

Precisely Predictable Dirac Observables

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Precisely Predictable Dirac Observables

by

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To the memory of F. Rellich, R.S. Phillips, C.B. Morrey, and T. Kato

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Preface

In this book we are attempting to offer a modification of Dirac's theory of the electron we believe to be free of the usual paradoxa, so as perhaps to be acceptable as a clean quantum-mechanical treatment.

While it seems to be a fact that the classical mechanics, from Newton to Einstein's theory of gravitation, offers a very rigorous concept, free of contradictions and able to accurately predict motion of a mass point, quantum mechanics, even in its simplest cases, does not seem to have this kind of clarity. Almost it seems that everyone of its fathers had his own wave equation.

For the quantum mechanical 1-body problem (with vanishing potentials) let us focus on 3 different wave equations¹:

(I) The Klein-Gordon equation

$$(1) \quad \partial^2 \psi / \partial t^2 + (1 - \Delta) \psi = 0, \quad \Delta = \text{Laplacian} = \sum_1^3 \partial^2 / \partial x_j^2.$$

This equation may be written as

$$(2) \quad (\partial / \partial t - i\sqrt{1 - \Delta})(\partial / \partial t + i\sqrt{1 - \Delta})\psi = 0.$$

Here it may be noted that the operator $1 - \Delta$ has a well defined positive square root as unbounded self-adjoint positive operator of the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3)$.

(II) The Dirac equation is of the form (" = 1/2 of (I)")

$$(3) \quad (\partial / \partial t + iH_D)\psi = 0,$$

where H_D is a square root of $1 - \Delta$, but not the above positive one; rather, Dirac introduces some hypercomplex units² $\alpha_1, \alpha_2, \alpha_3, \beta$ such that $\alpha_j \alpha_l + \alpha_l \alpha_j = 2\delta_{jl}$, $\alpha_j \beta + \beta \alpha_j = 0$, $\beta^2 = 1$. Then he defines

¹We use units of length, time and energy making $c = m = e = \hbar = 1$, cf. footnote 1 of ch.1.

$H_D = \alpha.D + \beta$ with $D = (D_1, D_2, D_3)$ $D_j = -i\partial/\partial x_j$, and then gets $H_D^2 = 1 - \Delta$, so that, indeed, H_D is a square root of $1 - \Delta$.

(III) The Schrödinger equation arises if we “approximate” $\sqrt{1 - \Delta} \approx 1 - \frac{1}{2}\Delta$, resulting in the equation

$$(4) \quad (\partial/\partial t + i(-\frac{1}{2}\Delta + 1))\psi = 0 ,$$

where the last term - corresponding to the rest mass of the particle - usually is eliminated by a substitution $e^{it}\psi \rightarrow \psi$, so that we then get

$$(5) \quad (\partial/\partial t + iH_S)\psi = 0 \text{ with } H_S = -\frac{1}{2}\Delta .$$

If there is an electromagnetic field present, represented by a scalar electrostatic \mathbf{V} and a 3-vector electromagnetic potential \mathbf{A} , we get

$$(6) \quad H_D = \alpha(D - \mathbf{A}) + \beta + \mathbf{V} ,$$

and

$$(7) \quad H_S = \frac{1}{2} \sum (D_j - \mathbf{A}_j)^2 + \mathbf{V} ,$$

as Dirac or Schrödinger “Hamiltonian”.

We have presented above 3 wave equations to exhibit their interrelation: Most discussions of elementary quantum mechanics deal either with the Schrödinger equation or the Dirac equation, or with both. But it is clear at once, that the approximation $\sqrt{1+x} \approx 1 + \frac{1}{2}x$ is good only for very small x . This means that also the approximation between the operators (6) and (7) can be useful only for very small momenta³. So, only one - either Schrödinger or Dirac - can reflect the real world, one should think. Why then do both equations enjoy their existence, parallel to each other?

One feels tempted to declare the Dirac equation as the *true wave equation of the 1-body problem*. Indeed, first of all, the spectrum of the operator H_D of (6) exhibits the split of basic hydrogen states, known as *fine structure*, while the operator H_S only has these as states of higher multiplicity⁴, ignoring the fine structure split.

Next, looking at both equations from a mathematical aspect, one finds that

²Such α_j, β may be represented by self-adjoint 4×4 -matrices with complex coefficients, making (3) a (hyperbolic symmetric) system of 4 linear first order PDE-s in 4 unknown functions. A variety of such representations are in use.

³The rest energy of an electron is $\approx 500000eV$, while the energies of the various bound states of the hydrogen atom range around $10eV$. So, for the spectral lines of H the relative error should be around 10^{-4} , perhaps good enough for even the accuracies of spectral measurements.

⁴For more details cf. sec.3.0.

eq. (3) with H_D of (6) is a *true wave equation* while eq.(5) with H_S of (7) does not have this property. More precisely, eq. (3) is a *first order hyperbolic system* (of 4 equations in 4 unknown functions). It exhibits a finite propagation speed, and a geometrical optics. “Finite propagation speed” means that a disturbance at $t = 0$ (at a point x^0) propagates only within a cone $|x - x^0| \leq ct$ (with a constant $c > 0$) - it cannot be felt outside that cone. “Geometrical optics” means that, approximately, - with an error depending on wave length (i.e., momentum) - the time-propagation may be described by letting an initial configuration (at $t = 0$) propagate along “light rays” - that is, along a certain field of orbits. Evidently then, for the Dirac equation, this field of orbits will be given by the classical field of motion. Rather, one then will find two such fields of orbits, reflecting the fact that eq. (3) really takes care of two particles - electron and positron, propagating along different orbits.

But this parallel becomes even more striking because - as we will discuss later on (cf. sec.4.6) - the Dirac equation’s geometrical optics does not only define the classical orbits of propagation of the two particles, but also assigns a *magnetic moment* riding on each particle - that is, a 3-vector changing along the propagation, exactly as indicated by equations valid for a magnetic moment (of Bohr strength) in the electromagnetic field of the potentials \mathbf{A}, \mathbf{V} . In other words, this geometrical optics also represents the electron spin.

Finally, the Dirac equation remains invariant (rather co-variant) under Lorentz transforms - i.e., it is compatible with theory of relativity. In comparison to the above, the Schrödinger equation does not have above properties. It lives in a mathematical environment of its own, is not a hyperbolic equation, in particular. One might list in its favour that it allows a simple generalization to multiple particle problems: For a system of N particles with masses m_j and charges e_j (without other outside fields) one just uses the equation

$$(8) \quad (\partial/\partial t + iH_S^N)\psi = 0 \text{ with } H_S = -\frac{1}{2} \sum_1^N \frac{1}{m_j} \Delta_j + \mathbf{V} ,$$

involving $3N$ independent variables $x_l^j : j = 1, \dots, N, l = 1, 2, 3$, with $\Delta_j = \sum_{l=1}^3 \partial_{x_l^j}^2$ and $\mathbf{V} = \sum_{j,k} \frac{e_j e_k}{|x^j - x^k|}$.

Moreover, it appears that the Schrödinger equation seems to be firmly entrenched as equation of the *harmonic oscillator* (i.e., equ. (5) with $H_S = \frac{1}{2} \{-\partial_x^2 + \omega^2 x^2\}$), in one variable x , with a “frequency” $\omega = 2\pi\nu$, and indispensable for quantum field theory, involving theory of “light quant’s” - that is, particles *other than electrons*).

For a system of electrons and protons however, the Schrödinger equation should survive only as an approximation, not as the real thing.

From the above perspective, with all its beautiful agreements, it then appears as a very disturbing fact that the Dirac equation was plagued by a variety of systematic difficulties seemingly leading into rather bad contradictions. The aim of the present book is to eliminate these: We will try to show that they appear only due to a *deficient (or incomplete) interpretation of quantum mechanical prediction*.

What then are the theoretical foundations of quantum mechanical prediction? While in classical mechanics one may accurately predict the status of a physical system, once its initial status (at $t = 0$) is precisely determined, this is not so in quantum mechanics. Given an initial status, the data at a future time may be predicted only with a certain *probability*. The accuracy of such prediction is limited. In particular, the Heisenberg uncertainty principle states that location and momentum of a particle cannot both be predicted with infinite precision.

