume the existence of an antiunitary map C (the "*charge conjugation*") such that the transformed Dirac operator $-CHC^{-1}$ restricted to the Hilbert space $C\mathfrak{H}_-$ can be interpreted as the Dirac operator for an antiparticle. Then we denote

$$\mathfrak{F}_+^{(1)} \equiv \mathfrak{H}_+, \qquad \mathfrak{F}_-^{(1)} \equiv C\mathfrak{H}_-. \tag{10.2}$$

In order to be concrete, the one-particle Hilbert spaces $\mathfrak{F}_\pm^{(1)}$ are both considered subspaces of $\mathfrak{H} = L^2(\mathbb{R}^3)^4$ with the ordinary scalar product, i.e., $\mathfrak{F}_\pm^{(1)}$ consist of four component square integrable functions f. We shall write $f_s(\boldsymbol{x}) \equiv f(\boldsymbol{x}, s)$, $s = 1, .., 4$, where $\boldsymbol{x}$ is the space variable of the particle, s its spinor index. Unlike our earlier notation the spinor index s is written as an ordinary variable in order to avoid the clustering of indices in the n particle case. Furthermore we shall use the notation

$$x = (\boldsymbol{x}, s), \quad \boldsymbol{x} \in \mathbb{R}^3, \quad s \in \{1, 2, 3, 4\}. \tag{10.3}$$

Example: Let $H = H(e)$, the Dirac operator in a sufficiently weak external electromagnetic field. In this case C is the charge conjugation as defined in Sect. 1.4.6, and $CH(e)C^{-1} = -H(-e)$. The Hilbert space $\mathfrak{F}_+^{(1)}$ is the subspace of positive energies $\mathfrak{H}_{\text{pos}}$, and $\mathfrak{F}_-^{(1)} = C\mathfrak{H}_{\text{neg}}$. The decomposition (10.1) clearly depends on the external field and so does the whole construction below. A difficulty arises if the field is so strong that electron bound states dive below the $E = 0$ threshold, so that particles and antiparticles cannot be simply separated

by the sign of energy. In this case the splitting (10.1) has to be done in a more subtle way.

2. The n-particle subspaces. The Hilbert space $\mathfrak{F}_+^{(n)}$ of states describing n particles is defined as the *antisymmetrized* tensor product[1] of n copies of $\mathfrak{F}_+^{(1)}$. It can be described by forming antisymmetrized products of the one-particle basis vectors: Let $\{f_j \mid j = 1, 2, \ldots\}$ be a basis in $\mathfrak{H}_+$. Choose n basis vectors corresponding to the indices $j_1, \ldots, j_n$ and consider the function

$$\frac{1}{\sqrt{n!}} \sum_{\text{Permutations } \sigma} \operatorname{sgn}(\sigma)\, f_{\sigma(j_1)}(x_1)\, f_{\sigma(j_2)}(x_2) \cdots f_{\sigma(j_n)}(x_n), \tag{10.4}$$

which depends on n variables

$$x_i = (\boldsymbol{x}_i, s_i), \quad \boldsymbol{x}_i \in \mathbb{R}^3, \quad s_i \in \{1, 2, 3, 4\}, \quad i = 1, \ldots, n. \tag{10.5}$$

Next consider functions $\psi^{(n)}$ which are finite linear combinations of the vectors (10.4). The $\psi^{(n)}$ are antisymmetric in the arguments x_i, i.e., for arbitrary $i \neq k$ we find

$$\psi^{(n)}(x_1, .., x_j, .., x_k, .., x_n) = -\psi^{(n)}(x_1, .., x_k, .., x_j, .., x_n). \tag{10.6}$$

Finally, define a scalar product by

$$(\psi^{(n)}, \phi^{(n)})_n =$$

$$\sum_{s_1, \ldots, s_n = 1}^{n} \int_{\mathbb{R}^{3n}} d^3x_1 \cdots d^3x_n\, \overline{\psi^{(n)}(x_1, .., x_n)}\, \phi^{(n)}(x_1, .., x_n). \tag{10.7}$$

Definition 10.1. *The n-particle space $\mathfrak{F}_+^{(n)}$ is the closure of the set of finite linear combinations of the vectors (10.4) with respect to the norm associated with the scalar product (10.7).*

If $\{f_j\}$ is an orthonormal basis in $\mathfrak{H}_+$, then the vectors (10.4) form an orthonormal basis of $\mathfrak{F}_+^{(n)}$.

Similarly, we define the Hilbert space $\mathfrak{F}_-^{(m)}$ of m antiparticles as the antisymmetric m-fold tensor product of $\mathfrak{F}_-^{(1)}$. The wavefunction describing m antiparticles is antisymmetric in the variables $y_k = (\boldsymbol{y}_k, t_k)$, $k = 1, \ldots, m$, where $\boldsymbol{y}_k$ is the space variable of the k-th antiparticle, t_k its spinor index.

3. Arbitrary numbers of particles. In order to be able to treat various numbers of particles and antiparticles simultaneously, we define the Dirac field Fock space as the direct sum

[1] [RS 72], Sect. II.4.

$$\mathfrak{F} = \bigoplus_{n,m=0}^{\infty} \mathfrak{F}^{(n,m)}, \qquad \mathfrak{F}^{(n,m)} = \mathfrak{F}_+^{(n)} \otimes \mathfrak{F}_-^{(m)}, \tag{10.8}$$

where $\mathfrak{F}_\pm^{(0)} = \mathbb{C}$. The Fock space consists of sequences ψ of functions $\psi^{(n,m)}$,

$$\psi = (\psi^{(n,m)})_{n,m=0,1,2,\ldots}, \tag{10.9}$$

where $\psi^{(n,m)} \in \mathfrak{F}^{(n,m)}$ depends on $(x_1, \ldots, x_n; y_1, \ldots, y_m)$ and is antisymmetric in particle and antiparticle variables separately. The scalar product of the vectors $\psi = (\psi^{(n,m)})$ and $\phi = (\phi^{(n,m)})$ is given by

$$(\psi, \phi)_{\mathfrak{F}} = \sum_{n,m=0}^{\infty} (\psi^{(n,m)}, \phi^{(n,m)})_{nm}, \tag{10.10}$$

$$(\psi^{(n,m)}, \phi^{(n,m)})_{nm} =$$

$$\sum_{s_1,\ldots,t_m=1}^{4} \int_{\mathbb{R}^{3(n+m)}} d^3x_1 \cdots d^3y_m \, \overline{\psi^{(n,m)}(x_1, .., y_m)} \, \phi^{(n,m)}(x_1, .., y_m). \tag{10.11}$$

The usual interpretation is the following: A normalized state $\psi \in \mathfrak{F}$ describes a physical system with a variable number of particles, the probability that there are just n particles and m antiparticles at a given time is

$$\|\psi^{(n,m)}\|_{nm}^2 \equiv (\psi^{(n,m)}, \psi^{(n,m)})_{nm}. \tag{10.12}$$

A state of the form

$$\Omega = (e^{i\lambda}, 0, 0, \ldots) \in \mathfrak{F}, \quad \lambda \in \mathbb{R}, \tag{10.13}$$

describes the possibility that there are no particles at all and is called "*vacuum*".

10.1.2 Creation and Annihilation Operators

1. Particles. For any $f \in \mathfrak{H}_+$, we define in $\mathfrak{F}$ the "*particle annihilation operator*" $a(f)$, which maps each subspace $\mathfrak{F}^{(n+1,m)}$ into $\mathfrak{F}^{(n,m)}$,

$$\big(a(f)\psi\big)^{(n,m)}(x_1, .., x_n; y_1, .., y_m) =$$

$$= \sqrt{n+1} \sum_{s=1}^{4} \int_{\mathbb{R}^3} d^3x \, \overline{f(x)} \, \psi^{(n+1,m)}(x, x_1, .., x_n; y_1, .., y_m), \tag{10.14}$$

where $x = (\boldsymbol{x}, s)$ as in Eq. (10.3). Next we define the "*particle creation operator*" mapping $\mathfrak{F}^{(n-1,m)}$ into $\mathfrak{F}^{(n,m)}$,

$$\big(a^*(f)\psi\big)^{(n,m)}(x_1, .., x_n; y_1, .., y_m) =$$

$$= \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (-1)^{j+1} \, f(x_j) \, \psi^{(n-1,m)}(x_1, .., \hat{x}_j, .., x_n; y_1, .., y_m). \tag{10.15}$$

(The hat indicates that the corresponding argument has to be omitted). A little calculation shows the "*canonical anticommutation relations*" (CAR)

$$\{a(f_1), a(f_2)\} = \{a^*(f_1), a^*(f_2)\} = 0,$$

$$\{a(f_1), a^*(f_2)\} = (f_1, f_2)\mathbf{1}, \tag{10.16}$$

for $f_1, f_2 \in \mathfrak{H}_+$. Here (f_1, f_2) denotes the ordinary scalar product in $L^2(\mathbb{R}^3)^4$. Moreover, we find that $a^*(f)$ is the adjoint of $a(f)$,

$$a^*(f) = \big(a(f)\big)^*, \tag{10.17}$$

and that $a(f)$ and $a^*(f)$ are bounded operators on $\mathfrak{F}$,

$$\|a^*(f)\psi\|^2 + \|a(f)\psi\|^2 = \big(\psi, \{a(f), a^*(f)\}\psi\big)_{\mathfrak{F}} = \|f\|^2 \, \|\psi\|^2. \tag{10.18}$$

For the vacuum state Ω we obtain

$$a(f)\Omega = 0 \in \mathfrak{F}, \qquad \big(a^*(f)\Omega\big)^{(n,m)} = \begin{cases} f & \text{for } (n,m) = (1,0), \\ 0 & \text{otherwise.} \end{cases} \tag{10.19}$$

For any $\psi \in \mathfrak{F}$

$$a(f)^2 \, \psi = \tfrac{1}{2} \, \{a(f), a(f)\} \, \psi = 0, \tag{10.20}$$

which shows that ψ contains at most one particle in the state f. This is the famous "*Pauli exclusion principle*".

2. Antiparticles. For any $g \in \mathfrak{H}_-$ we define the "*antiparticle annihilation operator*"

$$\big(b(g)\psi\big)^{(n,m)}(x_1, .., x_n; y_1, .., y_m) =$$

$$(-1)^n \sqrt{m+1} \sum_{t=1}^{4} \int_{\mathbb{R}^3} d^3y \, \overline{[Cg](y)} \, \psi^{(n,m+1)}(x_1, .., x_n; y, y_1, .., y_m), \tag{10.21}$$

and the "*antiparticle creation operator*"

$$\big(b^*(g)\psi\big)^{(n,m)}(x_1, .., x_n; y_1, .., y_m) =$$

$$\frac{(-1)^n}{\sqrt{m}} \sum_{k=1}^{m} (-1)^{k+1} \, [Cg](y_k) \, \psi^{(n,m-1)}(x_1, .., x_n; y_1, .., \hat{y}_k, .., y_m), \tag{10.22}$$

where C is the charge conjugation. Note that b depends linearly on g, while the mapping $g \to b^*(g)$ is antilinear. We find that for g, g_1, $g_2 \in \mathfrak{H}_-$ the operators $b(g)$ and $b^*(g)$ are bounded and satisfy the CAR

$$\{b(g_1), b(g_2)\} = \{b^*(g_1), b^*(g_2)\} = 0,$$

$$\{b(g_1), b^*(g_2)\} = (Cg_1, Cg_2)\mathbf{1} = (g_2, g_1)\mathbf{1} = \overline{(g_1, g_2)}\mathbf{1}, \tag{10.23}$$

(note that C is antiunitary!) and in addition

$$\{a^{\times}(f), b^{\times}(g)\} = 0, \tag{10.24}$$

(where "$^{\times}$" means either "*" or "no *"). As before,

$$b^*(g) = \big(b(g)\big)^*, \tag{10.25}$$

$$b(g)\Omega = 0, \qquad \big(b^*(g)\Omega\big)^{(n,m)} = \begin{cases} Cg & \text{for } (n,m) = (0,1), \\ 0 & \text{otherwise.} \end{cases} \tag{10.26}$$

The equations $a(f)\psi = 0$, $b(g)\psi = 0$ for all $f \in \mathfrak{H}_+$, $g \in \mathfrak{H}_-$, imply $\psi = \alpha\Omega$, with $\alpha \in \mathbb{C}$, i.e., the vacuum is unique up to a constant.

10.1.3 The Algebra of Field Operators

In $\mathfrak{H} = \mathfrak{H}_+ \oplus \mathfrak{H}_-$ we denote the projections onto the subspaces $\mathfrak{H}_\pm$ by $P_\pm$. For any $f \in \mathfrak{H}$ we define a "*field operator*" $\Psi(f)$ on the Fock space $\mathfrak{F}$ by

$$\Psi(f) = a(P_+ f) + b^*(P_- f). \tag{10.27}$$

Obviously, $\Psi(f)$ is bounded. It annihilates a particle and creates an antiparticle. The mapping $f \to \Psi(f)$ is antilinear. The adjoint operator $\Psi^*(f)$ depends linearly on f and is given by

$$\Psi^*(f) = a^*(P_+ f) + b(P_- f). \tag{10.28}$$

In terms of the field operators the CAR (10.16), (10.23), (10.24) become

$$\{\Psi(f_1), \Psi(f_2)\} = \{\Psi^*(f_1), \Psi^*(f_2)\} = 0,$$

$$\{\Psi(f_1), \Psi^*(f_2)\} = (f_1, f_2)\,\mathbf{1}, \quad \text{all } f_1,\, f_2 \in \mathfrak{H}. \tag{10.29}$$

We easily find

$$\|\Psi(f)\,\psi\|^2 + \|\Psi^*(f)\,\psi\|^2 = (\psi, \{\Psi(f), \Psi^*(f)\}\psi) = \|f\|^2\|\psi\|^2, \tag{10.30}$$

and hence

$$\|\Psi(f)\| = \|\Psi^*(f)\| = \|f\|. \tag{10.31}$$

The mapping $f \to \Psi(f)$ is often referred to as the "second quantized Dirac field". In a "naive" field theory, the operators $\Psi(f)$ satisfying the CAR would have been interpreted as annihilation operators. Instead Eq. (10.27) reflects Dirac's original idea formulated in his "hole theory". In this intuitive picture the vacuum Ω describes the "Dirac sea". It consists of infinitely many electrons with negative energies which completely fill up the negative energy continuum. Hence by the Pauli principle, only electrons with positive energies can be created. The "annihilation" $\Psi(P_- f)$ of one of the electrons with negative energy amounts to the creation of a "hole" in the Dirac sea. But the holes can be interpreted as particles with the same mass, but the opposite charge, i.e., as antiparticles.

10.1.4 Irreducibility of the Fock Representation

One often takes the abstract "C^* algebra" generated by the field operators Ψ as a starting point. A *representation* of the CAR is given by some Hilbert space $\mathfrak{G}$ and an antilinear mapping Φ from $\mathfrak{H}$ into the bounded operators in $\mathfrak{G}$ satisfying (10.29). Given Φ we define annihilation operators by writing — in analogy to Eqs. (10.27) and (10.28) — $c(f) \equiv \Phi(f)$ for $f \in \mathfrak{H}_+$ and $d(g) = \Phi^*(g)$ for $g \in \mathfrak{H}_-$. If there exists a vector $\Omega \in \mathfrak{G}$ such that $c(f)\Omega = d(g)\Omega = 0$ for all $f \in \mathfrak{H}_+$ and $g \in \mathfrak{H}_-$, then Ω is called the vacuum of the representation. The field operators in the Fock space $\mathfrak{G} = \mathfrak{F}$ given above may be regarded as a special representation with a vacuum vector. This representation is distinguished by the property of being irreducible, i.e., there is no proper subspace of $\mathfrak{F}$, which is left invariant by all field operators.

Let $\{f_j \mid j = 1, 2, \ldots\}$ (resp. $\{g_k \mid k = 1, 2, \ldots\}$) be an orthonormal basis of $\mathfrak{H}_+$ (resp. $\mathfrak{H}_-$). In the expression

$$a^*(f_{j_1})\, a^*(f_{j_2}) \cdots a^*(f_{j_n})\, b^*(g_{k_1})\, b^*(g_{k_2}) \cdots b^*(g_{k_m})\, \Omega \in \mathfrak{F} \tag{10.32}$$

the indices can be assumed ordered, $j_1 < \ldots < j_n$, $k_1 < \ldots < k_m$ (by the CAR, any transposition of creation operators only changes the sign). A Fock space vector of this type can be identified in a natural way with a state describing n particles and m antiparticles for every n, m: It is easily verified that (10.32) can be written as the product of (10.4) with an analogous expression involving the antiparticle states $Cg_{k_1}, \ldots, Cg_{k_m}$. But these products form a basis of the Hilbert space $\mathfrak{F}_+^{(n)} \otimes \mathfrak{F}_-^{(m)}$, because the f's and g's form a basis of $\mathfrak{H}$. Hence the states obtained in this way for $n, m = 0, 1, 2, \ldots$ form an orthonormal basis of the Fock space $\mathfrak{F}$. The set

$$\mathfrak{D} = \{\psi \in \mathfrak{F} \mid \psi \text{ is a finite linear combination of basis vectors of the form (10.32)}\} \tag{10.33}$$

is a useful dense domain which will be needed below for the definition of various operators in $\mathfrak{F}$.

Consider any subspace $\mathfrak{F}_1$ of $\mathfrak{F}$ which is invariant with respect to all field operators. The corresponding projection operator P_1 commutes with all creation and annihilation operators. Hence $a(f)P_1\Omega = P_1 a(f)\Omega = 0$, for all $f \in \mathfrak{H}_+$, and $b(g)P_1\Omega = 0$, for all $g \in \mathfrak{H}_-$. This implies $P_1\Omega = \alpha\Omega$, because the vacuum is unique up to a constant. Hence $P_1\psi = \alpha\psi$ for all states ψ of the form (10.32), i.e., $P_1 = \alpha \mathbf{1}$ on a dense set. But since P_1 is closed we find $P_1 = \alpha \mathbf{1}$ on $\mathfrak{F}$. (In fact, we have shown that any closed operator commuting with all field operators is a multiple of 1). Finally, since P_1 is a projection, we find $\alpha^2 = \alpha$ which implies $\mathfrak{F}_1 = \{0\}$ or $\mathfrak{F}_1 = \mathfrak{F}$. Hence we have proven

Theorem 10.2. There is no proper subspace of the Fock space $\mathfrak{F}$ which is invariant with respect to all field operators $\Psi(f)$ and $\Psi^*(f)$, $f \in \mathfrak{H}$, i.e., the Fock representation is irreducible.

The next theorem states that the irreducible representations of the CAR with a vacuum vector are equivalent to the Fock representation.

Theorem 10.3. Let $\Phi(f)$ and $\Phi^*(f)$ be another representation of the CAR which is irreducible on a Hilbert space $\mathfrak{G}$. Define

$$c(f) = \Phi(f), \quad d(g) = \Phi^*(g), \quad \text{for all } f \in \mathfrak{H}_+ \text{ and all } g \in \mathfrak{H}_-. \tag{10.34}$$

The representation Φ has a vacuum vector $\Omega' \in \mathfrak{G}$ satisfying

$$c(f)\Omega' = 0 = d(g)\Omega', \quad \text{for all } f \in \mathfrak{H}_+ \text{ and all } g \in \mathfrak{H}_-, \tag{10.35}$$

if and only if there is a unitary transformation $\mathbb{U} : \mathfrak{F} \to \mathfrak{G}$ such that

$$\Phi(f) = \mathbb{U}\Psi(f)\mathbb{U}^*, \quad \text{for all } f \in \mathfrak{H}, \tag{10.36}$$

where $\Psi(f)$ are the field operators defined in (10.27).

Proof. The unitary operator $\mathbb{U}$ is easily obtained by extension of the mapping which sends the basis vector (10.32) of $\mathfrak{F}$ to

$$c^*(f_{j_1})\, c^*(f_{j_2}) \cdots c^*(f_{j_n})\, d^*(g_{k_1})\, d^*(g_{k_2}) \cdots d^*(g_{k_m})\, \Omega' \in \mathfrak{G}. \tag{10.37}$$

Conversely, given $\mathbb{U}$, we can obtain a new vacuum vector as $\Omega' = \mathbb{U}\Omega$. □

10.2 Operators in Fock Space

10.2.1 Implementation of Unitary Operators

For any unitary operator U which leaves the one-particle subspaces $\mathfrak{H}_\pm$ invariant we can define a Fock space operator as follows.

Consider the mapping

$$\Psi(f) \to \Phi(f) = \Psi(Uf), \quad \text{all } f \in \mathfrak{H}. \tag{10.38}$$

Obviously, the operators $\Phi(f)$ and $\Phi^*(f)$ act irreducibly on the Fock space and satisfy the CAR, because $(f_1, f_2) = (Uf_1, Uf_2)$. Using the assumption $U\mathfrak{H}_\pm = \mathfrak{H}_\pm$ we find that any vector of the form

$$\Omega' = e^{i\theta}\Omega, \quad \text{with arbitrary } \theta \in [0, 2\pi), \tag{10.39}$$

satisfies (10.35). Hence Ω' is a vacuum vector for the new field operators Φ. By Theorem 10.3 we conclude that there is a unitary operator $\mathbb{U}$ in the Fock space such that

$$\Psi(Uf) = \mathbb{U}\Psi(f)\mathbb{U}^*. \tag{10.40}$$

Usually, one chooses $\theta = 0$ and hence $\mathbb{U}\Omega = \Omega$.

For the argument above it has been crucial that U leaves the subspaces $\mathfrak{H}_\pm$ invariant. The implementation of unitary operators in the general case will be described in Sect. 10.3 below.

10.2.2 The Time Evolution

In the Hilbert space $\mathfrak{H}$ of the Dirac equation the time evolution is described by the unitary group $\exp(-\mathrm{i}Ht)$, where H is the Dirac operator (for simplicity, we assume that H does not depend on time t, leaving the more general case to a discussion in Sect. 10.4). Obviously, the time evolution leaves the one-particle subspaces invariant, because $\mathfrak{H}_\pm$ are defined as spectral subspaces of H. Hence we can apply the results of the preceding section and find that for each $t \in \mathbb{R}$ there is a unitary operator $\mathbb{U}_t$ in the Fock space such that

$$\Psi(f) \to \Psi_t(f) = \Psi(e^{-\mathrm{i}Ht} f) = \mathbb{U}_t \Psi(f) \mathbb{U}_t^*. \tag{10.41}$$

The choice of $\mathbb{U}_t$ is made unique by the condition

$$\mathbb{U}_t \Omega = \Omega \qquad \text{all } t \in \mathbb{R}. \tag{10.42}$$

It is easily verified that the operators $\mathbb{U}_t$, form a unitary group,

$$\mathbb{U}_0 = \mathbf{1}, \qquad \mathbb{U}_s \mathbb{U}_t = \mathbb{U}_{s+t}, \qquad \text{all } s, t. \tag{10.43}$$

The strong continuity of $e^{-\mathrm{i}Ht}$ implies the norm continuity of $\Psi_t(f)$ by (10.31). For $f \in \mathfrak{D}(H)$ we find, using the antilinearity of Ψ and (10.31),

$$\begin{aligned} \left\| \tfrac{1}{h}\left[\Psi_{t+h}(f) - \Psi_t(f)\right] - \Psi_t(-\mathrm{i}Hf) \right\| &= \left\| \Psi\left(e^{-\mathrm{i}Ht}\left[\tfrac{1}{h}(e^{-\mathrm{i}Hh} - \mathbf{1}) + \mathrm{i}H\right] f\right) \right\| \\ &= \left\| \left[\tfrac{1}{h}(e^{-\mathrm{i}Hh} - \mathbf{1}) + \mathrm{i}H\right] f \right\| \to 0, \quad \text{as } h \to 0. \end{aligned} \tag{10.44}$$

Hence $\Psi_t(f)$ is even differentiable in t with respect to the operator norm,

$$\frac{d}{dt} \Psi_t(f) = \mathrm{i}\, \Psi_t(Hf), \quad \text{all } f \in \mathfrak{D}(H). \tag{10.45}$$

Using (10.27) we find that the operators

$$a_t^*(f) = a^*(e^{-\mathrm{i}Ht} f), \quad b_t^*(g) = b^*(e^{-\mathrm{i}Ht} g), \quad f \in \mathfrak{H}_+,\ g \in \mathfrak{H}_- \tag{10.46}$$

are norm differentiable for f and g in $\mathfrak{D}(H)$,

$$\frac{d}{dt} a_t^*(f) = -\mathrm{i}\, a_t^*(Hf), \qquad \frac{d}{dt} b_t^*(g) = \mathrm{i}\, b_t^*(Hf). \tag{10.47}$$

Now, let ψ be a basis vector of the form (10.32). We choose the bases $\{f_j\}$ and $\{g_k\}$ to be contained in the domain of the Dirac operator H. We conclude

$$\begin{aligned} \mathrm{i}\frac{d}{dt}\Big|_{t=0} \mathbb{U}_t \psi &= \mathrm{i}\frac{d}{dt}\Big|_{t=0} a_t^*(f_{j_1}) \ldots a_t^*(f_{j_n})\, b_t^*(g_{k_1}) \ldots b_t^*(g_{k_m})\, \Omega \\ &= +a^*(Hf_{j_1}) \ldots a^*(f_{j_n})\, b^*(g_{k_1}) \ldots b^*(g_{k_m})\, \Omega + \ldots \\ &\quad + a^*(f_{j_1}) \ldots a^*(Hf_{j_n})\, b^*(g_{k_1}) \ldots b^*(g_{k_m})\, \Omega - \\ &\quad - a^*(f_{j_1}) \ldots a^*(f_{j_n})\, b^*(Hg_{k_1}) \ldots b^*(g_{k_m})\, \Omega - \ldots \\ &\quad - a^*(f_{j_1}) \ldots a^*(f_{j_n})\, b^*(g_{k_1}) \ldots b^*(Hg_{k_m})\, \Omega. \end{aligned} \tag{10.48}$$

This shows that the operator

$$\mathbb{H} = \mathrm{i}\frac{d}{dt}\bigg|_{t=0} \mathbb{U}_t \quad \text{on} \quad \mathfrak{D}(\mathbb{H}) = \{\phi \in \mathfrak{F} \mid \lim_{t\to 0} \tfrac{1}{t}(\mathbb{U}_t - 1)\,\phi \text{ exists}\} \tag{10.49}$$

is densely defined, because the dense set $\mathfrak{D}$ of finite linear combinations of the basis vectors (10.32) is contained in $\mathfrak{D}(\mathbb{H})$. We conclude that $\mathbb{U}_t$ is strongly differentiable on a dense set, hence $\mathbb{U}_t$ is a strongly continuous unitary group and its infinitesimal generator is $\mathbb{H}$. Using the CAR one can show with a little calculation that

$$\mathbb{H}\psi = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\Big((f_i, Hf_j)a^*(f_i)a(f_j) - (g_j, Hg_i)b^*(g_i)b(g_j) \Big)\,\psi. \tag{10.50}$$

This expression shows that $\mathbb{H}$ is semibounded, because $-H$ is semibounded from below on $\mathfrak{H}_-$. The operator $\mathbb{H}$ implements H into the Fock space. It is sometimes called the "second quantized Dirac operator". We collect our results in the following theorem.

Theorem 10.4. The time evolution $\exp(-\mathrm{i}Ht)$ can be implemented as a unitary group $\mathbb{U}_t = \exp(-\mathrm{i}\mathbb{H}t)$ with a positive self-adjoint generator $\mathbb{H}$ which is given by (10.50).

We see that the energy of a state ψ in the Fock space is always positive. The problem with the unphysical negative energies obviously has disappeared. The negative energy states of the one-particle theory are regarded as states of antiparticles with positive energy. Note, however, that the particles and antiparticles in the system described by $\psi \in \mathfrak{F}$ do not interact with each other. Of course this is only a rough approximation to a more complete theory involving the quantization of the field describing the interaction. Nevertheless, the external field theory is used in a number of situations (e.g., laser physics, heavy ion collisions), where the external field is so strong that it dominates the behavior of the system.

10.2.3 Number and Charge Operators

On the dense domain $\mathfrak{D}$ of finite linear combinations of basis vectors (10.32) we can define the "*number operator*"

$$N = \sum_{j=1}^{\infty}\big(a^*(f_j)\,a(f_j) + b^*(g_j)\,b(g_j)\big), \tag{10.51}$$

and the "*charge operator*"

$$Q = \sum_{j=1}^{\infty}\big(a^*(f_j)\,a(f_j) - b^*(g_j)\,b(g_j)\big). \tag{10.52}$$

Both N and Q are independent of the chosen orthonormal bases. A short calculation shows that vectors ψ of the form (10.32) are eigenvectors of both N and Q with $N\psi = (n+m)\psi$ and $Q\psi = (n-m)\psi$, where n and m are the numbers of particles and antiparticles in ψ. Since these vectors form a complete orthonormal basis we see that N and Q both have a purely discrete spectrum and are unbounded. The eigenspace $\mathfrak{F}_q$ of Q belonging to an eigenvalue $q \in \mathbb{Z}$ is called the charge-q sector.

Obviously, the charge operator Q corresponds to the identity $\mathbf{1}$ in $\mathfrak{H}$ in the same way as $\mathbb{H}$ corresponds to H. Similarly, the number operator N corresponds to the unitary involution $\tau = \operatorname{sgn} H$. The unitary transformations generated by $\mathbf{1}$ in $\mathfrak{H}$ are the global gauge transformations $f \to e^{i\theta} f$, which leave the Dirac equation invariant. In Fock space, they are implemented by $\exp(i\theta Q)$.

10.2.4 One-Particle Operators

The operators H, $\operatorname{sgn} H$, $\mathbf{1}$ considered above leave the subspaces $\mathfrak{H}_\pm$ invariant. Now we consider a bounded operator $A : \mathfrak{H} \to \mathfrak{H}$ which need not have this property. Let us consider first the simplest case where A is a trace-class operator. We define

$$A\Psi^*\Psi = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}(e_i, Ae_j)\,\Psi^*(e_i)\,\Psi(e_j) = \sum_{i=1}^{\infty}\Psi^*(Ae_j)\,\Psi(e_j), \tag{10.53}$$

where $\Psi(e) = a(P_+e) + b^*(P_-e)$ is the second-quantized Dirac field, and the $\{e_j\}_{j=1}^{\infty}$ form an orthonormal base (ONB) of $\mathfrak{H}$. The definition does not depend on the choice of the ONB. Writing the trace-class operator in the form[2]

$$A = \sum_{k=1}^{\infty}\lambda_k\,(g_k, \cdot)\,f_k, \tag{10.54}$$

($\lambda_k \geq 0$ are the singular values of A and where $\{f_k\}$, $\{g_k\}$ are ONBs in $\mathfrak{H}$) and choosing $e_j = f_j$ in (10.53) we find

$$A\Psi^*\Psi = \sum_{k=1}^{\infty}\lambda_k\,\Psi^*(g_k)\,\Psi(f_k). \tag{10.55}$$

Eq. (10.31) implies immediately that the sum converges in the operator norm and

$$\|A\Psi^*\Psi\| \leq \sum_{k=1}^{\infty}\lambda_k \equiv \|A\|_1 \qquad \text{(the trace norm)}. \tag{10.56}$$

Hence for trace-class operators A the expression $A\Psi^*\Psi$ defines a bounded operator in $\mathfrak{F}$. With the help of some little calculations one finds for trace-class operators A, B the relations

[2] [RS 72], Thm VI.17 (normal form of compact operators).

$$A^*\Psi^*\Psi = (A\Psi^*\Psi)^*, \tag{10.57}$$

$$[A\Psi^*\Psi, B\Psi^*\Psi] = C\Psi^*\Psi, \quad \text{where } C = [A, B], \tag{10.58}$$

$$[A\Psi^*\Psi, \Psi^*(f)] = \Psi^*(Af), \qquad [A\Psi^*\Psi, \Psi(f)] = -\Psi(A^*f). \tag{10.59}$$

One can define the exponential $\exp(it\, A\Psi^*\Psi)$ by its norm-convergent power series and finds

$$e^{it\, A\Psi^*\Psi}\Psi(f)\, e^{-it\, A\Psi^*\Psi} = \Psi(e^{-itA}f). \tag{10.60}$$

Next we express $A\Psi^*\Psi$ in terms of creation and annihilation operators. Using Eqs. (10.27), (10.28) we find

$$A\Psi^*\Psi = Aa^*a + Aa^*b^* + Aba + Abb^*, \tag{10.61}$$

where the summands are defined in the obvious way: Choosing orthonormal bases $\{f_j \mid j = 1, 2, \ldots\}$ of $\mathfrak{H}_+$ and $\{g_k \mid k = 1, 2, \ldots\}$ of $\mathfrak{H}_-$ we have

$$Aa^*a \equiv \sum_{i,j} (f_i, A\, f_j)\, a^*(f_i)\, a(f_j) \equiv A_{+}a^*a, \tag{10.62}$$

$$Aa^*b^* \equiv \sum_{j,k} (f_j, A\, g_k)\, a^*(f_j)\, b^*(g_k) \equiv A_{+-}a^*b^*, \tag{10.63}$$

$$Aba \equiv \sum_{k,j} (g_k, A\, f_j)\, b(g_k)\, a(f_j) \equiv A_{-+}ba, \tag{10.64}$$

$$Abb^* \equiv \sum_{k,l} (g_k, A\, g_l)\, b(g_k)\, b^*(g_l) \equiv A_{-}bb^*. \tag{10.65}$$

Here we denote by $A_{+} = P_{+}AP_{+}$, $A_{+-} = P_{+}AP_{-}$, etc., the matrix elements of A with respect to the decomposition (10.1) of the Hilbert space.

It is easy to see that the operators $\mathbb{H}$, N, and Q defined in the previous section all have a vanishing expectation value in the vacuum state Ω. Calculating the vacuum expectation value $(\Omega, A\Psi^*\Psi\Omega)$ of the trace-class operator A, we see immediately that only the last summand in (10.61) can give a non-vanishing contribution

$$\begin{aligned}(\Omega, Abb^*\Omega) &= \sum_{k,l} (g_k, Ag_l)(\Omega, b(g_k)\, b^*(g_l)\Omega) \\ &= \sum_{k} (g_k, Ag_k) = \operatorname{tr} A_{-}.\end{aligned} \tag{10.66}$$

Hence, if A is not trace-class, not even the vacuum belongs to the domain of the formally defined operator $A\Psi^*\Psi$. In this case we have to modify the definition (10.53). For any expression consisting of a sum of products of the creation/annihilation operators $a^{(*)}$ and $b^{(*)}$ we introduce the procedure of "normal ordering": In each product all creation operators are moved to the left of the annihilation operators. For each transposition which is necessary to

perform this rearrangement the product is multiplied with a factor (-1). The procedure is denoted by double dots, e.g.,

$$:Abb^*: = -\sum_{k,l}(g_k, Ag_l)\, b^*(g_l)\, b(g_k) \tag{10.67}$$

Using the CAR we find $:Abb^*: = Abb^* - \operatorname{tr} A_-$ and hence

$$(\Omega\,,\, :A\Psi^*\Psi:\Omega) = 0. \tag{10.68}$$

Now we are able to relax the trace-class condition. We first consider the operator Aa^*a, assuming that A is bounded. It is easy to see that the action on a basis vector

$$\psi = a^*(f_{j_1}) \cdots a^*(f_{j_n})\,\phi, \quad \text{where} \quad \phi = b^*(g_{k_1}) \cdots b^*(g_{k_m})\,\Omega \tag{10.69}$$

is simply given by a sum of n terms

$$\begin{aligned} Aa^*a\psi = {} & a^*(Af_{j_1})\, a^*(f_{j_2}) \cdots a^*(f_{j_n})\,\phi + \ldots \\ & \ldots + a^*(f_{j_1})\, a^*(f_{j_2}) \cdots a^*(Af_{j_n})\,\phi. \end{aligned} \tag{10.70}$$

An analogous calculation can be done for $:Abb^*:$. This shows that the operators Aa^*a and $:Abb^*:$ are both well defined on the dense domain (10.33).