Note, the initial concept of quantum mechanical prediction grew out of observation of spectral lines of light emitted by excited atoms. Schrödinger found that the spectral lines emitted by hydrogen atoms could be explained by looking at the linear operator $H = -\Delta - \frac{c}{|x|}$, with a suitable constant c , under suitable conditions at ∞ . This operator has a sequence of negative eigenvalues $\lambda_0 < \lambda_1 < \dots$ with $\lim \lambda_j = 0$. The energies corresponding to the spectral lines of hydrogen then coincided with the differences of the (energy states) λ_j .

Based on this fact (and other similar ones) mathematicians brought into play a general spectral theory of unbounded self-adjoint operators on a separable Hilbert space \mathcal{H} . In the above we have $\mathcal{H} = L^2(\mathbb{R}^3)$ and the self-adjoint operator H in a suitable domain, such that $\psi, H\psi \in \mathcal{H}$. Based on an earlier theory of Hilbert this was mainly started by J.v.Neumann [JvN1,2] and F.Riesz [Rie1], and developed into a field where many authors contributed⁵.

J.v.Neumann, in his book [JvN], then also attempted to design a precise formal scheme of prediction, perhaps generally accepted, as follows.

The status of a system (like an atom) is fully described by specifying a unit vector ψ of some given separable Hilbert space \mathcal{H} . This vector ψ is called the physical state of the system; it contains all the data available.

The properties or quantities which can be predicted are called “observables”. Each observable is represented by an unbounded self-adjoint linear operator A acting on (a dense subdomain of) \mathcal{H} . Such a self-adjoint operator possesses a spectral resolution $\{E(\lambda) : -\infty < \lambda < \infty\}$

⁵cf. H.Weyl [Wey1], and the books of M.H.Stone [Sto1], B. Sz.-Nagy [Na1], E.C.Titchmarsh [Til,2]; especially note also the split of approaches, either abstract or specifically adapted to differential operators.

such that $A = \int_{-\infty}^{\infty} \lambda dE(\lambda)$ (with a Stieltjes integral over the measure $dE(\lambda)$). [Or, in simpler terms, A has an orthonormal eigenvector expansion or a corresponding integral expansion, or both - for different parts of its spectrum.]

Physics then tries to predict the outcome of a measurement of an observable in a given physical state. The result of such measurement always must be a point of the spectrum $Sp(A)$ of A . If $\lambda \in Sp(A)$ is measured, and λ is an isolated point-eigenvalue, then, after the measurement, the system is assumed to be in a state ψ_1 which is an eigenvector of A to eigenvalue λ , regardless of its earlier state ψ -i.e., we have $A\psi_1 = \lambda\psi_1$. If such eigenvalue λ is simple (of multiplicity 1) then the probability of measuring the value λ for A is given by $|\langle \psi_1, \psi \rangle|^2$ with the inner product $\langle \cdot, \cdot \rangle$ of \mathcal{H} . In general, the probability of measuring a value of A in the (open) interval $(\lambda_1, \lambda_2) \subset \mathbb{R}$ is given by $\langle \psi, (E(\lambda_2 - 0) - E(\lambda_1 + 0))\psi \rangle$. Thus the expectation value of the measurement will be given by $\langle \psi, A\psi \rangle = \int \lambda d\langle \psi, E(\lambda)\psi \rangle$.

As time propagates we may either keep all observables constant (independent of t), and let the state propagate as a solution of the wave equation $\partial u / \partial t + iHu = 0$ (where H denotes an observable - an unbounded self-adjoint operator on \mathcal{H} - representing the total energy of the system, and called the Hamiltonian of the system). Or else we may let the states stay constant and let all observables propagate according to the law $A \rightarrow A_t = e^{iHt} A e^{-iHt}$ - noting that $e^{\pm iHt}$ are unitary operators on \mathcal{H} . Both procedures will give the same prediction results. The two above procedures are called the ‘‘Schrödinger representation’’ and ‘‘Heisenberg representation’’, respectively.

In particular, prediction of a measurement of the total energy H - an observable - is independent of time: We get $H_t = e^{iHt} H e^{-iHt} = H$, for all t , reflecting conservation of energy.

In the above it was assumed that the potentials \mathbf{A}, \mathbf{V} are independent of time.

For the Dirac equation one usually uses the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$, called the *configuration space* and the total energy observable $H = H_D$ of (6). Then it is common to work with a variety of *dynamical observables*, all derived from important quantities of classical Physics, such as location, momentum, angular momentum, spin, current, The difficulties in Dirac’s theory then arise from the fact that (i) that equation $\dot{\psi} + iH_D\psi = 0$ must serve as wave equation for two different particles - electron and positron - while (ii) prediction (or observation)

of most dynamical observables (except energy and angular momentum) tends to mix up states belonging to either particle.

Here now we come in with our proposal of *repair or modification* of v. Neumann's procedure:

*First of all, one should not attempt to work with a collection of observables as large as v. Neumann does. All dynamical observables are differential operators (perhaps of order 0, i.e., multiplications by a function of polynomial growth). We propose to work with an algebra of **pseudodifferential operators**⁶ we call strictly classical, and allow only self-adjoint operators within that algebra as observables. We will give a physical motivation for this restriction in ch.2.*

Secondly, working with the time-propagation $A \rightarrow A_t = e^{iHt} A e^{-iHt}$, of observables (with constant states), we want this time propagation to depend smoothly on t , in a manner to be specified. This condition alone will amount to further restrictions on observables, seemingly too strong, because this excludes many dynamical observables. However, the dynamical observables excluded are just the ones leading into contradictions.

*We resolve this difficulty by introducing an algebra \mathcal{P} of precisely predictable observables. - The elements of \mathcal{P} are (strictly classical) ψ -do-s, and they have a smooth A_t , and J. v. Neumann's principles of predicting measurements, laid out above, should be applied only to precisely predictable observables. Moreover then, for an observable A which is not precisely predictable - such as location, for example - we discuss some principles of finding precisely predictable approximations, that is, observables in \mathcal{P} with expectation value close to that of A . Such an approximation either may work for all states ψ . Or else, it may work only for certain states - for example, if the particle is not too close to the origin, or if it is known with certainty that the particle is an electron - not a positron. At any rate, then, there is a **built in error** for the prediction of expectation value. For example, location has a built-in error of the order of the Compton wave length of the*

⁶Pseudodifferential operators arise if we interpolate among the differential polynomials $a(x, D) = \sum_{\theta} a_{\theta}(x) D^{\theta}$ defined for a function $a(x, \xi) = \sum_{\theta} a_{\theta}(x) \xi^{\theta}$, polynomial in ξ , using a procedure to allow definition of an operator $a(x, D)$ also for more general functions $a(x, \xi)$, not polynomials in ξ . This will be done in such a way that the well known composition formulas for products of differential polynomials - the so-called "Leibniz formulas" - still are valid in a generalized form. For details cf. ch.1.

electron, in agreement with the fact that location of an electron cannot be predicted more accurately than its wave length - since in some experiments the electron appears as a wave.

As another important observation: The elements of our precisely predictable algebra \mathcal{P} may be *almost decoupled* by a unitary pseudodifferential operator U roughly similar to the Foldy-Wouthuysen transform (cf. [Th1], sec.3.3.9 or [DV1]). Now, under some mathematical restrictions on the potentials \mathbf{A}, \mathbf{V} this decoupling (unitary pseudodifferential-) operator U may be refined in such a way that it precisely decouples the Hamiltonian operator⁷ H_D . Using this refined Foldy-Wouthuysen decoupling, we then define a further restriction $\mathcal{PX} \subset \mathcal{P}$ as the subalgebra of operators precisely decoupled by (the refined) U , and then use \mathcal{PX} as algebra of precisely predictable observables.

This then will give an orthogonal split $\mathcal{H} = \mathcal{H}_e \oplus \mathcal{H}_p$ of the Hilbert space \mathcal{H} into a space \mathcal{H}_e of electronic states and a space \mathcal{H}_p of positronic states. And, moreover, a precisely predictable observable A preserves this split - such operator A is reduced by above decomposition; A maps $\mathcal{H}_e \rightarrow \mathcal{H}_e$ and $\mathcal{H}_p \rightarrow \mathcal{H}_p$.

Following the v. Neumann principle thus modified will remove all difficulties of Dirac's theory. Moreover, we also investigate the behaviour of the algebras \mathcal{P} and \mathcal{PX} under a Lorentz transform of the coordinate system, finding a kind of covariance of these algebras (with features to be explained (ch.6)). [The algebras \mathcal{PX} are not uniquely characterized, by the way, leaving something open for physical intuition, but also something in the way of a straight covariance.]

Finally, in ch.7, we undertake a study of certain precisely predictable approximations of observables not in \mathcal{P} . Such approximations are not uniquely determined either. Still, since it is proposed to use the spectral theory of these approximations as substitute for the non-corrected observable, their spectral theory will be of interest, and it is hoped that it will not be too different from that of the original observable. This is confirmed, indeed. In fact, for the two observables we studied explicitly - location and electrostatic potential - it was found that the approximation is unitarily equivalent to the original observable, so that only a unitary map - not too far away from 1 is in the way.

In conclusion of this preliminary discussion we might note that a similar notion of precisely predictable observables seems possible for gauge theories à la

⁷In other words, then the Dirac equation splits precisely into one equation for the electron, and another one for the positron - both are strictly classical hyperbolic (2×2 -systems of) pseudodifferential equations.

Yang-Mills (cf.[FS]). Especially we may think of the two problems in nuclear physics involving special representations of the Liegroups $SU(2, \mathbb{C})$ and $SU(3, \mathbb{C})$ of Weinberg-Salam ([Sa1],[Wb1]) and Gell-Man ([GM1]) used for discussion of weak and strong interactions - that is for their corresponding Dirac-type equations. (cf.[Ca1]). However the simplest such case would deal with 8×8 - or 12×12 - matrices, and we have not attempted approaching it, so far.

No such approach seems possible for the Schrödinger equation - at least not as a directly analogous generalization. In fact, the Heisenberg representation $A \rightarrow A_t = e^{iHt} A e^{-iHt}$ has very different properties for a second order differential operator H .

However, we might make a distinction here between the case of equ. (8), where the Schrödinger equation serves as a non-relativistic approximation only, and the special case of the harmonic oscillator. In the first case, where we deal with an *approximation only*, a distinction of precisely predictable observables may be out of place anyhow. But the Schrödinger equation of the harmonic oscillator has been used in Quantum Field theory as a (precise) wave equation of the *Photon* - a particle of *spin* 0.

We address this case in ch.8. Interestingly, an algebra of precisely predictable observables arises, but with the property that these observables are precisely predictable only at periodic times. This might be compared with the fact that total energy $H_D(t)$ for a Dirac problem with time-dependent potentials also is *not* precisely predictable, except at the precise time t , but not earlier or later.

Assuming that a time-constant field \mathbf{A}, \mathbf{V} is superimposed with a field of an oscillation - an electromagnetic wave - then also $H(t)$ may be precisely predictable only at periodic time-intervals. This, of course, would be a situation where an atom emits (or absorbs) a photon, thereby changing its total energy. [And then, it seems that time is also quantized - in the sense that only very special moments can serve for precise observations.]

In fact, if we must admit that the outcome of our measurements can be precisely predicted only at periodically occurring distinct times, then at once we might be free from all concerns about so-called quantum jumps, because continuity at a set of discrete points is a meaningless thing.

All in all, our improvement of v.Neumann's "principles of quantum mechanics" remains confined to a rather special set of problems. We must leave it to others to perhaps use some of these ideas to design a fitting more general concept.

We have tried to anticipate the fact that this book might meet readers of very different orientations. While, generally, we have tried to offer a mathematically rigorous theory, including an introduction into (our kind of) pseudodifferential

operators, we have tried to put lengthy and technical proofs into footnotes, or somewhat out of the way, as not to bore others willing to accept the statements. We have neglected to include an introduction into rigorous spectral theory of self-adjoint differential operators in Hilbert space, although frequent use is made of such things, referring to the large mathematical literature, already more than half a century old. Regarding pseudodifferential operators, we did not include existence proofs of evolution operators, and the global Egorov theorem for hyperbolic systems of pseudodifferential equations we developed in our book [Co5] is only discussed for the Dirac operator, a very special symmetric hyperbolic operator, although this is often used for more general such problems. Neither did we discuss the proofs for global coordinate changes for ψ do-s, although, again, this is used. Again, we did not include a general discussion of composition of Fourier integral operators, although the evolution operator of H_D is a Fourier integral operator. But for the special compositions of FIOps we require, this is not needed. A sort of “Egorov-type argument” always is sufficient for us. It avoids the nonlinear PDE-s arising while obtaining newly-generated phase functions, focusing instead on some kind of (linear) “Hamiltonian flow” in each case. In fact, we are making it a special point, to be able to avoid Fourier integral operator calculus throughout this book – just as well as we resist the temptation to translate our theory from Euclidean space \mathbb{R}^3 to differentiable manifolds, following a popular trend.

In conclusion: After looking over a multitude of introductions into Quantum Theory - notably Dirac’s theory of the electron - given by Physicists and Mathematicians, our personal orientation, emphasizing physical interest, spectral theory and theory of pseudodifferential operators has lead us to a lookout over Quantum Theory which seems distinctly different, in some respects. While we must admit that we did not attempt a complete review of all relevant physical literature⁸, we find it worthwhile to hereby attempt a presentation to the general public - for inspection and comments.

Our “Thanks” must be expressed to anybody - known or unknown - who encouraged us, especially the editor of this series, and the publisher, and to Stefan Cordes who helped in many respects.

Heinz Otto Cordes
August 2006

⁸Reference to older attempts dealing with Dirac paradoxes may be found in Thaller’s book [Th1]; For arguments for or against v.Neumann’s principles one might look into the papers of [DV]; also, the paper [GZA] of T. Gill et al. was recently brought to our attention.

Chapter 2

Why Should Observables be Pseudodifferential?

2.0 Introduction

The present chapter will be irrelevant¹ for the mathematical deployment in succeeding chapters. We offer this material only to provide a motivation for our claim that a Dirac observable should be a self-adjoint *pseudodifferential* operator.

We shall consider the action of translations, rotations, and dilations on ψ do-s - or, rather, on general bounded operators $A : \mathcal{H}_s \rightarrow \mathcal{H}_{s-m}$. We shall find that these actions are *smooth*, both in configuration space and in momentum space, **if and only if** A is a ψ do of order m , not quite in $Op\psi c_m$ but in a slightly larger such class, also equipped with *some* calculus of ψ do-s.

Note, the property “smooth” appears here as a mathematical idealization: **An observable certainly should be “insensitive” against small errors in positioning our coordinate system - both in configuration space and in momentum space - and this also should hold for small rotational errors or dilational ones - if its prediction is to make any sense at all.** The idealization appears here as a replacement of “insensitive against small errors” by “smooth under translational, rotational and dilational action”.

To explain in more detail, what this means: Consider the linear operators $T_z : u(x) \rightarrow u(x - z) = (T_z u)(x)$, and, $S_o : u(x) \rightarrow u(ox) = (S_o u)(x)$, and, $R\tau : u(x) \rightarrow u(\tau x) = (R_\tau u)(x)$, for general $z \in \mathbb{R}^3$, $0 < \tau \in \mathbb{R}$, and a general (real

¹Exception: We are making some practical application in sec.2.4, useful for a side-result in ch.3.

3×3 -rotation matrix $o \in \text{SO}_3(\mathbb{R})$. Note, we have $T_z = e^{-izD}$ - formally a ψ do (with symbol $e^{-ix\xi}$) but certainly, T_z is *not* a strictly classical ψ do - except for $z = 0$. Similarly, the operators S_o , R_τ do not belong to $\text{Op}\psi c$, except for $\tau = 1$ or $o = 1$.