Unfortunately, the situation is more complicated for Aa^*b^*. For simplicity, let us assume that A_{+-} is a compact operator from $\mathfrak{H}_-$ to $\mathfrak{H}_+$. Hence there exist orthonormal bases $\{u_j\}_{j=1}^{\infty}$ in $\mathfrak{H}_+$ and $\{v_j\}_{j=1}^{\infty}$ in $\mathfrak{H}_-$ such that

$$A_{+-} = \sum_j \lambda_j\, (v_j, \cdot)\, u_j, \qquad \lambda_j \geq 0. \tag{10.71}$$

(The numbers λ_j^2 are the eigenvalues of the positive operator $A_{+-}^* A_{+-}$). With these bases in the definition (10.63) of Aa^*b^* we obtain

$$Aa^*b^* = \sum_j \lambda_j\, a^*(u_j)\, b^*(v_j). \tag{10.72}$$

Using the CAR we calculate

$$\begin{aligned} \|Aa^*b^*\Omega\|^2 &= \sum_{k.j} \lambda_k \lambda_j (\Omega, b(v_k)a(u_k)a^*(u_j)b^*(v_j)\Omega) \\ &= \sum_k \lambda_k^2 (\Omega, b(v_k)b^*(v_k)\Omega) = \sum_k \lambda_k^2. \end{aligned} \tag{10.73}$$

Hence Ω is in the domain of Aa^*b^* if and only if $\sum_k \lambda_k^2 < \infty$, which is equivalent to A_{+-} being a Hilbert-Schmidt operator. The same consideration with A^* lets us require the Hilbert-Schmidt property also for[3] A_{-+}^* and hence for A_{-+}. Having defined Aa^*b^* on Ω and noting that Aa^*b^* commutes with all creation operators, we can extend the definition to all finite linear combinations of basis vectors of the form (10.32).

[3] We use the simplified notation $A_{-+}^* = (A_{-+})^*$, etc. The reader should be careful with this notation, because $(A_{-+})^* = (A^*)_{+-}$.

10.3 Bogoliubov Transformations

10.3.1 Unitary Implementation in the General Case

Any unitary transformation $U: \mathfrak{H} \to \mathfrak{H}$ induces a transformation of the field operators by

$$\Psi(f) \to \Psi'(f) = \Psi(Uf), \quad \text{for all } f \in \mathfrak{H}. \tag{10.74}$$

This implies for the corresponding annihilation operators

$$a'(f) = a(U_+ f) + b^*(U_{-+} f), \quad \text{all } f \in \mathfrak{H}_+, \tag{10.75}$$

$$b'(g) = a^*(U_{+-} g) + b(U_- g), \quad \text{all } g \in \mathfrak{H}_-, \tag{10.76}$$

where $U_+ = P_+ U P_-$, $U_{+-} = P_+ U P_-$, etc. Obviously, the new field operators $\Psi'(f)$ again satisfy the CAR (10.29).

Definition 10.5. *The transformation U is called "unitarily implementable", if there exists a unitary operator $\mathbb{U}$ such that*

$$\Psi'(f) = \mathbb{U}\Psi(f)\mathbb{U}^*. \tag{10.77}$$

According to Theorem 10.3 the unitary implementability of U is equivalent to the existence of a vacuum vector $\Omega' \in \mathfrak{F}$ for the new annihilation operators

$$a'(f)\Omega' = b'(g)\Omega' = 0 \quad \text{all } f \in \mathfrak{H}_+, \text{ and all } g \in \mathfrak{H}_-. \tag{10.78}$$

If such a vector exists, then it is a scalar multiple of $\mathbb{U}\Omega$.

10.3.2 Even and Odd Parts of Unitary Operators

Here we discuss some mathematical properties of unitary operators which will be useful later. As always we assume that $\mathfrak{H}$ is a Hilbert space with a unitary involution τ which induces a splitting $\mathfrak{H} = \mathfrak{H}_+ \oplus \mathfrak{H}_-$ (Chapter 5). In the present context we have $\tau = \operatorname{sgn} H$ but the results of this section also hold in the general case.

Any unitary operator U in $\mathfrak{H}$ can be decomposed into an even (or diagonal) part U_{even} which commutes with τ and an odd (or off-diagonal) part U_{odd} which anticommutes with τ,

$$U = \begin{pmatrix} U_+ & U_{+-} \\ U_{-+} & U_- \end{pmatrix} = U_{\text{even}} + U_{\text{odd}}. \tag{10.79}$$

The unitarity condition for U can be rewritten as

$$U^*U = \mathbf{1} = U^*_{\text{even}} U_{\text{even}} + U^*_{\text{odd}} U_{\text{odd}}, \tag{10.80}$$

$$\mathbf{0} = U^*_{\text{even}} U_{\text{odd}} + U^*_{\text{odd}} U_{\text{even}}, \tag{10.81}$$

$$UU^* = \mathbf{1} = U_{\text{even}} U^*_{\text{even}} + U_{\text{odd}} U^*_{\text{odd}}, \tag{10.82}$$

$$\mathbf{0} = U_{\text{even}} U_{\text{odd}}^* + U_{\text{odd}} U_{\text{even}}^*, \tag{10.83}$$

From this we conclude immediately,

$$U_{\text{odd}} \operatorname{Ker} U_{\text{even}} \subset \operatorname{Ker} U_{\text{even}}^* = U_{\text{odd}} U_{\text{odd}}^* \operatorname{Ker} U_{\text{even}} \subset U_{\text{odd}} \operatorname{Ker} U_{\text{even}},$$

where we have successively applied Eqs. (10.81), (10.82), and (10.83). This implies

$$U_{\text{odd}} \operatorname{Ker} U_{\text{even}} = U \operatorname{Ker} U_{\text{even}} = \operatorname{Ker} U_{\text{even}}^*. \tag{10.84}$$

Now, let us assume that U_{odd} is compact (for unitarily implementable operators U we shall even show that U_{odd} is Hilbert-Schmidt). Then, if 1 is an eigenvalue of $U_{\text{odd}}^* U_{\text{odd}}$, it is isolated and has finite multiplicity. Hence

$$\operatorname{Ker} U_{\text{even}} = \operatorname{Ker} U_{\text{even}}^* U_{\text{even}} = \operatorname{Ker} (\mathbf{1} - U_{\text{odd}}^* U_{\text{odd}}) \tag{10.85}$$

is finite-dimensional and (10.84) implies that U_{even} is a Fredholm operator with

$$\operatorname{ind} U_{\text{even}} \equiv \dim \operatorname{Ker} U_{\text{even}} - \dim \operatorname{Ker} U_{\text{even}}^* = 0. \tag{10.86}$$

Hence the matrix elements U_+ and U_- are also Fredholm with

$$\operatorname{ind} U_+ = -\operatorname{ind} U_-. \tag{10.87}$$

Since by Eq. (5.26) U_{even} maps $(\operatorname{Ker} U_{\text{even}})^\perp$ onto $(\operatorname{Ker} U_{\text{even}}^*)^\perp$, we find that U_{even}^{-1} is well defined and bounded on $(\operatorname{Ker} U_{\text{even}}^*)^\perp$. We extend its definition to all of $\mathfrak{H}$ by setting

$$U_{\text{even}}^{-1} = \begin{cases} (U_{\text{even}}^* U_{\text{even}})^{-1} U_{\text{even}}^* & \text{on } (\operatorname{Ker} U_{\text{even}}^*)^\perp, \\ 0 & \text{on } \operatorname{Ker} U_{\text{even}}^*, \end{cases} \tag{10.88}$$

and obtain from (10.83)

$$U_{\text{even}}^{-1} U_{\text{odd}} U_{\text{even}}^* = -U_{\text{odd}}^* \quad \text{on } (\operatorname{Ker} U_{\text{even}}^*)^\perp. \tag{10.89}$$

For the matrix elements of U this implies, e.g.,

$$U_+^{-1} U_{+-} U_-^* = -U_{-+}^* \quad \text{on } (\operatorname{Ker} U_-^*)^\perp. \tag{10.90}$$

In the next section the operator $\mathrm{i} U_{\text{odd}} U_{\text{even}}^{-1}$ will be used. We show that it is self-adjoint. From (10.81) and (10.82) we conclude that $U_{\text{even}} U_{\text{even}}^* U_{\text{odd}} = U_{\text{odd}} U_{\text{even}}^* U_{\text{even}}$, and on $(\operatorname{Ker} U_{\text{even}})^\perp$

$$(U_{\text{even}} U_{\text{even}}^*)^{-1} U_{\text{odd}} = U_{\text{odd}} (U_{\text{even}}^* U_{\text{even}})^{-1}. \tag{10.91}$$

Hence, on $(\operatorname{Ker} U_{\text{even}}^*)^\perp$ we calculate, using Eq. (10.89)

$$\begin{aligned} (\mathrm{i} U_{\text{odd}} U_{\text{even}}^{-1})^* &= -\mathrm{i} (U_{\text{even}}^{-1})^* U_{\text{odd}}^* = \mathrm{i} (U_{\text{even}}^{-1})^* U_{\text{even}}^{-1} U_{\text{odd}} U_{\text{even}}^* \\ &= \mathrm{i} (U_{\text{even}} U_{\text{even}}^*)^{-1} U_{\text{odd}} U_{\text{even}}^* = \mathrm{i} U_{\text{odd}} (U_{\text{even}}^* U_{\text{even}})^{-1} U_{\text{even}}^* \\ &= \mathrm{i} U_{\text{odd}} U_{\text{even}}^{-1}. \end{aligned} \tag{10.92}$$

10.3.3 The Shale-Stinespring Criterion

In this section we want to prove the main mathematical result of this chapter: A unitary operator U can be implemented in Fock space if and only if U_{odd} is Hilbert-Schmidt. We divide this problem into two steps. Necessity will be proven in Theorem 10.7. In Theorem 10.6 we prove sufficiency by explicitly constructing the action of the unitary implementer $\mathbb{U}$ on the vacuum Ω. Before doing so we have to define the exponential $\exp(Aa^*b^*)$ of the (unbounded) operator Aa^*b^*, where $A : \mathfrak{H}_- \to \mathfrak{H}_+$ is Hilbert-Schmidt. As in Eq. (10.72) we write

$$Aa^*b^* = \sum_j \lambda_j\, a^*(u_j)\, b^*(v_j), \quad \lambda_j \geq 0, \quad \sum_j \lambda_j^2 < \infty, \tag{10.93}$$

with orthonormal bases $\{u_j\}_{j=1}^{\infty}$ in $\mathfrak{H}_+$ and $\{v_j\}_{j=1}^{\infty}$ in $\mathfrak{H}_-$. The sum is well defined on vectors ψ in the dense set $\mathfrak{D}$ given by Eq. (10.33). Since the summands in (10.93) commute, we can write

$$e^{Aa^*b^*} = \prod_j e^{\lambda_j\, a^*(u_j)\, b^*(v_j)} = \prod_j \big(1 + \lambda_j\, a^*(u_j)\, b^*(v_j)\big) \tag{10.94}$$

(in the last step we have used the Pauli principle $a^*(u_j)^2 = b^*(v_j)^2 = 0$). Hence

$$\begin{aligned} \left\| e^{Aa^*b^*}\, \Omega \right\|^2 &= \prod_j \big((1 + \lambda_j\, a^*(u_j)\, b^*(v_j))\Omega, (1 + \lambda_j\, a^*(u_j)\, b^*(v_j))\Omega \big) \\ &= \prod_j (1 + \lambda_j^2). \end{aligned} \tag{10.95}$$

This expression is finite since by the Hilbert-Schmidt property $\sum_j \lambda_j^2 < \infty$. Hence $e^{Aa^*b^*}$ is well defined on the vacuum state. Since $e^{Aa^*b^*}$ commutes with any creation operator, this operator is also well defined on the basis vectors (10.32) and hence on $\mathfrak{D}$, the set of all finite linear combinations of these basis vectors. In the Appendix we list some useful commutation formulas for operators of this type.

Now we are prepared to formulate our first result.

Theorem 10.6. If the operators U_{+-}, U_{-+} are Hilbert-Schmidt, then U is unitarily implementable and

$$\mathbb{U}\Omega = k\, e^{i\theta} \prod_{l=1}^{L} a^*(f_l) \prod_{m=1}^{M} b^*(g_m)\, e^{Aa^*b^*}\, \Omega, \qquad \theta \in [0, 2\pi), \tag{10.96}$$

where

$$A = (U_{\text{odd}} U_{\text{even}}^{-1})_{+-} = U_{+-} U_{-}^{-1}, \tag{10.97}$$

$$k = \sqrt{\det\,(1 - U_{+-} U_{+-}^*)} = \sqrt{\det\,(1 - U_{-+} U_{-+}^*)}. \tag{10.98}$$

Here $\{f_l\,|, l = 1, \ldots, L\}$ and $\{g_m\,|, m = 1, \ldots, M\}$ are orthonormal bases of the finite dimensional subspaces $\operatorname{Ker} U_+^*$ and $\operatorname{Ker} U_-^*$, respectively, and the products are in the natural order of the indices. The operator $\mathbb{U}$ can be made unique by choosing $\theta = 0$.

Proof. 1. Let us determine the normalization constant k. We must have

$$1 = \left\| k \prod_{l=1}^{L} a^*(f_l) \prod_{m=1}^{M} b^*(g_m)\, e^{Aa^*b^*}\, \Omega \right\|^2 = k^2 \prod_j (1 + \lambda_j^2). \tag{10.99}$$

The last expression can be written as the determinant

$$\prod_j (1 + \lambda_j^2) = \det(1 + A^*A) = \det(1 + AA^*). \tag{10.100}$$

If A is given by (10.97), we can use Eqs. (10.80)-(10.83) to obtain

$$1 + A^*A = (U_-U_-^*)^{-1} = (1 - U_{-+}U_{-+}^*)^{-1}, \tag{10.101}$$

$$1 + AA^* = (U_+^*U_+)^{-1} = (1 - U_{+-}U_{+-}^*)^{-1}, \tag{10.102}$$

from which we conclude Eq. (10.98) immediately.

2. By Theorem 10.3 we have to show that there is a vacuum Ω' for the new field operators a', b', cf. Eqs. (10.75), (10.76). Clearly we choose

$$\Omega' = \prod_{l=1}^{L} a^*(f_l) \prod_{m=1}^{M} b^*(g_m)\, e^{Aa^*b^*}\, \Omega. \tag{10.103}$$

We first prove $a'(f)\Omega' = 0$ for $f \in \operatorname{Ker} U_+ \subset \mathfrak{H}_+$. We find from (10.76)

$$a'(f) = b^*(U_{-+}f) = \sum_{m=1}^{M} c_m b^*(g_m). \tag{10.104}$$

Here $U_{-+}f$ is in $\operatorname{Ker} U_-^*$ and has been expanded into the basis $\{g_m\}_{m=1}^M$. If we now apply $a'(f)$ to Ω', then each of the summands in (10.104) can be combined with the corresponding term in the product (10.103) to yield a factor $b^*(g_m)^2 = 0$. The proof of $b'(g)\Omega' = 0$, all $g \in \operatorname{Ker} U_-$ is similar.

3. Now, let $f \in (\operatorname{Ker} U_+)^\perp$. Hence $U_{-+}f$ is orthogonal to $\operatorname{Ker} U_-^*$ and U_+f is orthogonal to $\operatorname{Ker} U_+^*$. Hence, if $a'(f) = a(U_+f) + b^*(U_{-+}f)$ is applied to (10.103), it can be commuted through all the products in front of $e^{Aa^*b^*}$. But using Eq. (10.167) we obtain

$$\big(a(U_+f) + b^*(U_{-+}f)\big)e^{Aa^*b^*}\,\Omega = \big(b^*(A^*U_+f) + b^*(U_{-+}f)\big)e^{Aa^*b^*}\,\Omega, \tag{10.105}$$

and using (10.97), (10.90), we obtain

$$A^*U_+f = [(U_{\text{odd}}U_{\text{even}}^{-1})^*\,U_{\text{even}}]_{-+}f = -U_{-+}f, \tag{10.106}$$

which finally proves $a'(f)\Omega' = 0$. The proof of $b'(g)\Omega' = 0$ for $g \in (\operatorname{Ker} U_-)^\perp$ is analogous. □

The next theorem shows that the Hilbert-Schmidt condition is not only sufficient, but also necessary.

Theorem 10.7. The unitary transformation U in $\mathfrak{H}$ is unitarily implementable if and only if U_{+-} and U_{-+} are Hilbert-Schmidt operators.

Proof. The if-part is the content of Theorem 10.6, it remains to prove the Hilbert-Schmidt property for unitarily implementable operators.

Let $\{f_j\}_{j=1}^{\infty}$ be an orthonormal basis (ONB) of $\mathfrak{H}_+$ which contains an ONB of $\operatorname{Ker} U_+^*$ as a subset. Similarly, let $\{g_k\}_{k=1}^{\infty}$ be an ONB of $\mathfrak{H}_-$ containing an ONB of $\operatorname{Ker} U_-^*$. With these bases we form an ONB of the Fock space $\mathfrak{F}$ according to Eq. (10.32).

If U is unitarily implementable, then $\Omega' = \mathbb{U}\Omega \in \mathfrak{F}$, with $\|\Omega'\| = 1$, is the unique vacuum vector for the field operators (10.75), (10.76). Since any element of $\mathfrak{F}$ is a linear combination of the basis vectors (10.32), we can write

$$\Omega' = \{(\Omega')^{(n,m)}\}_{n,m=0,1,2,\ldots}, \quad \text{where} \tag{10.107}$$

$$(\Omega')^{(n,m)} = \sum_{\substack{j_1,\ldots,j_n \\ k_1,\ldots,k_m}} \alpha^{(n,m)}_{j_1,\ldots,k_m}\, a^*(f_{j_1}) \ldots a^*(f_{j_n})\, b^*(g_{k_1}) \ldots b^*(g_{k_m})\, \Omega, \tag{10.108}$$

with suitable coefficients $\alpha^{(n,m)}_{\ldots}$. Using (10.75) we find for all $f \in \operatorname{Ker} U_+^*$

$$a^*(f)\Omega' = \mathbb{U}^* a'^*(f)\mathbb{U}\Omega' = a'^*(U_+^* f)\Omega' = a'^*(0)\Omega' = 0. \tag{10.109}$$

Similarly, $b^*(g)\Omega' = 0$ for $g \in \operatorname{Ker} U_-^*$. The coefficients in (10.108) are clearly given by

$$\alpha^{(n,m)}_{j_1,\ldots,k_m} = (a^*(f_{j_1}) \ldots b^*(g_{k_m})\, \Omega, \Omega'). \tag{10.110}$$

If f_l is a basis vector of $\operatorname{Ker} U_+^*$ with $l \notin \{j_1, \ldots, j_n\}$, then the coefficient (10.110) also occurs in the expansion of the vector $a^*(f_l)\Omega'$, and we can also write

$$\alpha^{(n,m)}_{j_1,\ldots,k_m} = (a^*(f_l) a^*(f_{j_1}) \ldots b^*(g_{k_m})\, \Omega, a^*(f_l)\Omega'), \tag{10.111}$$

which is zero by Eq. (10.109). With a similar consideration for the basis vectors of $\operatorname{Ker} U_-^*$ we conclude

$$(\Omega')^{(n,m)} = 0 \quad \text{if } n < N \equiv \dim \operatorname{Ker} U_+^*, \text{ or } m < M \equiv \dim \operatorname{Ker} U_-^*. \tag{10.112}$$

The numbers N and M have to be finite, because otherwise all the coefficients $\alpha^{(n,m)}_{\ldots}$ would be zero in contradiction to $\|\Omega'\| = 1$. We can therefore renumber the basis vectors such that $\{f_j\}_{j=1}^{N}$ and $\{g_k\}_{k=1}^{M}$ are the ONB's of $\operatorname{Ker} U_+^*$ and $\operatorname{Ker} U_-^*$. Using this notation we find

$$(\Omega')^{(N,M)} = \delta \prod_{j=1}^{N} a^*(f_j) \prod_{k=1}^{M} b^*(g_k)\, \Omega, \tag{10.113}$$

where δ is a norming factor. From $(a'(f)\Omega')^{(N+r,M+s)} = 0$ and Eq. (10.75) we obtain for all $f \in \mathfrak{H}_+$

$$a(U_+f)(\Omega')^{(N+r+1,M+s)} = -b^*(U_{-+}f)(\Omega')^{(N+r,M+s-1)}. \tag{10.114}$$

Therefore, $(\Omega')^{(N+r,M+s-1)} = 0$ implies $(\Omega')^{(N+r+1,M+s)} = 0$ for all $r \geq 0$ and $s \geq 0$. With the help of Eq. (10.112) we infer $(\Omega')^{(N+r+j,M+j)} = 0$ for all $r > 0$ and $j \geq 0$. Similarly, $b'(g)\Omega' = 0$ implies $(\Omega')^{(N+j,M+r+j)} = 0$. Combining these results yields

$$(\Omega')^{(N+r,M+s)} = 0 \quad \text{for } r \neq s. \tag{10.115}$$

The only nonzero components of Ω' are $(\Omega')^{(N+j,M+j)}$, $j \geq 0$. For example, in view of Eq. (10.108) we can write

$$(\Omega')^{(N+1,M+1)} = \sum_{j=N+1}^{\infty} \sum_{k=M+1}^{\infty} \gamma_{jk} a^*(f_j) b^*(g_k) (\Omega')^{(N,M)}. \tag{10.116}$$

The coefficients γ_{jk} must satisfy the condition

$$\sum_{j,k} |\gamma_{jk}|^2 < \infty, \tag{10.117}$$

otherwise (10.116) would not be normalizable. We further conclude from (10.116) that $k \neq 0$ in Eq. (10.113), otherwise all components of Ω' would vanish. Eq. (10.116) can be written as

$$(\Omega')^{(N+1,M+1)} = K a^* b^* \, (\Omega')^{(N,M)}, \tag{10.118}$$

with

$$Kg = \sum_{j=N+1}^{\infty} \sum_{k=M+1}^{\infty} \gamma_{jk} \, f_j \, (g_k, g) \quad \text{for all } g \in (\operatorname{Ker} U_-^*)^{\perp}. \tag{10.119}$$

K maps $(\operatorname{Ker} U_-^*)^{\perp}$ onto $(\operatorname{Ker} U_+^*)^{\perp}$ and is Hilbert-Schmidt because of (10.117).

Now we are ready to prove that U_{+-} is Hilbert-Schmidt. We calculate

$$\begin{aligned} 0 = \big(b'(g)\Omega'\big)^{(N+1,M)} &= \big(b(U_-g)\Omega' + a^*(U_{+-}g)\Omega'\big)^{(N+1,M)} \\ &= \big(b(U_-g)\, K a^* b^* + a^*(U_{+-}g)\big)(\Omega')^{(N,M)}, \end{aligned} \tag{10.120}$$

and

$$\begin{aligned} & b(U_-g)\, K a^* b^* \, (\Omega')^{(N,M)} \\ &= \sum_{\substack{j=N+1 \\ k=M+1}}^{\infty} \gamma_{jk} \, a^*(f_j) \left[\{b(U_-g), b^*(g_k)\} - b^*(g_k) b(U_-g)\right] (\Omega')^{(N,M)}. \end{aligned} \tag{10.121}$$

For $g \in (\operatorname{Ker} U_-)^{\perp}$ we have $U_-g \in (\operatorname{Ker} U_-^*)^{\perp}$, using the CAR and (10.113) we find that

$$b(U_-g)\,(\Omega')^{(N,M)} = 0 \quad \text{for all } g \in (\operatorname{Ker} U_-)^\perp. \tag{10.122}$$

Finally, using the CAR (10.23),

$$\begin{aligned} b(U_-g)\,Ka^*b^*\,(\Omega')^{(N,M)} &= \sum_{\substack{j=N+1\\k=M+1}}^{\infty} \gamma_{jk}\, a^*(f_j)\,(g_k, U_-g)(\Omega')^{(N,M)} \\ &= a^*(KU_-g)\,(\Omega')^{(N,M)}. \end{aligned} \tag{10.123}$$

Therefore

$$a^*(KU_-g)\,(\Omega')^{(N,M)} = -a^*(U_{+-}g)\,(\Omega')^{(N,M)}, \tag{10.124}$$

for all $g \in (\operatorname{Ker} U_-)^\perp$. We have $KU_-g,\ U_{+-}g \in (\operatorname{Ker} U_+^*)^\perp$, hence Eqs. (10.113) and (10.124) imply $a^*(KU_-g)\,\Omega = -a^*(U_{+-}g)\,\Omega$ which leads to

$$U_{+-}g = -KU_-g \quad \text{for all } g \in (\operatorname{Ker} U_-)^\perp. \tag{10.125}$$

This shows that U_{+-} is a Hilbert-Schmidt operator on $(\operatorname{Ker} U_-)^\perp$. Since U_{+-} is of finite rank on $\operatorname{Ker} U_-$ (by Eq. (10.84) we have $U_{+-}\operatorname{Ker} U_- = \operatorname{Ker} U_+^*$, which is finite dimensional), we conclude that U_{+-} is a Hilbert-Schmidt operator on $\mathfrak{H}_- = \operatorname{Ker} U_- \oplus (\operatorname{Ker} U_-)^\perp$.

Similarly, the equation $(a'(f)\Omega')^{(N,M+1)} = 0$ with $f \in (\operatorname{Ker} U_+)^\perp$ proves the Hilbert-Schmidt property for the operator U_{-+}. □

10.3.4 Unitary Groups, Schwinger Terms, and Indices

If A is a bounded operator with A_{odd} Hilbert-Schmidt, then $e^{\mathrm{i}At}$ can be defined by a norm-convergent power series and it is easy to see that the odd part converges even in the Hilbert-Schmidt norm (using $\|B_1B_2\|_2 \le \|B_1\|\|B_2\|_2$ if B_1 is bounded and B_2 is Hilbert-Schmidt). Hence $[e^{\mathrm{i}At}]_{\text{odd}}$ is a Hilbert-Schmidt operator. If A is self-adjoint, the Shale-Stinespring criterion implies that the unitary operators $e^{\mathrm{i}At}$ can be implemented in Fock space. The theorem below states that the implementers can be chosen to form a strongly continuous unitary group in the Fock space.

Theorem 10.8. Let A be bounded and self-adjoint with $A_{+-} = A_{-+}^*$ being Hilbert-Schmidt. Then $:A\Psi^*\Psi:$ is well defined and essentially self-adjoint on $\mathfrak{D}(N)$ (the domain of the number operator N). If $\mathbb{A}$ is the unique self-adjoint extension in $\mathfrak{F}$, then the unitary group $\exp(\mathrm{i}\mathbb{A}t)$ implements $\exp(\mathrm{i}At)$, i.e.,

$$e^{\mathrm{i}\mathbb{A}t}\,\Psi(f)\,e^{-\mathrm{i}\mathbb{A}t} = \Psi(e^{\mathrm{i}At}f) \quad \text{for all } t. \tag{10.126}$$

Proof. See [86], Proposition 2.1. □

For trace-class operators A, Eq. (10.126) follows from (10.60), because then $\mathbb{A} = :A\Psi^*\Psi: = A\Psi^*\Psi - \operatorname{tr} A_-$.

It is perhaps surprising that for two operators commuting at the one-particle level the Fock space implementers do not necessarily commute. If A and B are trace-class operators we can apply the CAR to obtain the result

$$[A\Psi^*\Psi, B\Psi^*\Psi] = C\Psi^*\Psi, \qquad \text{where } C = [A, B]. \tag{10.127}$$

Inserting $A\Psi^*\Psi = :A\Psi^*\Psi: + \operatorname{tr} A_-$, etc., gives immediately

$$[:A\Psi^*\Psi:, :B\Psi^*\Psi:] = :C\Psi^*\Psi: + \operatorname{tr} C_-. \tag{10.128}$$

From $C_- = A_{-+}B_{+-} - B_{-+}A_{+-} + [A_-, B_-]$ and $\operatorname{tr}[A_-, B_-] = 0$ we find the formula

$$[\mathbb{A}, \mathbb{B}] = \mathbb{C} + s(A, B)\mathbf{1}, \tag{10.129}$$

where

$$s(A, B) = \operatorname{tr}(A_{-+}B_{+-} - B_{-+}A_{+-}) \tag{10.130}$$

is called the "*Schwinger term*". By the Baker-Campbell-Hausdorff formula we find

$$e^{\mathrm{i}\mathbb{A}}e^{\mathrm{i}\mathbb{B}} = e^{-s(A,B)/2}\, e^{\mathrm{i}(\mathbb{A}+\mathbb{B})}, \qquad \text{if } [A, b] = 0. \tag{10.131}$$

For operators A, B satisfying the assumptions of Theorem 10.8, Eq. (10.131) remains true, and Eq. (10.129) still holds on $\mathfrak{D}(N)$.

For the following we assume that $A = A^*$ is bounded with A_{odd} being Hilbert-Schmidt. Let U be a unitarily implementable operator in $\mathfrak{H}$ commuting with A. Then both $\exp(\mathrm{i}\mathbb{A}t)$ and $\mathbb{V}_t \equiv \mathbb{U}\exp(\mathrm{i}\mathbb{A}t)\mathbb{U}^*$ implement the unitary group $e^{\mathrm{i}At}$. But since the implementers are unique up to a phase, $\mathbb{V}_t$ must be equal to $e^{\mathrm{i}\theta(t)}e^{\mathrm{i}\mathbb{A}t}$. The group property implies $\theta(t) = \gamma t$ with some real γ. Thus $\mathbb{U}\mathbb{A}\mathbb{U}^* = \mathbb{A} + \gamma\mathbf{1}$ is the generator of $\mathbb{V}_t$. Writing $\Omega' = \mathbb{U}\Omega$ we calculate, using Eq. (10.68)

$$0 = (\Omega, \mathbb{A}\Omega) = (\Omega', \mathbb{U}^*\mathbb{A}\mathbb{U}\Omega') = (\Omega', \mathbb{A}\Omega') + \gamma, \tag{10.132}$$

i.e., $\gamma = -(\Omega', \mathbb{A}\Omega')$. This implies the formula

$$\mathbb{U}\, e^{\mathrm{i}\mathbb{A}t}\, \mathbb{U}^* = e^{-\mathrm{i}t(\Omega', \mathbb{A}\Omega')}\, e^{\mathrm{i}\mathbb{A}t} \quad (\text{where } [U, A] = 0,\ \Omega' = \mathbb{U}\Omega). \tag{10.133}$$

We are now ready to prove

Theorem 10.9. Let U be unitarily implementable. An implementer $\mathbb{U}$ maps each charge-k sector $\mathfrak{F}_k$ onto $\mathfrak{F}_{k-q(U)}$, where $q(U)$ is the Fredholm-index of U_+,

$$q(U) = \operatorname{ind} U_+ = -\operatorname{ind} U_-. \tag{10.134}$$

If A satisfies the assumptions of Theorem 10.8, then

$$q(e^{\mathrm{i}\mathbb{A}t}) = 0. \tag{10.135}$$

Proof. The gauge group e^{it} is unitarily implemented by e^{iQt}, where Q is the charge operator. If U is implementable, then Eq. (10.133) implies

$$\mathbb{U} e^{iQt} = e^{-it(\mathbb{U}\Omega, \mathbb{A}\mathbb{U}\Omega)} e^{iQt} \mathbb{U}. \tag{10.136}$$

Since Q has integer eigenvalues, $e^{2\pi iQ} = \mathbf{1}$, and hence

$$q(U) \equiv (\mathbb{U}\Omega, \mathbb{A}\mathbb{U}\Omega) \tag{10.137}$$

is an integer. This number depends only on U, because the implementers are unique up to a phase which cancels in the scalar product (10.137). Now Eq. (10.136) implies for all $k \in \mathbb{Z}$ that $\mathbb{U}$ maps the eigenspace $\mathfrak{F}_k$ of Q (the charge-k sector) onto $\mathfrak{F}_{k-q(U)}$.

Now, if $\mathbb{U} = e^{i\mathbb{A}t}$, then $[\mathbb{A}, Q] = 0$ by Eq. (10.129). Hence

$$q(e^{iAt}) = (e^{i\mathbb{A}t}\Omega, Qe^{i\mathbb{A}t}\Omega) = (\Omega, Q\Omega) = 0. \tag{10.138}$$

Next we use the explicit form for $\mathbb{U}\Omega$ obtained in Theorem 4.7. First we note that $e^{Aa^*b^*}\Omega$ is a charge-0 state, because the operator Aa^*b^* creates particles and antiparticles only in pairs. Hence the charge of $\mathbb{U}\Omega$ is completely determined by the difference of the number of particle and antiparticle creation operators in the product

$$\prod_{l=1}^{L} a^*(f_l) \prod_{m=1}^{M} b^*(g_m) \tag{10.139}$$

appearing in (10.96). Obviously, the charge is

$$\begin{aligned} -q(U) = L - M &= \dim \operatorname{Ker} U_+^* - \dim \operatorname{Ker} U_-^* \\ &= \dim \operatorname{Ker} U_- - \dim \operatorname{Ker} U_-^* = \operatorname{ind} U_- = -\operatorname{ind} U_+. \end{aligned} \tag{10.140}$$

This proves the theorem. □

10.3.5 Example: The Shift Operator

An elementary mathematical example of a unitary transformation generating a charged vacuum is the shift operator T. For some physically more relevant examples we refer to the literature cited in the notes.

In $\mathfrak{H} = \mathfrak{H}_+ \oplus \mathfrak{H}_-$ choose an orthonormal basis (ONB) $\{e_j \mid j \in \mathbb{Z}\}$ such that $\{e_j \mid j \geq 0\}$ is an ONB in $\mathfrak{H}_+$, and $\{e_j \mid j < 0\}$ is an ONB in $\mathfrak{H}_-$. Then

$$Te_j = e_{j+1}, \quad \text{all } j \in \mathbb{Z}, \tag{10.141}$$

defines a unitary operator in $\mathfrak{H}$, called "right shift". One finds immediately that

$$T_{+-} = e_0(e_{-1}, \cdot), \qquad T_{-+} = 0 \tag{10.142}$$

are Hilbert-Schmidt operators. This shows that T is unitarily implementable in $\mathfrak{F}$. Moreover, T maps $\mathfrak{H}_+$ into $\mathfrak{H}_+$, and $\operatorname{Ker} T_+ = \{0\}$.

The operator $T^* = T^{-1}$ is the "shift to the left". From $T^* e_0 = e_{-1} \in \mathfrak{H}_-$ we conclude that $\operatorname{Ker} T_+^* = \{e_0\}$, i.e.,

$$\operatorname{ind} T_+ = -1. \tag{10.143}$$

Similarly one verifies $\operatorname{Ker} T_- = \{e_{-1}\}$, $\operatorname{Ker} T_-^* = \{0\}$, hence $\operatorname{ind} T_- = 1$, as expected. We conclude from Theorem 10.9 that the unitarily implemented shift operator $\mathbb{T}$ maps the vacuum into the charge-1 sector. The heuristics is of course the following: B moves a state from the negative energies to $\mathfrak{H}_+$ without leaving a hole in the Dirac sea. Hence the vacuum is turned into a single-particle state. We can directly verify this in the following calculation. Writing

$$Q = \sum_{j \geq 0} \{a^*(e_j)\, a(e_j) - b^*(e_{-j-1})\, b(e_{-j-1})\}, \tag{10.144}$$

and using Eqs. (10.75)–(10.77) gives

$$\begin{aligned} \mathbb{T} Q \mathbb{T}^* &= \sum_{j \geq 1} \{a^*(e_j)\, a(e_j) - b^*(e_{-j})\, b(e_{-j})\} - a(e_0)\, a^*(e_0) \\ &= Q - \mathbf{1}. \end{aligned} \tag{10.145}$$

In particular, this implies

$$(\mathbb{T}\Omega, Q\mathbb{T}\Omega) = (\Omega, (Q + \mathbf{1})\Omega) = 1, \tag{10.146}$$

which is in accordance with our previous observations.