In the simplest case (of $\mathcal{H}_s = \mathcal{H}$ - i.e., $s = 0$ - , and a bounded operator $A : \mathcal{H} \rightarrow \mathcal{H}$) we consider the 4 operator families²

$$(2.0.1) \quad \{A_z = T_z^{-1}AT_z : z \in \mathbb{R}^3\}, \text{ and } , \{A_\zeta = e^{-i\zeta x}Ae^{i\zeta x} : \zeta \in \mathbb{R}^3\},$$

and,

$$(2.0.2) \quad \{A_o = S_o^{-1}AS_o : o \in \text{SO}_3(\mathbb{R})\}, \text{ and } , \{A_\tau = R_\tau^{-1}AR_\tau : 0 < \tau < \infty\}.$$

Each of these families involves certain parameters. In (2.0.1) there are the 3 parameters $z_1, z_2, z_3 \in \mathbb{R}$ (or $\zeta_1, \zeta_2, \zeta_3 \in \mathbb{R}$), in (2.0.2) we have the coefficients o_{jl} of the orthogonal matrix o , leaving 3 (real) degrees of freedom, since we may write $o = e^a$ with a real antisymmetric 3×3 -matrix $a = -a^T$. (Or, in the second case of (0.2), we have the single (real) parameter $\tau > 0$.) So, we may ask whether partial derivatives (of all orders) for these parameters exist - then we will say that the corresponding *action* (of the operator T_z or $e^{-i\zeta x}$ or S_o or R_τ on the operator A) is *smooth*. And, to be precise, we want these partial derivatives to exist in operator norm of the Hilbert space \mathcal{H} . [That is, for example, we want that $\|\partial A_z / \partial z_1 - \Delta A_z / \Delta z_1\| \rightarrow 0$ as $\Delta z_1 \rightarrow 0$, with $\Delta A_z = A_{z+\Delta z_1(1,0,0)} - A_z$, etc., with operator norm $\|\cdot\|$ of \mathcal{H} .]

The point we are trying to make then is this:

All the above 4 actions are smooth if and only if the bounded operator $A : \mathcal{H} \rightarrow \mathcal{H}$ is a pseudodifferential operator of order 0, with symbol belonging to a class we call ψs_0 , where $\psi s_0 \supset \psi c_0$ is a bit larger, but still allows some calculus of ψ do-s.

For simplicity we get restricted to ψ do-s with complex-valued symbol - even presenting some major arguments only for the 1-dimensional case, with trivial extensions to arbitrary dimensions. We only want to make the point, that it may be *physically significant* to restrict theory of observables to ψ do-s, while not

²Clearly this involves 4 Lie-group representations on the algebra $L(\mathcal{H})$. For the second (2.0.1) the Fourier transform $A_\zeta^\wedge = F^*A_\zeta F$ may be written as $(A_\zeta)^\wedge = T_\zeta^{-1}A^\wedge T_\zeta$, since we have $T_\zeta = F^*e^{-i\zeta x}F$. Thus this amounts to translation smoothness in phase space, while the first (2.0.1) expresses the same for configuration space. The smoothnesses of (2.0.2) automatically imply (and are implied by) the corresponding smoothnesses in phase space, as a simple calculation shows.

allowing more general abstract linear operators of our Hilbert space \mathcal{H} . For the first (perhaps hardest) step we only use the Heisenberg group and the Hilbert space \mathcal{H} , postponing a refined treatment to later sections. Otherwise, the results developed here are of no significance for our discussions in later chapters, so that reading may be skipped or postponed.

2.1 Smoothness of Lie Group Action on ψ do-s

Consider first an arbitrary bounded operator A of $\mathcal{H} = L^2(\mathbb{R}^3)$. Assume that we have

$$(2.1.1) \quad e^{izD} e^{-i\zeta x} A e^{i\zeta x} e^{-izD} = A_{z,\zeta} \in C^\infty(\mathbb{R}^6, L(\mathcal{H})) .$$

To discuss this condition: Note, that the operators $T_z = e^{-izD}$ form the group of translation operators - We find that $T_z u(x) = u(x - z)$. This is a Lie-subgroup of the group of unitary operators. It is strongly continuous in z - we have $T_z u \rightarrow T_{z_0} u$ in strong L^2 -convergence, as $z \rightarrow z_0$, for every $u \in \mathcal{H}$. However, T_z is **not** uniformly continuous - we do not have $\|T_z - T_{z_0}\| \rightarrow 0$ as $z \rightarrow z_0$, as easily seen³.

Quite similarly, the group $\{e^{i\zeta x} : \zeta \in \mathbb{R}^3\}$ of (unitary) multiplication operators again is strongly continuous but not uniformly continuous⁴. The Fourier transform of the multiplication group is the translation group again. Both groups $\{T_z\}$ and $\{e^{i\zeta x}\}$ together generate what is called the Heisenberg group.

Then we must emphasize: by (2.1.1) we mean that the family $A_{z,\zeta}$ is operator norm continuous in $L(\mathcal{H})$, not only strongly continuous. And in addition, that all partial derivatives for z_j and ζ_j (of any order) exist in norm convergence, and also are norm continuous.

Now we want to prove:

Theorem 2.1.1 *An operator $A \in L(\mathcal{H})$ satisfies (2.1.1) if and only if it is a ψ do in $Op\psi t_0$. Here $\psi t_0 = CB^\infty(\mathbb{R}^6)$ denotes the space of $C^\infty(\mathbb{R}^6)$ -functions having all derivatives bounded. For such a function the ψ do $A = a(x, D)$ is defined in the usual way - either (1.0.15) or (1.2.1)⁵.*

³Consider the family $u_\varepsilon(x) = \prod_1^3 \varphi_\varepsilon(x_j)$, $\varphi_\varepsilon(t) = (\varepsilon^2 \pi)^{-1/4} e^{-t^2/2\varepsilon^2}$ of unit vectors in \mathcal{H} . Show that $\|T_z u_\varepsilon - T_{z_0} u_\varepsilon\|^2 \rightarrow 2$ as $\varepsilon \rightarrow 0$, $\varepsilon > 0$ for every fixed z, z_0 with $z \neq z_0$, so that $\|T_z - T_{z_0}\| = 2$, as $z \neq z_0$, follows.

⁴Get $\|(e^{i\zeta x} - e^{i\zeta_0 x})u\| = 2\|u \sin(\frac{1}{2}(\zeta - \zeta_0)x)\| \geq \|u\|$ whenever $u \in \mathcal{H}$ vanishes outside a (non-empty) open x -set where $|\sin \frac{1}{2}(\zeta - \zeta_0)x| \geq \frac{1}{2}$. Such open x -sets exists whenever $\zeta \neq \zeta_0$ since the sine reaches ± 1 for some points x . Hence we get $\|e^{i\zeta x} - e^{i\zeta_0 x}\| \geq 1$ whenever $\zeta \neq \zeta_0$.

⁵(1.0.14) will work too, but the distribution $a^{\vee 2}(x, x - \cdot)$ no longer has the nice properties as for an $a \in \psi c$. [For example, the translation operator T_z itself has symbol $t_z(x, \xi) = e^{iz\xi} \in \psi t_0$, but its integral kernel is $\delta(x - y - z)$ - with a singularity at $x - y = z$ different from 0.]

Proof. First of all, the ψ do-s $A = a(x, D)$ all are bounded operators of \mathcal{H} . [Of course⁶, we have stated theorem 1.1.4 only for $a \in \psi c_0$, but the reader may inspect the proof given, to find that **only the boundedness** of a few derivatives (up to order 8) was used, and not the more stringent conditions (1.0.13), defining ψc_0 .]

Furthermore, for such $A = a(x, D)$, we find that

$$(2.1.2) \quad A_{z, \zeta} = a(x + z, \zeta + D) .$$

In other words, $A_{z, \zeta}$ is also a ψ do in $Op\psi t_0$ with symbol $a_{z, \zeta} = a(x + z, \xi + \zeta)$. Indeed, $(e^{-i\zeta x} A e^{i\zeta x} u)(x) = \frac{1}{8\pi^3} e^{-i\zeta x} \int d\xi \int dy e^{i\xi(x-y)} a(x, \xi) u(y) e^{i\zeta y}$
 $= \frac{1}{8\pi^3} \int d\xi \int dy e^{i(\xi-\zeta)(x-y)} a(x, \xi) u(y) dy = a(x, \zeta + D) u(x)$. Similarly, $T_{-z} A T_z u(x) = a(x + z, D) u(x)$, confirming (2.1.2).

With formula (2.1.2) things are clear now: If $a \in \psi t_0$ then all derivatives of a exist in uniform convergence over \mathbb{R}^6 . Using (2.1.2) and (1.4.5) (for ψt_0) we thus conclude that, indeed, all derivatives (for z and ζ) of $A_{z, \zeta}$ exist in operator norm, so that (2.1.1) holds.

Vice versa, assume now that an operator $A \in L(\mathcal{H})$ satisfies (2.1.1). Then our attempt to show that $A \in Op\psi t_0$ will require that we specify a symbol $a \in \psi t_0$ such that $A = a(x, D)$. Let us play a bit with the (norm-smooth) family $A_{z, \zeta}$.

For a translucent argument we get restricted to the case of a 1-dimensional operator - that is, we consider the case of an operator $A \in L(\mathcal{H})$, $\mathcal{H} = L^2(\mathbb{R})$, so that only one (real) x - and ξ -variable⁷ is involved. Then we arrive at a formula expressing the symbol $a(x, \xi)$ of A in terms of $A_{z, \zeta}$ by writing

$$(2.1.3) \quad a(z, \zeta) = \int dx d\xi \gamma_2(-x) \gamma_2(-\xi) b(x + z, \xi + \zeta) ,$$

with $b(x, \xi) = (1 + \partial_x)^2 (1 + \partial_\xi)^2 a(x, \xi)$, and the Greens function

$$(2.1.4) \quad \gamma_m(t) = e^{-t} \frac{t^{m-1}}{(m-1)!} \text{ as } t \geq 0, = 0, \text{ as } t < 0$$

of the differential operator $(1 + \partial_t)^m$ in $(-\infty, \infty)$ - that is, we have $(1 + \partial_t)^m \gamma_m(t) = \delta(t)$ with the Dirac delta function δ , and (2.1.3) simply expresses this fact.

Note that $b(x, \xi)$ is the symbol of the operator

$$(2.1.5) \quad B = (1 + i \text{ ad}_D)^2 (1 - i \text{ ad}_D)^2 A$$

⁶Incidentally, as to be used later on, this also holds for (1.4.5): Again our proof there does not use the Leibniz formulas, but only the special Beals-formulas for the symbol of $a^s(x, D) = \Lambda_s a(x, D) \Lambda_s^{-1}$, but they already work for $a \in \psi t_0$. Hence it follows that $a_s(x, \xi) \in \psi t_0$, and thus also $a(x, D) \in L(\mathcal{H}_s)$, for all s .

⁷For 3 dimensions one simply must replace the function $\gamma_2(-x)$ in (2.1.3) by the product $\gamma_2(-x_1) \gamma_2(-x_2) \gamma_2(-x_3)$, and the differential operator $(1 + \partial_x)^2$ by $\prod_1^3 (1 + \partial_{x_j})^2$, and similarly for ξ . Then we get fl. (2.1.7) again with W replaced by a product of 3 1-dimensional operators.

where we have written “ $ad_X A = [X, A]$ ”. If $A \in Op\psi t_0$ then clearly $B \in Op\psi t_0$ as well.

By (2.1.2) we get $B_{z,\zeta} = b_{z,\zeta}(x, D)$ where $b_{z,\zeta}(x, \xi) = b(x + z, \xi + \zeta)$. Using this we may write (2.1.3) in the form

$$(2.1.6) \quad a(z, \zeta) = \int dx d\xi \lambda(x, \xi) b_{z,\zeta}(x, \xi) \quad \text{with} \quad \lambda(x, \xi) = \gamma_2(-x)\gamma_2(-\xi).$$

Formally the right hand side of (2.1.6) looks like a trace: Using formula (1.2.1) it is clear that $b_{z,\zeta}(x, \xi)e^{ix\xi}$ is the integral kernel of the operator $\sqrt{2\pi}B_{z,\zeta}F^*$, while $\lambda(x, \xi)e^{ix\xi}$ similarly would be the integral kernel of the operator $\sqrt{2\pi}\lambda(x, D)F^* = \sqrt{2\pi}\gamma_2(-x)\gamma_2(-D)F^*$. Note that $\lambda(x, \xi)$ is real, by definition. So, the right hand side of (2.1.6) - i.e.,

$= \int dx d\xi (a(x, \xi)e^{ix\xi}) \overline{(\lambda(x, \xi)e^{ix\xi})}$ - then should represent the trace of the product $2\pi(B_{z,\zeta}F^*)(\lambda(x, D)F^*)^* = 2\pi B_{z,\zeta}\lambda(x, D)^* = 2\pi B_{z,\zeta}\gamma_2(-D)\gamma_2(-x)$. So, this gives the formula

$$(2.1.7) \quad a(z, \zeta) = \text{trace}\{B_{z,\zeta}W^*\},$$

with the integral operator

$$(2.1.8) \quad W = \frac{1}{2\pi}\gamma_2(-x)\gamma_2(-D) = \gamma_2(-x)\left(\frac{1}{(1+ix)^2}\right)^*.$$

For the derivation of (2.1.7) we have used that $\gamma_2^\wedge(\xi) = \frac{1}{\sqrt{2\pi}(1+i\xi)^2}$.

The point is that (i) formulas (2.1.7),(2.1.8) indeed express the symbol a of a ψ do $A \in Op\psi t_0$ explicitly in terms of the operator family $B_{z,\zeta}$ generated by B of (2.1.5), while (ii) the operator W of (2.1.9) turns out to be⁸ of *trace class* (cf. [Ka1]), so that indeed the traces and above formula make sense. Moreover, (iii) even for a general bounded operator A of \mathcal{H} satisfying (2.1.1), we find the family $B_{z,\zeta}$ smooth as well, so that formula (2.1.7) defines a complex-valued function $a(z, \zeta) \in \psi t_0$, using the fact that the trace class is an ideal of the algebra $L(\mathcal{H})$, where the function $\text{trace}\{CX^*\}$ is a continuous function of C for $C \in L(\mathcal{H})$ with operator norm, as long as the operator X belongs to trace class.

⁸According to ch.X, sec’s 1.3-1.4 of [Ka1] an operator X is of trace class whenever it can be shown that $X = YZ$ where Y and Z are of Schmidt class (i.e., they are integral operators with kernel in $L^2(\mathbb{R}^2)$ for our 1-dimensional case.) But we may write the operator W as a product UV of Schmidt operators as follows: W has integral kernel $w(x, y) = \frac{\gamma_2(-x)}{(1+i(x-y))^2}$. Just introduce $Uu(x) = \int dz \frac{\gamma_1(x-z)}{1+iz}u(z)dz$, and note that $U^{-1} = (1+ix)(1+\partial_x)$, so that $W = U((1+ix)(1+\partial_x)W) = UV$. The integral kernel of U is squared integrable, since γ_1 (of (2.1.4)) and $\frac{1}{1+ix}$ both are L^2 -functions. Similarly, V has the kernel $(1+ix)(1+\partial_x)\frac{\gamma_2(-x)}{(1+i(x-y))^2}$, also in $L^2(\mathbb{R}^2)$, so that U and V both are Schmidt operators. Hence W is of trace class, and so then is $B_{z,\zeta}W^*$, since the trace class is an adjoint invariant ideal of $L(\mathcal{H})$.