10.4 Particle Creation and Scattering Theory

The splitting of the Hilbert space of the Dirac equation into a one-particle and a one-antiparticle space can be made explicit in the case of free particles (see Section 1.4.2), but is extremely difficult in the presence of external fields. If the field is even time-dependent, then also the Fock space would depend on time, because its construction is based on the positive/negative spectral subspaces of the Dirac operator $H(t)$.

We assume that the hypotheses of Theorem 4.9 are satisfied, hence there is a unitary propagator $U(t, s)$ in $\mathfrak{H} = L^2(\mathbb{R}^3)^4$. At some initial time, say $t = 0$, we can split the Hilbert space into $\mathfrak{H} = \mathfrak{H}_+ \oplus \mathfrak{H}_-$ as in Eq. (10.1), and build a Fock space from the vacuum Ω, which is characterized by $a(P_+ f)\Omega = b(P_- f)\Omega = 0$. At time t we can write

$$\mathfrak{H} = U(t, 0)\mathfrak{H}_+ \oplus U(t, 0)\mathfrak{H}_-, \tag{10.147}$$

and the corresponding projection operators are given by

$$P_\pm(t) = U(t, 0)\, P_\pm\, U(0, t). \tag{10.148}$$

There is a vacuum vector Ω_t, given by

$$a(P_+(t)U(t,0)f)\Omega_t = b(P_-(t)U(t,0)f)\Omega_t = 0, \tag{10.149}$$

and a Fock space given as the closure of the linear hull of the vectors

$$\prod_{j,k} a^*(U(t,0)f_j)\, b^*(U(t,0)g_k)\, \Omega_t, \tag{10.150}$$

where $\{f_j\}_{j=1}^{\infty}$ is a basis in $\mathfrak{H}_+$ and $\{g_k\}_{k=1}^{\infty}$ in $\mathfrak{H}_-$.

In this formulation the Fock representation depends on time while the field operators remain unchanged ("Schrödinger picture"). This means that at each instant of time the interpretation of particles and antiparticles changes. In order to avoid these difficulties and to obtain a particle interpretation for all times, one tries to describe the whole theory in a fixed Fock space. If all particles are asymptotically free (scattering theory), then it seems to be reasonable to choose the free particle Fock space.

We denote by $\mathfrak{F}_0$ the Fock space associated with the free Dirac operator H_0. Its construction is based on the splitting of the one-particle Hilbert space $\mathfrak{H}$ into $\mathfrak{H}_{\text{pos}}$ and $\mathfrak{H}_{\text{neg}}$, the spectral subspaces of H_0 which are defined in Sect. 1.4.2. We obtain field operators which satisfy the CAR

$$\{a_0(f_1), a_0^*(f_2)\} = (f_1, f_2)\mathbf{1}, \quad f_j \in \mathfrak{H}_{\text{pos}}, \qquad \text{etc.} \tag{10.151}$$

Let $\mathfrak{H}_+$ and $\mathfrak{H}_-$ be the the positive and negative energy subspaces of the Dirac operator with an external field. We can build a new Fock space $\mathfrak{F}$ starting with the splitting $\mathfrak{H} = \mathfrak{H}_+ \oplus \mathfrak{H}_-$. This defines field operators and CAR for interacting particles. But now we want to describe the particles in an external field within the framework of the original free particle Fock space $\mathfrak{F}_0$. For this we have to represent the "interacting field algebra" in $\mathfrak{F}_0$, i.e., we look for operators $a(f)$, $b(g)$ in $\mathfrak{F}_0$ such that

$$\{a(f_1), a^*(f_2)\} = (f_1, f_2)\mathbf{1}, \quad f_j \in \mathfrak{H}_+, \qquad \text{etc.} \tag{10.152}$$

One can describe interacting particles within this framework, if it is possible to implement the time evolution $\exp(-\mathrm{i}Ht)$ of a particle in an external field as a unitary operator in the free particle Fock space. By Theorem 10.7, it is necessary and sufficient that the operators

$$P_{\text{pos}} \exp(-\mathrm{i}Ht)\, P_{\text{neg}}, \qquad P_{\text{neg}} \exp(-\mathrm{i}Ht)\, P_{\text{pos}} \tag{10.153}$$

are Hilbert-Schmidt. This of course restricts the class of external fields which can be described by this method.

10.4.1 The S-Matrix in Fock Space

It is not clear whether it is always useful to implement the whole time evolution in the Fock space of free particles. Scattering theory, however, describes asymptotically free states and the scattering operator S maps free incoming states onto free outgoing states. Therefore the free particle Fock space $\mathfrak{F}_0$ is a natural framework for the implementation of scattering theory, at least if we

assume that the operators $P_{\text{pos}} S P_{\text{neg}}$ and $P_{\text{neg}} S P_{\text{pos}}$ have the Hilbert-Schmidt property.

One of the most interesting phenomena which can be described as a scattering process in QED is the possibility of pair creation from the vacuum. If the scattering operator is implementable, then $|(\Omega, \mathbb{S}\Omega)|^2$ is the probability that a system which is in the vacuum state for $t \to -\infty$ is still in the vacuum state for $t \to +\infty$, i.e., after the scattering by the external field. Hence

$$p = 1 - |(\Omega, \mathbb{S}\Omega)|^2 \tag{10.154}$$

is the probability of pair creation from the vacuum.

Remark. Particles are usually created in pairs as a consequence of the charge conservation. Let $H = H_0 + \lambda V$ and assume that the scattering operator $S(\lambda)$ depends continuously (in operator norm) on the coupling constant λ. (Note that S given by Eq. (8.163) is even analytic in λ). In the set $F(\mathfrak{H}_+)$ of all Fredholm operators on $\mathfrak{H}_+$ the operator $S_+(\lambda)$ is therefore connected by a norm-continuous path with the identity operator $S(0) = \mathbf{1}$. By the topological invariance of the Fredholm index, all operators in the same path component of $F(\mathfrak{H}_+)$ have the same index,

$$\operatorname{ind} S_+(\lambda) = \operatorname{ind} \mathbf{1} = 0. \tag{10.155}$$

By Theorem 10.9, if $S(\lambda)$ is unitarily implementable, the implementer $\mathbb{S}$ leaves all charge sectors invariant, $q(S(\lambda)) = 0$, and therefore

$$\mathbb{S}Q = Q\mathbb{S}. \tag{10.156}$$

If the external field does not depend on time, then S commutes with the free Dirac operator and hence it leaves the spectral subspaces $\mathfrak{H}_{+,-}$ invariant. Therefore, $S_{+-} = S_{-+} = 0$, and we conclude the following theorem which states that static external fields are unable to create pairs.

Theorem 10.10. Let V be a static external field such that the scattering operator S exists and is unitary. Then S is unitarily implementable in Fock space and

$$\mathbb{S}\Omega = \Omega, \tag{10.157}$$

i.e., the probability of pair creation is zero.

However, a scattering operator can also be defined for time dependent fields. Criteria for the Hilbert-Schmidt property of the operators S_{+-} and S_{-+} are given in Sect. 8.5, Theorem 8.25.

Theorem 10.11. Let $H = H_0 + \lambda V(t)$ and let $S(\lambda)$ be the scattering operator for the pair (H, H_0). Assume that $S_{+-}(\lambda)$ and $S_{-+}(\lambda)$ are Hilbert-Schmidt

operators for all $\lambda \in \mathbb{C}$. Then the map $\lambda \to \mathbb{S}(\lambda)\psi$ is holomorphic on $\mathbb{R}$ for any ψ which is a finite linear combination of the basis vectors (10.32).

Proof. See the Notes □

10.4.2 Spontaneous Pair Creation

Originally, the notion of "spontaneous pair creation" should describe a jump in the probability of pair creation if the external field strength exceeds a critical threshold (below that threshold no pair creation is expected). However, our considerations above give no hint for the existence of such a phenomenon within the present framework. For static fields, the notion of spontaneous pair creation makes no sense at all, because in this case there is no pair creation at all, no matter how strong the external field might be. For time dependent fields the Fock space scattering operator $\mathbb{S}$ depends analytically on the coupling constant λ of the external field. Therefore, also $(\Omega, \mathbb{S}(\lambda)\Omega)$ is analytic in λ, i.e., there is no sudden change in the probability of pair creation if the strength of the external field is varied.

One possibility of treating spontaneous pair creation comes from the adiabatic switching formalism. One considers time dependent fields with a large probability of pair creation from the vacuum. Following Nenciu [336] we say that a spontaneous pair creation appears, if the probability of pair creation is still large in the adiabatic limit, i.e., if the field varies very slowly in time. Let the potential be of the form

$$V_{\lambda,\epsilon} = \lambda e^{-\epsilon^2 t^2} V, \tag{10.158}$$

where V is a time independent potential such that the Fock space scattering operator $\mathbb{S}(V_{\lambda,\epsilon})$ exists for all $\lambda, \epsilon > 0$. It is believed there exist potentials for which there is a critical threshold λ_c, such that

$$\lim_{\epsilon \to 0} (\Omega, \mathbb{S}(V_{\lambda,\epsilon})\Omega) \quad \begin{cases} = 1 & \text{for } \lambda < \lambda_c, \\ < k < 1 & \text{for } \lambda > \lambda_c. \end{cases} \tag{10.159}$$

In the "overcritical" case $\lambda > \lambda_c$, one would say that "spontaneous pair creation" occurs. The existence of the overcritical case has not been shown yet, although some partial results were obtained (see the Notes). The discontinuity with respect to the coupling constant λ only occurs in the adiabatic limit $\epsilon \to 0$. For any fixed $\epsilon > 0$, the probability of pair creation is a smooth function of λ, by Theorem 10.11. If the scattering operator $\mathbb{S}(V_{\lambda,0})$ exists for all λ, then the probability of pair creation is even zero for all λ by Theorem 10.10.

Theorem 10.12. A static field is undercritical, if during the switching the eigenvalues emerging from the upper (resp. lower) continuum do not reach the lower (resp. upper) continuum.

Proof. See the Notes. □

It has been conjectured that a field is overcritical if the electron eigenvalues dive into the positron continuum (or vice versa) during switching the field on and off.

Appendix

We list some useful formulas with Aa^*a, Aa^*b^*, etc., where A is bounded with A_{odd} being Hilbert-Schmidt. We have

$$(Aa^*b^*)^* = A^*ba, \qquad (Aba)^* = A^*a^*b^*, \tag{10.160}$$

$$(Aa^*a)^* = A^*a^*a, \qquad (Abb^*)^* = A^*bb^*. \tag{10.161}$$

On the domain $\mathfrak{D}$ given by Eq. (10.33) we define the exponentials

$$e^{Aa^*b^*} = \sum_{n=0}^{\infty} \frac{1}{n!} (Aa^*b^*)^n, \quad \text{etc.}, \tag{10.162}$$

where (choosing orthonormal bases $\{f_j \mid j = 1, 2, \ldots\}$ of $\mathfrak{H}_+$ and $\{g_k \mid k = 1, 2, \ldots\}$ of $\mathfrak{H}_-$)

$$(Aa^*b^*)^n =$$

$$\sum_{\substack{j_1 \cdots j_n \\ k_1 \cdots k_n}} (f_{j_1}, Ag_{k_1}) \cdots (f_{j_n}, Ag_{k_n})\, a^*(f_{j_1}) b^*(g_{k_1}) \cdots a^*(f_{j_n}) b^*(g_{k_n}) =$$

$$\sum_{\substack{j_1 \cdots j_n \\ k_1 \cdots k_n}} (f_{j_1}, Ag_{k_1}) \cdots (f_{j_n}, Ag_{k_n})\, a^*(f_{j_1}) \cdots a^*(f_{j_n}) b^*(g_{k_n}) \cdots b^*(g_{k_1}). \tag{10.163}$$

In case of mixed creation and annihilations operators we define besides the ordinary n-th power

$$(Aa^*a)^n =$$

$$\sum_{\substack{i_1 \cdots i_n \\ j_1 \cdots j_n}} (f_{i_1}, Af_{j_1}) \cdots (f_{i_n}, Af_{j_n})\, a^*(f_{i_1}) a(f_{j_1}) \cdots a^*(f_{i_n}) a(f_{j_n}) \tag{10.164}$$

the "normally ordered" operators

$$:(Aa^*a)^n: \equiv$$

$$\sum_{\substack{i_1 \cdots i_n \\ j_1 \cdots j_n}} (f_{i_1}, Af_{j_1}) \cdots (f_{i_n}, Af_{j_n})\, a^*(f_{i_1}) \cdots a^*(f_{i_n}) a(f_{j_n}) \cdots a(f_{j_1}) \tag{10.165}$$

$$:e^{Aa^*a}: \equiv \sum_{n=0}^{\infty} \frac{1}{n!} :(Aa^*a)^n: \quad \text{etc.}, \tag{10.166}$$

in which all creation operators appear to the left of the annihilation operators. A little calculation shows the following commutation relations for all $f \in \mathfrak{H}_+$ and $g \in \mathfrak{H}_-$

$$[e^{Aa^*b^*}, a(f)] = -b^*(A^*f)\, e^{Aa^*b^*}, \tag{10.167}$$

$$[e^{Aa^*b^*}, b(g)] = a^*(Ag)\, e^{Aa^*b^*}, \tag{10.168}$$

$$[e^{Aa^*b^*}, a^*(f)] = [e^{Aa^*b^*}, b^*(g)] = 0, \tag{10.169}$$

$$[e^{Aba}, a^*(f)] = b(Af)\, e^{Aba}, \tag{10.170}$$

$$[e^{Aba}, b^*(g)] = -a(A^*g)\, e^{Aba}, \tag{10.171}$$

$$[e^{Aba}, a(f)] = [e^{Aba}, b(g)] = 0, \tag{10.172}$$

$$:e^{(A-1)a^*a}: a^*(f) = a^*(Af) :e^{(A-1)a^*a}:, \tag{10.173}$$

$$:e^{(A-1)a^*a}: a(Af) = a(f) :e^{(A-1)a^*a}:, \tag{10.174}$$

$$[:e^{(A-1)a^*a}:, b^*(g)] = [:e^{(A-1)a^*a}:, b(g)] = 0, \tag{10.175}$$

$$:e^{(1-A)bb^*}: b^*(g) = b^*(A^*g) :e^{(1-A)bb^*}:, \tag{10.176}$$

$$:e^{(1-A)bb^*}: b(Ag) = b(g) :e^{(1-A)bb^*}:, \tag{10.177}$$

$$[:e^{(1-A)bb^*}:, a(f)] = [:e^{(1-A)bb^*}:, a^*(f)] = 0. \tag{10.178}$$

Notes

Chapter 1

Section 1.1. The Klein-Gordon equation was already known to E. Schrödinger in 1926 but he found it gave the wrong solutions to the hydrogen problem. ("Z.B. führt das relativistische Keplerproblem, wenn man es genau nach der eingangs gegebenen Vorschrift durchrechnet, merkwürdigerweise auf halbzahlige Teil quanten." [407], p. 372). Subsequently, this equation was rediscovered by several authors [104, 145, 146, 180, 272, 277]. The Dirac equation appeared first in Dirac's paper [113]; see also [114]. Sect. 1.1 follows essentially the presentation in Dirac's famous book [Di 76]. Similar considerations can be found in nearly any physics book dealing with the Dirac equation. A still very readable introduction is Pauli's article for Handbuch der Physik [358], or [Pa 90]. Concerning the square-root Klein-Gordon equation Dirac remarks: "...although it takes into account the relation between energy and momentum required by relativity, (it) is yet unsatisfactory from the point of view of relativistic theory, because it is very unsymmetrical between p_0 and the other p's, so much so that one cannot generalize it in a relativistic way to the case when there is a field present." ([Di 76], p.255). The bad behavior under Lorentz transformations, when external fields are introduced by "minimal coupling", is discussed in more detail in [434]. More about the history of the Dirac equation can be found in the book [SW 72] and in [323, 324, 325].

Section 1.2. Some standard books on linear functional analysis as it is needed for quantum mechanics are, for example, [Ka 80, RS 72, We 80]. There are several excellent textbooks on the mathematical foundations of quantum mechanics, e.g., [Th 79]. More details on the material in this section can be found in [Pr 71].

Section 1.3. The association of observables with operators is the one made implicitly in most textbooks. Problems arising with the position observable will be discussed in Sects. 1.7 and 1.8. The choice of the standard position operator lets $|\psi|^2$ become the position probability density. This was also an implicit motivation for our choice of Hilbert space: A normalized state describes a particle which is "somewhere" in space with probability one.

Section 1.4. The Foldy-Wouthuysen transformation owes its name to [148]. In this paper the authors aim at finding the transformation in presence of external fields. This results in a formal perturbation series for the Dirac operator in the parameter $1/c^2$. We shall not follow this approach here because even now there is no rigorous formulation of this method (see the notes to Sect. 6.1). For free particles the diagonal form of H_0 already appears in [369]. Further details and references are given in the notes to Sect. 5.6.

A detailed proof of the domain properties, the self-adjointness and the spectrum of the Dirac operator (Sect. 1.4.4) is contained in [We 80], Sect. 10.6; see also [Ka 80], Sect. V.5.4.

The interpretation of the negative energy states usually involves the notion of the "Dirac sea" which consists of the negative energy continuum filled up with electrons. The positrons then appear as "missing electrons with negative energy", i.e., as holes in the Dirac sea. This heuristic explanation has surely inspired the quantum field theoretic point of view which today is commonly accepted in the physics community despite the mathematical difficulties it presents. We did not present the "hole theory" at this point because we want to stay conceptually within the usual quantum mechanics as long as possible. An appreciation of the hole

theory and its impact on physics is contained in [475]. The difficulties with negative energies have inspired various new approaches to relativistic quantum mechanics among which we mention a stochastic interpretation [368], an approach using an algebra of pseudodifferential operators [95, 96], and a formulation in terms of a proper time parameter which is proposed for spin-1/2 particles in [363, 377]; see also [126]. The proper time formalism is related to ideas used by Schwinger [411] for calculating propagators in the presence of external fields.

The reader might wish to compare the spectral transformation of the Dirac operator given in Sect. 1.4.5 with that for the free Schrödinger operator which is given, e.g., in [AJS 77], Eq. (5.95). The spectral transformation U_{sp} is not widely used because it is simpler to use the "almost spectral transformation" $\mathcal{W}$ of Sect. 1.4.1 [386].

Section 1.5. A discussion of the time evolution kernel in the spirit of this section is given in [367]. The most important distributions appearing in this context are discussed in the appendix. For details see [Ja 69], Sect. IV, and [386]. The integral kernel of the operator $\exp\{-t\sqrt{p^2+m^2}\}$ is calculated, e.g., in [290], Eq. (2.13), from where we obtained our expression for $K(t,\boldsymbol{x})$ by analytic continuation.

We did not mention the path integral representations of the evolution kernel (propagator). There are three different approaches to path integrals for particles with spin. These constructions are based on random walk in a spinor space [239], representations of the homotopy group (paths on multiply connected spaces) [410] (see also [112]), and on holonomy [35, 364].

Section 1.6. Breit [69, 70] was the first to notice that Dirac's velocity operator $c\boldsymbol{\alpha}$ has the eigenvalues $+c$ and $-c$. The Zitterbewegung was discovered by Schrödinger [408] and investigated subsequently by many authors, e.g., [31, 34, 196, 224, 227, 244, 361]. Concerning the older literature see the review article by Hönl [226]. The asymptotic damping of the Zitterbewegung according to the Riemann Lebesgue lemma can be found in [292]. The notation for the operators $\boldsymbol{F}$ and G is that of Enss and Thaller in [129], where the behavior of these operators is investigated in the presence of external fields, see also Sect. 8.2.4. Ref. [129] also contains a more general result on the invariance of the domain of the position operator. For the Schrödinger equation the non-invariance (!) of the domain of $\boldsymbol{x}$ is discussed in [371]; see also [128]. General techniques for defining commutators on invariant domains are introduced in [155]; see also the discussion of Nelson's theorem in Sect. 2.3.

Section 1.7. Concerning the huge amount of literature on relativistic observables, in particular the possible choices of position operators, we refer to the review article by Kálnay [283]. Observables restricted to the positive energy subspace are considered in [369]; also the Newton-Wigner operator appears in this paper for the first time. Newton and Wigner [340] take a different point of view. Their basic assumption is that localization in a finite region is a property which a relativistic particle with positive energy can have. They derive their position operator as the unique operator for which this localization property satisfies the assumptions of Sect. 1.7.3. Their approach was put on a sound mathematical basis by Wightman [474]. This reference contains the proof of Theorem 1.5 (in fact of a more general result).

Section 1.8. The result on causality and localization in final form is due to Hegerfeldt and Ruijsenaars [208]. In their paper a slightly more general theorem is proven; there are also similar results for scattering states in the presence of external fields. A similar causality problem can be shown to arise for exponentially decaying wavepackets [207]. Instantaneous spreading from compact regions was already shown in [206] for quite general notions of localization; cf. also [360]. Of course this result also holds for nonrelativistic systems, where e.g. $\lambda(p) = p^2/2m$. For the Newton-Wigner operator and some other notions of localization this phenomenon has been known for some time [144, 158, 362]. In fact, Newton and Wigner [340] had already noticed the missing Lorentz invariance of their notion of localization, which is a related problem: Take a particle which is NW-localized in a finite region of space with respect to a particular Lorentz frame of reference. In general, the particle will not be localized in a finite region with respect to another Lorentz frame related to the first by a boost.

The detection probability of acausal events associated with the Newton-Wigner localization was estimated by Ruijsenaars [391], who found that this probability is practically negligible. An explicit example is given in [384]. The remarks concerning the compact support of wavefunctions are from [445]. More recently, the assumptions, implications and meaning of Hegerfeldt's "paradox" were discussed in [119, 255] with the result that the effect cannot be used to transmit signals.

Section 1.9. The results in this section are not specific to the Dirac equation. It is a quite general phenomenon that the quantum mechanical motion is for large times close to the motion of an ensemble of classical particles with a statistical distribution of initial positions and momenta. More about stationary phase methods can be found, e.g., in [RS 79], Appendix 1 to XI.3, and in [Pe 83], Chap. 1.3. A more general version of Theorem 1.8 is due to Hörmander [228].

Chapter 2

Section 2.1. Concerning the definition of Lorentz transformations and the underlying principles we mention the paper of Berzi and Gorini [50], in which a derivation of Lorentz transformations is based on the principle of relativity, the homogeneity of space-time and the isotropy of space. This paper also contains references to earlier work on Lorentz transformations. In particular, Zeeman [503] has shown that the Lorentz transformations together with dilations form the group of causal automorphisms of space time. A one-to-one mapping τ of the Minkowsky space M onto itself is called causal if $x < y :\Leftrightarrow (x^0 < y^0$ and $\langle y-x, y-x\rangle > 0)$ is equivalent to $\tau(x) < \tau(y)$, for all $x, y \in M$ (neither linearity nor continuity of τ is assumed). Zeeman proved that any causal automorphism is of the form $\tau(x) = \Lambda x + a$, with some real r, four-vector a, and some Lorentz transformation Λ with $\Lambda^{00} \geq 0$ (for this result dim $M > 2$ is crucial).

In the examples of Sect. 2.1.3 and throughout the book we use the active point of view. This means that a Lorentz transformation changes the state of the physical system under consideration without changing the state of the observer. An alternative but equivalent interpretation is the Lorentz transformation as a change of the observer: After the transformation the system is still the same but it is seen from a different inertial frame. This "passive" point of view would result in a different sign for the velocity or the rotation angle in the matrix Λ. Similarly, while $\exp(-iHt)$ is the time evolution of a quantum particle as seen from an observer who changes his position in time (because he is getting older), an active time translation of a state Ψ is given by $\exp(+iHt)\Psi$.

Section 2.2. A good explanation of the relativistic invariance of a quantum system is given in [Si 68]. As a general reference for further reading on this and related topics we also recommend [Va 85]. The Wigner-Bargmann theorem was first formulated in Wigner's book ([Wi 31], pp. 251–254; [Wi 59], pp. 233–236), but there the theorem is not proved in full detail. The complete proof is due to Bargmann [29]. More on the history of this theorem and further references can be found in [419].

Section 2.3. The existence of a dense invariant domain for a unitary representation of a Lie group has been shown by Gårding [199]. The reader should compare our proof in Sect. 2.3.1 with the proof of Stone's theorem (see for example [We 80], Sect. 7.6). The counterexample in Sect. 2.4 is due to E. Nelson. It is discussed in [RS 72], Sect. VIII.5. Nelson's theorem of Sect. 2.4 is proved in [332]. See [155] for related results. In Sect. 2.5 we prove the essential self-adjointness of Q using Konrady's trick, which is described in detail in [RS 75], pp. 174–176. In this book one can also find further possibilities of proving this result, analogous to the various ways of proving essential self-adjointness of the anharmonic oscillator Hamiltonian.

Section 2.4. It was again Bargmann who solved the problem of lifting projective representations [28] of Lie groups and applied these results to the Poincaré group. A modern but very abstract proof of the results in Sect. 2.4.2 can be found in [Si 68], Sect. 2.

Section 2.5. This section provides an example for the use of Clifford algebras in the theory of representations of Lie groups. The classical approach presented here is sufficient for our purposes. See [Rü 70] for additional information on the group SL(2) and its representations; for a classical treatment of spinors see [Co 53]. Among the more recent books on the Poincaré group we mention [KN 86]. A modern presentation of the deep results on "spin geometry" (which are beyond the scope of this book) can be found, e.g., in the book of Lawson and Michelson [LM 89]. The elementary proof of Lemma 2.25 is due to Pauli [357]; see also [179].

The formulas in the Appendix are obtained by lengthy calculations. See [304] from where we took in particular Eq. (2.218) in Sect. 2.D.

Chapter 3

Section 3.1. Wigner gave a classification of the irreducible representations of the Poincaré group (the "inhomogeneous Lorentz group") in his classic paper [477]; see also [30]. This was the first analysis of a group with no non-trivial finite dimensional unitary representations. Further studies of Poincaré transformations including the discrete transformations were done in a series of papers by Shirokov [421, 422, 423, 424, 425] and Joos [249]. See [182] for some recent work on that subject. The mathematical theory of induced representations is mainly due to Mackey [305], [Ma 68]. A systematic theory of induced projective representations in the presence of antiunitary operators has been formulated by Parthasarathy [354] and applied to the Poincaré group. Induced representations and their application to physics are also treated in [BR 86]. A physics book on this subject is [Oh 88].

Sections 3.2–3. The presentation of the material in these sections has been inspired in part by [341]. Almost all the results have an analog for particles with spin other than 1/2. Details concerning the representations for particles with higher spin can be found in the literature, for example in the books [Co 53, VW 77, BR 86, Oh 88]. Classical papers on relativistic wave equations are [30, 478]. See also the references in [Co 53]. Various representations of the Poincaré group and the meaning of the wave equations are investigated in [471]. However, the higher spin equations have gone a little bit out of fashion, since Velo and Zwanziger observed that in some cases the wavefunctions of particles with spin ≥ 1 propagate faster than light in an external electromagnetic field [452, 453]. The Foldy-Wouthuysen transformation can be defined for particles with any spin as the transformation linking the covariant realization with the Wigner realization [303]. A new interpretation of the Dirac equation, based on an analysis of the representations of the Poincaré group in stochastic phase space is attempted in [368].

Section 3.4. The results in this section are essentially due to Wigner [477]; see also [425, 479, 480].

Chapter 4

Section 4.2. Scalar potentials which increase as $|\boldsymbol{x}| \to \infty$ (e.g., like a harmonic oscillator) have been used as models of quark confinement [234, 373, 374, 375, 420, 427, 433, 441]. Increasing electrostatic potentials are known to give a continuous scattering spectrum with the Dirac equation (see Sects. 4.6.6 and 4.7.1). The potential describing anomalous magnetic moment coupling was introduced by Pauli; see [358], p. 157. The anomalous electric moment terms are treated in [140, 396].

Section 4.3. The problem of self-adjointness of Dirac operators has a long history. In fact, for some time most of the mathematical investigations of Dirac operators dealt with this and related questions [254]. Theorem 4.2 was obtained by Kato in his book [Ka 80], Sect. V.5.4.

Arai [17, 18] showed that Kato's result is optimal for matrix-valued potentials (cf. the remark in Sect. 4.3.1). It follows from results of Weidmann [467] that the Dirac operator with a Coulomb potential γ/r is essentially self-adjoint if and only if $\gamma \leq c\sqrt{3}/2$ (a proof of this fact had already appeared in unpublished lecture notes of F. Rellich in Göttingen, 1953, "Eigenwerttheorie partieller Differentialgleichungen"). These proofs make use of the spherical symmetry of the potential. Results of this type cannot be shown with the help of the Kato Rellich Theorem, because the relative bound of $1/r$ with respect to H_0 is exactly two [355]. The first part of Theorem 4.4, namely that $|\phi_{\rm el}(x)| < c\sqrt{3}/2r$ implies essential self-adjointness of the Dirac operator $H_0 + \phi_{\rm el}\mathbf{1}$, was proved by Schmincke [404]. In this case the domain of the self-adjoint extension is just the domain of H_0, as shown in [286, 287]; see also [19, 265]. A new proof of this result is given in [456]. For the Coulomb potential γ/r the Dirac operator is not essentially self-adjoint if $\gamma > c\sqrt{3}/2$ [331, 467] (see also Sect. 4.6.6). But there are several self-adjoint extensions. Schmincke [403] and Wüst [490, 491, 492] investigated a self-adjoint extension in the case $\gamma < c$, which is distinguished by the property that all states in the domain of Dirac operator have finite potential energy. On the other hand, Nenciu [333, 334] required that all states in the domain of the self-adjoint extension have finite kinetic energy. Klaus and Wüst showed that the self-adjoint extensions considered by Wüst and Nenciu are the same [270] and have the same essential spectrum as the free Dirac operator [271]. So all these authors have contributed to the second part of Theorem 4.4. More recently, Vogelsang investigated distinguished self-adjoint extensions for larger coupling constants [457, 458]. In this case, however, the physical meaning of the extensions is less clear [331] (for $\gamma > c$ or $Z > 137$ the radially symmetric problem displays an oscillatory limit circle case), in particular, the behavior of the eigenvalues is ambiguous [79]. The breakdown of self-adjointness at high nuclear charges is related to a "collapse to the center" [366], allowing the particle to reach the singularity in a finite time.

Most of the investigations mentioned so far dealt almost exclusively with electrostatic potentials. More general matrix-valued potentials are considered in [333] and in a series of papers by Arai and Yamada [17, 18, 19, 498]. They prove essential self-adjointness, the existence of distinguished self-adjoint extensions and invariance of the essential spectrum for a class of matrix-valued potentials. Ref. [18] contains a generalization of Theorem 4.4 to a matrix potential of the form $\beta\phi_{\rm sc} + \phi_{\rm el} + i\beta\alpha \cdot x\phi_{\rm am}$ with a $1/r$-singularity. Potentials of this type occur in the description of particles with anomalous magnetic moments. In a Coulomb field, however, a particle with an anomalous magnetic moment would feel a $1/r^2$ singularity; see Sect. 5.3.

The essential self-adjointness of the Dirac operator on a domain of functions with support away from the origin (Theorem 4.2) shows that one cannot introduce relativistic point interactions in three dimensions in the same way as in the nonrelativistic theory. The Schrödinger operator is not essentially self-adjoint on that domain, and point interactions can be associated to its self-adjoint extensions [AGHH 88]. In one dimension, however, point interactions can be defined also for the Dirac operator; see [170]. Further treatments of the relativistic δ-potentials can be found in [116, 117, 120, 137]. Periodic point interactions serve as an explicitly soluble model in solid state physics; see [108, 109, 110], where relativistic effective masses are calculated.

In 1972, Jörgens [251] proved essential self-adjointness of the Dirac operator for all matrix potentials with elements in $L^3_{\rm loc}$, which shows that only the local behavior of the potential affects the question of essential self-adjointness, and that the smoothness required in Theorem 4.3 is not really necessary. The proof of Theorem 4.3 is a slight generalization of the proof for Dirac operators with magnetic fields given in [212], Proposition 1.1. A similar result appears in a paper of Chernoff [89]. It is proven there with a different method, which can be used for Dirac operators on Riemannian manifolds; see also [90, 483]. In one dimension or for radial Dirac operators Theorem 4.2 also follows from [133], p. 538, and [467], Theorem 5.1.

Many center Coulomb potentials are treated in [41, 203, 257, 265, 334, 457].

Section 4.4. In this section we consider only smooth gauge transformations. Gauge transformations of singular magnetic vector potentials are discussed in [289] in the context of

Schrödinger operators. The gauge invariance of the Dirac equation is treated in [390] in the context of the implementation of scattering theory in Fock space. The remark after Lemma 4.11 is due to Arai [18].

Section 4.5. In 1928, O. Klein discovered oscillatory solutions inside a potential step where a nonrelativistic solution would decay exponentially [273]. He determined the reflection and transmission coefficients for a rectangular step potential $\phi_0\theta(x)$. Subsequently F. Sauter investigated Klein's paradox for a smooth potential, which gave the same qualitative result, but with a much smaller transmission coefficient [398]. Klein's paradox is also described in the book of Bjorken and Drell [BD 64], but in their "plane wave treatment" of the problem is a serious error, as was pointed out first by Dosch, Jensen and Müller [121]. Bjorken and Drell considered a solution as "transmitted" which in fact corresponds to an incoming particle. Obviously they neglected the fact that the velocity of the transmitted wave is opposite to its momentum (which is typical for negative energy solutions, cf. Sect. 1.5, and was already noted by Klein). They concluded that more is reflected than comes in, which is incorrect and contradicts, e.g., the unitarity of time evolution. Unfortunately the same error is contained also in many papers which treat that subject on a formal level. The most comprehensive and mathematically complete analysis of the Klein paradox up to now has been given by Bongaarts and Ruijsenaars [59, 60]. Their goal was to treat that phenomenon in the context of quantum field theory. They arrived at the negative conclusion that the scattering operator for that situation cannot be implemented in the Fock space.

The one-dimensional Dirac operator with a step-like potential is of certain interest in solid state physics, where it can be used to model the transition between two periodic structures [110].

Scalar step potentials occur as soliton solutions of the mKdV equation (Chap. 9); see the Notes to Sects. 9.4 and 10.3.

Section 4.6. The angular momentum decomposition of the Dirac equation is treated in most textbooks, but usually only at a formal level. An extensive and rigorous discussion is contained in [376]. The separation of Dirac operators in other coordinate systems is carried through in [93, 402]. The partial wave expansion in the presence of a magnetic monopole is considered in [262, 489]. The radial Dirac operator for an electrostatic potential is treated, e.g., in [71, 198, 381]. More general first order systems of ordinary differential equations are investigated in [467, 468] by methods similar to those for Sturm-Liouville problems. These results can be applied immediately to the radial Dirac operator. Lemma 4.15 is proved in [18]. The absence of eigenvalues for increasing spherically symmetric electrostatic potentials is shown in [130, 135, 204, 216, 447]. Further results which are relevant for the radial Dirac operator are contained in [201, 215]. The radial Dirac operator with a scalar potential is treated in [433] (see also Sect. 4.2.). This is a special case of a supersymmetric system; see Chap. 5. A systematic study of the spectral theory of one-dimensional Dirac and Sturm-Liouville operators allowing a detailed comparison of all aspects is the goal of the book [LS 91].