In other words, we find that (2.1.7) constitutes a left-inverse of the map $a(x, \xi) \rightarrow A = a(x, D)$ defined for $a \in \psi t_0$. We already noted that formula (2.1.7) defines a symbol in ψt_0 for every operator A satisfying (2.1.1). Therefore, in order to show that this left-inverse actually is an inverse, we only must prove that $a(z, \zeta) \equiv 0$ - with a defined by (2.1.7), for some $A \in L(\mathcal{H})$ satisfying (2.1.1), implies that $A = 0$. But then we get $\text{trace}\{B_{z, \zeta} W^*\} = \text{trace}\{B W_{z, \zeta}^*\} = 0$ for all z, ζ , by the general rules for traces. Also, for the formal ψ do $W = \frac{1}{2\pi} \lambda(x, D)$ we get (just as (2.1.2))

$$(2.1.9) \quad W_{z, \zeta} = \frac{1}{2\pi} g_2(-x - z) \gamma_2(-\zeta - D) .$$

Then, given two arbitrary C_0^∞ -functions ω, χ get

$$(2.1.10) \quad \int dz d\zeta W_{z, \zeta} (1 - \partial_z)^2 \omega(z) (1 - \partial_\zeta)^2 \omega(\zeta) = \omega(-x) \chi(-D) ,$$

using partial integration and that $(1 + \partial_t)^2 \gamma_2(t) = \delta(t)$. Applying this we get

$$(2.1.11) \quad \text{trace}(\bar{\omega}(x) B \bar{\chi}(D)) = 0 \quad \text{for all } \omega, \chi \in C_0^\infty .$$

Expressing this with the distribution kernel $k_B(x, y)$ of B we get $\int k_B(x, x - z) \omega(x) \chi(z) dx d\zeta = 0$ for all $\omega, \chi \in C_0^\infty$, implying $B = 0$, hence $A = 0$, q.e.d.

Our above theorem only is a preliminary result, involving the special translation group in configuration space and momentum space, and the Hilbert space $\mathcal{H} = \mathcal{H}_0$, and operators of order 0. In the sections, below, we shall extend this in various directions.

2.2 Rotation and Dilation Smoothness

We are still with zero-order ψ do-s with symbol in ψt_0 (and with scalar-valued symbol). The class $Op\psi t_0$ was seen to be identical with the class of bounded operators of $\mathcal{H} = L^2$ which are translation smooth, both in configuration space and in momentum space - i.e., the operator A and its Fourier transform $A^\wedge = F^* A F$ both are translation smooth - we have cdn.(2.1.1) We now ask about the subset $\Psi\mathcal{G}\mathcal{S}$ of $Op\psi t_0$ of operators which also are smooth with respect to the action of rotations and dilations. That is, we request that, for the two families of substitution operators $\mathcal{G}\mathcal{R} = \{S_o : o \in \mathbf{SO}_3\}$ and $\mathcal{G}\mathcal{D} = \{R_\tau : \tau \in \mathbb{R}_+\}$ we have

$$(2.2.1) \quad S_o^* A S_o \in C^\infty(\mathbf{SO}_3, L(\mathcal{H})) ,$$

and

$$(2.2.2) \quad R_\tau^* A R_\tau \in C^\infty(\mathbb{R}_+, L(\mathcal{H})) .$$

Here we use the operators $S_o u(x) = u(ox)$, and, $R_\tau u(x) = \tau^{3/2} u(\tau x)$, respectively. Both are unitary operators, and the classes \mathcal{GR} and \mathcal{GD} are Lie groups, of course. Again the two conditions mean that the two conjugations (by S_o or by R_τ) are smoothly depending on the parameters $o \in \mathbf{SO}_3$ and $\tau > 0$, respectively, with derivatives existing and continuous in operator norm⁹ of $L(\mathcal{H})$.

First of all, in that respect, we notice that

$$(2.2.3) \quad FS_o = S_o^* F \quad , \quad \text{and} \quad , \quad FR_\tau = R_\tau^* F .$$

This implies that $A \in \text{Op}\psi t_0$ satisfies (2.2.1) (or (2.2.2)) if and only if $A^\wedge = F^* A F$ does. So, we need not distinguish between these conditions in configuration space or momentum space: If they hold in one of these spaces, then they do hold in the other one as well. If (2.2.1) or (2.2.2) hold then we will say that A is “rotation smooth” (“dilation smooth”).

Furthermore, after sec.2.1, if A is translation and rotation and dilation smooth then we already know that A has a symbol in ψt_0 and may work with it - this makes things easier, and reduces the theorem below to a series of calculations.

Theorem 2.2.1 *An operator $A \in L(\mathcal{H})$ is smooth in the sense of all four above groups $\{e^{-izD}\}$ and $\{e^{i\xi x}\}$ and $\{S_o\}$ and $\{R_\tau\}$ if and only if $A = a(x, D)$ with symbol $a(x, \xi) \in \psi t_0$ satisfying the following “condition ψs_0 ”:*

Define the (first order linear) partial differential operators

$$(2.2.4) \quad \varepsilon_{jl} = \xi_j \partial_{\xi_l} - x_l \partial_{x_j} \quad , \quad j, l = 1, 2, 3,$$

and then

$$(2.2.5) \quad \eta_{jl} = \varepsilon_{jl} - \varepsilon_{lj} \quad \text{as} \quad j \neq l \quad , \quad \eta_{00} = \sum_1^3 \varepsilon_{jj} .$$

Every finite application of the η_{jl} to the symbol $a(x, \xi)$ must still belong to ψt_0 .

The proof of this theorem consists of studying the action of the two corresponding Lie-algebras onto our symbols $a(x, \xi)$. This will be left to the reader. For details, see [Co5],ch.8, sec.5.

The class of all symbols $a(x, \xi) \in \psi t_0$ satisfying cnd. ψs_0 will be denoted by ψs_0 , henceforth. The classes ψs and ψs_m are defined similarly to ψc , ψc_m :

⁹Note that again, the operators S_o and R_τ are only strongly continuous - not uniformly continuous in their parameters o or τ .

ψ_s is the class of all polynomials in x, ξ with coefficients in ψ_{s_0} . Also, $\psi_{s_m} = \langle x \rangle^{m_2} \langle \xi \rangle^{m_2} \psi_{s_0}$. One confirms that

$$(2.2.6) \quad \psi_{c_m} \subset \psi_{s_m} \subset \psi_{t_m} ,$$

and that ψ_{s_m} may be described as the subset of ψ_{t_m} of all $a(x, \xi)$ such that

every finite application of the operators η_{jl} still belongs to ψ_{t_m} .

Investigating the type of symbol in ψ_{s_m} we note first: These symbols (at least) satisfy the (Hoermander-type) conditions (1.2.2) locally, in the following sense:

Proposition 2.2.2 *For $a \in \psi_{s_m}$ we have (1.2.2) whenever either $|x|$ or $|\xi|$ belongs to a bounded set. That is,*

$$(2.2.7) \quad a_{(\iota)}^{(\theta)}(x, \xi) = O((1 + |\xi|)^{m_1 - |\theta|}) , \text{ as } |x| \leq c ,$$

and,

$$(2.2.8) \quad a_{(\iota)}^{(\theta)}(x, \xi) = O((1 + |x|)^{m_2 - |\iota|}) , \text{ as } |\xi| \leq c .$$

Proof. Focus on (2.2.7) (and assume $m = 0$). For $a \in \psi_{s_0}$ and $|x| \leq c$ get

$$\lambda_{00}a = \sum \xi_j a_{|\xi_j} = \eta_{00}a + O(1) = O(1) , \quad \lambda_{jl}a = \xi_j a_{|\xi_l} - \xi_l a_{|\xi_j} = \eta_{jl}a + O(1) = O(1) .$$

Thus,

$|\xi|^2 a_{|\xi_j} = \xi_j \lambda_{00}a - \sum_l \xi_l \lambda_{jl}a = O(|\xi|)$, implying $a_{|\xi_j} = O(\langle \xi \rangle^{-1})$. This procedure may be iterated to get (2.2.7). Similarly for general m and for (2.2.8), q.e.d.

As one consequence of this proposition we note that, for a symbol $a \in \psi_s$, the integral kernel $k_A(x, y) = (2\pi)^{-3/2} a^{\vee 2}(x, x - y)$ of $A = a(x, D)$ (appearing in fla. (1.0.14)) has regained the properties it had for a symbol of the class ψ_{c_m} : It is C^∞ except at $x = y$ and for large $|y|$, $k(x^0, y)$ behaves like a function in \mathcal{S} . This follows from prop.1.1.1, since, evidently, $a(x, \xi)$ is of polynomial growth in ξ for a given fixed x .

It is possible to state more precise global estimates for the symbols in ψ_{s_m} - where we again get restricted to $m = 0$ with similar facts for general m left to the reader.