Section 4.7. Theorem 4.20 and its proof is given in [132, 134]. In the latter paper it is shown that essentially the same proof allows one to include an additional magnetic vector potential which in the spheres B_n can be approximated by a gradient vector field in the mean square sense. The paradoxical result that the spectrum in the relativistic case consists of the whole real axis but is discrete in the nonrelativistic case poses the question in which sense these situations are connected in the nonrelativistic limit $c \to \infty$. Titchmarsh [448] studied the Dirac operator with the electrostatic potential $\lambda|x|$ and showed that the analytic continuation of the Green function has poles which for large values of c are close to the eigenvalues of the corresponding Schrödinger operator. The question has also been treated by Veselić [454], who showed for a large class of potentials bounded from below that the transition from the continuous spectrum to a discrete spectrum can be interpreted in terms of a spectral concentration. Hence it is clear that the Schrödinger bound states are turned into resonances for the Dirac operator. This phenomenon is also treated by G. Hachem [200] for a linearly increasing electromagnetic field.

The diving of Dirac eigenvalues into the lower continuum at some critical value of the coupling constant is another source of resonances associated with the Dirac equation. This phenomenon, which has no nonrelativistic counterpart, is of particular interest for modeling "spontaneous pair creation" in the field of superheavy nuclei generated during heavy ion collisions, see Chap. 9.

The techniques of describing resonances for the nonrelativistic Schrödinger equation are based on the method of complex scaling due to Aguilar and Combes [5], [RS 78], Sect. XII.6, and on the semiclassical analysis of Helffer and Sjöstrand [214]. The two methods, if both can be applied to a potential, give the same resonances [210]. Both approaches were applied to the Dirac equation. R. Weder [465] and P. Seba [413] generalized the method of complex scaling to Dirac operators. B. Parisse [352, 353] gave a definition of resonances in the semiclassical limit and proved that the dimension of the space of resonance functions is even. Resonances for the Dirac equation as poles of an analytically continued S-matrix have been investigated further by Balslev and Helffer [26] with the help of stationary scattering theory. Their method is based on an extension of the limiting absorption principle for Dirac operators (see also [455, 458], and in particular [65]).

The relativistic virial theorem was proven for the Dirac equation for the first time in [8], p. 247ff. A more general version of Theorem 4.21 has been obtained by Kalf [252]. His conditions include the Coulomb singularities described in Theorem 4.4. At a more formal level the relativistic virial theorem is treated also in [68, 178, 185]. As in nonrelativistic quantum mechanics, the virial theorem can be used to prove the absence of bound states in the continuum [253]. A more powerful method is based on Carleman inequalities and the unique continuation property [47, 48, 49, 63, 245]. The unique continuation property states that solutions of the equation $H\psi = \lambda\psi$ that vanish on an open subset vanish identically. In particular, any eigensolution with compact support is identically zero. In [63] it is shown that the unique continuation property holds for Dirac operators $H_0 + V$ in three dimensions with $V \in L^{7/2}_{\mathrm{loc}}$.

The spectrum of the Dirac operator — at least for potentials that are small at infinity — is expected to consist of finitely degenerate eigenvalues in the gap $(-mc^2, mc^2)$, with possible accumulation points only at $\pm mc^2$ and an absolutely continuous spectrum outside. This is also shown for a large class of potentials in [65] by a method based on the Mourre estimate (see also [64] and the references therein).

Further results on the number of eigenvalues can be found in [266, 278, 436]. New and precise estimates are obtained by Ivrii [231]. The behavior of the eigenvalues near the threshold to the continuous spectrum was investigated in more detail by Klaus [267].

In recent years the semiclassical point of view has become increasingly important also for the spectral theory of Dirac operators; see, e.g., [213] (in particular pp. 266–267) and [231, 232, 233], which are concerned with the counting of eigenfunctions in an interval. The book [Le 90] contains a section on the asymptotic distribution, as $\hbar \to 0$, of the discrete eigenvalues of Dirac operators. Semiclassical methods (WKB) are also employed in [317, 352, 462], treating the double (multiple) well problem. The classical limit of the Dirac equation was treated in some detail also by K. Yajima [494, 495, 496].

Chapter 5

Section 5.1. Supersymmetry has its origin in particle physics and quantum field theory [472] as a symmetry between bosons and fermions; see [Fe 85] for a commented collection of relevant papers. E. Witten initiated studies of systems with a finite number of degrees of freedom [481]; for some early applications to quantum mechanical models see, e.g., [98, 263, 395] and the references therein.

In this chapter we present "$N = 1$ supersymmetry", also known as "factorization" or "commutation methods" [106, 405]. As a method for factorizing differential operators some "supersymmetric ideas" can be traced back literally for centuries — not under this name, of

course. A historical review is given in [429]. Meanwhile there are many examples of the use of supersymmetric methods in differential geometry and quantum mechanics. Some applications of supersymmetry to differential geometry can be found, e.g., in [61, 184, 378, 482], [Gi 84] (see the references to Sect. 5.7). Here the index of the Dirac operator is of special importance, because it provides a link between the analysis of operators and topological properties of spin manifolds. Special quantum mechanical systems which have been studied with supersymmetric methods include quantum mechanics in a magnetic field or Yang-Mills-Higgs fields and the Coulomb problem (see the Notes to Sects. 5.5, 5.11 and Chapter 7).

Section 5.2. The standard representation described in Sect. 5.2 was used by Cirincione and Chernoff [92] in their treatment of the nonrelativistic limit (Chapter 6). The basic commutation results in Sect. 5.2.3 are proven in [106] by different means. Nelson's trick in connection with the polar decomposition is described in [443]. For some background on closed operators we refer to the books on linear operators in Hilbert spaces, e.g., [Ka 80, We 80]. The properties of the matrix elements of unitary operators in the standard representation are described in some detail in Sect. 10.3.2.

Section 5.3. Theorem 5.31 is taken from [173], where it is applied to the problem of electrons with an anomalous magnetic moment in a Coulomb potential. Implicitly, the results of Sect. 5.3.2 were already contained in [467] (see also [468]). The first rigorous treatment of Dirac particles with anomalous magnetic moments in singular potentials is due to Behncke [39, 40, 41], who proved the essential self-adjointness and some spectral properties of the Dirac operator with techniques from the theory of ordinary differential equations. These results are extended to multi-center problems in [257]. Possible resonances in the electron–positron problem due to anomalous moments are discussed in [32, 33]. The occurrence of resonances seems to be indicated by the shape of the effective (energy-dependent) potential arising after an iteration of the Dirac equation with anomalous magnetic moment.

Sections 5.4 and 5.5. The supersymmetric structure of the Dirac equation is implicit in many investigations of the special situations listed in this section, see, e.g., [321, 385, 450, 464]. Writing the Klein-Gordon equation as a first-order system is a very natural procedure and had already been suggested for a transparent interpretation by Feshbach and Villars [141]. A point of view which is similar to our approach is taken in [466]. Among the further mathematical literature on the Klein-Gordon equation we mention [300, 329, 401]. Unfortunately, we have no occasion to discuss Dirac-type operators over Riemannian manifolds, which also provide us with realizations of supersymmetric Dirac operators [92]; see the Notes to Sect. 5.7.

Section 5.6. Our treatment of the Foldy-Wouthuysen transformation differs from those usually found in the textbooks, e.g., [Das 73, Me 70]. The Foldy-Wouthuysen (FW) transformation was introduced in an effort to understand how the Dirac theory approaches its nonrelativistic limit [148]. Independently, Pryce [369] and Tani [439, 440] found the same transformation in a different context; see also [247]. Foldy used this transformation for a systematic "canonical" description of covariant wave equations [147]; another variant was proposed in [88]. At that time the canonical form of the Dirac equation after an FW transformation was considered to have significant conceptual advantages. This and the beautiful interpretation of the relativistic correction terms arising by the FW method elicited considerable interest in this transformation; see the references in the review article of deVries [111]. There were generalizations [131, 279] and applications to some of the special situations listed in Sect. 5.5 [87, 348]. The FW transformation has even been considered as a Lorentz transformation. This is not quite correct. It is not a Lorentz transformation, but in momentum space the FW transformation is related to a Lorentz transformation to the rest frame, because it gives just the relation between the covariant representation and the Wigner representation of Lorentz transformations [303] (see Sect. 3.3). The generalization of the FW transformation to supersymmetric quantum mechanics is given in [443]. A further generalization is obtained in [183] and [75]. See also [37, 319] for some related work.

The Cini-Touschek transformation [91], which had already been given by Mendlowitz [312], has been used for a discussion of the ultrarelativistic limit $c \to 0$ of the Dirac equation. Other related transformations are given, e.g., in [38, 42, 311, 321, 397, 463].

Section 5.7. In this book we describe the index theory of Dirac operators on an elementary but abstract level. In the literature, the index has been studied most extensively for Dirac operators on compact manifolds. Some of our results apply to this case as well, because Dirac operators on manifolds also have the structure of the abstract Dirac operators considered here, see, e.g., [92]. In this context appears the famous Atiyah-Singer index theorem (see, e.g., [BB 85, LM 89]), which links the index of Fredholm operators with certain topological invariants ($\hat{A}$ genera). Hence Dirac operators have become an important tool in modern geometry. Unfortunately, these topics are beyond the scope of this book. In quantum mechanics, index theory has been applied by Callias [82], who derived an index formula for the Dirac operator with an external Yang-Mills-Higgs field (Sect. 5.11.3). This problem requires the discussion of Dirac operators on open (i.e., non-compact) manifolds [10, 62]. Some important investigations studying this problem with respect to applications in quantum theory are [9, 149, 150, 153, 217, 218, 240, 241, 242, 243, 297, 299, 344, 470], see also the review article of Niemi and Semenoff [343]. Important mathematical contributions to index theory on open spaces are further given in [10, 11, 13, 14, 16, 45, 55, 73, 175, 184, 320, 378, 426]; see also the books [Gi 84, Ro 88]. The Notes to Sect. 5.11 contain references for the index problem in magnetic fields and the Yang-Mills-Higgs fields describing fermion monopole and fermion vortex interactions. The index has also been studied with the help of supersymmetric scattering theory (Chap. 8), e.g., [15, 56, 61, 77, 149].

Section 5.8. The connection between index theory and Krein's spectral shift function was found in [56, 57, 159] and in [149]; see also [61]. Our presentation mainly follows [171]. For the connection of Krein's spectral shift function with scattering theory, see also Sect. 8.1.3. The spectral shift function is related to Fredholm determinants, or modified Fredholm determinants; see Sect. 5.10. The axial anomaly is the origin of the breaking of the chiral symmetry of the Lagrangian in gauge field theory with fermions; see, e.g., [67, 82, 506]. We recommend [393] as an elementary introduction to anomalies and their occurrence in quantum field theory from a mathematical point of view. For more references and applications to physics see [BW 85]. We have introduced the Atiyah-Patodi-Singer η invariant or "spectral asymmetry" following the definition of [56], which is very convenient in the present framework but differs slightly from earlier definitions [21, 125].

Section 5.9. The topological invariance of the Fredholm index is a classical result; see, e.g., [Ka 80], Sect. IV.5.3. Theorem 5.28 is taken from [171], where a slightly more general result is proven. This paper also contains the derivation of Eqs. (5.182) and (5.183) from the assumptions of the theorem. A similar result holds for the invariance of the resolvent regularized index; see [56], where these results are applied to various physical problems.

Section 5.10. For the connection of Krein's spectral shift function and Fredholm determinants, see, e.g., [274], [BW 83]. Fredholm determinants are used to calculate the index of one-dimensional Dirac operators in [159] and [56]; see also Sect. 9.4.2. For higher dimensional systems, modified Fredholm determinants [Si 79] have to be used to overcome the singularity of the Green function for $x = y$. This idea was used in [56] to calculate the index of the Dirac operator in a two dimensional magnetic field. For background information on (modified) Fredholm determinants, see, e.g., [GK 69, Si 79] and [275].

Section 5.11. The index of the Dirac operator in one space dimension with a scalar potential is investigated in [7, 56, 66, 82, 159, 217, 218, 229, 298, 431]. We give an explicit calculation based on stationary scattering theory (Jost function techniques) in Sect. 9.4.2. This approach follows [159] and [56]. For the two dimensional magnetic field problem we refer to [6, 56, 57, 160, 171, 235, 264]; see also Sect. 7.2.3 and [CFKS 87] (in particular Ch. 6.4). The difference between the L^2 index and the Witten index has been related to the η invariant in [12]. Callias' index formula is obtained in [82]; his results and methods are discussed and generalized, e.g.,

in [11, 16, 62]. As further examples of index calculations for Dirac operators we mention the fermion-vortex system [223, 238, 470], the Yang-Mills-Higgs monopole [82, 342, 351, 469, 501] and the instanton background field [72, 237]. The above examples are also discussed in the review article [343].

Chapter 6

Section 6.1. Pauli was the first to study the connection between the Dirac theory and its nonrelativistic approximation by separating the "large" and "small" components of the wavefunction [358]. For the early literature on this subject, see [51] or [BS 59]. We mention [417], where Eq. (6.73) is derived for a special case using formal expansions of wavefunctions. Pauli's method was developed further in [302], still at a formal level, and more rigorously by Schoene [406], who investigated in particular the convergence of the solutions in the nonrelativistic limit. The spherically symmetric case is studied rigorously by Titchmarsh in [449], spherically symmetric scattering problems are treated in [379, 380].

A completely different approach was taken by Foldy and Wouthuysen [148], who developed a formal scheme of applying successively Foldy-Wouthuysen (FW) transformations in order to obtain operator perturbations of the nonrelativistic Pauli operator H_{P} of order $1/c^2$ and higher. In principle, this method gives an expansion of the Dirac operator into powers of $1/c^2$. This method became the most popular one [111] and can be found in most textbooks on relativistic quantum mechanics. However, even the first order perturbation of H_{P} is so singular that it destroys completely all spectral properties of H_{P}. For example, all bound states of H_{P} dissolve into a continuous spectrum [167]. Mathematically, one is actually forced to consider H_{P} as a small perturbation of the $1/c^2$ term. Adding higher order corrections makes the situation even worse. The divergence of the Foldy-Wouthuysen series for a special case is also noted in [54]. Nevertheless, the first order corrections of eigenvalues obtained in this formal way are correct and agree with the expressions obtained in Theorem 6.9. Therefore it should be clear that the "operator perturbations" cannot not be taken literally. The FW corrections are not meaningful in an operator sense and should only be considered if applied to wavefunctions with energies in a neighborhood of the bound state energy under consideration. We refer to [183] for further clarification. Attempts to understand the status of the FW method are also made in [75, 163, 167, 282].

The resolvent approach which is presented here was suggested first by Veselić [454]. He derived the analyticity of the resolvent by perturbation theoretic arguments. A similar approach was used by Hunziker [225] for a larger class of potentials. The explicit expansion of the resolvent into powers of $1/c$ was obtained for the first time in [164] and [166]. The last paper also contains estimates on the convergence radius of the expansion. The convergence of solutions of the Dirac equation in the nonrelativistic limit is also considered in [92, 330].

Section 6.2. For the complicated systems in atomic and molecular physics the calculation of relativistic corrections is of great practical importance. Many-body analogues of the Dirac equation can be used to deduce formulas for the first-order relativistic corrections. It is perhaps not meaningful to calculate higher-order corrections or the exact solution of the many-particle Dirac equation, because in higher orders one expects contributions from QED which cannot be described by the Dirac equation alone. More on the applications of Dirac-type equations in many-particle systems can be found, e.g., in the books [Das 73], [Ma 83], [Py 86], or in [280]. As a review of the various methods used in the perturbation theory of relativistic corrections we recommend [281, 282].

The problem of finding relativistic corrections to bound state energies was solved rigorously and for a large class of potentials by Gesztesy, Grosse and Thaller [166]. Formula (6.73) was known before only in some special cases [417, 449]. The result is folklore in the form of Eq. (6.79), although the derivation of (6.79) had been based on heuristic and formal arguments [148] (see also the discussion of the Foldy-Wouthuysen method in the notes to Sect. 6.1). The approach in [166] uses perturbation theory of resolvents and the explicit $1/c^2$

expansion to obtain the result (6.73), but only in the case of nondegenerate eigenvalues. The analyticity of eigenvalues had already been stated by Hunziker [225] without giving the proof in the degenerate case. Theorem 6.8 for degenerate eigenvalues was proven first by Wiegner [473]. Some essential simplifications of the method have been obtained by Grigore, Nenciu and Purice [183], who independently gave a proof in the degenerate case. Our presentation here follows closely their elegant exposition.

The method of finding relativistic corrections to nonrelativistic quantities by the resolvent method is extended to the Breit-Fermi Hamiltonian for two-fermion systems in [165]. One dimensional Dirac operators with a periodic potential are considered in [74]. In this case the first order corrections of the energy band edges are again given by Eq. (6.72).

Relativistic corrections for the scattering matrix are derived in [75]; the scattering amplitude is considered in [183]. For exponentially decaying potentials the holomorphy of the scattering matrix at fixed energy is derived in [75] in the framework of Kuroda's stationary scattering theory. Again, the first order correction to the nonrelativistic S-matrix can be obtained explicitly. Unfortunately the resulting expression is too complicated to be reproduced here. Ref. [183] requires a weaker decay of the potential, which implies only differentiability of the scattering amplitude instead of holomorphy. This is, however, sufficient to obtain first order corrections of the scattering amplitude. The nonrelativistic limit of stationary scattering theory and the analyticity of resonances in $1/c$ is investigated in [26]. Among earlier results on the nonrelativistic limit of Dirac scattering theory we mention the proof of strong convergence of wave operators as $c \to \infty$, in [493].

The explicit form of the correction terms arising from the FW method and given in Eq. (6.79) has always been a strong argument in favor of the Dirac equation. A more detailed discussion of their physical interpretation is given, e.g., in the book [Ro 61] (Sects. I.7 and IV. 22), which also contains a derivation of the Thomas precession (Appendix B).

Chapter 7

Section 7.1. For a review of recent results in the theory of Schrödinger operators with magnetic fields we refer to [CFKS 87], Sect. 6.

The principle of minimal coupling is a straightforward and simple concept for the implementation of magnetic fields, but it requires the introduction of an unobservable and nonunique vector potential. A formulation of quantum mechanics which does not make use of vector potentials was given by Grümm [194].

We want to stress that our general assumption on the smoothness of the magnetic field is certainly too strong. Many of the results presented in this and the following sections were proven under more general conditions in the cited literature.

We solve the Dirac equation in a homogeneous magnetic field with a supersymmetric method which is well known for harmonic oscillators [CFKS 87], Sect. 6.3, Example 1a. Indeed, the square of the Dirac operator gives a Schrödinger operator with a harmonic oscillator potential. The reader is also referred to Sect. 7.4, where the Coulomb problem is solved by similar methods.

An interesting example of an external magnetic field for which the Dirac equation can be solved exactly is the (abelian) magnetic monopole. Dirac himself introduced the hypothesis of a magnetic monopole in 1931 [115]. Since the magnetic field of a monopole (=magnetic charge) is not divergence-free, it cannot be represented by a magnetic vector potential defined everywhere and without singularities. Instead, the monopole vector potential has a singular "string" extending from the location of the monopole to infinity along some path. This corresponds to the image of a monopole as one end of an infinitely long and infinitely thin solenoid. The infinite string of magnetic flux produces a phase shift in the wavefunction when it is encircled (Aharonov-Bohm effect). In order to make it invisible in a scattering experiment, Dirac had to assume the quantization condition $eg/\hbar c = n/2$, where n is some integer, g is the charge of the monopole, and e is the electric charge of the particle in the

field of the monopole. Hence, if at least one monopole exists, then all electric charges must be integer multiples of an "elementary charge". Up to now there is no experimental evidence for the existence of a magnetic monopole, but the possible explanation of charge quantization has drawn some interest to the theoretical investigation of monopoles. Some early work on this subject containing explicit solutions of the Dirac equation in the external field of a monopole is [27, 202].

In 1975, Wu and Yang [488] proposed a singularity-free description of monopoles in the mathematical framework of gauge theory. The main idea is to cover the Euclidean space by two overlapping regions and to define for each region a vector potential with string situated outside of its respective region. The conditions that (1) their curl equals the magnetic field of the monopole in each region and that (2) in the overlapping region the vector potentials are related by a smooth gauge transformation again implies Dirac's quantization condition. For an abelian magnetic monopole this idea exactly describes a nontrivial connection on a principal $U(1)$ fiber bundle. The quantum mechanical wave functions are sections on this fiber bundle. In [489] Wu and Yang carry out a partial wave analysis similar to the one in Sect. 4.6. This is possible because, owing to the spherical symmetry of the problem, the angular momentum operator $\boldsymbol{J} = \boldsymbol{x} \wedge (\boldsymbol{p} - (e/c)\boldsymbol{A}) + \boldsymbol{S} + (eg/c)\boldsymbol{e}_r$ is conserved [177, 291]. Wu and Yang showed that only the angular part of the wavefunction has to be a section and they called the angular momentum eigensections "monopole harmonics". The radial Dirac operator for zero angular momentum ($\boldsymbol{J} = 0$) is not essentially self-adjoint but admits a one-parameter family of self-adjoint extensions [80, 81, 499]. In [260, 261, 262] the authors add an infinitesimal anomalous magnetic moment in order to regularize the problem. In [100] the abelian monopole is considered as the limit of a non-abelian $SU(2)$ monopole. Depending on the chosen regularization, the Dirac equation may or may not have a bound state. For higher partial waves the Dirac equation has only scattering solutions. The solution of the Pauli equation with a monopole is constructed by a supersymmetric method in [101]. For a review of further aspects of the monopole problem we refer the reader to [97]; see also [499] and the references therein. More on the Dirac equation with non-abelian monopoles can be found, e.g., in [81, 236, 306, 500]. See also the Notes to Sect. 5.11.

Section 7.2. Theorem 7.3 and the method of its proof is due to Aharonov and Casher [6]; see also [235] for related results, and Chap. 6.4 of [CFKS 87]. The result of Aharonov-Casher is the explicit determination of the L^2 index of the Dirac operator on a noncompact manifold.

The ground state solution in three dimensions (Example 7.4) was found by Loss and Yau [296]. Their goal was to investigate the stability of matter in the presence of magnetic fields. By a result of Fröhlich, Lieb and Loss [156], the existence of zero energy bound states implies that nonrelativistic single electron atoms collapse when the nuclear charge exceeds some critical threshold.

The result of Theorem 7.5 is obtained in [264] using a path integral approach. The first non-perturbative and rigorous treatment is contained in [56], Example 4.5. See [12] for a differential geometric proof relating the difference between the L^2 index and the Witten index to the η invariant. Further references are [57, 160, 171]. In odd dimensions the index is zero and one should consider instead spectral flows of families of Dirac operators [76].

Section 7.3. Infinitely degenerate ground states in two dimensions (Sect. 7.2.3) were also found by Avron and Seiler [23]. They discuss this phenomenon in connection with the paramagnetic inequality (see [CFKS 87], Sect. 6.6) $\inf \sigma(H(A)+V) \leq \inf \sigma(H_0+V)$, which they prove for a polynomial B and arbitrary potentials V. The paramagnetic inequality is formulated in [221]. It is clear that it is not true for general fields $\boldsymbol{A}$ and V, because there are counterexamples; see [24] and the discussion at the end of [209].

Theorem 7.6 is taken from [212]. The method of proof of Theorem 7.7 has been applied by Leinfelder [289] to the Schrödinger equation (see also [CFKS 87], Theorem 6.1) and by Miller and Simon to the Dirac equation [313, 314]. These papers also contain the results related to cylindrical symmetry (Theorem 7.10). The proof of Theorem 7.8 is due to Helffer, Nourrigat and Wang. It can be found, together with a discussion of the assumptions (A_r) and various other interesting results in [212]. Schrödinger operators which have a compact

resolvent under similar conditions on the magnetic field are treated in [211]. Some new results on the number of eigenvalues were obtained by Ivrii [231, 232, 233]. Theorem 7.9 is due to Kalf [253]. A more general result for a wide class of external fields is obtained in [49].

Section 7.4. The eigenvalues and eigenfunctions of the Dirac-Coulomb problem are of course well known and can be found, e.g., in the textbooks [BS 59, Ro 61, LL 82]. The Dirac-Coulomb problem has been of central importance ever since the invention of the Dirac equation, because it provides the basis for relativistic atomic physics. Historically, the solutions of the radial Dirac equation for the hydrogen atom were first worked out independently by Darwin [102] and Gordon [181].

The solution of the Coulomb problem using supersymmetric methods is due to Sukumar [435]. Similar methods are applied in [22, 52, 99, 432, 486]. The factorization technique presented here is quite similar to a construction for second order differential equations due to Schrödinger [409] and Infeld and Hull [230]. A review of the history of the factorization method (which starts in fact with Darboux, Jacobi, and Frobenius) is contained in [429].

The supersymmetric relation between the solutions with positive and negative spin-orbit quantum number κ is just the action of the BJL operator, the relativistic analog of the Pauli-Runge-Lenz vector [Th 79]. The BJL operator is considered in a short note by Johnson and Lippmann [246] and discussed in detail by Biedenharn [52, 53]. In his investigation, Biedenharn uses a transformation which brings Temple's operator Γ to a diagonal form. For the radial Dirac equation the Biedenharn transformation is essentially identical to the transformation **A** defined in Sect. 7.4.1. The supersymmetric form of the Coulomb-Dirac equation can also be found in [52]. The Biedenharn transformation has been interpreted as the quantum analog of the Sommerfeld transformation. This is a Lorentz transformation to a moving frame in which the classical relativistic orbits appear to be closed ellipses (in the original reference frame the perihelion of the ellipse is advancing). In this sense the moving frame is the "most nonrelativistic" frame for the Coulomb problem [53]. Temple's operator appears in [Te 48] and [307].

The Coulomb scattering phases and continuum eigenfunctions were obtained by Mott [322]. His result for the scattering cross section contains an error; the correct form appears in [310]. Our presentation of the Coulomb scattering problem is motivated by [487] (see also [430]), which contains a partially group theoretic derivation of the Coulomb scattering phase shifts. In this work the operator B was used to derive the relation between δ_κ and $\delta_{-\kappa}$.

We also mention some other treatments of the Coulomb-Dirac problem, e.g., [25, 94, 222, 250, 293, 461]. Further investigations of the relativistic Coulomb scattering problem are [118, 122, 152, 248, 382, 484, 485].

Based on the results of Sukumar, H. Grosse [189] derived some results on the level order for Dirac operators. He proved that the degenerate Dirac-Coulomb eigenvalues split under a perturbation $V(r)$ in such a way that the eigenvalue with negative κ is above (or below) the eigenvalue with positive κ if $\Delta V(r) > 0$ (or < 0). Similar results for a mixed scalar and electrostatic potential are obtained in [349]. The applications of factorization methods to the level ordering problem for Schrödinger operators are described in [36].

There are only a few other exactly solvable problems with spherical symmetry [BG 90]. Explicit solutions were obtained for a magnetic monopole field (see the Notes to Sect. 7.1) and for the Coulomb field combined with a magnetic monopole [205]. A supersymmetric solution of the Dirac oscillator equation ($H = c\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta mc^2 + imc\omega\beta\boldsymbol{\alpha} \cdot \boldsymbol{x}$) is described in [370] (see also the references therein). The Dirac equation can also be solved for a scalar Coulomb potential $V = -\beta g/r$ [428]; one obtains the eigenvalues

$$E_{n,\pm} = \pm mc^2 \left\{ 1 - \frac{g^2/c^2}{\left(n + \sqrt{\kappa^2 + g^2/c^2}\right)^2} \right\}^{\frac{1}{2}} .$$

Concerning the definition of the Dirac operator and the behavior of the eigenvalues for $|\gamma| \geq c$ see, e.g., [79, 331, 365, 366], and Sects. 4.3.3 and 5.3.2.

Chapter 8

Section 8.1. There are numerous mathematical books on scattering theory; see e.g. [AJS 77, RS 79, BW 83, Pe 83], where the foundations of scattering theory and the various notions of asymptotic completeness are treated in more detail. In particular, [Pe 83] contains more information on the beautiful geometric characterization of bound and scattering states. The quantum mechanical applications in these books deal almost exclusively with the Schrödinger equation. In this chapter we describe the time-dependent geometric approach to the problem of asymptotic completeness for the Dirac equation [129]. This approach was developed for the Schrödinger equation by V. Enss [127]. The alternative approach of stationary scattering theory is used, e.g., in [123, 124, 197, 328, 359, 446, 497] and, more recently, in [26]. While the time-dependent scattering theory seems better suited to treating the existence and completeness of a scattering theory, the technically more demanding stationary approach allows one to obtain more precise results on the spectrum, the resolvent and, e.g., resonances [26]. Finally we note that a presentation of scattering theory which is useful for the practical calculations of physicists can be found, for example, in the books [Pi 79, Sc 79].

Section 8.2. We describe in this section the theory of asymptotic observables as developed by V. Enss for the Schrödinger equation [128] and adapted for the Dirac equation in [129] (an independent but closely related investigation is contained in [327]). The results are proved in this section under some convenient restrictions. The general proofs in the presence of an additional singular short-range field can be found in [129]. This paper also contains the results on invariant domains and Zitterbewegung; see the Notes to Sect. 1.6. The asymptotic observable theory for the Schrödinger equation is described in [CFKS 87, Pe 83] and [127]. Our use of asymptotic observables aims at a proof of asymptotic completeness, but there might well be practical applications. In fact, the algebraic solution of the nonrelativistic Coulomb scattering problem [190] is essentially based on asymptotic observables.

Section 8.3 The asymptotic completeness of the Dirac scattering system with short-range interactions was established for the first time in the framework of stationary scattering theory; the time-dependent proof given here is contained as a special case in [129]. The existence of wave operators in the case of Coulomb fields was proven for the first time in [118]. Asymptotic completeness as stated in Theorem 8.21 is proven in [326] for a more general class of long-range electric fields. A comparatively simple proof for Coulomb-type potentials based on the theory of asymptotic observables is given in [129, 327]. Long-range scalar potentials are treated in [442], where the explicit form of the modification (8.113) was given for the first time.

Section 8.4. Theorem 8.22 is taken from [444]; see also [443]. In order to appreciate the use of Theorem 8.22 in the proof of Theorem 8.23 let us briefly discuss the direct proof given in [295]. There is the following difficulty. In order to apply the Cook argument, Eq. (8.124), which works well in the nonrelativistic case, one has to verify that $\| \alpha \cdot A(x) \exp(-\mathrm{i}H(0)t)\psi \|$ decays integrably in time for ψ in a suitable dense subset of scattering states. But this is wrong, because $A(x)$ decays only like $|x|^{-1/2-\delta}$, at least if we choose the transversal gauge. Usually it is impossible to make $A(x)$ short-range by some other clever choice of gauge (see the remark in Sect.7.1.2).

In the literature on this subject the Coulomb gauge $\operatorname{div} A = 0$ is used almost exclusively instead of the transversal gauge, which is best adapted to scattering theory. Therefore, previous results were obtained only by introducing modifications of the wave operators [46, 327].

In situations like the Aharonov-Bohm effect the free asymptotics (e.g., plane waves for the asymptotic description of stationary scattering states) are used together with the Coulomb gauge, although the vector potential is long-range. But in this case the calculations are justified, because in two dimensions and for rotationally symmetric fields the Coulomb gauge happens to coincide with the transversal gauge.

Asymptotic completeness is also true in relativistic and nonrelativistic quantum mechanics if one adds a short-range electric potential to the magnetic field.

A discussion of classical scattering theory with magnetic fields is given in [294].

Section 8.5. For more details on the scattering theory for Dirac operators under the convenient assumptions made in this section, see [386]. Theorem 8.25 is proven in [416]; earlier proofs under more restrictive conditions on the potentials are given in [350, 390]. In [308, 309], Matsui calculates the index of the operator S_+ under conditions ensuring that S_{+-} and S_{-+} are compact. The Fredholm index $\mathrm{ind}\, S_+$ (if S can be implemented in Fock space, Sect. 10.3) describes the shift of the vacuum charge during scattering (vacuum polarization) [85]. More precisely, the implemented scattering operator maps the charge-q sector of the fermionic Fock space onto the charge-$(q - \mathrm{ind}\, S_+)$ sector. For massive particles, Matsui found that the index is always zero, whereas for massless particles, $\mathrm{ind}\, S_+$ equals the instanton number $(8\pi^2)^{-1} \int F \wedge F$ of the external field. See [78, 392] for some related work.

Chapter 9

Section 9.1. For the theory of solitons of the KdV equation and its relation to the Schrödinger equation we refer the reader to one of the excellent textbooks on that topic, e.g., [AS 81, DEGM 82, EvH 83, NMPZ 84, Ne 85, Ma 86, Le 87, Ma 88, BDT 88, DJ 89, LS 91]. The idea of relating a (nonlinear) differential equation to the commutator of certain operators (a Lax pair) appears in [288]. The Lax approach for the KdV/Schrödinger equation is described in Chap. 3 of [EvH 83] in a way similar to our presentation in Sects. 9.1 and 9.2. In [316], Miura shows that the solutions of the KdV and mKdV equations are related by "a remarkable nonlinear transformation". The relation mKdV/Dirac became clear in [1], where it was shown that for a potential which obeys the mKdV equation the eigenvalues of the Dirac operator remain time independent. A Lax pair for mKdV equation (Theorem 9.2) was given by Tanaka [438]. In Sect. 9.1.3 we gave a description of the Miura transformation showing its close connection to supersymmetry. This was first exploited in [4, 106].

Section 9.2. Besides the mKdV equation discussed here, there is another mKdV equation, referred to as the mKdV$_+$ equation, $\phi_t + 6\phi^2\phi_x - \phi_{xxx} = 0$, in which the nonlinear term has the opposite sign. The mKdV$_+$ equation is related to a non-self-adjoint Dirac operator with a complex potential $Q = -\mathrm{i}\sigma_2\partial_x + \mathrm{i}(\sigma_3 \mathrm{Re}\,\phi + \sigma_1 \mathrm{Im}\,\phi)$. (This operator is unitarily equivalent to the operator considered in [346, 438]). It is obvious that the purely imaginary solutions of the mKdV$_+$ equation are related to the real solutions of Eq. (9.39). The connection with the KdV equation is given by the complex Miura transformation $V = \phi^2 \pm \mathrm{i}\phi_x$. The mKdV$_+$ equation has real, nonsingular, "particle-like" soliton solutions which vanish as $|x| \to \infty$. These solitons can be obtained with the help of inverse scattering theory from the imaginary discrete eigenvalues of Q. In soliton theory, the mKdV$_+$ solitons are much better known than the kink-like solitons discussed in Sect. 9.5. The following is a short list of references concerning the mKdV$_+$-equation: [219, 256, 258, 276, 346, 437, 438, 451, 459].

The KdV and mKdV equations are special cases of the general AKNS-ZS evolution equations [2, 502]. There is an entire hierarchy of higher order KdV- and mKdV-type equations for which completely analogous results can be obtained [3, 136]. The hierarchies are related by supersymmetry [169]. Moreover, one expects that the mKdV hierarchy reduces somehow to the KdV hierarchy in the nonrelativistic limit [383].

For many results within the Lax approach and the AKNS-formalism it is not necessary that the generator of the isospectral transformations is self-adjoint. An example is the hyperbolic sine-Gordon equation where the Hamiltonian in the Lax pair is again the Dirac operator Q, but where the operator $B(t)$ is a non self-adjoint integral operator. There is also an analog of the Miura transformation relating the hyperbolic sine-Gordon equation to a KdV-type integro-differential equation [161].

Section 9.3. The construction of solutions of the modified KdV equation given a solution of the ordinary KdV equation is due to Gesztesy and Simon [172] (see also [161, 162, 169]). In this section we closely follow their exposition. The paper [169] contains many references to earlier work and related results. The proof of Theorem 9.4 requires some results on critical and subcritical Schrödinger operators; see [174] for details. In [161, 169] it is shown that Theorem 9.4 extends to the entire mKdV hierarchy. Related results on the construction of mKdV solutions from KdV solutions are contained in [105, 460, 505], and [BDT 88], Sect. 38.

Section 9.4. The scattering theory for the Dirac equation with an electromagnetic step potential is considered in [60]. General systems with different asymptotics to the right and left are treated in [103]. One dimensional scattering theory for the Schrödinger equation is described in [159]; the results pertaining to supersymmetry are also relevant for the Dirac equation. Scattering theory for the Dirac equation with scalar potentials is treated in some detail in [169] and [162]

In Sect. 9.4.2 we follow mainly [56, 159]; see also [339], p. 505. The result Eq. (9.116) was first derived by Callias [82], and since then by many authors using various methods; see, e.g., [7, 66, 217, 218, 229, 298, 343, 431].

Section 9.5. We refer to [107, 157, 259] and the textbooks on solitons and the inverse scattering transform cited above for more details on the material of Sect. 9.5.1 and possible generalizations.

The n-soliton solutions of the Dirac equation were obtained for the first time by Ohmiya [347] and later independently by Grosse [187], using the inverse scattering transform method (Sect. 9.5.1), which can also be applied to the Dirac equation [154, 195]. In [188] solitons of a coupled system of mKdV equations are derived by relating them to the Dirac equation with a scalar and a pseudoscalar potential. Ref. [186] discusses applications of the mKdV equation to physical models of polyacethylene.

In Sects. 9.5.2 and 9.5.3 we construct the soliton solutions of the mKdV equation using the supersymmetric method developed in [169] and [162]. These authors apply this method also to more general soliton-like solutions of the KdV equation as well as periodic solutions and relate it to the corresponding solutions of the KdV equation. Refs. [4, 169] and in particular [168] (see also the references therein) also discuss singular KdV and mKdV solutions.

Chapter 10

Section 10.1. The main physical ideas about the theory of the electron–positron field interacting with an external electromagnetic field are contained in papers of Feynman [142], Salam and Matthews [394], and Schwinger [412], and are described, e.g., in the book [Th 58]. The external field problem in QED has gained some interest in physics for its possible application to laser physics [315] and to heavy ion collisions [372], [GMR 85]. During these processes strong time-dependent electric fields occur which are assumed to "spontaneously" create electron–positron pairs out of the vacuum. The strength of the electromagnetic field excludes the application of perturbation theory in QED. Neglecting the field created by the electron leads to the external field problem, which is accessible to rigorous and nonperturbative methods. More on the physics of strong external fields in QED can be found in [FGS 91]

There are several mathematical approaches to the external field problem. The method of Capri [83] and Wightman [476] is based on the retarded and advanced Green functions and the associated Yang-Feldman-Källen integral equations, smeared out with a test function. In this chapter we follow an approach by Friedrichs [Fr 52]. This method starts with an operator of the one-particle Hilbert space and tries to obtain a physically meaningful operator by implementing it into the Fock space, if possible. A related method is the C^* algebraic approach of I. E. Segal which is described in [58]. It was shown by Ruijsenaars [387] that the Capri-Wightman approach and the Friedrichs-Segal approach lead to the same scattering

operator. Another approach based on perturbation theory and renormalization is due to Bellissard [43, 44]; see also [386].

Among the mathematical standard textbooks on quantum electrodynamics and field theory we mention [Fr 52, Be 66, StW 64, Jo 65, Th 80, Sch 89, BLOT 90].

We want to note that in the physics literature the field operators are treated in a different way, with second quantized fields depending on space-time or momentum coordinates, and the CAR formally given by $\{a(x), a^*(y)\} = \delta(x-y)$. The connection between the "unsmeared" annihilation/creation operators $a(x)$, $a^*(x)$, etc., and the operators $a(f)$, $a^*(f)$ defined here, is given for example by $a(f) = \int f(x)a(x)dx$, etc. Hence the unsmeared field operators are regarded as "operator valued distributions". But while the annihilation operator $a(x)$ is a densely defined operator in the Fock space, the domain of the adjoint $a^*(x)$ consists only of the zero vector. In Fock space, $a^*(x)$ can only be interpreted as a quadratic form, and products of unsmeared creation/annihilation operators usually have no clear meaning. Therefore, these expressions can only be used in formal calculations; from a mathematical point of view we prefer the "smeared" field operators. This also gives a more satisfying physical interpretation: While $a^*(x)$ creates an "electron at the point x" (which is an ill defined concept), $a^*(f)$ creates an electron in the state f (which has a clear meaning).

Section 10.2. This section contains mainly standard results. We want to mention that the relativistic covariance of the theory is not quite clear at this point. If H is the Dirac operator with an external field, then a Poincaré transformation would not commute with $\operatorname{sgn} H$ and the question of implementability is nontrivial (see the next section). Moreover, the transformed Dirac operator has a different potential; hence the splitting of the one-particle Hilbert space in positive/negative energy subspaces will be different. But then the whole Poincaré transformed theory has to be defined in a different Fock space.

One might think of describing everything in the same Fock space, for example, in the Fock space of free particles. Here the one-particle Hilbert space is split into the eigenspaces of $\operatorname{sgn} H_0$, which are left invariant under proper Poincaré transformations. Hence we can implement the Poincaré group in the same way as described in this section for the time evolution $\exp(iH_0t)$. However, the interacting time evolution does not commute with $\operatorname{sgn} H_0$ and hence the implementability implies restrictions on the external field (see the next section). In particular, the interacting time evolution cannot be implemented in the free Fock space if the field contains a magnetic vector potential. Hence the implementability of the time evolution has no covariant meaning. It is concluded in [143] that a particle interpretation in the Fock space has only an asymptotic meaning for particles which asymptotically become free.

Section 10.3. A fundamental result for the theory presented here is the Hilbert-Schmidt criterion for the implementability of a unitary transformation in Fock space. This result is due to Shale and Stinespring [418]; proofs can be also found in [Be 66], [20, 220, 284, 388, 389, 414, 415], [Sch 89]; see also [151, 268].

The Shale-Stinespring theorem can be used to investigate the implementability of the time evolution in the free particle Fock space [58, 284, 285, 414]. In [220] it is shown for spin-0 particles in a static external field that the time evolution cannot be implemented in the free particle Fock space if the external field contains a magnetic vector potential. Ruijsenaars [386] showed this result also in the spin-1/2 case. In addition, he proves that the interacting time evolution is not implementable for any type of interaction which is not electric or pseudoelectric. In these cases no interaction Hamiltonian can be defined in the free particle Fock space.

An explicit construction of the implementable unitary transformation (Bogoliubov transformation) in Fock space is given by Ruijsenaars [388]. Our Theorem 10.6 is a special case of this result. Further generalizations, suitable for treating spin-0 and spin-1/2 particles with the same formalism, are given in [389]. In [387] these results are used to establish the connection between the formal Feynman-Dyson expansion and the unitarily implemented scattering operator.

In [269], regular external fields are considered, defined by the property that the "interacting" creation and annihilation operators realize a representation of the CAR in the free particle Fock space. A field is regular if $P_+ - P_+^0$ is a Hilbert-Schmidt operator. In [269], conditions for static regular fields satisfying this assumption are given, and in [338] it is shown that no static magnetic field is regular. Also Klaus and Scharf [269] give an explicit construction of the implemented unitary operator, and they use a normal form similar to that of Ruijsenaars to investigate the vacuum polarization [268]. This implies the possibility that the vacuum defined by the interacting creation and annihilation operators corresponds to a charged state in the free particle Fock space. This phenomenon occurs for (static) external fields which are strong enough to cause transitions from electron to positron states (e.g., if the lowest bound state reaches the negative energy subspace). The physical effect is that the vacuum in the neighborhood of the strong field becomes charged thereby partially screening the field ("vacuum polarization").

Meanwhile there are several rigorous investigations of this effect. In [84, 85] the charge $q(U)$ of the unitarily transformed vacuum is related to the index of U_+. Matsui [308, 309] showed that the index of the scattering operator S_+ for massless Dirac particles in a time dependent external field (such that S_{odd} is compact) is given by the instanton number of the field. The implementation of (chiral) gauge transformations of the 2 and $2n$-dimensional Dirac theory is investigated in [86, 392], where index formulas for chiral transformations are derived (in particular for "kink-like" transformations with nonzero winding number). A very readable introduction to the connections of these problems with the axial (or chiral) anomaly in quantum field theory is given in [393].

We also mention that external fields with nontrivial topology lead to models with fractional charges [236]; see, e.g., [343] for a review of the applications to physics. Consider, e.g., a one-dimensional kink-like scalar potential with different asymptotics $\pm m$ to the right and left (like the soliton fields of Chap. 9). It can be shown [191] that the regularized charge operator in the corresponding Fock space has half-integer eigenvalues. Moreover, the CAR in this Fock space cannot be represented in the Fock space of particles in a constant scalar potential. Hence this model provides an example of nonequivalent representations of the CAR. Further investigations dealing with related problems and the implementability of gauge, axial gauge and chiral transformations are [192, 193]. Dirac particles in one dimension on an interval with boundary conditions (point interactions) are considered in [137, 138]. Time-dependent problems are discussed, e.g., in [139, 345].

Theorem 10.8 and the related results are taken mainly from the corresponding sections in [86], see also the references therein. Some earlier related work on related problems is, e.g., [151, 301].

Section 10.4. The implementability of the scattering operator [43, 44] was shown for a class of smooth electric and pseudo-electric fields with small coupling constants. A wider class of time-dependent fields, for which the scattering operator of the Dirac equation is unitarily implementable, was found in [350]. A simpler proof is given in [390] for external fields which are smooth test functions decaying rapidly in all space and time variables. In [416] the H-S criterion for the external field in Theorem 8.23 is proven (even under slightly more general assumptions); see also [Sch 89], Sect. 2.5. Attempts to generalize these results to external fields decaying more slowly in time are made in [356]. The possibilities of implementing the whole time evolution of a system in a time-dependent external field are discussed by Fierz and Scharf [143]. For regular fields the equivalence of various representations is shown. However, magnetic fields are again excluded; only time-dependent electric fields are regular. Hence this formalism cannot be covariant, and the authors conclude that a particle interpretation has only an asymptotic meaning.

One would expect that the Klein paradox has a resolution in quantum electrodynamics. However, the external field theory described here is not the appropriate framework for the description of this problem because it turns out that the scattering operator for a high potential step ($> 2mc^2$) cannot be implemented in the Fock space [59]. It seems as if in a

complete treatment of the Klein paradox the interaction of electrons and positrons should not be neglected, but I am not aware of any mathematically rigorous solution to this problem.

The proof of the analytic dependence of the scattering operator on the coupling constant, Theorem 10.11, is due to Ruijsenaars [387] and Seipp [416]. Theorem 10.11 follows from Theorems 2.3 and 2.4 of [387] and the observation that no branch point can arise on the real axis [416]. The stronger version stated as Theorem 6 in [416] (see also [399]) is not proven there, since it is not clear whether the implemented scattering operator is bounded for complex λ in a neighborhood of the real axis. Let us finally mention [400], where the probability of pair creation is described in the limit of large coupling constants.

The notion of spontaneous pair creation was developed to explain the phenomena during heavy ion collisions. It is expected to occur if a superheavy nucleus (modeled by a uniformly charged sphere) is formed with nuclear charge so large, that the $2p_{1/2}$-state has dived into the lower continuum. Zel'dovich and Popov [504] have interpreted this resonance phenomenon in terms of a creation process. This point of view has gained much interest in the physics literature, see [GMR 85] for a fairly complete presentation including the earlier literature on that subject and a comparison with the experiments.

The possible description of a spontaneous pair creation in the adiabatic limit was proposed by Nenciu [336]. A review of these ideas is also given in [335]. The proof of Theorem 10.12 can be found in [336]. Parts of the conjectures of the first papers are proven by Nenciu in [337]. The intuition behind this is the following. If a strong attractive (overcritical) potential is slowly switched on, the lowest bound state emerges from the positive spectral subspace, is transported through the spectral gap, and finally dives into the lower continuum. Here it becomes a positron scattering state in the absolutely continuous negative energy subspace. Adiabatically this scattering state has enough time to spread and hence only a small portion of it will be transported back through the gap when the potential is finally turned off. Thus the scattering operator belonging to the adiabatically time dependent potential maps a state from the positive to the negative energy subspace. Thus we expect a nonvanishing probability for pair creation in the adiabatic limit, despite the fact that for a static external potential there is no pair creation at all. No pair creation occurs, if the field is undercritical and the ground state does not reach the lower continuum during adiabatic switching. Hence in the adiabatic limit we expect a discontinuity of the probability of pair creation as a function of the coupling strength of the potential.

Books

Some famous books on quantum mechanics for physicists which also contain information on the Dirac equation are, e.g., [BS 59, Da 65, Di 76, Ei 69, Ku 62, Mb 70, Me 70, Pa 90, Sch 68, SLT 64] (of course, this list is incomplete). Books dealing mainly with relativistic quantum mechanics are, e.g., [BG 90, BD 64, CS 63, Das 73, Fe 61, Ke 76, LL 82, Ma 63, Pi 79, Ro 61, Sc 79]. The applications of relativistic quantum mechanics in atomic and molecular physics are the topic of [Ma 83, Py 86]. Nonrelativistic quantum mechanics from the mathematical point of view is presented, e.g., in [AJS 77, CFKS 87, Pr 71, Th 79], more mathematical background can be found in [Ka 80, RS 72, RS 75, RS 78, RS 79, We 80]. Dirac operators on manifolds are not studied here, we refer to [Ba 81, Bl 81, CFKS 87, LM 89, Ro 88, GM 91]. The other books deal with more specialized topics and are cited in the text or in the notes.

[AGHH 88] S. Albeverio, F. Gesztesy, R. Høegh-Krohn, H. Holden: *Solvable Models in Quantum Mechanics*, Springer Verlag, Berlin, Heidelberg, New York 1988 — Notes 4.3

[AJS 77] W. O. Amrein, J. M. Jauch, and K. B. Sinha: *Scattering Theory in Quantum Mechanics*, Benjamin, Inc., Reading, Massachusetts 1977 — Notes 1.4, 8.1

[AS 81] M. J. Ablowitz and H. Segur: *Solitons and the Inverse Scattering Transform*, Siam Studies in Applied Mathematics, Siam, Philadelphia 1981 — Notes 9.1

[Ba 81] H. Baum: *Spin Strukturen und Dirac Operatoren über pseudoriemannschen Mannigfaltigkeiten*, Teubner Texte zur Mathematik, Bd. 41, B. G. Teubner, Leipzig 1981

[BB 85] B. Boos and D. Bleecker: *Topology and Analysis, The Atiyah-Singer Index Formula and Gauge Theoretic Physics*, Springer Verlag, New York, Berlin 1985 — Notes 5.7

[BDT 88] R. Beals, P. Deift, C. Tomei: *Direct and Inverse Scattering on the Line*, Mathematical Surveys and Monographs 28, Amer. Math. Soc., Providence, Rhode Island, 1988 — Notes 9.1, 9.3

[BD 64] J. D. Bjorken and S. D. Drell: *Relativistic Quantum Mechanics*, MacGraw-Hill, New York 1964 — Notes 4.5

[Be 66] F. A. Berezin: *The Method of Second Quantization*, Academic Press, New York, London 1966 — Notes 10.1, 10.3

[BG 90] V. G. Bagrov and D. M. Gitman: *Exact Solutions of Relativistic Wave Equations*, Mathematics and Its Applications (Soviet Series) Vol. 39, Kluwer Academic Publishers, Dordrecht, Boston, London 1990 — Notes 7.3

[BLOT 90] N. N. Bogoliubov, A. A. Logunov, A. T. Oksak, and I. T. Todorov: *General Principles of Quantum Field Theory*, Kluwer Academic Publishers, Dordrecht 1990 — Notes 10.1

[Bl 81] D. Bleecker: *Gauge Theory and Variational Principles*, Global analysis, pure and applied, no. 1, Addison-Wesley, London 1981

[Br 65] H. Bremermann: *Distributions, Complex Variables, and Fourier Transforms*, Addison-Wesley, Reading, Massachusetts, 1983

[BR 86] A. O. Barut and R. Raczka: *Theory of Group Representations and Applications*, 2nd edition, World Scientific, Singapore 1986 — Notes 3.1, 3.2–3

[BS 59] H. A. Bethe and E.E. Salpeter: *Quantum Mechanics of One- and Two-Electron Atoms*, Academic Press, New York 1959 and Plenum, New York 1977 — Notes 6.1, 7.4

[BW 83] H. Baumgärtel and M. Wollenberg: *Mathematical Scattering Theory*, Akademie Verlag, Berlin 1983 — Notes 5.10, 8.1

[BW 85] W. A. Bardeen, A. R. White (eds.): *Symposion on Anomalies, Geometry, Topology*, World Scientific, Singapore 1985 — Notes 5.8

[CFKS 87] H. L. Cycon, R. G. Froese, W. Kirsch, and B. Simon: *Schrödinger Operators*, Springer Verlag, Berlin 1987 — Notes 5.11, 7.1, 7.2, 7.3, 8.2

[Ch 46] C. Chevalley: *Theory of Lie Groups*, Princeton University Press, Princeton 1946

[Co 53] E. M. Corson: *Introduction to Tensors, Spinors, and Relativistic Wave Equations*, Blackie and Son, Glasgow 1953 — Notes 2.5, 3.2–3

[CS 63] E. Corinaldesi and F. Strocchi: *Relativistic Wave Mechanics*, North-Holland, Amsterdam 1963

[Das 73] T. P. Das: *Relativistic Quantum Mechanics of Electrons*, Harper and Row, New York 1973 — Notes 5.6, 6.2

[Da 65] A. S. Davydov: *Quantum Mechanics*, Pergamon Press, Oxford 1965

[DEGM 82] R. K. Dodd, J. C. Eilbeck, J. D. Gibbon, H. C. Morris: *Solitons and Nonlinear Wave Equations*, Academic Press, New York 1982 — Notes 9.1

[Di 76] P. A. M. Dirac: *The Principles of Quantum Mechanics*, 4th edition, Oxford University Press, London 1976 — Notes 1.1

[DJ 89] P. G. Drazin, R. S. Johnson: *Solitons: An Introduction*, Cambridge texts in applied mathematics, Cambridge University Press, New York 1989 — Notes 9.1

[Ei 69] J. A. Eisele: *Modern Quantum Mechanics with Applications to Elementary Particle Physics*, Wiley, New York 1969

[EvH 83] V. Eckhaus, A. v. Harten: *The Inverse Scattering Transformation and the Theory of Solitons*, North-Holland, Amsterdam, New York, Oxford 1983 — Notes 9.1

[Fe 61] R. P. Feynman: *Quantum Electrodynamics*, Benjamin, New York 1961

[Fe 85] S. Ferrara: *Supersymmetry*, Vols. 1 and 2, North Holland, Amsterdam and World Scientific, Singapore 1987 — Notes 5.1

[FGS 91] E. S. Fradkin, D. M. Gitman, S. M. Shvartsman: *Quantum Electrodynamics with Unstable Vacuum*, Springer Series in Nuclear and Particle Physics, Springer Verlag, Berlin, Heidelberg, New York 1991 — Notes 10.1

[Fr 52] K. O. Friedrichs: *Mathematical Aspects of the Quantum Theory of Fields*, Interscience Publ., New York 1952 — Notes 10.1

[Gi 84] P. B. Gilkey: *Invariance Theory, the Heat Equation, and the Atiyah-Singer Index Theorem*, Publish or Perish, Wilmington 1984 — Notes 5.1, 5.7

[GK 69] I. C. Gohberg and M. G. Krein: *Introduction to the Theory of Linear Nonselfadjoint Operators*, Translations of Mathematical Monographs Vol. 18, American Mathematical Society, Providence, Rhode Island 1969 — Notes 5.10

[GM 91] J. E. Gilbert and M. A. M. Murray: *Clifford Algebras and Dirac Operators in Harmonic Analysis*, Cambridge studies in advanced mathematics Vol. 26, Cambridge University Press, Cambridge 1991

[GMR 85] W. Greiner, B. Müller, and J. Rafelski: *Quantum Electrodynamics of Strong Fields*, TMP, Springer Verlag, Berlin, Heidelberg 1985 — Notes 10.1, 10.4

[GR 80] I. S. Gradshteyn and I. M. Ryzhik: *Table of Integrals, Series and Products*, Corrected and enlarged edition, Academic Press, New York 1980

[Ha 82] P. Hartman: *Ordinary Differential Equations*, 2nd ed., Birkhäuser, Boston 1982

[He 78] S. Helgason: *Differential Geometry, Lie Groups, and Symmetric Spaces*, Academic Press, New York 1978

[HR 63] E. Hewitt and K. A. Ross: *Abstract Harmonic Analysis I*, Springer Verlag, Berlin, Göttingen, Heidelberg, 1963

[Ja 69] E. M. de Jager: *Applications of Distributions in Mathematical Physics*, 2nd Edition, Mathematisch Centrum Amsterdam, 1969 — Notes 1.5

[Jo 65] R. Jost: *The General Theory of Quantized Fields*, Amer. Math. Soc., Providence, Rhode Island 1965 — Notes 10.1

[Ka 80] T. Kato: *Perturbation Theory of Linear Operators*, 2nd edition, Springer Verlag, Berlin, Heidelberg, New York 1980 — Notes 1.2, 1.4, 4.3, 5.2, 5.9

[Ke 76] J. Kessler: *Polarized Electrons*, TMP, Springer Verlag, Berlin, Heidelberg 1976

[KN 86] Y. S. Kim and M. E. Noz: *Theory and Applications of the Poincaré Group*, D. Reidel 1986 — Notes 2.5

[Ku 62] B. Kurşunoğlu: *Modern Quantum Theory*, W. H. Freeman, San Francisco 1962

[Le 87] B. M. Levitan: *Inverse Sturm-Liouville Problems*, VNU Science Press, Utrecht 1987 — Notes 9.1

[Le 90] S. Levendorskiĭ: *Asymptotic Distribution of Eigenvalues of Differential Operators*, Mathematics and Its Applications (Soviet Series) Vol. 53, Kluwer Academic Publishers, Dordrecht, Boston, London 1990 — Notes 4.7

[LL 82] L. D. Landau and E. M. Lifschitz: *Course of Theoretical Physics, Vol. 4, Quantum Electrodynamics*, 2nd ed. by W. B. Berestetzki, E. M. Lifshitz and L. P. Pitajewski, Pergamon Press, Oxford 1982 — Notes 7.4

[LM 89] H. B. Lawson, Jr. and M.-L. Michelson: *Spin Geometry*, Princeton University Press, Princeton, New Jersey 1989 — Notes 2.5, 5.7

[LS 91] B. M. Levitan and I. S. Sargsjan: *Sturm-Liouville and Dirac Operators*, Mathematics and Its Applications (Soviet Series) Vol. 59, Kluwer Academic Publishers, Dordrecht, Boston, London 1991 — Notes 4.6, 9.1

[Ma 63] W. Macke: *Quanten und Relativität, Ein Lehrbuch der Theoretischen Physik*, Akademische Verlagsgesellschaft, Leipzig 1963

[Ma 68] G. Mackey: *Induced Representations of Groups and Quantum Mechanics*, Benjamin, New York 1968 — Notes 3.1

[Ma 83] G. L. Malli (ed.): *Relativistic Effects in Atoms, Molecules, and Solids*, Nato ASI Series B: Physics, Vol. 87, Plenum Press, New York, London 1983 — Notes 6.2

[Ma 86] V. A. Marchenko: *Sturm-Liouville Operators and Applications* (Operator Theory: Advances and Applications Vol. 22), Birkhäuser Verlag, Basel, Boston, Stuttgart 1986 — Notes 9.1

[Ma 88] V. A. Marchenko: *Nonlinear Equations and Operator Algebras* (Mathematics and Its Applications, Soviet Series), D. Reidel Publishing Company, Dordrecht, Boston, Lancaster, Tokyo, 1988 — Notes 9.1

[Mb 70] E. Merzbacher: *Quantum Mechanics*, 2nd ed., Wiley, New York 1970

[Me 70] A. Messiah: *Quantum Mechanics*, Vol.2, North-Holland, Amsterdam 1970 — Notes 5.6

[Ne 85] A. C. Newell: *Solitons in Mathematics and Physics*, Society for Industrial and Applied Mathematics, Philadelphia 1985 — Notes 9.1

[NMPZ 84] S. Novikov, S. V. Manakov, L. P. Pitaevskii, and V. E. Zakharov: *Theory of Solitons* (Contemporary Soviet Mathematics), Consultants Bureau, New York, London, 1984 — Notes 9.1

[Oh 88] Y. Ohnuki: *Unitary Representations of the Poincaré group and Relativistic Wave Equations*, World Scientific, Singapore, New Jersey, Hongkong 1988 — Notes 3.1, 3.2–3

[Pa 90] W. Pauli: *Die allgemeinen Prinzipien der Wellenmechanik*, N. Straumann ed., Springer Verlag, Berlin 1990 — Notes 1.1

[Pe 83] P. A. Perry: *Scattering Theory by the Enss Method*, Mathematical Reports, Vol. 1, Harwood, New York 1983 — Notes 1.9, 8.1, 8.2

[Pi 79] H. M. Pilkuhn: *Relativistic Particle Physics*, Springer Verlag, Berlin, Heidelberg, New York 1979 — Notes 8.1

[Pr 71] E. Prugovecki: *Quantum Mechanics in Hilbert Space*, Academic press, New York, San Francisco, London 1971 — Notes 1.2

[Py 86] P. Pykkö: *Relativistic Theory of Atoms and Molecules*, Lecture Notes in Chemistry, Vol. 41, Springer Verlag, Berlin, Heidelberg, New York 1986 — Notes 6.2

[Ro 61] M. E. Rose: *Relativistic Electron Theory*, Wiley, New York 1961 — Notes 6.2, 7.4

[Ro 88] J. Roe: *Elliptic Operators, Topology and Asymptotic Methods*, Longmann Scientific and Technical 1988 — Notes 5.7

[RS 72] M. Reed and B. Simon: *Methods of Modern Mathematical Physics I, Functional Analysis*, Academic Press, New York, San Francisco, London 1972, 2nd edition 1980 — Notes 1.2, 2.3

[RS 75] M. Reed and B. Simon: *Methods of Modern Mathematical Physics II, Fourier Analysis, Self-Adjointness*, Academic Press, New York, San Francisco, London 1975 — Notes 2.3

[RS 78] M. Reed and B. Simon: *Methods of Modern Mathematical Physics IV, Analysis of Operators*, Academic Press, New York, San Francisco, London 1978 — Notes 4.7

[RS 79] M. Reed and B. Simon: *Methods of Modern Mathematical Physics III, Scattering Theory*, Academic Press, New York, San Francisco, London 1979 — Notes 1.9, 8.1

[Rü 70] W. Rühl: *The Lorentz Group and Harmonic Analysis*, Benjamin, New York 1970 — Notes 2.5

[Sc 79] M. D. Scadron: *Advanced Quantum Theory*, Springer Verlag, Berlin, Heidelberg, New York 1979 — Notes 8.1

[Sch 68] L. I. Schiff: *Quantum Mechanics*, 3rd ed., McGraw-Hill, New York 1968

[Sch 89] G. Scharf: *Finite Quantum Electrodynamics*, Springer Verlag, Berlin, Heidelberg, New York 1989 — Notes 10.1, 10.3, 10.4

[Si 68] D. J. Simms: *Lie Groups and Quantum Mechanics*, Lecture Notes in Mathematics 52, Springer Verlag, Berlin, Heidelberg, New York 1968 — Notes 2.2, 2.4

[Si 79] B. Simon: *Trace Ideals and their Applications*, London Math. Soc. Lecture Notes Series, Vol. 35, Cambridge Univ. Press, 1979 — Notes 5.10

[SLT 64] A. A. Sokolov, J. M. Loskutov and I. M. Ternov: *Quantenmechanik*, Akademie Verlag, Berlin 1964

[StW 64] R. F. Streater and A. S. Wightman: *PCT, Spin and Statistics and all that*, Benjamin, 1964 — Notes 10.1

[SW 72] A. Salam and E. P. Wigner (eds.): *Aspects of Quantum Theory*, Cambridge University Press 1972 — Notes 1.1

[Te 48] G. Temple: *The General Principles of Quantum Mechanics*, Methuen and Co, New York 1948 — Notes 7.4

[Th 58] W. Thirring: *Principles of Quantum Electrodynamics*, Academic Press, New York 1958 — Notes 10.1

[Th 79] W. Thirring: *Lehrbuch der Mathematischen Physik 3, Quantenmechanik von Atomen und Molekülen*, Springer Verlag, Wien, New York 1979 — Notes 1.2, 7.4

[Th 80] W. Thirring: *Lehrbuch der Mathematischen Physik 4, Quantenmechanik großer Systeme*, Springer Verlag, Wien, New York 1980 — Notes 10.1

[Va 85] V. S. Varadarajan: *Geometry of Quantum Theory*, 2nd edition, Springer Verlag, Berlin, Heidelberg, New York 1985 — Notes 2.2

[VW 77] G. Velo and A. S. Wightman eds.: *Invariant Wave Equations*, Proceedings Erice 1977, Lecture Notes in Physics 73, Springer Verlag, Berlin, Heidelberg, New York 1978 — Notes 3.2–3

[We 80] J. Weidmann: *Linear Operators in Hilbert Spaces*, Springer Verlag, Berlin, Heidelberg, New York 1980 (german edition: Teubner, Stuttgart 1976) — Notes 1.2, 1.4, 2.3, 5.2

[Wi 31] E. P. Wigner: *Gruppentheorie*, Vieweg, Braunschweig 1931 — Notes 2.2

[Wi 59] E. P. Wigner: *Group Theory*, Academic Press, New York 1959 — Notes 2.2

Articles

1. Ablowitz, M., Kaup, D., Newell, A. C. and Segur, H., Nonlinear evolution equations of physical significance, Phys. Rev. Lett. **31**, 125–127 (1973) — Notes 9.1.
2. Ablowitz, M., Kaup, D. J., Newell, A. C. and Segur, H., The inverse scattering transform—Fourier analysis for nonlinear problems, Studies Appl. Math. **53**, 249–315 (1974) — Notes 9.2.
3. Ablowitz, M. J., Kruskal, M. and Segur, H., A note on Miura's transformation, J. Math. Phys. **20**, 999–1003 (1979) — Notes 9.2.
4. Adler, M. and Moser, J., On a class of polynomials connected with the Korteweg-de Vries equation, Commun. Math. Phys. **61**, 1–30 (1978) — Notes 9.1.
5. Aguilar, J. and Combes, J. M., A class of analytic perturbations for one-body Schrödinger Hamiltonians, Commun. Math. Phys. **22**, 280–294 (1971) — Notes 4.7.
6. Aharonov, Y. and Casher, A., Ground state of a spin-1/2 charged particle in a two dimensional magnetic field, Phys. Rev. **A19**, 2461–2462 (1979) — Notes 5.11, 7.2.
7. Akhoury, R. and Comtet, A., Anomalous behaviour of the Witten index — exactly soluble models, Nucl. Phys. **B246**, 253–278 (1984) — Notes 5.11, 9.4.
8. Albeverio, S., On the bound states in the continuum of N-body systems and the virial theorem, Ann. Phys. **71**, 167–276 (1972) — Notes 4.7.
9. Alvarez-Gaume, L., Supersymmetry and the Atiyah-Singer index theorem, Commun. Math. Phys. **90**, 161–173 (1983) — Notes 5.7.
10. Anghel, N., Remark on Callias' index theorem, Rep. Math. Phys. **28**, 1–6 (1989) — Notes 5.7.
11. Anghel, N., L^2-Index formulae for perturbed Dirac operators, Commun. Math. Phys. **128**, 77–97 (1990) — Notes 5.7, 5.11.
12. Anghel, N., The two-dimensional magnetic field problem revisited, J. Math. Phys. **31**, 2091–2093 (1990) — Notes 5.11, 7.2.
13. Anghel, N., Index theory for short ranged fields in higher dimensions, preprint (1991) — Notes 5.7.
14. Arai, A., Asymptotic analysis of fundamental solutions of Dirac operators on even-dimensional Euclidean spaces, J. Math. Anal. Appl. **126**, 186–208 (1987) — Notes 5.7.
15. Arai, A., Some remarks on scattering theory in supersymmetric quantum mechanics, J. Math. Phys. **28**, 472–476 (1987) — Notes 5.7.
16. Arai, A., On regularized indices of a class of Dirac operators on euclidean spaces, preprint (1990) — Notes 5.7, 5.11.
17. Arai, M., On essential self-adjointness of Dirac operators, RIMS Kokyuroku, Kyoto Univ. **242**, 10–21 (1975) — Notes 4.3.
18. Arai, M., On essential self-adjointness, distinguished self-adjoint extension and essential spectrum of Dirac operators with matrix valued potentials, Publ. RIMS, Kyoto Univ. **19**, 33–57 (1983) — Notes 4.3, 4.4, 4.6.
19. Arai, M. and Yamada, O., Essential self-adjointness and invariance of the essential spectrum for Dirac operators, Publ. RIMS, Kyoto Univ. **18**, 973–985 (1982) — Notes 4.3.
20. Araki, H., On quasi-free states of CAR and Bogoliubov automorphisms, Publ. RIMS. **6**, 385–442 (1971) — Notes 10.3.
21. Atiyah, M. F., Patodi, V. K. and Singer, I. M., Spectral asymmetry and Riemannian Geometry. I–III., Math. Proc. Camb. Phil. Soc. **77**, 43–69 (1975), **78**, 405–432 (1975), and **79**, 71–99 (1976) — Notes 5.8.

22. Auvil, P. R. and Brown, L. R., The relativistic hydrogen atom: A simple solution, Am. J. Phys. **46**, 679–681 (1978) — Notes 7.4.
23. Avron, J. E. and Seiler, R., Paramagnetism for nonrelativistic electrons and euclidean massless Dirac particles, Phys. Rev. Lett. **42**, 931–934 (1979) — Notes 7.3.
24. Avron, J. and Simon, B., A counter-example to the paramagnetic conjecture, Phys. Lett. **75A**, 41–42 (1979) — Notes 7.3.
25. Bacry, H. and Richard, J. L., Partial group theoretical treatment for the relativistic hydrogen atom, J. Math. Phys. **8**, 2230–2233 (1967) — Notes 7.4.
26. Balslev, E. and Helffer, B., Limiting absorption principle and resonances for the Dirac operator, preprint Aarhus Universiteit (1991) — Notes 4.7, 6.1, 8.1.
27. Banderet, P., Zur Theorie singulärer Magnetpole, Helv. Phys. Acta. **19**, 503–522 (1946) — Notes 7.1.
28. Bargmann, V., On unitary ray representations of continuous groups, Ann. Math. **59**, 1–46 (1954) — Notes 2.4.
29. Bargmann, V., Note on Wigner's Theorem on Symmetry Operations, J. Math. Phys. **5**, 862–868 (1964) — Notes 2.2.
30. Bargmann, V. and Wigner, E. P., Group theoretical discussion of relativistic wave equations, Proc. Natl. Acad. Sci. USA **34**, 211–223 (1948) — Notes 3.1, 3.2–3.
31. Barut, A. O. and Bracken, A. J., The Zitterbewegung and the internal geometry of the electron, Phys. Rev. **D23**, 2454–2463 (1981) — Notes 1.6.
32. Barut, A. O. and Kraus, J., Resonances in $e^+ - e^-$ system due to anomalous magnetic moment interactions, Phy. Letters. **59 B**, 175–178 (1975) — Notes 5.3.
33. Barut, A. O. and Kraus, J., Solution of the Dirac equation with Coulomb and magnetic moment interactions, J. Math. Phys. **17**, 506–508 (1976) — Notes 5.3.
34. Barut, A. O. and Pavsic, M., Quantisation of the classical relativistic Zitterbewegung in the Schrödinger picture, Classical Quantum Gravity. **4**, L131–L136 (1987) — Notes 1.6.
35. Batenburg, P. and Schakel, A. M. J., A geometrical interpretation of spin, Modern Phys. Lett. A. **4**, 1355–1363 (1989) — Notes 1.5.
36. Baumgartner, B., Level comparison theorems, Ann. Phys. **168**, 484–526 (1986) — Notes 7.4.
37. Beckers, J. and Debergh, N., Supersymmetry, Foldy-Wouthuysen transformations, and relativistic oscillators, Phys. Rev. **D42**, 1255–1259 (1990) — Notes 5.6.
38. Beckers, J. and Jaspers, M., Dirac theory and its Melosh quantum mechanical representation, Phys. Rev. **D23**, 499–502 (1981) — Notes 5.6.
39. Behncke, H., The Dirac equation with an anomalous magnetic moment, Math. Z. **174**, 213–225 (1980) — Notes 5.3.
40. Behncke, H., Dirac equation with an anomalous magnetic moment. II, in: *Ordinary and Partial Differential Equations*, p. 77–85, W. N. Everitt and B. D. Sleeman eds., Lecture Notes in Math. 964, Springer, 1982 — Notes 5.3.
41. Behncke, H., Spectral properties of the Dirac equation with anomalous magnetic moment, J. Math. Phys. **26**, 2556–2559 (1985) — Notes 4.3, 5.3.
42. Bell, J. S., The melosh transformation and the Pryce-Tani-Foldy-Wouthuysen transformation, Acta Phys. Austriaca Suppl. **13**, 395–445 (1974) — Notes 5.6.
43. Bellissard, J., Quantized fields in interaction with external fields. I. Exact solutions and perturbative expansions, Commun. Math. Phys. 41, 235–266 (1975) — Notes 10.1, 10.4.
44. Bellissard, J., Quantized fields in external fields. II. Existence theorems, Commun. Math. Phys. **46**, 53–74 (1976) — Notes 10.1, 10.4.
45. Berline, N. and Vergne, M., A proof of Bismut local index theorem for a family of Dirac operators, Topology. **26**, 435–463 (1987) — Notes 5.7.
46. Berthier, A. M. and Collet, P., Wave operators for momentum dependent long-range potential, Ann. Inst. H. Poncaré. **26**, 279–293 (1977) — Notes 8.4.
47. Berthier, A. and Georgescu, V., Sur la propriété de prolongement unique pour l'opérateur de Dirac, C. R. Acad. Sci. Paris Ser. A **291**, 603–606 (1980) — Notes 4.7.
48. Berthier, A. and Georgescu, V., Sur le spectre ponctuel de l'opérateur de Dirac, C. R. Acad. Sci. Paris Sér. I. **297**, 335–338 (1983) — Notes 4.7.