Theorem 2.2.3 *For $a \in \psi_{s_0}$ we have the estimates¹⁰*

$$(2.2.9) \quad a_{(\theta)}^{(\iota)}(x, \xi) = O\left(\left\{\frac{|x|}{|\xi|}\right\}^j\right) \text{ for all } -|\theta| \leq j \leq |\iota| ,$$

for all θ, ι .

To prove this theorem we need the following

Lemma 2.2.4 For $a(x, \xi) \in C_0^\infty(\mathbb{R}^6)$ define $a_{pq} = \eta_{pq}a$, $p, q = 0, \dots, 3$ where we extend (2.2.5) by setting

$$(2.2.10) \quad \eta_{p0} = \partial_{x_p}, \quad \eta_{0q} = \partial_{\xi_q}, \quad \eta_{pp} = 0, \quad p, q = 1, 2, 3.$$

Then there exist symbols $\gamma^{1j}pq \in \psi_{c_{e^1-e^2}}$ and $\gamma_{pq}^{2j} \in \psi_{c_{e^2-e^1}}$ such that

$$(2.2.11) \quad a|_{x_j} = \sum_{p,q=0}^3 \gamma_{pq}^{1j} a_{pq}, \quad a|_{\xi_j} = \sum_{p,q=0}^3 \gamma_{pq}^{2j} a_{pq}.$$

This lemma follows with the argument of prop.2.2.2, writing down terms a bit more carefully. It is clear then that the lemma allows to generate a factor $\langle x \rangle / \langle \xi \rangle$ (or $\langle \xi \rangle / \langle x \rangle$) in the general estimates for symbols, so that we get (2.2.11) and the theorem.

Finally, in this section, let us come back to the question about calculus of ψ do-s within $Op\psi$ s. It is clear from (2.2.7) that we have a “local calculus of ψ do-s” in the sense of Hoermander [Hoe1]. That is, the Leibniz formulas (1.0.8), (1.0.9) are valid locally - i.e., we have asymptotic convergence of the series for c and a_* in compact x -subsets (with respect to ξ) or vice versa, giving asymptotic operator convergences in the sense of [Ho1] (cf.also, [Co5],IV) - that is, in the sense of smoother and smoother remainders.

Note also, the classes ψ_{s_0} , ψ_s as well as the operator classes $Op\psi_{s_0}$, $Op\psi_s$ form algebras, under their corresponding products - pointwise or operator product.

In matters of global calculus of ψ do-s it turns out that, at least, we have asymptotically convergent Leibniz formulas for products AK , KA and commutator $[K, A]$ if $A = a(x, D) \in Op\psi_{s_m}$, but $K = k(x, D) \in Op\psi'_{c'_m}$, in the following sense.

Proposition 2.2.5 We have

$$(2.2.12) \quad k(x, D)a(x, D) = c_1(x, D), \quad a(x, D)k(x, D) = c_2(x, D),$$

$$[k(x, D), a(x, D)] = c_3(x, D),$$

where

$$c_1(x, \xi) = \sum_{|\iota| \leq N} \frac{(-i)^{|\iota|}}{\iota!} k^{(\iota)}(x, \xi) a_{(\iota)}(x, \xi) + R_N^1(x, \xi),$$

¹⁰The class of symbols $a(x, \xi)$ satisfying estimates (2.2.9) is known as the Weinstein-Zelditch class (cf.[We1],[Ze1]).

$$(2.2.13) \quad c_2(x, \xi) = \sum_{|\iota| \leq N} \frac{(-i)^{|\iota|}}{\iota!} a^{(\iota)}(x, \xi) k_{(\iota)}(x, \xi) + R_N^2(x, \xi) ,$$

$$c_3(x, \xi) = \sum_{j=0}^N \frac{(-i)^j}{j!} \{k, a\}_j(x, \xi) + R_N^3(x, \xi) .$$

In (2.2.13) the terms $k^{(\iota)} a_{(\iota)}$, $a^{(\iota)} k_{(\iota)}$, with $|\iota| = j$, and the “higher order Poisson brackets”

$$(2.2.14) \quad \{k, a\}_j = \nabla_\xi^j k \cdot \nabla_x^j a - \nabla_\xi^j a \cdot \nabla_x^j k$$

belong to $\psi s_{m+m'-re^1-r'e^2}$ for all $r, r' = 0, 1, \dots$ with $r + r' = j$, while $R_N^l \in \psi s_{m+m'-re^1-r'e^2}$ for all $r, r' = 0, 1, \dots$, with $r + r' = N + 1 - \text{for } l = 1, 2, 3$.

The proof is discussed in [Co5],ch.8, prop.7.4.

2.3 General Order and General \mathcal{H}_s -Spaces

In this section we shall consider smoothness under the Heisenberg group as in sec.2.1, but for operators $A \in L(\mathcal{H}_s)$, with one of the weighted Sobolev spaces of sec.1.4 . Moreover, one may remove the restriction to ψ do-s of order 0 and also characterize the classes $Op\psi c_m$, for general $m \in \mathbb{R}^2$ by looking at translation smoothness for operators in $L(\mathcal{H}_s, \mathcal{H}_t)$ - rather $L(\mathcal{H}_s, \mathcal{H}_{s-m})$, for any fixed $s \in \mathbb{R}^2$, as we will find.

Observe first that - clearly - the class $Op\psi t_0$ is an algebra - it coincides with the class of smooth operators considered in sec.2.1, above, and they trivially form an (adjoint invariant) algebra. Moreover, we note that the translation operator $T_z = e^{-izD}$ and the multiplication operator $e^{i\zeta x}$ both belong to the algebra $Op\psi t_0$. As a consequence, it follows from corollary 1.4.2 that e^{-izD} and $e^{i\zeta x}$ both form groups of bounded linear operators in every weighted Sobolev space¹¹ \mathcal{H}_s . Thus we might ask whether a similar characterization of the smooth operators also is possible for the spaces \mathcal{H}_s .

Recall from sec.1.4: our Sobolev space \mathcal{H}_s carries the norm $\|u\|_s = \|\Lambda_s u\|_{L^2}$ with $\Lambda_s = \langle x \rangle^{s_2} \langle D \rangle^{s_1}$, so that Λ_s and $\Lambda_s^{-1} = \Lambda_{-s}^* = \langle D \rangle^{-s_1} \langle x \rangle^{-s_2}$ provide isometries $\Lambda_s : \mathcal{H}_s \rightarrow \mathcal{H}$ and $\Lambda_{-s}^* : \mathcal{H} \rightarrow \mathcal{H}_s$.

While examining operators in $L(\mathcal{H}_s)$ we then should keep in mind that

$$“A \in L(\mathcal{H}_s)” \text{ means the same as } “A_s = \Lambda_s A \Lambda_{-s}^* \in L(\mathcal{H})” .$$

¹¹Of course the operators $e^{-izD}, e^{i\zeta x} \in L(\mathcal{H}_s)$ no longer may be expected to be unitary, but they will be bounded.