49. Berthier, A. and Georgescu, V., On the point spectrum for Dirac operators, J. Func. Anal. **71**, 309–338 (1987) — Notes 4.7, 7.3.
50. Berzi, V. and Gorini, V., Reciprocity principle and the Lorentz transformations, J. Math. Phys. **10**, 1518–1524 (1969) — Notes 2.1.
51. Bethe, H. A. and Salpeter, E. E., Quantum mechanics of one- and two-electron systems, in: *Handbuch der Physik, Vol. 35, Atome I*, p. 88–436, S. Flügge ed., Springer, 1957 — Notes 6.1.
52. Biedenharn, L. C., Remarks on the relativistic Kepler problem, Phys. Rev. **126**, 845–851 (1962) — Notes 7.4.
53. Biedenharn, L. C., The "Sommerfeld Puzzle" revisited and resolved, Found. Physics. **13**, 13–34 (1983) — Notes 7.4.
54. Biedenharn, L. C. and Horwitz, L. P., Chiral two-component spinors and the factorization of Kramers's equation., Found. Phys. **14**, 953–961 (1984) — Notes 6.1.
55. Bismut, J. M. and Freed, D. S., The analysis of elliptic families II. Dirac operators, eta invariants, and the holonomy theorem, Commun. Math. Phys. **107**, 103–163 (1986) — Notes 5.7.
56. Bollé, D., Gesztesy, F., Grosse, H., Schweiger, W. and Simon, B., Witten index, axial anomaly, and Krein's spectral shift function in supersymmetric quantum mechanics, J. Math. Phys. **28**, 1512–1525 (1987) — Notes 5.7, 5.8, 5.9, 5.10, 5.11, 7.2, 9.4.
57. Bollé, D., Gesztesy, F., Grosse, H. and Simon, B., Krein's spectral shift function and Fredholm determinants as efficient methods to study supersymmetric quantum mechanics, Lett. Math. Phys. **13**, 127–133 (1987) — Notes 5.8, 5.11, 7.2.
58. Bongaarts, P. J. M., The electron-positron field, coupled to external electromagnetic potentials as an elementary C^* algebra theory, Ann. Phys. **56**, 108–139 (1970) — Notes 10.1, 10.3.
59. Bongaarts, P. J. M. and Ruijsenaars, S. N. M., The Klein paradox as a many particle problem, Ann. Phys. **101**, 289–318 (1976) — Notes 4.5.
60. Bongaarts, P. J. M. and Ruijsenaars, S. N. M., Scattering theory for one-dimensional step potentials, Ann. Inst. H. Poincaré **A26**, 1–17 (1977) — Notes 4.5, 9.4.
61. Borisov, N. V., Müller, W. and Schrader, R., Relative index theorems and supersymmetric scattering theory, Commun. Math. Phys. **114**, 475–513 (1988) — Notes 5.1, 5.7, 5.8.
62. Bott, R. and Seeley, R., Some remarks on the paper of Callias, Commun. Math. Phys. **62**, 235–245 (1978) — Notes 5.7, 5.11.
63. Boutet de Monvel-Berthier, A., An optimal Carleman-type inequality for the Dirac operator, in: *Stochastic Processes and their Applications*, p. 71–94, S. Albeverio ed., Math. Appl., 61, Kluwer Acad. Publ., 1990 — Notes 4.7.
64. Boutet de Monvel-Berthier, A., Manda, D. and Purice, R., The commutator method for form relatively compact perturbations, Lett. Math. Phys. (to appear) (1991) — Notes 4.7.
65. Boutet de Monvel-Berthier, A., Manda, D. and Purice, R., Limiting absorption principle for the Dirac operator, Ann. Inst. H. Poincaré (to appear) (1991) — Notes 4.7.
66. Boyanowsky, D. and Blankenbecler, R., Fractional indices in supersymmetric theories, Phys. Rev. **D30**, 1821–1824 (1984) — Notes 5.11, 9.4.
67. Boyanowsky, D. and Blankenbecler, R., Axial and parity anomalies and vacuum charge: A direct approach, Phys. Rev. **D31**, 3234–3250 (1985) — Notes 5.8.
68. Brack, M., Virial theorems for relativistic spin-1/2 and spin-0 particles, Phys. Rev. **D27**, 1950–1953 (1983) — Notes 4.7.
69. Breit, G., An interpretation of Dirac's theory of the electron, Proc. Nat. Acad. Sci. USA **14**, 553–559 (1928) — Notes 1.6.
70. Breit, G., On the interpretation of Dirac's alpha matrices, Proc. Nat. Acad. Sci. USA **17**, 70–73 (1931) — Notes 1.6.
71. Breit, G. and Brown, G. E., Perturbation methods for Dirac radial equations, Phys. Rev. **76**, 1307–1310 (1949) — Notes 4.6.

72. Brown, L. S., Carlitz, R. D. and Lee, C., Massless excitations in pseudoparticle fields, Phys. Rev. D. **16**, 417–422 (1977) — Notes 5.11.
73. Brüning, J. and Seeley, R., An index theorem for first order regular singular operators, Am. J. Math. **110**, 659–714 (1988) — Notes 5.7.
74. Bulla, W., Gesztesy, F. and Unterkofler, K., On relativistic energy band corrections in the presence of periodic potentials, Lett. Math. Phys. **15**, 313–324 (1988) — Notes 6.2.
75. Bulla, W., Gesztesy, F. and Unterkofler, K., Holomorphy of the scattering matrix with respect to $1/c^2$ for Dirac operators and an explicit treatment of relativistic corrections, Commun. Math. Phys. **144**, 391–416 (1992) — Notes 5.6, 6.1, 6.2.
76. Bunke, U., On the spectral flow of families of Dirac operators with constant symbol, preprint (1991) — Notes 7.2.
77. Bunke, U., Relative index theory, preprint (1991) — Notes 5.7.
78. Bunke, U. and Hirschmann, T., The index of the scattering operator on the positive spectral subspace, preprint (1991) — Notes 8.5.
79. Burnap, C., Brysk, H. and Zweifel, P. F., Dirac Hamiltonian for strong Coulomb fields, Nuovo Cimento **64B**, 407–419 (1981) — Notes 4.3, 7.4.
80. Callan, C. G., Jr. and Das, S. R., Boundary conditions on the monopole Dirac equation, Phys. Rev. Lett. **51**, 1155–1158 (1983) — Notes 7.1.
81. Callias, C. J., Spectra of fermions in monopole fields - Exactly soluble models, Phys. Rev. **D16**, 3068–3077 (1977) — Notes 7.1.
82. Callias, C., Axial anomalies and index theorems on open spaces, Commun. Math. Phys. **62**, 213–234 (1978) — Notes 5.7, 5.8, 5.11, 9.4.
83. Capri, A., Electron in a given time-dependent electromagnetic field, J. Math. Phys. **10**, 575–580 (1969) — Notes 10.1.
84. Carey, A. L., Hurst, C. A. and O'Brien, D. M., Automorphisms of the canonical anticommutation relations and index theory, J. Func. Anal. **48**, 360–393 (1982) — Notes 10.3.
85. Carey, A. L. and O'Brien, D. M., Absence of vacuum polarization in Fock space, Lett. Math. Phys. **6**, 335–340 (1982) — Notes 8.5, 10.3.
86. Carey, A. L. and Ruijsenaars, S. N. M., On fermion gauge groups, current algebras, and Kac-Moody algebras, Acta Appl. Math. **10**, 1–86 (1987) — Notes 10.3.
87. Case, K. M., Some generalizations of the Foldy-Wouthuysen transformation, Phys. Rev. **95**, 1323–1328 (1954) — Notes 5.6.
88. Chakrabarti, A., Canonical form of the covariant free particle equations, J. Math. Phys. **4**, 1215–1222 (1963) — Notes 5.6.
89. Chernoff, P. R., Essential self-adjointness of powers of generators of hyperbolic equations, J. Func. Anal. **12**, 401–414 (1973) — Notes 4.3.
90. Chernoff, P. R., Schrödinger and Dirac operators with singular potentials and hyperbolic equations, Pacific J. Math. **72**, 361–382 (1977) — Notes 4.3.
91. Cini, M. and Touschek, B., The relativistic limit of the theory of spin 1/2 particles, Nuovo Cimento **7**, 422–423 (1958) — Notes 5.6.
92. Cirincione, R. J. and Chernoff, P. R., Dirac and Klein-Gordon equations: Convergence of solutions in the nonrelativistic limit, Commun. Math. Phys. **79**, 33–46 (1981) — Notes 5.2, 6.1.
93. Cook, A. H., On separable solutions of Dirac's equation for the electron, Proc. R. Soc. London. **A383**, 247–278 (1982) — Notes 4.6.
94. Cordero, P., Hojman, S., Furlan, P. and Ghirardi, G. C., Algebraic treatment of nonrelativistic and relativistic equations and its relation to the theory of differential equations, Il Nuovo Cimento **3A**, 807–820 (1971) — Notes 7.4.
95. Cordes, H. O., A pseudo-algebra of observables for the Dirac equation, manuscripta math. **45**, 77–105 (1983) — Notes 1.4.
96. Cordes, H. O., A pseudodifferential Foldy Wouthuysen transform, Comm. Part. Diff. Eq. **8**, 1475–1485 (1983) — Notes 1.4.
97. Craigie, N. S., Some remarkable spin physics with monopoles and fermions, Journal de Physique. **46**, C2/95–106 (1985) — Notes 7.1.

98. Crombrugghe, M. d. and Rittenberg, V., Supersymmetric quantum mechanics, Ann. Phys. **151**, 99–126 (1983) — Notes 5.1.
99. Cunningham, M. J., An $O(2,1) \times O(3)$ solution to a generalized quantum mechanical Kepler problem, J. Math. Phys. **13**, 1108–1112 (1972) — Notes 7.4.
100. D'Hoker, E. and Farhi, E., The abelian monopole fermion system and its self-adjoint extensions as a limit of a nonabelian system, Phys. Lett. **B127**, 360–364 (1983) — Notes 7.1.
101. D'Hoker, E. and Vinet, L., Supersymmetry of the Pauli equation in the presence of a magnetic monopole, Phys. Lett. **137B**, 72–76 (1984) — Notes 7.1.
102. Darwin, C., The wave equation of the electron, Proc. Roy. Soc. (London). **A118**, 654–680 (1928) — Notes 7.4.
103. Davies, E. B. and Simon, B., Scattering theory for systems with different spatial asymptotics to the left and right, Commun. Math. Phys. **63**, 277–301 (1978) — Notes 9.4.
104. De Donder, T. and van den Dungen, H., La quantification déduite de la gravifique einsteinienne, Comptes Rendus de l'academie des sciences. **182**, 22–24 (1926) — Notes 1.1.
105. de Jager, E. M. and Spannenburg, S., Prolongation structures and Bäcklund transformations for the matrix Korteweg-de Vries and the Boomeron equation, J. Phys. A.: Math. Gen. **18**, 2177–2189 (1985) — Notes 9.3.
106. Deift, P. A., Applications of a commutation formula, Duke Math. J. **45**, 267–310 (1978) — Notes 5.1, 9.1.
107. Deift, P. and Trubowitz, E., Inverse scattering on the line, Commun. pure appl. Math. **32**, 121–251 (1979) — Notes 9.5.
108. Detcheva, V., Kandilarov, B. D., Khristov, T. and Metodieva, M., One-dimensional dirac equation approach to the effective mass concept in diatomic crystals, Phys. Stat. Sol. (b). **152**, 163–169 (1989) — Notes 4.3.
109. Detcheva, V., Kandilarov, B. D., Metodieva, M. and Lungarova, M., Effective masses in a simple relativistic energy-band scheme, Czech. J. Phys. **B 39**, 696–701 (1989) — Notes 4.3.
110. Detcheva, V., Kandilarov, B. D., Metodieva, M. and Primatarowa, M. T., Dirac equation approach to scattering from interface potential steps and existence of interface states, Helv. Phys. Acta. **63**, 908–921 (1990) — Notes 4.3, 4.5.
111. deVries, E., Foldy-Wouthuysen transformations and related problems, Fortschr. d. Physik. **18**, 149–182 (1970) — Notes 5.6, 6.1.
112. Dewitt-Morette, c., Elworthy, K. D., Nelson, B. C. and Sammelman, G. S., A stochastic scheme for constructing solutions of the Schrödinger equation, Ann. Inst. H. Poincaré **A32**, 327–341 (1980) — Notes 1.5.
113. Dirac, P. A. M., The quantum theory of the electron, Proc. Roy. Soc. (London). **A117**, 610–624 (1928) — Notes 1.1.
114. Dirac, P. A. M., The quantum theory of the electron, II, Proc. Roy. Soc. (London). **A118**, 351–361 (1928) — Notes 1.1.
115. Dirac, P. A. M., Quantised singularities in the electromagnetic field, Proc. Roy. Soc. **133**, 60–72 (1931) — Notes 7.1.
116. Dittrich, J., Exner, P. and Seba, P., Dirac operators with a spherically symmetric δ-shell interaction, J. Math. Phys. **30**, 2875–2882 (1989) — Notes 4.3.
117. Dittrich, J., Exner, P. and Seba, P., Dirac Hamiltonian with Coulomb potential and spherically symmetric shell contact interaction, in: *Proceedings of the conference on order, disorder and chaos in quantum systems*, Dubna (USSR) 1989, p. 209–219, P. Exner and N. Neidhardt eds., Operator Theory: Advances and Applications, Vol. 46, Birkhäuser Verlag, Basel, Boston, Berlin (1990) — Notes 4.3.
118. Dollard, J. and Velo, G., Asymptotic behaviour of a Dirac particle in a Coulomb field, Il Nuovo Cimento **45**, 801–812 (1966) — Notes 7.4, 8.3.
119. Domingos, J. M. and Caldeira, M. H., Localization and noncausal behaviour of relativistic quantum particles, Il Nuovo Cimento **106B**, 623–626 (1991) — Notes 1.8.
120. Dominguez-Adame, F., Exact solutions of the Dirac equation with surface delta interactions, J. Phys. A: Math. Gen. **23**, 1993–1999 (1990) —

121. Dosch, Jensen and Müller, Einige Bemerkungen zum Klein'schen Paradoxon, Physica Norvegica. **5**, 151–162 (1971) — Notes 4.5.
122. Durgapal, P. and Onley, D. S., Coulomb wave expansion in electron scattering, Phys. Rev. **C24**, 7–15 (1981) — Notes 7.4.
123. Eckardt, K. J., On the existence of wave operators for Dirac operators, manuscripta math. 11, 359–371 (1974) — Notes 8.1.
124. Eckardt, K. J., Scattering theory for Dirac operators, Math. Z. **139**, 105–131 (1974) — Notes 8.1.
125. Eguchi, T., Gilkey, P. B. and Hanson, A. J., Gravitation, gauge theories and differential geometry, Phys. Rep. **66**, 213–393 (1980) — Notes 5.8.
126. Ellis, J. R., 'Proper time' and the Dirac equation, J. Phys. A: Math. Gen. 14, 2917–2925 (1981) — Notes 1.4.
127. Enss, V., Geometric methods in spectral and scattering theory of Schrödinger operators, in: *Rigorous Atomic and Molecular Physics*, p. G. Velo and A. S. Wightman eds., Plenum, 1981 — Notes 8.1, 8.2.
128. Enss, V., Asymptotic observables on scattering states, Commun. Math. Phys. **89**, 245–268 (1983) — Notes 1.6, 8.2.
129. Enss, V. and Thaller, B., Asymptotic observables and Coulomb scattering for the Dirac equation, Ann. Inst. H. Poincaré **45**, 147–171 (1986) — Notes 1.6, 8.2, 8.3.
130. Erdélyi, A., Note on a paper of Titchmarsh, Quart. J. Math. Oxford. **14**, 147–152 (1963) — Notes 4.6.
131. Eriksen, E., Foldy-Wouthuysen transformation. Exact solution with generalization to the two-particle problem, Phys. Rev. 111, 1011–1016 (1958) — Notes 5.6.
132. Evans, W. D., On the decomposition method and the spectrum of the Dirac operator, Proc. London. Math. Soc. **21**, 651–673 (1970) — Notes 4.7.
133. Evans, W. D., On the unique self-adjoint extension of the Dirac operator and the existence of the Green matrix, Proc. London Math. Soc. **20**, 537–557 (1970) — Notes 4.3.
134. Evans, W. D., Spectral Theory of the Dirac operator, Math. Z. **121**, 1–23 (1971) — Notes 4.7.
135. Evans, W. D. and Harris, B. J., Bounds for the point spectra of separated Dirac operators, Proc. Roy. Soc. Edinburgh Sect. A **88**, 1–15 (1980) — Notes 4.6.
136. Falkensteiner, P. and Grosse, H., A hierarchy of systems of non-linear equations, J. Phys. A: Math. Gen. **19**, 2983–2989 (1986) — Notes 9.2.
137. Falkensteiner, P. and Grosse, H., Quantization of fermions interacting with point-like external fields, Lett. Math. Phys. **14**, 139–148 (1987) — Notes 4.3, 10.3.
138. Falkensteiner, P. and Grosse, H., Unitary implementability of gauge transformations for the Dirac operator and the Schwinger term, J. Math. Phys. **28**, 850–854 (1987) — Notes 10.3.
139. Falkensteiner, P. and Grosse, H., Fermions in interaction with time-dependent fields, Nucl. Phys. **B305**, 126–142 (1988) — Notes 10.3.
140. Feinberg, G., Effects of an electric dipole moment of the electron on the hydrogen energy levels, Phys. Rev. **112**, 1637–1642 (1958) — Notes 4.2.
141. Feshbach, H. and Villars, F., Elementary relativistic wave mechanics of spin 0 and spin 1/2 particles, Rev. Mod. Phys. **10**, 24–45 (1958) — Notes 5.4, 5.
142. Feynman, R. P., The theory of positrons, Phys. Rev. **76**, 749–759 (1949) — Notes 10.1.
143. Fierz, H. and Scharf, G., Particle interpretation for external field problems in QED, Helv. Phys. Acta. **52**, 437–453 (1979) — Notes 10.2, 10.4.
144. Fleming, G. N., Nonlocal properties of stable particles, Phys. Rev. **139**, B963–B968 (1965) — Notes 1.8.
145. Fock, V., Zur Schrödingerschen Wellenmechanik, Z. Physik. **38**, 242–250 (1926) — Notes 1.1.
146. Fock, V., Über die invariante Form der Wellen- und der Bewegungsgleichungen für einen geladenen Massenpunkt, Z. Physik. **39**, 226–232 (1926) — Notes 1.1.
147. Foldy, L. L., Synthesis of covariant particle equations, Phys. Rev. **102**, 568–581 (1956) — Notes 5.6.

148. Foldy, L. L. and Wouthuysen, S. A., On the Dirac theory of spin-1/2 particles and its nonrelativistic limit, Phys. Rev. **78**, 29–36 (1950) — Notes 1.4, 5.6, 6.1, 6.2.
149. Forgacs, P., O'Raifeartaigh, L. and Wipf, A., Scattering theory, U(1) anomaly and index theorems for compact and non-compact manifolds, Nucl. Phys. **B293**, 559–592 (1987) — Notes 5.7, 5.8.
150. Forte, S., Spectral asymmetry and vacuum charge in three-dimensional closed and open space, Nucl. Phys. **B301**, 69–92 (1988) — Notes 5.7.
151. Fredenhagen, K., Implementation of automorphisms and derivations of the CAR algebra, Commun. Math. Phys. **52**, 255–266 (1977) — Notes 10.3.
152. Friar, J. L. and Wallace, S. J., Alternative partial wave representations for ultrarelativistic Dirac potential scattering, Phys. Rev. **C25**, 2583–2590 (1982) — Notes 7.4.
153. Friedan, D. and Windey, P., Supersymmetric derivation of the Atiyah-Singer index and the chiral anomaly, Nucl. Phys. **B235**, 395–416 (1984) — Notes 5.7.
154. Frolov, I. S., Inverse scattering problem for a Dirac system on the whole axis, Sov. Math. Dokl. **13**, 1468–1472 (1972) — Notes 9.5.
155. Fröhlich, J., Application of commutator theorems to the integration of representations of Lie algebras and commutation relations, Commun. Math. Phys. **54**, 135–150 (1977) — Notes 1.6, 2.3.
156. Fröhlich, J., Lieb, E. and Loss, M., Stability of Coulomb systems with magnetic fields. I. The one electron atom, Commun. Math. Phys. **104**, 251–270 (1986) — Notes 7.2.
157. Gardner, C. S., Greene, J. M., Kruskal, M. D. and Miura, R. M., Korteweg-de-Vries equation and generalizations. VI. Methods for exact solution, Commun. pure appl. Math. **27**, 97–133 (1974) — Notes 9.5.
158. Gerlach, B., Gromes, D. and Petzold, J., Eine kritische Analyse der Ladungsdichte des Klein-Gordon-Feldes, Z. Physik. **202**, 401–411 (1967) — Notes 1.8.
159. Gesztesy, F., Scattering theory for one-dimensional systems with nontrivial spatial asymptotics, in: *Schrödinger operators*, p. 93–102, E. Balslev ed., Lecture Notes in Mathematics 1218, Springer, 1986 — Notes 5.8, 5.10, 5.11, 9.4.
160. Gesztesy, F., On stationary two-body scattering theory in two dimensions, in: *Models and Methods in Few-Body Physics*, p. 609–629, L. S. Ferreira, A. C. Fonseca and L. Streit eds., Lecture Notes in Physics 273 Springer Verlag, 1987 — Notes 5.11, 7.2.
161. Gesztesy, F., Some Applications of Commutation Methods, in: *Proceedings of the Nordic Summer School in Mathematics*, p. 93–117, H. Holden and A. Jensen eds., Lecture Notes in Physics 345, Springer, 1989 — Notes 9.2, 9.3.
162. Gesztesy, F., On the modified Korteweg-deVries equation, in: *Differential Equations with Applications in Biology, Physics and Engineering*, p. 139–183, J. Goldstein, F. Kappel and W. Schappacher eds., Lecture notes in pure and applied mathematics, Vol. 133, Marcel Dekker, New York, Basel, Hong-Kong, 1991 — Notes 9.3, 9.4, 9.5.
163. Gesztesy, F., Grosse, H. and Thaller, B., Spectral concentration in the nonrelativistic limit, Phys. Lett. **116B**, 155–157 (1982) — Notes 6.1.
164. Gesztesy, F., Grosse, H. and Thaller, B., An efficient method for calculating relativistic corrections for spin-1/2 particles, Phys. Rev. Lett. **50**, 625–628 (1983) — Notes 6.1.
165. Gesztesy, F., Grosse, H. and Thaller, B., Relativistic corrections to bound-state energies for two-fermion systems, Phys. Rev. **D30**, 2189–2193 (1984) — Notes 6.2.
166. Gesztesy, F., Grosse, H. and Thaller, B., A rigorous approach to relativistic corrections of bound state energies for spin-1/2 particles, Ann. Inst. H. Poincaré **40**, 159–174 (1984) — Notes 6.1, 6.2.
167. Gesztesy, F., Grosse, H. and Thaller, B., First-order relativistic corrections and spectral concentration, Adv. Appl. Math. **6**, 159–176 (1985) — Notes 6.1.
168. Gesztesy, F. and Schweiger, W., Rational KP and mKP-solutions in Wronskian form, Rep. Math. Phys. (to appear) (1992) — Notes 9.5.
169. Gesztesy, F., Schweiger, W. and Simon, B., Commutation methods applied to the mKdV-equation, Trans. Amer. Math. Soc. **324**, 465–525 (1991) — Notes 9.2, 9.3, 9.4, 9.5.

170. Gesztesy, F. and Seba, P., New analyticaly solvable models of relativistic point interactions, Lett. Math. Phys. **13**, 345–358 (1987) — Notes 4.3.
171. Gesztesy, F. and Simon, B., Topological invariance of the Witten index, J. Func. Anal. **79**, 91–102 (1988) — Notes 5.8, 5.9, 5.11, 7.2.
172. Gesztesy, F. and Simon, B., Constructing Solutions of the mKdV-equation, J. Func. Anal. **89**, 53–60 (1990) — Notes 9.3.
173. Gesztesy, F., Simon, B. and Thaller, B., On the self-adjointness of Dirac operators with anomalous magnetic moment, Proc. of the Amer. Math. Soc. **94**, 115–118 (1985) — Notes 5.3.
174. Gesztesy, F. and Zhao, Z., On critical and subcritical Sturm-Liouville operators, J. Func. Anal. **98**, 311–345 (1991) — Notes 9.3.
175. Getzler, E., A short proof of the local Atiyah-Singer index theorem, Topology. **25**, 111–117 (1986) — Notes 5.7.
176. Gleason, A. M., Groups without small subgroups, Ann. Math. **56**, 193–212 (1952) —
177. Goldhaber, A. S., Role of spin in the monopole problem, Phys. Rev. **140**, B1407–B1414 (1965) — Notes 7.1.
178. Goldman, S. P. and Drake, G. W. F., Relativistic sum rules and integral properties of the Dirac equation, Phys. Rev. **A25**, 2877–2881 (1982) — Notes 4.7.
179. Good, R. H., Properties of the Dirac matrices, Rev. Mod. Phys. **27**, 187–211 (1955) — Notes 2.5.
180. Gordon, W., Der Compton Effekt nach der Schrödingerschen Theorie, Z. Physik. **40**, 117–133 (1926) — Notes 1.1.
181. Gordon, W., Die Energieniveaus des Wasserstoffatoms nach der Diracschen Quantentheorie des Elektrons, Z. Physik. **48**, 11–14 (1928) — Notes 7.4.
182. Grigore, D. R., Irreducible representations of the Poincaré group including inversions, Fortschr. d. Physik. **39**, 101–130 (1991) — Notes 3.1.
183. Grigore, D. R., Nenciu, G. and Purice, R., On the nonrelativistic limit of the Dirac Hamiltonian, Ann. Inst. H. Poincaré **51**, 231–263 (1989) — Notes 5.6, 6.1, 6.2.
184. Gromov, M. and H. B. Lawson, J., Positive scalar curvature and the Dirac operator on complete Riemannian manifolds, Publ. Math. IHES. **58**, 295–408 (1983) — Notes 5.1, 5.7.
185. Groot, E. H. d., The virial theorem and the Dirac H atom, Am. J. Phys. **50**, 1141–1143 (1982) — Notes 4.7.
186. Grosse, H., Solitons in solid state physics, Acta Phys. Austriaca. Suppl. **26**, 393–399 (1984) — Notes 9.5.
187. Grosse, H., Solitons of the modified KdV equations, Lett. Math. Phys. **8**, 313–319 (1984) — Notes 9.5.
188. Grosse, H., New solitons connected to the Dirac equation, Phys. Rep. **134**, 297–304 (1986) — Notes 9.5.
189. Grosse, H., On the level order for Dirac operators, Phys. Lett. **B197**, 413–417 (1987) — Notes 7.4.
190. Grosse, H., Grümm, H. R., Narnhofer, H. and Thirring, W., Algebraic theory of Coulomb scattering, Acta Phys. Austriaca. **40**, 97–103 (1974) — Notes 8.2.
191. Grosse, H. and Karner, G., Quantization in presence of external soliton fields, Phys. Lett. **172**, 231–234 (1986) — Notes 10.2, 10.3.
192. Grosse, H. and Karner, G., Implementability of gauge transformations and quantization of fermions in external fields, J. Math. Phys. **28**, 371–375 (1987) — Notes 10.3.
193. Grosse, H. and Opelt, G., Fractional charges in external field problems and the inverse scattering method, Nucl. Phys. **B285**, 143–161 (1987) — Notes 10.3.
194. Grümm, H. R., Quantum mechanics in a magnetic field, Acta Phys. Austriaca. **53**, 113–131 (1981) — Notes 7.1.
195. Grébert, B., Formule de trace et problème de diffusion inverse pour l'opérateur de Dirac sur la droite réelle, C. R. Acad. Sci. Paris, Sér. I. **309**, 21–24 (1989) — Notes 9.5.
196. Guertin, R. F. and Guth, E., Zitterbewegung in relativistic spin-0 and -1/2 hamiltonian theories, Phys. Rev. **D7**, 1057–1068 (1973) — Notes 1.6.

197. Guillot, J. C. and Schmidt, G., Spectral and scattering theory for Dirac operators, Arch. Rat. Mech. Anal. **55**, 193–206 (1974) — Notes 8.1.
198. Gustafson, K. E. and Rejto, P. A., Some essentially self-adjoint Dirac operators with sperically symmetric potentials, Israel J. Math. **14**, 63–75 (1973) — Notes 4.6.
199. Gårding, L., Note on continuous representations of Lie groups, Proc. Nat. Acad. Sci. USA. **33**, 331–332 (1947) — Notes 2.3.
200. Hachem, G., Théorie spectrale de l'opérateur de Dirac dans un champ électromagnétique à croissance linéaire à l'infini, Thèse d'état, Université Paris-Nord (1988) — Notes 4.7.
201. Halvorsen, S. G. and Shaw, J. K., Spiral motion for components of a Dirac system of limit circle type, Proc. Roy. Soc. Edinburgh Sect. A **97**, (1984) — Notes 4.6.
202. Harish-Chandra, Motion of an electron in the field of a magnetic pole, Phys. Rev. **74**, 883–887 (1948) — Notes 7.1, 7.4.
203. Harrell, E. M. and Klaus, M., On the double-well problem for Dirac operators, Ann. Inst. H. Poincaré. **A38**, 153–166 (1983) — Notes 4.3.
204. Harris, B. J., Bounds for the eigenvalues of separated Dirac operators, Proc. Roy. Soc. Edinburgh Sect. A **95**, 341–366 (1983) — Notes 4.6.
205. Hautot, A., Motion in radial magnetic fields, J. Math. Phys. **14**, 2011–2017 (1973) — Notes 7.4.
206. Hegerfeldt, G. C., Remark on causality and particle localization, Phys.Rev. **D10**, 3320–3321 (1974) — Notes 1.8.
207. Hegerfeldt, G. C., Violation of causality in relativistic quantum theory?, Phys. Rev. Lett. **54**, 2395–2398 (1985) — Notes 1.8.
208. Hegerfeldt, G. C. and Ruijsenaars, S. N. M., Remarks on causality, localization, and spreading of wave packets, Phys. Rev. **D22**, 377–384 (1980) — Notes 1.8.
209. Helffer, B., Effet d'Aharonov Bohm sur un état borné de l'équation de Schrödinger, Commun. Math. Phys. **119**, 315–329 (1988) — Notes 7.3.
210. Helffer, B. and Martinez, A., Comparaison entre les diverses notions de résonances., Acta Phys. Helv. **60**, 992–1003 (1987) — Notes 4.7.
211. Helffer, B. and Mohammed, A., Sur le spectre essentiel des opérateurs de Schrödinger avec champ magnétique, Ann. Inst. Fourier. **38**, 95–113 (1988) — Notes 7.3.
212. Helffer, B., Nourrigat, J. and Wang, X. P., Sur le spectre de l'equation de Dirac (dans $\mathbb{R}^3$ ou $\mathbb{R}^2$) avec champ magnetique., Ann. Sci. Ecole Norm. Sup. **22**, 515–533 (1989) — Notes 4.3, 7.3.
213. Helffer, B. and Robert, D., Calcul fonctionnel par la transformée de Mellin et applications, J. Func. Anal. **53**, 246–268 (1983) — Notes 4.7.
214. Helffer, B. and Sjöstrand, J., Résonaces en limite semi-classique, Mémoire no. 24/25 de la SMF, Supplément du bulletin de la SMF. **114**, Fasc. 3 (1986) — Notes 4.7.
215. Hinton, D. B., Mingarelli, A. B., Read, T. T. and Shaw, J. K., On the number of eigenvalues in the spectral gap of a Dirac system, Proc. Edinburgh Math. Soc. (2). **29**, 367–378 (1986) — Notes 4.6.
216. Hinton, D. B. and Shaw, J. K., Absolutely continuous spectra of Dirac systems with long range, short range and oscillating potentials., Quart. J. Math. Oxford Ser. (2). **36**, 183–213 (1985) — Notes 4.6.
217. Hirayama, M., Supersymmetric quantum mechanics and index theorem, Prog. Theor. Phys. **70**, 1444–1453 (1983) — Notes 5.7, 5.11, 9.4.
218. Hirayama, M., Topological invariants for Dirac operators on open spaces, Phys. Rev. **D33**, 1079–1087 (1986) — Notes 5.7, 5.11, 9.4.
219. Hirota, R., Exact solutions of the modified Korteweg-de Vries equation for multiple collisions of solitons, J. Phys. Soc. Japan. **33**, 1456–1458 (1971) — Notes 9.2.
220. Hochstenbach, W. J. M. A., Field theory with an external potential, Commun. Math. Phys. **51**, 211–217 (1976) — Notes 10.3.
221. Hogreve, H., Schrader, R. and Seiler, R., A conjecture on the spinor functional determinant, Nucl. Phys. **B142**, 525–534 (1978) — Notes 7.3.

222. Hojman, S., Algebraic method for solving the Dirac equation with a Coulomb potential, Il Nuovo Cimento **4A**, 676–682 (1971) — Notes 7.4.
223. Hosoda, M., Shimizu, T. and Yamakoshi, H., APS-index for the fermion-vortex system, Prog. Theor. Phys. **76**, 538–547 (1986) — Notes 5.11.
224. Huang, K., On the Zitterbewegung of the Dirac electron, Am. J. Phys. **20**, 479–484 (1952) — Notes 1.6.
225. Hunziker, W., On the nonrelativistic limit of the Dirac theory, Commun. Math. Phys. **40**, 215–222 (1975) — Notes 6.1, 6.2.
226. Hönl, H., Feldmechanik des Elektrons und der Elementarteilchen, Ergeb. d. Exakten Naturwiss. **26**, 291–382 (1952) — Notes 1.6.
227. Hönl, H. and Papapetrou, A., Über die innere Bewegung des Elektrons. III, Z. Physik. **116**, 153–183 (1940) — Notes 1.6.
228. Hörmander, L., The existence of wave operators in scattering theory, Math. Z. **146**, 69–91 (1976) — Notes 1.9.
229. Imbimbo, C. and Mukhi, S., Topological invariance in supersymmetric theories with a continuous spectrum, Nucl. Phys. **B242**, 81–92 (1984) — Notes 5.11, 9.4.
230. Infeld, L. and Hull, T. E., The factorization method, Rev. Mod. Phys. **23**, 21–68 (1951) — Notes 7.4.
231. Ivrii, V. Y., Estimates for the spectrum of the Dirac operator, Soviet Math. Dokl. **36**, 599–602 (1988) — Notes 4.7, 7.3.
232. Ivrii, V. Y., Asymptotic behavior of eigenvalues for the two-dimensional Dirac operator with a strong magnetic field, Dokl. Akad. Nauk SSSR. **311**, 1102–1105 (1990) — Notes 4.7, 7.3.
233. Ivrii, V. Y., Exact spectral asymptotics for the Dirac operator with a strong magnetic field. (In Russian), Dokl. Akad. Nauk SSSR. **310**, 788–792 (1990) — Notes 4.7, 7.3.
234. Iyer, V. P. and Sharma, L. K., Scalar potentials in the Dirac equation and quark confinement, Phys. Lett. **102B**, 154–156 (1981) — Notes 4.2.
235. Jackiw, R., Fractional charge and zero modes for planar systems in a magnetic field, Phys. Rev. D. **29**, 2375–2377 (1984) — Notes 5.11, 7.2.
236. Jackiw, R. and Rebbi, C., Solitons with fermion number 1/2, Phys. Rev. **D13**, 3398–3409 (1976) — Notes 7.1, 10.3.
237. Jackiw, R. and Rebbi, C., Spinor analysis of Yang-Mills theory, Phys. Rev. **D16**, 1052 (1977) — Notes 5.11.
238. Jackiw, R. and Rossi, P., Zero modes of the vortex-fermion system, B190. **681–691**, (1981) — Notes 5.11.
239. Jacobson, T., Bosonic path integral for spin-1/2 particles, Phys. Lett. **B216**, 150–154 (1989) — Notes 1.5.
240. Jaffe, A. and Lesniewski, A., Supersymmetric quantum fields and infinite dimensional analysis, in: *Proceedings of the Cargèse Summer School, July 1987* (1988) — Notes 5.7.
241. Jaffe, A., Lesniewski, A. and Lewenstein, M., Ground state structure in supersymmetric quantum mechanics, Ann. Phys. **178**, 313–329 (1987) — Notes 5.7.
242. Jaffe, A., Lesniewski, A. and Weitsman, J., Index of a family of Dirac operators on loop space, Commun. Math. Phys. **112**, 75–88 (1987) — Notes 5.7.
243. Jaroszewicz, T., Gauge anomalies and scattering theory, Phys. Rev. **D34**, 3141–3148 (1986) — Notes 5.7.
244. Jehle, H., Relationship of flux quantization and charge quantization and the electromagnetic coupling constant, Phys. Rev. **D3**, 306–345 (1971) — Notes 1.6.
245. Jerison, D., Carleman inequalities for the Dirac and Laplace operators and unique continuation, Adv. in Math. **62**, 118–134 (1986) — Notes 4.7.
246. Johnson, M. H. and Lippman, B. A., Relativistic Kepler problem, Phys. Rev. **78**, 329 (1950) — Notes 7.4.
247. Johnson, M. H. and Lippmann, B. A., Relativistic motion in a magnetic field, Phys. Rev. **77**, 702–705 (1950) — Notes 5.6.
248. Johnson, W. R. and Deck, R. T., Continuum Coulomb wave function, J. Math. Phys. **3**, 319–324 (1962) — Notes 7.4.

249. Joos, H., Zur Darstellungstheorie der inhomogenen Lorentzgruppe als Grundlage quantenmechanischer Kinematik, Fortschr. d. Phys. **10**, 65–146 (1962) — Notes 3.1.

250. Josephson, J., An alternative formulation for the analysis and interpretation of the Dirac hydrogen atom, Found. Phys. **10**, 243–266 (1980) — Notes 7.4.

251. Jörgens, K., Perturbations of the Dirac operator, in: *Proceedings of the conference on the theory of ordinary and partial differential equations*, Dundee (Scotland) 1972, p. 87–102, W. N. Everitt and B. D. Sleeman eds., Lecture Notes in Mathematics 280, Springer Verlag, Berlin (1972) — Notes 4.3.

252. Kalf, H., The virial theorem in relativistic quantum mechanics, J. Func. Anal. **21**, 389–396 (1976) — Notes 4.7.

253. Kalf, H., Non-existence of eigenvalues of Dirac operators, Proc. Roy. Soc. Edinburgh. **A89**, 309–317 (1981) — Notes 4.7, 7.3.

254. Kalf, H., Schmincke, U. W., Walter, J. and Wüst, R., On the spectral theory of Schrödinger and Dirac operators with strongly singular potentials, in: *Proceedings of the Conf. Spectral Theory and Differential Equations*, Dundee (Scotland), p. 182–226, Springer Lecture Notes in Mathematics 448, Berlin, Heidelberg, New York (1974) — Notes 4.3.

255. Kaloyerou, P. N., Comments on the Hegerfeldt "paradox", Phys. Lett. **A129**, 285–290 (1988) — Notes 1.8.

256. Kametaka, Y., Korteweg-de Vries equation IV. Simplest generalization, Proc. Japan Acad. **45**, 661–665 (1969) — Notes 9.2.

257. Karnarski, B., Generalized Dirac-operators with several singularities, J. Op. Theor. **13**, 171–188 (1985) — Notes 4.3, 5.3.

258. Kato, T., On the Cauchy problem for the (generalized) Korteweg-de Vries equation, in: *Studies in Applied Mathematics*, p. 93–128, V. Guillemin ed., Adv. Math. Suppl. Studies 18, Academic Press, 1983 — Notes 9.2.

259. Kay, I. and Moses, H. E., Reflectionless transmission through dielectrics and scattering potentials, J. Appl. Phys. **27**, 1503–1508 (1956) — Notes 9.5.

260. Kazama, Y., Electric and magnetic dipole moments of the bound system of a Dirac particle and a fixed magnetic monopole, Phys. Rev. **D16**, 3078–3085 (1977) — Notes 7.1.

261. Kazama, Y. and Yang, C. N., Existence of bound states for a charged spin-1/2 particle with an extra magnetic moment in the field of a fixed magnetic monopole, Phys. Rev. **D15**, 2300–2307 (1977) — Notes 7.1.

262. Kazama, Y., Yang, C. N. and Goldhaber, A. S., Scattering of a Dirac particle with charge Ze by a fixed magnetic monopole, Phys. Rev. **D15**, 2287–2299 (1977) — Notes 7.1.

263. Khare, A. and Maharana, J., Supersymmetric quantum mechanics in one, two, and three dimensions, Nucl. Phys. **B244**, 409–420 (1984) — Notes 5.1.

264. Kihlberg, A., Salomonson, P. and Skagerstam, B. S., Witten's index and supersymmetric quantum mechanics, Z. Phys. **C28**, 203–209 (1985) — Notes 5.11, 7.2.

265. Klaus, M., Dirac operators with several Coulomb singularities, Helv. Phys. Acta. **53**, 463–482 (1980) — Notes 4.3.

266. Klaus, M., On the point spectrum of Dirac operators, Helv. Phys. Acta. **53**, 453–462 (1980) — Notes 4.7.

267. Klaus, M., On coupling constant thresholds and related eigenvalue properties of Dirac operators, J. Reine Angew. Math. **362**, 197–212 (1985) — Notes 4.7.

268. Klaus, M. and Scharf, G., The regular external field problem in quantum electrodynamics, Helv. Phys. Acta. **50**, 779–802 (1977) — Notes 10.3.

269. Klaus, M. and Scharf, G., Vacuum polarization in Fock space, Helv. Phys. Acta. **50**, 803–814 (1977) — Notes 10.3.

270. Klaus, M. and Wüst, R., Characterization and uniqueness of distinguished self-adjoint extensions of Dirac operators, Commun. Math. Phys. **64**, 171–176 (1979) — Notes 4.3.

271. Klaus, M. and Wüst, R., Spectral properties of Dirac operators with singular potentials, J. Math. Anal. Appl. **72**, 206–214 (1979) — Notes 4.3.

272. Klein, O., Elektrodynamik und Wellenmechanik von Standpunkt des Korrespondenzprinzips, Z. Physik. **41**, 407–442 (1927) — Notes 1.1.
273. Klein, O., Die Reflexion von Elektronen an einem Potentialsprung nach der relativistischen Dynamik von Dirac, Z. Physik. **53**, 157–165 (1928) — Notes 4.5.
274. Krein, M. G., On certain new studies in the perturbation theory for self-adjoint operators, in: *Topics in Differential and Integral Equations and Operator Theory*, p. 107–172, I. Gohberg ed., Birkhäuser Verlag, 1983 — Notes 5.10.
275. Krein, M. G., On perturbation determinants and a trace formula for certain classes of pairs of operators, Amer. Math. Soc. Transl. (2). **145**, 39–84 (1989) — Notes 5.10.
276. Kruzhkov, S. N. and Faminskii, A. V., Generalized solutions of the Cauchy problem for the Korteweg-de Vries equation, Math. USSR Sbornik. **48**, 391–421 (1984) — Notes 9.2.
277. Kudar, J., Zur vierdimensionalen Formulierung der undulatorischen Mechanik, Annalen d. Phys. **81**, 632–636 (1926) — Notes 1.1.
278. Kurbenin, O. I., The discrete spectra of the Dirac and Pauli operators, in: *Topics in Mathematical Physics, Vol.3, Spectral Theory*, p. 43–52, M. S. Birman ed., Consultants Bureau, 1969 — Notes 4.7.
279. Kursunoglu, B., Transformation of relativistic wave equations, Phys. Rev. **101**, 1419–1424 (1956) — Notes 5.6.
280. Kutzelnigg, W., The relativistic many body problem in molecular theory, Phys. Scripta. **36**, 416–431 (1987) — Notes 6.2.
281. Kutzelnigg, W., Perturbation theory of relativistic corrections I., Z. Phys. D - Atoms, Molecules and Clusters. **11**, 15–28 (1989) — Notes 6.2.
282. Kutzelnigg, W., Perturbation theory of relativistic corrections II, Z. Phys. D - Atoms, Molecules and Clusters. **15**, 27–50 (1990) — Notes 6.1, 6.2.
283. Kálnay, A. J., The Localization Problem, in: *Problems in the Foundations of Physics, Vol. 4*, p. 93–110, M. Bunge ed., Springer, 1971 — Notes 1.7.
284. Labonté, G., On the nature of "strong" Bogoliubov transformations for fermions, Commun. Math. Phys. **36**, 59–72 (1974) — Notes 10.3.
285. Labonté, G., On the particle interpretation for the quantized fields in external field problems, Canad. J. Physics. **53**, 1533–1559 (1975) — Notes 10.3.
286. Landgren, J. J. and Reitö, P. A., An application of the maximum principle to the study of essential self-adjointness of Dirac operators. I, J. Math. Phys. **20**, 2204–2211 (1979) — Notes 4.3.
287. Landgren, J. J., Reitö, P. A. and Klaus, M., An application of the maximum principle to the study of essential self-adjointness of Dirac operators. II, J. Math. Phys. **21**, 1210–1217 (1980) — Notes 4.3.
288. Lax, P. D., Integrals of nonlinear equations of evolution and solitary waves, Commun. Pure Appl. Math. **21**, 467–490 (1968) — Notes 9.1.
289. Leinfelder, H., Gauge invariance of Schrödinger operators and related spectral properties, J. Op. Theory. **9**, 163–179 (1983) — Notes 4.4, 7.3.
290. Lieb, E. H. and Yau, H. T., The stability and instability of relativistic matter, Commun. Math. Phys. **118**, 177–213 (1988) — Notes 1.5.
291. Lipkin, H. J., Peshkin, M. and Weisberger, W. I., Magnetic charge quantization and angular momentum, Ann. Phys. **53**, 203–214 (1969) — Notes 7.1.
292. Lock, J. A., The Zitterbewegung of a free localized Dirac particle, Am. J. Phys. **47**, 797–802 (1979) — Notes 1.6.
293. Lombardi, J. R., Relativistic hydrogen atom in the momentum representation, Phys. Rev. **A27**, 1275–1278 (1983) — Notes 7.4.
294. Loss, M. and Thaller, B., Scattering of particles by long-range magnetic fields, Ann. Phys. **176**, 159–180 (1987) — Notes 8.4.
295. Loss, M. and Thaller, B., Short-range scattering in long-range magnetic fields: The relativistic case, J. Diff. Eq. **73**, 225–236 (1988) — Notes 8.4.
296. Loss, M. and Yau, H. T., Stability of Coulomb systems with magnetic fields III. Zero energy bound states of the Pauli operator, Commun. Math. Phys. **104**, 283–290 (1986) — Notes 7.2.

297. Lott, J., The Eta function and some new anomalies, Phys. Lett. **145B**, 179–180 (1984) — Notes 5.7.
298. Lott, J., Vacuum charge and the eta-function, Commun. Math. Phys. **93**, 533–558 (1984) — Notes 5.11, 9.4.
299. Lott, J., A proof of the axial anomaly, Commun. Math. Phys. **97**, 371–379 (1985) — Notes 5.7.
300. Lundberg, L. E., Spectral and scattering theory for the Klein-Gordon equation, Commun. Math. Phys. **31**, 243–257 (1973) — Notes 5.4, 5.
301. Lundberg, L. E., Quasi-free "second quantization", Commun. Math. Phys. **50**, 103–112 (1976) — Notes 10.3.
302. Löwdin, P. O., Studies in perturbation theory VIII. Separation of Dirac equation and study of the spin-orbit coupling and Fermi contact terms, J. Mol. Spectr. 14, 131–144 (1964) — Notes 6.1.
303. Léon, J., Quirós, M. and Mittelbrunn, J. R., Group content of the Foldy-Wouthuysen transformation and the nonrelativistic limit for arbitrary spin, J. Math. Phys. **20**, 1068–1076 (1979) — Notes 3.2–3, 5.6.
304. Macfarlane, A. J., Dirac matrices and the Dirac matrix description of Lorentz transformations, Commun. Math. Phys. **2**, 133–146 (1966) — Notes 2.D.
305. Mackey, G., Induced representations of locally compact groups I, Ann. Math. **55**, 101–139 (1952) — Notes 3.1.
306. Marciano, W. J. and Muzinich, I. J., Exact solution of the Dirac equation in the field of a 't Hooft Polyakov monopole, Phys. Rev. Lett. **50**, 1035–1037 (1983) — Notes 7.1.
307. Martin, P. C. and Glauber, R. J., Relativistic theory of radiative orbital electron capture, Phys. Rev. **109**, 1307–1325 (1958) — Notes 7.4.
308. Matsui, T., The index of scattering operators of Dirac equations, Commun. Math. Phys. **110**, 553–571 (1987) — Notes 8.5, 10.3.
309. Matsui, T., The index of scattering operators of Dirac equations. 2, J. Func. Anal. **94**, 93–109 (1990) — Notes 8.5, 10.3.
310. McKinley, W. A. and Feshbach, H., The Coulomb scattering of relativistic electrons by nuclei, Phys. Rev. **74**, 1759–1763 (1948) — Notes 7.4.
311. Melosh, H. J., Quarks: Currents and constituents, Phys. Rev. **D9**, 1095–1112 (1974) — Notes 5.6.
312. Mendlowitz, H., High-energy electron-nuclear scattering, Phys. Rev. **102**, 527–529 (1956) — Notes 5.6.
313. Miller, K. C., Bound states of quantum mechanical particles in magnetic fields, Dissertation, Princeton University (1982) — Notes 7.3.
314. Miller, K. and Simon, B., Quantum magnetic Hamiltonians with remarkable spectral properties, Phys. Rev. Lett. 44, 1706–1707 (1980) — Notes 7.3.
315. Mitter, H., Quantum electrodynamics in laser fields, Acta Phys. Austriaca Suppl. 14, 397–468 (1975) — Notes 10.1.
316. Miura, R. M., Korteweg-deVries equation and generalizations I. A remarkable explicit nonlinear transformation, J. Math. Phys. **9**, 1202–1204 (1968) — Notes 9.1.
317. Mohamed, A. and Parisse, B., Approximation des valeurs propres de certaines perturbations singulières et application à l'opérateur de Dirac, preprint of the Département de Mathématiques, Université de Nantes (1991) — Notes 4.7.
318. Montgomery, D. and Zippin, L., Small subgroups of finite dimensional groups, Ann. Math. **56**, 213–241 (1952) —
319. Moreno, M., Martinez, R. and Zentella, A., Supersymmetry, Foldy-Wouthuysen transformation and stability of the Dirac sea, Modern Phys. Lett. A **5**, 949–954 (1990) — Notes 5.6.
320. Moscovici, H. and Stanton, R. J., Eta invariants of Dirac operators on locally symmetric manifolds, Invent. math. **95**, 629–666 (1989) — Notes 5.7.
321. Moss, R. E. and Okniński, A., Diagonal forms of the Dirac Hamiltonian, Phys. Rev. **D14**, 3358–3361 (1976) — Notes 5.5, 5.6.

322. Mott, N. F., The scattering of fast electrons by atomic nuclei, Proc. Roy. Soc. London. **A124**, 425–442 (1929) — Notes 7.4.
323. Moyer, D. F., Evaluations of Dirac's electron, 1928–1932, Am. J. Phys. **49**, 1055–1062 (1981) — Notes 1.1.
324. Moyer, D. F., Origins of Dirac's electron, 1925–1928, Am. J. Phys. **49**, 944–949 (1981) — Notes 1.1.
325. Moyer, D. F., Vindications of Dirac's electron, 1932–1934, Am. J. Phys. **49**, 1120–1125 (1981) — Notes 1.1.
326. Muthuramalingam, P., Scattering theory by Enss' method for operator valued matrices: Dirac operator in an electric field, J. Math. Soc. Japan. **37**, 415–432 (1985) — Notes 8.3.
327. Muthuramalingam, P. and Sinha, K. B., Existence and completeness of wave operators for the Dirac operator in an electromagnetic field with long range potentials, J. Indian Math. Soc. (N.S.). **50**, 103–130 (1986) — Notes 8.2, 8.3.
328. Najman, B., Scattering for the Dirac operator, Glasnik Matematički. 11, 63–80 (1976) — Notes 8.1.
329. Najman, B., Eigenvalues of the Klein-Gordon Equation, Proc. of the Edinburgh Math. Soc. **26**, 181–190 (1983) — Notes 5.5.
330. Najman, B., The nonrelativistic limit of the Klein-Gordon and Dirac equations, in: *Differential Equations with Applications in Biology, Physics and Engineering*, p. 291–299, J. Goldstein, F. Kappel and W. Schappacher ed., Lecture notes in pure and applied mathematics, Vol. 133, Marcel Dekker, New York, Basel, Hong-Kong, 1990 — Notes 6.1.
331. Narnhofer, H., Quantum Theory for $1/r^2$ - potentials, Acta Phys. Austriaca. **40**, 306–322 (1974) — Notes 4.3, 7.4.
332. Nelson, E., Analytic vectors, Ann. Math. **70**, 572–615 (1959) — Notes 2.3.
333. Nenciu, G., Self-adjointness and invariance of the essential spectrum for Dirac operators defined as quadratic forms, Commun. Math. Phys. **48**, 235–247 (1976) — Notes 4.3.
334. Nenciu, G., Distinguished self-adjoint extension for Dirac operator with potential dominated by multicenter Coulomb potentials, Helv. Phys. Acta. **50**, 1–3 (1977) — Notes 4.3.
335. Nenciu, G., Strong external fields in QED. Rigorous results, in: *Proceedings of the Predeal International Summer School in Heavi Ion Physics*, Predeal, Romania, p. 653–690, (1978) — Notes 10.4.
336. Nenciu, G., On the adiabatic limit for Dirac particles in external fields, Commun. Math. Phys. **76**, 117–128 (1980) — Notes 10.4.
337. Nenciu, G., Existence of the spontaneous pair creation in the external field approximation of Q.E.D., Commun. Math. Phys. **109**, 303–312 (1987) — Notes 10.4.
338. Nenciu, G. and Scharf, G., On regular external fields in quantum electrodynamics, Helv. Phys. Acta. **51**, 412–424 (1978) — Notes 10.3.
339. Newton, R. G., Inverse scattering. I. One dimension, J. Math. Phys. **21**, 493–505 (1980) — Notes 9.4.
340. Newton, T. D. and Wigner, E. P., Localized States for Elementary Systems, Rev. Mod. Phys. **21**, 400–406 (1949) — Notes 1.7.
341. Niederer, U. H. and O'Raifeartaigh, L., Realizations of the unitary representations of the inhomogeneous space-time groups I, II, Fortschritte d. Phys. **22**, 111–129, and 131–157 (1974) — Notes 3.2–3.
342. Niemi, A. J. and Semenoff, G. W., Spectral asymmetry on an open space, Phys. Rev. **D30**, 809–818 (1984) — Notes 5.11.
343. Niemi, A. J. and Semenoff, G. W., Fermion number fractionization in quantum field theory, Phys. Rep. **135**, 99–193 (1986) — Notes 5.7, 5.11, 9.4, 10.3.
344. Niemi, A. J. and Semenoff, G. W., Index theorems on open infinite manifolds, Nucl. Phys. **B269**, 131–169 (1986) — Notes 5.7.
345. Odaka, K. and Itoh, T., Particle picture in external fields, quantum holonomy, and gauge anomaly, Lett. Math. Phys. **15**, 297–303 (1988) — Notes 10.3.
346. Ohmiya, M., On the generalized soliton solutions of the modified Korteweg-de Vries equation, Osaka J. Math. **11**, 61–71 (1974) — Notes 9.2.

347. Ohmiya, M., The inverse scattering problem for the Dirac operator and the modified Korteweg-De Vries equation, Osaka J. Math. **16**, 249–269 (1979) — Notes 9.5.
348. Osche, G. R., Dirac and Dirac-Pauli equations in the Foldy Wouthuysen representation, Phys. Rev. **D15**, 2181–2185 (1977) — Notes 5.6.
349. Palladino, B. E. and Leal Ferreira, P., Level order in a relativistic potential model, Phys. Lett. B. **185**, 118–120 (1987) — Notes 7.4.
350. Palmer, J., Scattering automorphisms of the Dirac field, J. Math. Anal. Appl. **64**, 189–215 (1978) — Notes 8.5, 10.4.
351. Paranjape, M. and Semenoff, G., Spectral asymmetry, trace identities and the fractional fermion number of magnetic monopoles, Phys. Lett. **132B**, 369–373 (1983) — Notes 5.11.
352. Parisse, B., Résonances paires pour l'opérateur de Dirac, C. R. Acad. Sci. Paris, Série I. **310**, 265–268 (1990) — Notes 4.7.
353. Parisse, B., Résonances pour l'opérateur de Dirac, preprint (1991) — Notes 4.7.
354. Parthasarathy, K. R., Projective unitary antiunitary representations of locally compact groups, Commun. Math. Phys. **15**, 305–328 (1969) — Notes 3.1.
355. Parthasarathy, K. R., On the exact bound of the Coulomb potential with respect to the Dirac operator, Lett. Math. Phys. **2**, 413–415 (1978) — Notes 4.3.
356. Pasztor-Kraus, J., Scattering theory in external fields slowly decaying in time, Helv. Phys. Acta. **63**, 86–106 (1990) — Notes 10.4.
357. Pauli, W., Contributions mathématiques à la théorie des matrices de Dirac, Ann. Inst. Henri Poincaré. **6**, 109–136 (1936) — Notes 2.5.
358. Pauli, W., Die allgemeinen Prinzipien der Wellenmechanik, in: *Handbuch der Physik Vol. 5/1, Prinzipien der Quantentheorie*, p. 137–168, S. Flügge ed., Sect. 4.2, Springer, 1958 — Notes 1.1, 6.1.
359. Pearson, D. B., The Dirac operator with highly singular potentials, Commun. Math. Phys. **57**, 117–133 (1977) — Notes 8.1.
360. Perez, J. F. and Wilde, I. F., Localization and causality in relativistic quantum mechanics, Phys. Rev. **D16**, 315–317 (1977) — Notes 1.8.
361. Perkins, G. A., The direction of the Zitterbewegung: A hidden variable, Found. Phys. **6**, 237–248 (1976) — Notes 1.6.
362. Petzold, J., Probleme der Makrokausalität und Teilchendichte in der relativistischen Quantenmechanik, Annalen der Physik. **31**, 372–380 (1974) — Notes 1.8.
363. Piron, C. and Reuse, F., Relativistic dynamics for the spin 1/2 particle, Helv. Phys. Acta. **51**, 146 156 (1978) — Notes 1.4.
364. Polyakov, A. M., in: *Champs, cordes et phenomenes critiques* (Les Houches), 305–368, North Holland, Amsterdam 1990 — Notes 1.5.
365. Popov, On the properties of the discrete spectrum for Z close to 137, Sov. Phys. JETP. **33**, 665–673 (1971) — Notes 7.4.
366. Popov, V. S., "Collapse to the center" at $Z > 137$ and critical nuclear charge, Sov. J. Nucl. Phys. **12**, 235–243 (1971) — Notes 4.3, 7.4.
367. Prosser, R. T., Relativistic Potential Scattering, J. Math. Phys. 4, 1048–1054 (1963) — Notes 1.5.
368. Prugovečki, E., Dirac dynamics on stochastic phase spaces for spin 1/2 particles, Pep. Math. Phys. **17**, 401–417 (1980) — Notes 1.4, 3.2–3.
369. Pryce, M. H. L., The mass-centre in the restricted theory of relativity and its connexion with the quantum theory of elementary particles, Proc. Roy. Soc. Ser. A **195**, 62–81 (1948) — Notes 1.4, 1.7, 5.6.
370. Quesne, C., Supersymmetry and the Dirac oscillator, Int. J. Mod. Phys. A **6**, 1567–1589 (1990) — Notes 7.4.
371. Radin, C. and Simon, B., Invariant domains for the time-dependent Schrödinger equation, J. Diff. Equ. **29**, 289–296 (1978) — Notes 1.6.
372. Rafelski, J., Fulcher, L. P. and Klein, A., Fermions and bosons interacting with arbitrarily strong external fields, Phys. Reps. **38**, 227–361 (1978) — Notes 10.1.

373. Ram, B., Quark confining potential in relativistic equations, Am. J. Phys. **50**, 549–551 (1982) — Notes 4.2.
374. Ram, B. and Arafah, M., Bound-state Dirac eigenvalues for scalar potentials, Lett. al Nuovo Cimento **30**, 5–8 (1981) — Notes 4.2.
375. Ravndal, F., A harmonic quark bag model, Phys. Lett. **113B**, 57–60 (1982) — Notes 4.2.
376. Rejtö, P. A., On reducing subspaces for one-electron Dirac operators, Israel J. Math. **9**, 111–143 (1971) — Notes 4.6.
377. Reuse, F., A new relativistic model for the hydrogen atom, Helv. Phys. Acta. **51**, 157–166 (1978) — Notes 1.4.
378. Roe, J., An index theorem on open manifolds. I, II, J. Diff. Geom. **27**, 87–113, and 115–136 (1988) — Notes 5.1, 5.7.
379. Ronveaux, A., Nonrelativistic limit of the Dirac equation in the continuum, Lett. al Nuovo Cimento, Ser I. **4**, 703–706 (1970) — Notes 6.1.
380. Ronveaux, A., Longueur de diffusion en théorie de Dirac et de Schrödinger, C. R. Acad. Sc. Paris, Ser. **B272**, 1229–1231 (1971) — Notes 6.1.
381. Roos, B. W. and Sangren, W. C., Spectral theory of Dirac's radial relativistic wave equation, J. Math. Phys. **3**, 882–890 (1962) — Notes 4.6.
382. Rosen, B., Relativistic Coulomb scattering, J. Math. Phys. 4, 392–404 (1963) — Notes 7.4.
383. Rosenhouse, A. and Katriel, J., Isospectral transformations in relativistic and nonrelativistic mechanics, Lett. Math. Phys. **13**, 141–146 (1987) — Notes 9.2.
384. Rosenstein, B. and Usher, M., Explicit illustration of causality violoation: Noncausal relativistic wave-packet evolution, Phys. Rev. **D36**, 2381–2384 (1987) — Notes 1.8.
385. Roux, J. F., Exact diagonalization of the Hamiltonian of a Dirac particle with anomalous moment, interacting with an external magnetic field, J. Math. Phys. **25**, 2087–2089 (1984) — Notes 5.4, 5.
386. Ruijsenaars, S. N. M., Charged particles in external fields. I. Classical theory, J. Math. Phys. **18**, 720–737 (1977) — Notes 1.4, 8.5, 10.1, 10.3.
387. Ruijsenaars, S. N. M., Charged particles in external fields. II. The quantized Dirac and Klein-Gordon Theories, Commun. Math. Phys. **52**, 267–294 (1977) — Notes 10.1, 10.3, 10.4.
388. Ruijsenaars, S. N. M., On Bogoliubov transformations for systems of relativistic charged particles, J. Math. Phys. **18**, 517–526 (1977) — Notes 10.3.
389. Ruijsenaars, S. N. M., On Bogoliubov transformations. II. The general case, Ann. Phys. **116**, 105–134 (1978) — Notes 10.3.
390. Ruijsenaars, S. N. M., Gauge invariance and implementability of the S-operator for spin-0 and spin-1/2 particles in time dependent external fields, J. Func. Anal. **33**, 47–57 (1979) — Notes 4.4, 8.5, 10.4.
391. Ruijsenaars, S. N. M., On Newton Wigner localization and superluminal propagation speeds, Ann. Phys. **137**, 33–43 (1981) — Notes 1.8.
392. Ruijsenaars, S. N. M., Index formulas for generalized Wiener-Hopf operators and boson-fermion correspondence in 2N dimensions, Commun. Math. Phys. **124**, 553–593 (1989) — Notes 8.5, 10.3.
393. Ruijsenaars, S. N. M., Index theorems and anomalies: a common playground for mathematicians and physicists, CWI-Quarterly. **3**, 3–19 (1990) — Notes 5.8, 10.3.
394. Salam, A. and Matthews, P. T., Fredholm theory of scattering in a given time-dependent field, Phys. Rev. **90**, 690–694 (1953) — Notes 10.1.
395. Salomonsen, P. and Holten, J. W. v., Fermionic coordinates and supersymmety in quantum mechanics, Nucl. Phys. **B196**, 509–531 (1982) — Notes 5.1.
396. Salpeter, E. E., Some atomic effects of an electronic electric dipole moment, Phys. Rev. **112**, 1642–1648 (1958) — Notes 4.2.
397. Saroia, D., Rao, K. N. S. and Rao, A. V. G., New aspects of the Foldy-Wouthuysen and Cini-Touschek transformations, J. Phys. A: Math. Gen. **11**, 1185–1190 (1978) — Notes 5.6.
398. Sauter, F., Zum "Kleinschen Paradoxon", Z. Physik. **73**, 547–552 (1931) — Notes 4.5.

399. Scharf, G. and Seipp, H. P., Charged vacuum, spontaneous positron production and all that, Phys. Lett. **108B**, 196–198 (1982) — Notes 10.4.

400. Scharf, G. and Seipp, H. P., Strong-Coupling Theory of the Dirac equation, Nuovo Cimento **82A**, 1–34 (1984) — Notes 10.4.

401. Schechter, M., Wave operators for pairs of spaces and the Klein-Gordon equation, Aequat. Math. **20**, 38–50 (1980) — Notes 5.4, 5.

402. Schlüter, P., Wietschorke, P. and Greiner, K. H., The Dirac equation in orthogonal coordinate systems. I. The local representation. II. The two-centre Dirac equation, J. Phys. A: Math. Gen. **16**, 1999–2016, and 2017–2034 (1983) — Notes 4.6.

403. Schmincke, U. W., Distinguished selfadjoint extensions of Dirac operators, Math. Z. **129**, 335–349 (1972) — Notes 4.3.

404. Schmincke, U. W., Essential selfadjointness of Dirac operators with a strongly singular potential, Math. Z. **126**, 71–81 (1972) — Notes 4.3.

405. Schmincke, U. -., On Schrödingers factorization method for Sturm-Liouville operators, Proc. Roy. Soc. Edinburgh. **80A**, 67–84 (1978) —

406. Schoene, A. Y., On the nonrelativistic limits of the Klein Gordon and Dirac equations, J. Math. Anal. Appl. **71**, 36–47 (1979) — Notes 6.1.

407. Schrödinger, E., Quantisierung als Eigenwertproblem, Annalen d. Phys. **79**, 361–376 (1926) — Notes 1.1.

408. Schrödinger, E., Über die kräftefreie Bewegung in der relativistischen Quantenmechanik, Sitzungsber. Preuss. Akad. Wiss. Berlin, Phys.-math. Kl. **24**, 418–428 (1930) — Notes 1.6.

409. Schrödinger, E., A method of determining quantum-mechanical eigenvalues and eigenfunctions, Proc. Roy. Irish Acad. Sect. A **46**, 9–16 (1940) — Notes 7.4.

410. Schulman, L. S., A path integral for spin, Phys. Rev. **176**, 1558–1569 (1968) — Notes 1.5.

411. Schwinger, J., On gauge invariance and vacuum polarization, Phys. Rev. **82**, 664–679 (1950) — Notes 1.4.

412. Schwinger, J., Theory of quantized fields V., Phys. Rev. **93**, 615–628 (1954) — Notes 10.1.

413. Seba, P., The complex scaling method for Dirac resonances, Lett. Math. Phys. **16**, 51–59 (1988) — Notes 4.7.

414. Seiler, R., Quantum theory of particles with spin zero and one half in external fields, Commun. Math. Phys. **25**, 127–151 (1972) — Notes 10.3.

415. Seiler, R., Particles with spin≤ 1 in an external field, in: *Invariant Wave Equations*, p. 165–196, G. Velo and A. S. Wightman eds., Lecture Notes in Physics 73, Springer Verlag, 1978 — Notes 10.3.

416. Seipp, H. P., On the S-operator for the external field problem of QED, Helv. Phys. Acta. **55**, 1–28 (1982) — Notes 8.5, 10.4.

417. Sewell, G. L., An appropriate relation between the energy levels of a particle in a field of given potential energy, calculated in the relativistic and non-relativistic theories, Proc. Cambridge Phil. Soc. **45**, 631–637 (1949) — Notes 6.1, 6.2.

418. Shale, D. and Stinespring, W. F., Spinor representations of infinite orthogonal groups, J. Math. Mech. **14**, 315–322 (1965) — Notes 10.3.

419. Sharma, C. S. and Almeida, D. F., A direct proof of Wigners theorem on maps which preserve transition probabilities between pure states of quantum systems, Ann. Phys. **197**, 300–309 (1990) — Notes 2.2.

420. Sharma, L. K., Mehta, S. and Iyer, V. P., Solution of the Dirac equation for the general even power potential with application to particle spectroscopy, J. Math. Phys. **24**, 2521–2527 (1983) — Notes 4.2.

421. Shirokov, I. M., A group theoretical consideration of the basis of relativistic quantum mechanics, I. The general properties of the inhomogeneous Lorentz group, Soviet Physics JETP. **6** (**33**), 664–673 (1958) — Notes 3.1.

422. Shirokov, I. M., A group theoretical consideration of the basis of relativistic quantum mechanics, II. Classification of the irreducible representations of the inhomogeneous Lorentz group, Soviet Physics JETP. **6(33)**, 919–928 (1958) — Notes 3.1.

423. Shirokov, I. M., A group theoretical consideration of the basis of relativistic quantum mechanics, III. Irreducible representations of the classes P_0 and O_0, and the non-completely reducible representations of the inhomogeneous Lorentz group, Soviet Physics JETP. **6(33)**, 929–935 (1958) — Notes 3.1.

424. Shirokov, I. M., A group theoretical consideration of the basis of relativistic quantum mechanics, IV. Space reflections in quantum theory, Soviet Physics JETP. **34(7)**, 493–498 (1958) — Notes 3.1.

425. Shirokov, I. M., A group theoretical consideration of the basis of relativistic quantum mechanics, V. The irreducible representations of the inhomogeneous Lorentz group, including space inversion and time reversal, Soviet Physics JETP. **36(9)**, 620–626 (1959) — Notes 2.6, 3.1.

426. Singer, I. M., The η-invariant and the index, in: *Mathematical Aspects of String Theory*, p. 239–249, S. T. Yau ed., Advanced Series in Mathematical Physics **1**, World Scientific, 1987 — Notes 5.7.

427. Smith, P. F. and Lewin, J. D., Fermions in scalar and vector potentials, Il Nuovo Cimento **64A**, 421–452 (1981) — Notes 4.2.

428. Soff, G., Müller, B., Rafelski, J. and Greiner, W., Solution of the Dirac equation for scalar potentials and its implication in atomic physics, Zeitschr. f. Naturforsch. **A28**, 1389–1396 (1973) — Notes 7.4.

429. Stahlhofen, A., Erweiterung und neue Anwendungen der Infeld'schen Faktorisierung, Dissertation, Institut f. Theoret. Kernphysik, Universität Bonn, BRD (1986) — Notes 5.1, 7.4.

430. Stahlhofen, A. and Biedenharn, L. C., Group-theoretic approach to scattering: the Dirac-Coulomb problem and relativistic supersymmetry., in: *Proceedings of the 16th international colloquium on group theoretical methods in physics*, Varna 1987, p. 261–267, H. D. Doebner, J. D. Hennig and T. D. Palev eds., Lecture Notes in Physics 313, Springer Verlag (1988) — Notes 7.4.

431. Stone, M., Zero modes, boundary conditions and anomalies on the lattice and in the continuum, Ann. Phys. (NY). **155**, 56–84 (1984) — Notes 5.11, 9.4.

432. Su, J. Y., Simplified solutions of the Dirac-Coulomb equation, Phys. Rev. **A32**, 3251–3257 (1985) — Notes 7.4.

433. Su, R. K. and Ma, Z. Q., Confinement properties for the Dirac equation with scalar-like and vector-like potentials, J. Phys. A: Math. Gen. **19**, 1739–1743 (1986) — Notes 4.2, 4.6.

434. Sucher, J., Relativistic Invariance and the Square-Root Klein-Gordon Equation, J. Math. Phys. **4**, 17–23 (1963) — Notes 1.1.

435. Sukumar, C. V., Supersymmetry and the Dirac equation for a central Coulomb field, J. Phys. A: Math. Gen. **18**, L697–L701 (1985) — Notes 7.4.

436. Tamura, H., The asymptotic distribution of discrete eigenvalues for Dirac operators, J. Fac. Sci. Univ. Tokyo Sec. IA Math. **23**, 167–197 (1976) — Notes 4.7.

437. Tanaka, S., Modified Korteweg-de Vries equation and scattering theory, Proc. Japan Acad. **48**, 466–469 (1972) — Notes 9.2.

438. Tanaka, S., Some remarks on the modified Korteweg-de Vries equation, Publ. RIMS, Kyoto Univ. **8**, 429–437 (1973) — Notes 9.1, 9.2.

439. Tani, S., (in Japanese), Soryushiron Kenkyu. 1, 15 (1949) — Notes 5.6.

440. Tani, S., Connection between particle models and field theories, I, Prog. Theor. Phys. **6**, 267–285 (1951) — Notes 5.6.

441. Tegen, R., Relativistic harmonic oscillator potential for quarks in the nucleon, Ann. Phys. **197**, 439–455 (1990) — Notes 4.2.

442. Thaller, B., Relativistic scattering theory for long-range potentials of the nonelectrostatic type, Lett. Math. Phys. **12**, 15–19 (1986) — Notes 8.3.

443. Thaller, B., Normal forms of an abstract Dirac operator and applications to scattering theory, J. Math. Phys. **29**, 249–257 (1988) — Notes 5.2, 5.6.
444. Thaller, B., Scattering theory of a supersymmetric Dirac operator, in: *Differential Equations with Applications in Biology, Physics and Engineering*, p. 313–326, J. Goldstein, F. Kappel and W. Schappacher eds., Lecture notes in pure and applied mathematics, Vol. 133, Marcel Dekker, New York, Basel, Hong-Kong, 1991 — Notes 8.4.
445. Thaller, B. and Thaller, S., Remarks on the localization of Dirac particles, Il Nuovo Cimento **82A**, 222–228 (1984) — Notes 1.8.
446. Thompson, M., Eigenfunction expansions and the associated scattering theory for potential perturbations of the Dirac equation, Quart. J. Math. Oxford. **23**, 17–55 (1972) — Notes 8.1.
447. Titchmarsh, E. C., On the nature of the spectrum in problems of relativistic quantum mechanics, Quart. J. Math. Oxford. **12**, 227–240 (1961) — Notes 4.6.
448. Titchmarsh, E.. A problem in relativistic quantum mechanics, Proc. London. Math. Soc. **41**, 170–192 (1961) — Notes 4.7.
449. Titchmarsh, E. C., On the relation between the eigenvalues in relativistic and nonrelativistic quantum mechanics, Proc. Roy. Soc. **A 266**, 33–46 (1962) — Notes 6.1, 6.2.
450. Tsai, W., Energy eigenvalues for charged particles in a homogeneous magnetic field-an application of the Foldy-Wouthuysen transformation, Phys. Rev. **D7**, 1945–1948 (1973) — Notes 5.4, 5.
451. Tsutsumi, M., On global solutions of the generalized Korteweg-deVries equation, Publ. RIMS, Kyoto Univ. **7**, 329–344 (1972) —
452. Velo, G. and Zwanziger, D., Non causality and other defects of interaction Lagrangeans for particle with spin one and higher, Phys. Rev. **188**, 2218–2222 (1969) — Notes 3.2–3.
453. Velo, G. and Zwanziger, D., Propagation and quantization of Rarita-Schwinger waves in an external electromagnetic potential, Phys. Rev. **186**, 1337–1341 (1969) — Notes 3.2–3.
454. Veselić, K., The nonrelativistic limit of the Dirac equation and the spectral concentration, Glasnik Math. **4**, 231–240 (1969) — Notes 4.7, 6.1.
455. Vogelsang, V., Spektraltheorie der Diracgleichung für Potentiale mit großer Reichweite, Habilitationsschrift, Universität Göttingen (1984) — Notes 4.7.
456. Vogelsang, V., Remark on essential selfadjointness of Dirac operators with Coulomb potentials, Math. Z. **196**, 517–521 (1987) — Notes 4.3.
457. Vogelsang, V., Self-adjoint extensions of Dirac operators for non sperically symmetric potentials in Coulomb scattering, Int. Eq. and Op. Theor. **10**, 841–858 (1987) — Notes 4.3.
458. Vogelsang, V., Absolutely continuous spectrum of Dirac operators for long-range potentials, J. Func. Anal. **76**, 67–86 (1988) — Notes 4.3, 4.7.
459. Wadati, M., The modified Korteweg-de Vries equation, J. Phys. Soc. Japan. **34**, 1289–1296 (1973) — Notes 9.2.
460. Wahlquist, H. D. and Estabrook, F. B., Prolongation structures of nonlinear evolution equations, J. Math. Phys. **16**, 1–7 (1975) — Notes 9.3.
461. Waldenstrøm, S., On the Dirac equation for the hydrogen atom, Am. J. Phys. **47**, 1098–1100 (1979) — Notes 7.4.
462. Wang, X. P., Puits multiples pour l'opérateur de Dirac, Ann. Inst. H. Poincaré **42**, 269–319 (1985) — Notes 4.7.
463. Weaver, D. L., Some formal aspects of the Melosh and generalized unitary transformations of a class of massive-particle wave equations, Phys. Rev. **D12**, 2325–2329 (1975) — Notes 5.6.
464. Weaver, D. L., Exact diagonalization of relativistic Hamiltonians including a constant magnetic field, J. Math. Phys. **18**, 306–307 (1977) — Notes 5.4, 5.
465. Weder, R. A., Spectral properties of the Dirac Hamiltonian, Ann. Soc. Sci Bruxelles, Sér. I. **87**, 341–355 (1973) — Notes 4.7.

466. Weder, R., Self-adjointness and invariance of the essential spectrum for the Klein-Gordon equation, Helv. Phys. Acta. **50**, 105–115 (1977) — Notes 5.4, 5.
467. Weidmann, J., Oszillationsmethoden für Systeme gewöhnlicher Differentialgleichungen, Math. Z. **119**, 349–373 (1971) — Notes 4.3, 4.6, 5.3.
468. Weidmann, J., Absolut stetiges Spektrum bei Sturm-Liouville-Operatoren und Dirac-Systemen, Math. Z. **180**, 423–427 (1982) — Notes 4.6, 5.3.
469. Weinberg, E. J., Parameter counting for multimonopole solutions, Phys. Rev. **D20**, 936–944 (1979) — Notes 5.11.
470. Weinberg, E. J., Index calculations for the fermion-vortex system, Phys. Rev. **D24**, 2669–2673 (1981) — Notes 5.7, 5.11.
471. Weinberg, S., Feynman rules for any spin, Phys. Rev. **133**, B1318–B1332 (1964) — Notes 3.2–3.
472. Wess, J. and Zumino, B., Supergauge transformations in four dimensions, Nucl. Phys. **B70**, 39–50 (1974) — Notes 5.1.
473. Wiegner, A., Über den nichtrelativistischen Grenzwert der Eigenwerte der Diracgleichung, Diplomarbeit, Fernuniversität Hagen, BRD (1984) — Notes 6.2.
474. Wightman, A. S., On the Localizability of Quantum Mechanical Systems, Rev. Mod. Phys. **34**, 845–872 (1962) — Notes 1.7.
475. Wightman, A. S., The Dirac equation, in: *Aspects of Quantum Theory*, p. 95–115, A. Salam and E. P. Wigner eds., Cambridge University Press, 1972 — Notes 1.4.
476. Wightman, A. S., Invariant wave equations: General theory and applications to the external field problem, in: *Invariant Wave Equations*, p. 1–101, G. Velo and A. S. Wightman eds., Lecture Notes in Physics 73, Springer Verlag, 1978 — Notes 10.1.
477. Wigner, E., On unitary representations of the inhomogeneous Lorentz group, Ann. Math. **40**, 149–204 (1939) — Notes 2.6, 3.1.
478. Wigner, E. P., Relativistische Wellengleichungen, Z. Physik. **124**, 665–684 (1947) — Notes 3.2–3.
479. Wigner, E. P., Normal forms of antiunitary operators, J. Math. Phys. 1, 409–413 (1960) — Notes 2.6.
480. Wigner, E. P., Phenomenological distinction between unitary and antiunitary symmetry operators, J. Math. Phys. 1, 414–416 (1960) — Notes 2.6.
481. Witten, E., Dynamical breaking of supersymmetry, Nucl. Phys. **B188**, 513–554 (1981) — Notes 5.1.
482. Witten, E., Supersymmetry and Morse Theory, J. Diff. Geom. **17**, 661–692 (1982) — Notes 5.1.
483. Wolf, J. A., Essential self adjointness for the Dirac operator and its square, Indiana Univ. Math. J. **22**, 611–640 (1973) — Notes 4.3.
484. Wong, M. K. F., Coulomb scattering of fast electrons, Phys. Rev. **D26**, 927–930 (1982) — Notes 7.4.
485. Wong, M. K. F. and Yeh, E. H. Y., The Dirac Coulomb Green's function and its application to relativistic Rayleigh scattering, J. Math. Phys. **26**, 1701–1710 (1985) — Notes 7.4.
486. Wong, M. K. F. and Yeh, H. Y., Simplified solution of the Dirac equation with a Coulomb potential, Phys. Rev. **D25**, 3396–3401 (1982) — Notes 7.4.
487. Wu, J. S., Stahlhofen, A., Biedenharn, L. C. and Iachello, F., A group theoretical calculation of the S matrix for the Dirac-Coulomb problem, J. Phys. A: Math. Gen. **20**, 4637–4652 (1987) — Notes 7.4.
488. Wu, T. T. and Yang, C. N., Concept of nonintegrable phase factors and global formulation of gauge fields, Phys. Rev. D12, 3845–3857 (1975) — Notes 7.1.
489. Wu, T. T. and Yang, C. N., Dirac monopole without strings: monopole harmonics, Nucl. Phys. **B107**, 365–380 (1976) — Notes 7.1.
490. Wüst, R., A convergence theorem for selfadjoint operators applicable to Dirac operators with cutoff potentials, Math. Z. **131**, 339–349 (1973) — Notes 4.3.
491. Wüst, R., Distinguished self-adjoint extensions of Dirac operators constructed by means of cut-off potentials, Math. Z. **141**, 93–98 (1975) — Notes 4.3.

492. Wüst, R., Dirac Operators with strongly singular potentials, Math. Z. **152**, 259–271 (1977) — Notes 4.3.
493. Yajima, K., Nonrelativistic limit of the Dirac theory, scattering theory, J. Fac. Sci. Univ. Tokyo, Sec.IA. **23**, 517–523 (1976) — Notes 6.2.
494. Yajima, K., Classical scattering for relativistic particles, J. Fac. Sci. Univ. Tokyo Sect. IA. **29**, 599–610 (1982) — Notes 4.7.
495. Yajima, K., The quasi-classical approximation to Dirac equation. I, J. Fac. Sci. Univ. Tokyo Sect. IA. **29**, 161–194 (1982) — Notes 4.7.
496. Yajima, K., The quasi-classical approximation to Dirac equation. II, J. Fac. Sci. Univ. Tokyo Sect. IA. **29**, 371–386 (1982) — Notes 4.7.
497. Yamada, O., Eigenfunction expansions and scattering theory for Dirac operators, Publ. RIMS, Kyoto Univ. 11, 651–689 (1976) — Notes 8.1.
498. Yamada, O., Notes on the essential self-adjointness of Dirac operators, Memoirs Res. Inst. Sci. Eng., Ritsumeikan Univ. **40**, 1–8 (1981) — Notes 4.3.
499. Yamagishi, H., Fermion-monopole system reexamined, Phys. Rev. **D27**, 2383–2396 (1983) — Notes 7.1.
500. Yamagishi, H., Fermion-monopole system reexamined. II, Phys. Rev. **D28**, 977–988 (1983) — Notes 7.1.
501. Yamagishi, H., Magnetic monopoles and fractional Witten indices, Phys. Rev. **D29**, 2975–2976 (1984) — Notes 5.11.
502. Zakharov, V. E. and Shabat, A. B., Exact theory of self-focusing and one-dimensional self-modulation of waves in nonlinear media, Sov. Phys. JETP. **34**, 62–69 (1972) — Notes 9.2.
503. Zeeman, E. C., Causality implies the Lorentz group, J. Math. Phys. **5**, 490–493 (1964) — Notes 2.1.
504. Zel'dovich, Y. B. and Popov, V. S., Electronic structure of superheavy atoms, Usp. Fiz. Nauk **105**, 403–440 (1971), english translation in Sov. Phys. Usp. (USA). **14**, 673–694 (1972) (1971) — Notes 10.4.
505. Zheng, Y. and Chan, W. L., Gauge transformation and the higher order Korteweg-de Vries equation, J. Math. Phys. **29**, 308–314 (1988) — Notes 9.3.
506. Zumino, B., Wu, Y. S. and Zee, A., Chiral anomalies, higher dimensions and differential geometry, Nucl. Phys. **B239**, 477–507 (1984) — Notes 5.8.

Symbols

Symbol	Description	First occurrence
$\in$, $\notin$, $\subset$, $\supset$	element of, not element of, subset, superset of	
$\cup$, $\cap$, $\setminus$	union, intersection, difference of sets	
$\equiv$	definition of a new symbol	
$\cong$	isomorphic	
*	(superscript) adjoint of an operator A	
$\overline{z}$	complex conjugation	
$^\top$	(superscript) transposed of a matrix or vector	1.3.1
$^\perp$	(superscript) orthogonal complement of a set	5.2.3
$\cdot$ (dot)	scalar product in $\mathbb{R}^3$,	1.1
$\otimes$	direct product, tensor product	1.3.1, 2.1.5
$\odot$	semidirect product	2.1.5
$\oplus$	orthogonal direct sum	1.3.1
$\wedge$	exterior product of vectors	1.3.3
$\lvert z\rvert$, $\lvert \boldsymbol{x}\rvert$	modulus of a complex number z, length of a vector $\boldsymbol{x}$	
$\lVert\psi\rVert$, $\lVert A\rVert$	norm of a state, of an operator	1.2.1
$(\cdot,\cdot)$, $(\cdot,\cdot)_{\mathfrak{H}}$	scalar product (in Hilbert space $\mathfrak{H}$)	1.2.1, 1.4.5, 10.1.1
$(\cdot,\cdot)$, $(\cdot,\cdot,\cdots)$	pair of elements, n-tupel	1.1, 2.1.5
(a,b), $[a,b)$, etc.	intervals of real numbers	1.4.4
$[A,B]$	commutator $(= AB - BA)$	1.A, 5.1.2
$\{A,B\}$	anticommutator $(= AB + BA)$	1.A, 5.1.2
$\mathcal{G}/\mathcal{H}$	factor set	2.4.1, 3.1.1
$\langle y,x\rangle = y^\mu x_\mu$	metric in Minkowski space	2.1.1
$\langle\hat{\Psi},\hat{\Phi}\rangle$	transition probability	2.2.2
$\mathbf{1}$, $\mathbf{1}_n$	unit operator, unit matrix in n dimensions	1.1
$\mathbf{0}$	zero operator	1.1
∇	nabla operator	1.1
$\triangle = \nabla\cdot\nabla$	Laplace operator	1.1
A	operator for rel. kinematics	1.C, 8.2.1
$A(x)$	electromagnetic 4-vector potential	4.2.2
$A(Q)$	axial anomaly	5.8.2
$\tilde{A}$	part of an observable leaving $\mathfrak{H}_{\text{pos}}$ invariant	1.7.1
$\boldsymbol{A}$, $\boldsymbol{A}_{\text{pv}}$	vector potential, pseudovector potential	4.2
$\mathbf{A}$	transformation matrix	7.4.1
$\mathbb{A}$	operator in Fock space	10.3.4
a	4-vector of translations in Minkowski space	2.1.5

$\boldsymbol{a}$	vector for translations in $\mathbb{R}^3$	1.3.2
$a_\pm$	needed for FW-transformation	1.4.1, 5.6.1
$a(f)$, $a^*(f)$	annihilation, creation of particle in state f	10.1.2
Aa^*b^*, etc.	Fock space operators	10.2.4
$\boldsymbol{B}$	magnetic field strength	4.2.2
B_0	free BJL operator	1.C
B	BJL operator	7.4.4
$B(t)$, B, $B_\pm$	operator belonging to a Lax-pair	9.1.2
$b(g)$, $b^*(g)$	annihilation, creation of antiparticle in state g	10.1.2
C	charge conjugation	1.4.6, 10.1.1
C	Cayley tranform	5.6.3
CT	(subscript) Cini Touschek	5.6.2
$\mathbb{C}$	complex numbers	1.1
$\mathcal{C}_0^\infty$	infinitely differentiable functions with compact support	1.3.3
$\mathfrak{C}$	Hilbert space of covariant states	3.3.1
c	velocity of light	1.1
$c_n^\pm$	normalization constants	9.5.1
D	closed operator, component of a supercharge	5.2.2
$D_0(E)$	Coulomb ladder operator	7.4.1
$\mathfrak{D}$, $\mathfrak{D}(H)$	dense set, domain of an operator H	1.2.2
$\mathfrak{D}_G$	Gårding domain	2.3.1
D^γ	differential operator	8.4.2
$d^n\boldsymbol{x}$	Volume element	1.3.1
dg, $d\mu$, $d\mu(\dot{g})$	invariant measure on group or factor set	2.3.1, 3.1.1
$dE_A(\lambda)$	spectral measure	1.2.3
det	determinant of an operator	5.10
∂	partial differentiation	1.1
E	energy	1.1
$\boldsymbol{E}$	electric field strength	4.2.2
$E(B)$	localization operator	1.7.3
$E_A(\lambda)$	spectral family of A	1.2.3
e	Euler's number, neutral element of a group	2.2.3
e	elementary charge	1.4.6
$\boldsymbol{e}_r$, $\boldsymbol{e}_\vartheta$, $\boldsymbol{e}_\varphi$	unit vectors for polar coordinates	4.6.2
F	flux of a magnetic field	7.2.1
$F_{\mu\nu}$	electromagnetic field tensor	4.2.3
F_{ik}	components of magnetic field 2-form	7.1.1
$\hat{F}_{\mu\nu}$	Hodge dual of F	4.2.4
FW	(subscript) Foldy Wouthuysen	1.4.3, 1.7.2
$\mathcal{F}$	Fourier transformation	1.4.1
$\boldsymbol{F}$	operator for Zitterbewegung	1.6.1
$\mathfrak{F}$	Fockspace	10.1.1
$\mathfrak{F}_+^{(n)}$	n-particle Fockspace	10.1.1
$\mathfrak{F}_-^{(m)}$	m-antiparticle Fockspace	10.1.1
$\mathfrak{F}^{(n,m)}$	$n$particle/m antiparticle subspace of Fock space	10.1.1

G	operator for Zitterbewegung	1.6.5
$\mathcal{G}$	Lie group	2.2.3
$\mathcal{G}_q$	isotropy group of q	3.1.5
$\tilde{\mathcal{G}}$	covering group of a Lie group $\mathcal{G}$	2.3.3
g	metric tensor	2.1.1
g	gauge transformation	4.4.3
$\dot{g}$	coset $g\mathcal{K} = \{gk \mid k \in \mathcal{K}\} \subset \mathcal{G}/\mathcal{K}$	3.1.1
H	Dirac operator in an external field	4.1.1
H	abstract Dirac operator	5.1.2
$H(2)$	hermitian 2×2 matrices	2.5.1
H_0	free Dirac operator	1.1
$\dot{H}_0$, $\tilde{H}_0$	free Dirac operator on a smaller domain	1.4.4
H_∞	nonrelativistic limit of Dirac operator	6.1.3
$H_{\text{odd,even}}$	odd and even part of an abstract Dirac operator	5.1.2
$H(e)$	Dirac operator for charged particle	1.4.6, 10.1.1
$H(A)$	Dirac operator with magnetic field	7.1.1
H_{P}	Pauli operator	5.3.2, 6.1.4
H_{S}	Schrödinger operator	7.1.1
$H^1(\mathbb{R}^n)$	first Sobolev space	1.4.4
$H_\nu^{(1,2)}$	Hankel functions	1.5
$H(\boldsymbol{p}, \boldsymbol{x})$	Hamilton function	8.3.2
H	generator of x_0 translation	2.1.6
$\mathcal{H}$	closed subgroup, little group	2.4.1, 3.1.2
$\mathfrak{H}^{\text{cont}}$, $\mathfrak{H}^{\text{pp}}$, etc.	spectral subspaces	8.1.1
$\mathfrak{H}$	Hilbert space	1.2.1
$\mathfrak{H}_{\text{pos,neg}}$	subspaces with positive/negative energy	1.4.2
$\mathfrak{H}_\pm$	bosonic and fermionic subspaces	5.1.1
$\mathfrak{H}_\pm$	particle-antiparticle subspaces	10.1.1
$\mathbb{H}$	Dirac operator in Fock space	10.2.2
h($\boldsymbol{p}$)	Dirac operator in momentum space	1.4.1
h, h_{m_j,κ_j}, h_κ	radial Dirac operator	4.6.5, 7.4.1
$\hbar$	Planck's constant, usually $= 1$	1.1
I_h, $\hat{I}_h$	inner automorphism, dual action	3.1.4
$\mathrm{i} = \sqrt{-1}$	imaginary unit	1.1
i, j, k	3-indices (from 1 to 3) or spinor indices (from 1 to 4)	1.1
ind , ind_z , ind_t	index of an operator	5.7
J_ν	Bessel function	1.5
$\boldsymbol{J} = (J_1, J_2, J_3)$	angular momentum operator	1.3.3
J_j	generators of rotations	2.1.6
j	angular momentum quantum number	4.6.4
K	complex conjugation	2.6.1
K	spin orbit operator	1.C, 4.6.5
$K(\lambda)$	phase shift operator	8.1.3
K_ν	modified Bessel function	1.5
$K(t, \boldsymbol{x})$	evolution kernel in FW representation	1.5

Ker	kernel of an operator	5.2.3
$\mathcal{K}$	unitary transformation	1.4.5
$\mathcal{K}$	closed subgroup, isotropy group	3.1.1
$\mathfrak{K}$	spectral representation space of H_0	1.4.5
$\mathfrak{K}_{m_j,\kappa_j}$	angular momentum eigenspaces in $L^2(S^2)$	4.6.4
$L_{\mathcal{G}}$	Lie algebra of a Lie group $\mathcal{G}$	2.4.2
$\mathbf{L}$, $\mathbf{L}_X$	Lorentz transformations in spinor space	2.5.4
$\mathbf{L}_p$	4×4 matrix for the boost $q_0 \to p$	3.2.2
$L^1(\mathbb{R}^3)$	Lebesgue integrable functions	1.4.1
$L^2(\mathbb{R}^3)$	Hilbert space of quantum mechanics	1.3.1
$L^2(\mathbb{R}^3)^4$	Hilbert space of relativistic quantum mechanics	1.3.1
$\boldsymbol{L}$	orbital angular momentum operator	1.3.3
$\mathcal{L} = O(3,1)$	Lorentz group	2.1.2
$\mathcal{L}_+^\uparrow$, etc.	subgroups of the Lorentz group	2.1.4
$\tilde{\mathcal{L}}^\uparrow$	Lorentz covering group	2.5.4
$\tilde{\mathcal{L}}_+^\uparrow = SL(2)$	covering group of $\mathcal{L}_+^\uparrow$	2.5.1
M	supermass	5.1.3
M_{pos}	mass shell	2.1.3
$\mathfrak{M}$	Hilbert space of Mackey states	3.1.1
m	mass of a particle	1.1
m_j	angular momentum quantum number	4.6.4
mtr	matrix trace	5.7.2
N	number operator in Fock space	10.2.3
N_j	boost generators	2.1.6
$\boldsymbol{N}$	center of energy operator	1.3.3
$\boldsymbol{n}$	unit vector in $\mathbb{R}^3$	2.1.3
O_q	orbit of q	3.1.5
O	origin in $\mathbb{R}^3$	1.4.4
P	parity transformation	2.1.3
P	projection onto eigenspace	6.2.1
P^{cont}	projector on continuous spectral subspace	8.2.3
$P_{\text{pos,neg}}$	projectors on positive/negative energy	1.4.2
$P_\pm$	projectors on bosonic/fermionic subspaces	5.1.2
$P_\pm$	projectors on particle/antiparticle subspaces	10.1.3
P_l^m	associated Legendre polynomials	4.6.4
$\mathcal{P}$	Poincaré group	2.1.5
$\mathcal{P}_+^\uparrow$, etc.	subgroups of the Poincaré group	2.1.5
$\tilde{\mathcal{P}}$, $\tilde{\mathcal{P}}^\uparrow$, $\tilde{\mathcal{P}}_+^\uparrow$	Poincaré covering group	2.5.8
p	momentum 4-vector	2.1.3
$\boldsymbol{p}$	momentum variable, operator	1.3.2
p_j	generators of translations	2.1.6
Q	supercharge	5.1.2
Q	charge operator in Fock space	10.2.3
$Q^\pm$	projectors onto irreducible subspaces	3.1.7
Q'	associated supercharge	5.1.3

$q = (m, 0, 0, 0)$	momentum in rest system	2.1.3
$\mathbf{R}$, R_{ik}	rotation matrix	2.1.3
R^l, R^r	reflection coefficients	4.5
R_∞	resolvent in the nonrelativistic limit	6.1.3
$\boldsymbol{R}$	Pauli-Runge-Lenz vector	7.4.4
$\mathbb{R}$, $\mathbb{R}^3$	real numbers, Euclidean space	1.1
$\mathbb{R}^4$	Minkowski space	2.1.1
Ran	range of an operator	5.2.3
S	unitary operator occurring in polar decomposition	5.2.3
S	scattering operator	8.1.3
$S(\lambda)$	on-shell scattering operator	8.1.3
$\boldsymbol{S} = (S_1, S_2, S_3)$	spin angular momentum operator	1.3.3
$S(t, \boldsymbol{x})$	time evolution kernel	1.5
S^2	two dimensional unit sphere in $\mathbb{R}^3$	1.4.5
$SL(2)$	special linear group	2.5.1
$SO(3)$	rotation group	2.1.3
$SU(2)$	special unitary group	2.5.2
$\mathcal{S}(\mathbb{R}^3)$	rapidly decreasing functions (Schwartz functions)	1.4.4
$\mathbb{S}$	scattering operator in Fock space	10.3.1
s	eigenvalue of Temple's operator	7.4.1
sgn	sign function	1.4.5, 5.1.1
str	supertrace	5.7.2
supp	support of a function	1.8.3
sup	supremum	4.3.2
T	time reversal	2.1.3
T	reflection coefficient	5.4
T	unitary right shift	10.3.5
t	time parameter	1.1
t_0	initial time	1.2.1
tr	trace of an operator	1.1, 5.7.2
U	unitary transformation, abstract FW-transformation	5.6.1
$U(t, s)$	time evolution, propagator	4.4.1
U_θ	dilation operator	4.7.2
U_{FW}	Foldy-Wouthuysen transformation	1.4.3
$U(1)$	one-dimensional unitary group	2.2.4
U_{sp}	spectral transformation	1.4.5
$\mathbb{U}$	unitary transformation in Fock space	10.1.4, 10.2.1
$\mathbb{U}_t$	time evolution in Fock space	10.2.2
U_+, U_{+-}, etc.	matrix elements of U in standard representation	10.2.4
$\mathrm{u}(\boldsymbol{p})$	FW transformation in momentum space	1.4.1
$\boldsymbol{u}(\boldsymbol{p})$	classical velocity on positive energies	8.2.6
V	Cini Touschek transformation	5.6.2
$V(\boldsymbol{x})$	potential matrix	4.1.1
V_{cov}	potential in covariant Dirac equation	4.1.2
V_{lr}, V_{sr}	long-range and short-range part of V	8.2
$\boldsymbol{v}$	velocity vector	2.1.3

W	potential matrix	5.3.1
$\mathcal{W}$	related to spectral transformation of H_0	1.4.1
$W(Q)$	Witten index	5.8.2
$W_\kappa^\pm$	Coulomb-Jost solution	7.4.6
$W(t, \boldsymbol{p})$	classical action	8.3.2
$\mathfrak{W}$	Hilbert space of Wigner states	3.2.1
$\mathfrak{X}$	Hilbert space for group representation	3.1.1
x	coordinate of an event in $\mathbb{R}^4$	2.1.1
$\boldsymbol{x} = (x_1, x_2, x_3)$	coordinates in $\mathbb{R}^3$, position operator	1.3.2
$\tilde{\boldsymbol{x}}$	restricted position operator	1.7.1
$\boldsymbol{x}_{\mathrm{NW}}$	Newton Wigner operator	1.7.2
Y_l^m	spherical harmonics	4.6.4
$\mathbb{Z}$	integers	10.3.4
$z_\Psi(t)$	Zitterbewegung	1.6.3
$\boldsymbol{\alpha}$, α_i	Dirac matrices	1.1
β	Dirac matrix	1.1
Γ	Temple's operator	7.4.4
Γ_n	Gamma matrices	2.A
γ	coupling constant	4.7.3, 7.4.1
$\gamma(\boldsymbol{x})$	Dirac matrix	2.5.5
γ^ν, $\nu = 0, 1, 2, 3$	Gamma matrices	2.5.6
γ_5	Dirac matrix	1.A, 2.A
$\triangle$	Laplace operator	1.1
$\triangle(t, \cdot)$, $\triangle_\pm$, etc.	distributions associated to evolution kernel	1.5, 1.D
δ_{ik}	Kronecker delta	1.1
δ_{a}	anomalous electric moment	4.2.4
δ_κ	scattering phase shift	7.4.6
$\epsilon_{ikm}, \epsilon_{\mu\nu\rho\tau}$	antisymmetric tensor	1.3.3
ζ	Wigner state	3.2.1
θ	Heaviside step function	1.5
ϑ	polar angle	4.6.2
κ, κ_j	eigenvalue of spin-orbit operator K	4.6.4
κ_n	eigenvalue parameter	9.5.1
Λ	Lorentz transformation	2.1.2
Λ_p	transformation from a rest frame	2.1.3
$\Lambda_{\mathbf{L}}$	Lorentz transformation corresponding to $\mathbf{L} \in \tilde{\mathcal{L}}$	2.5.5
λ	spectral parameter, eigenvalue	1.2.3
$\lambda(\boldsymbol{p})$, $\lambda(\boldsymbol{p})$	relativistic energy as function of the momentum	1.4.1
μ, ν	4-indizes (ranging from 0 to 3)	2.1.1
μ_{a}	anomalous magnetic moment	4.2.3
ν	Coulomb distortion factor	7.4.6
ξ	Krein's spectral shift function	5.8.1
Π	Poincaré transformation	2.1.5
π, $\pi(g)$	the number π, or representation of a group	2.2.4
$\rho(H)$	resolvent set of H $(= \mathbb{C} \setminus \sigma(H))$	4.4.1

ρ	projective representation	2.2.3
σ	representation of the little group	3.1.2
$\sigma(A)$	spectrum of a self-adjoint operator A	1.2.3
$\sigma_{\text{ess}}(A)$	essential spectrum	4.3.4
$\sigma_{\text{a.c.}}(A)$	absolutely continuous spectrum	9.4.1
$\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$	Pauli matrices	1.1, 1.A
$\sigma^{\mu\nu}$	Dirac matrices	2.A
τ	representation of isotropy group	3.1.1
τ	unitary involution	5.1.1
Φ_{m_j,κ_j}	angular momentum eigenspinors	4.6.4
ϕ	Mackey state	3.1.1
ϕ_{sc}, ϕ_{el}, ϕ_{ps}	potential functions	4.2
φ	polar angle	4.6.2
$\boldsymbol{\varphi}$	rotation vector	2.1.3
$\chi(\lambda \in B)$	characteristic function	1.2.3
$\chi(A \in B)$	spectral measure of an operator A	1.2.3
$\chi(g)$	group character	3.1.3
$\hat{\Psi}$	ray in a Hilbert space	2.2.1
$\Psi(f)$, $\Psi^*(f)$	field operators in Fock space	10.1.3
Ψ_κ^{reg}	regular Coulomb wavefunction	7.4.6
ψ, ϕ	state, vector in a Hilbert space	1.2.1
ψ	wavefunction	1.1
$\tilde{\psi}$	covariant state	3.3.1
$\psi^{(n)}$	n-particle state	10.1.1
$\psi^{(n,m)}$	state in $\mathfrak{F}^{(n,m)}$	10.1.1
Ω	vacuum vector in Fock space	10.1.1
$\Omega_\pm$	wave operators	8.1.2
$\boldsymbol{\omega}$	boost vector	2.1.3
$\boldsymbol{\omega}$	Thomas precession	6.2.5
$\underset{\leftarrow}{\omega}$, $\underset{\rightarrow}{\omega}$	generalized eigenfunctions	4.5

Index