Note that Λ_s and Λ_{-s}^* are ψ do-s in $Op\psi c$. If $A = a(x, D)$ is a ψ do in $Op\psi t_0$ then we have calculated a symbol a_s for the operator A_s in 1.4 (footnote 23) - we found that

$$(2.3.1) \quad a_s(x, \xi) = (2\pi)^{-6} \int dy d\zeta a(x-y, \xi-\zeta) \left(\int dz e^{-iz\zeta} \left(\frac{\langle x-z \rangle}{\langle x \rangle} \right)^{-s_2} \right) \left(\int d\eta e^{-iy\eta} \left(\frac{\langle \xi-\eta-\zeta \rangle}{\langle \xi-\zeta \rangle} \right)^{s_1} \right),$$

where we must recall that all 4 integrals are finite parts: When evaluating them we must use the identity $e^{-ixy} = \langle x \rangle^{-2N} (1 - \Delta_x)^N e^{-ixy}$ and formal partial integration to convert (2.3.1) into an integral with integrand in L^1 which can be evaluated. Examining differentiability of $a_s(x, \xi)$ we note that - formally - a differentiation $\partial_x^\theta \partial_\xi^\nu$ may be carried out under the integral signs, giving

$$(2.3.2) \quad (a_s)_{(\theta)}^{(\nu)}(x, \xi) = (2\pi)^{-6} \int dy d\zeta a_{(\theta)}^{(\nu)}(x-y, \xi-\zeta) \left(\int dz e^{-iz\zeta} \left(\frac{\langle x-z \rangle}{\langle x \rangle} \right)^{-s_2} \right) \left(\int d\eta e^{-iy\eta} \left(\frac{\langle \xi-\eta-\zeta \rangle}{\langle \xi-\zeta \rangle} \right)^{s_1} \right),$$

Indeed, it is found that this operation is legal - the formal conversion gives

$$(2.3.3) \quad p(x, \xi) = (2\pi)^{-6} \int \frac{dy d\eta dz d\zeta}{(\langle y \rangle \langle \eta \rangle \langle z \rangle \langle \zeta \rangle)^{2N}} a_N(x-y, \xi-\zeta) e^{-iz\zeta} X_N(x, z) e^{-iy\eta} Y_N(\xi, \eta, \zeta)$$

with $a_N(x, \xi) = (1 - \Delta_x)^N (1 - \Delta_\xi)^N a(x, \xi)$, and,

$$(2.3.4) \quad X_N = \langle z \rangle^{2N} (1 - \Delta_z)^N \left\{ \frac{1}{\langle z \rangle^{2N}} \left(\frac{\langle x-z \rangle}{\langle x \rangle} \right)^{-s_2} \right\},$$

$$Y_N = \langle \eta \rangle^{2N} (1 - \Delta_\eta)^N \left\{ \frac{1}{\langle \eta \rangle^{2N}} \left(\frac{\langle \xi-\eta-\zeta \rangle}{\langle \xi-\zeta \rangle} \right)^{s_1} \right\}.$$

Again, N should be chosen sufficiently large, such that the integral converges absolutely. [Note the various applications of $1 - \Delta$ do not improve nor disimprove the estimates, but the various denominators $\langle y \rangle^{2N}$ eventually will create an L^1 -function.] Moreover, if $a \in \psi t_0$ then any arbitrary (x, ξ) -differentiation may be taken inside the integral (2.3.3), and it will not affect the L^1 -property of the integrand. So, it follows that $a_s \in \psi t_0$ whenever $a \in \psi t_0$.

This conclusion may be reversed. We clearly have $A = \Lambda_{-s}^* A_s \Lambda_s$. Hence we get the same formulas (2.3.3) and (2.3.4) with a and a_s (and $x \leftrightarrow \xi$) interchanged. We have proven:

Proposition 2.3.1 *We have $A = a(x, D) \in Op\psi t_0$ if and only if $A_s = \Lambda_s A \Lambda_{-s}^* \in Op\psi t_0$.*

Next let us also examine a possible relation between translation smoothness for A and A_s . In that respect we might examine the abstract meaning of condition (2.1.1):

Proposition 2.3.2 *For any fixed $s = (s_1, s_2) \in \mathbb{R}^2$ an operator $A \in L(\mathcal{H}_s)$ is smooth under conjugation with (both) e^{-izD} , $e^{i\zeta x} \in L(\mathcal{H}_s)$ - in the sense of (2.1.1) - \mathcal{H} replaced by \mathcal{H}_s - if and only if all commutators¹² $(ad_x)^\theta (ad_D)^\iota A$ belong to $L(\mathcal{H}_s)$, for any pair of multiindices θ, ι .*

Proof. For a Lie-group differentiability at the unit element $e = 0$ implies differentiability anywhere. For $A \in L(\mathcal{H})$ and $A_\zeta = e^{-i\zeta x} A e^{i\zeta x}$ we verify $\partial_{\zeta_j} \langle u, A_\zeta v \rangle|_{\zeta=0} = \partial_{\zeta_j} \langle e^{i\zeta x} u, A(e^{i\zeta x} v) \rangle|_{\zeta=0} = -i(\langle x_j u, Av \rangle - \langle u, Ax_j v \rangle)$ for $u, v \in C_0^\infty$. If the commutator $[x_j, A]$ exists as a well defined operator in $L(\mathcal{H})$ then the right hand side equals $-i\langle u, [x_j, A]v \rangle$. Moreover, then one easily verifies (by looking at the difference quotient of $\langle u, A_\zeta v \rangle$) that $\partial_{\zeta_j} A_\zeta|_{\zeta=0} = -i[x_j, A]$ exists in operator norm of \mathcal{H} . And this conclusion may be reversed: If $\partial_{\zeta_j} A_\zeta|_{\zeta=0}$ exists then also $[x_j, A]$ is well defined and belongs to $L(\mathcal{H})$. This argument may be iterated arbitrarily. By taking Fourier transforms one similarly finds a relation between differentiability of $e^{izD} A e^{-izD}$ and existence of iterated commutators $(ad_D)^\iota$. Q.E.D.

With prop. 2.3.2 it is now easy to relate conditions (2.1.1) for A and A_s :

Suppose that $A \in L(\mathcal{H}_s)$ satisfies $A_{z,\zeta} \in C^\infty(\mathbb{R}^6, L(\mathcal{H}_s))$. So, this amounts to the condition that $ad_x^\theta ad_D^\iota A \in L(\mathcal{H})$. Now consider $A_s = \Lambda_s A \Lambda_{-s}^* \in L(\mathcal{H})$. We have

$$(2.3.5) \quad [D_j, A_s] = ([D_j, \Lambda_s] \Lambda_{-s}^*) A_s + \Lambda_s [D_j, A] \Lambda_{-s}^* + A_s (\Lambda_s [D_j, \Lambda_{-s}^*]) \in L(\mathcal{H}) ,$$

because $[D_j, \Lambda_s] \Lambda_{-s}^* = s_2 \frac{x_j}{\langle x \rangle^2} \in L(\mathcal{H})$, and similar for $\Lambda_s [D_j, \Lambda_{-s}^*]$. Similarly we also get $[x_j, A_s] \in L(\mathcal{H})$. Moreover, the procedure may be iterated arbitrarily to get $ad_x^\theta ad_D^\iota A_s \in L(\mathcal{H})$ for all θ, ι . It follows that A_s satisfies the assumption of thm.2.1.1. Hence $A_s \in Op\psi t_0$. Then prop.2.3.1 implies that $A \in Op\psi t_0$. So, we have proven:

Theorem 2.3.3 *The class of all operators $A \in L(\mathcal{H}_s)$ with $A_{z,\zeta} \in C^\infty(\mathbb{R}^6, L(\mathcal{H}_s))$ coincides with the class $Op\psi t_0$ of ψ do-s with symbol in ψt_0 .*

Finally, let us also study the Heisenberg group action on an operator $A \in Op\psi t_m$. We defined ψt as the class of all polynomials $a(x, \xi) = \sum a_{\iota, \theta}(x, \xi) x^\theta \xi^\iota$, with coefficients $a_{\iota, \theta} \in \psi t_0$. Such symbol is said to have order $m = (m_1, m_2)$ if $\lambda_{-m} a(x, \xi) = \langle x \rangle^{-m_2} a(x, \xi) \langle \xi \rangle^{-m_1} \in \psi t_0$, and the class of such symbols is

¹²All operators ad_{x_j} and ad_{D_l} commute.

denoted by ψt_m . Clearly then we have $A = a(x, D) \in Op\psi t_m$ if and only if $A_0 = \langle x \rangle^{-m_2} A \langle D \rangle^{-m_1} \in Op\psi t_0$.

Under this aspect it is natural to consider the operator $A = a(x, D)$ as a map $A : \mathcal{H}_{(m_1, 0)} \rightarrow \mathcal{H}_{(0, -m_2)}$ because for $s = (m_1, 0)$, $s - m = (0, -m_2)$ the inequality $\|Au\|_s \leq c\|u\|$ means exactly the same as the inequality $\|A_0u\| \leq c\|u\|$, with L^2 -norm $\|\cdot\|$. Since $T_z = e^{-izD}$ and $e^{i\zeta x}$ have their meaning as groups mapping $\mathcal{H}_s \rightarrow \mathcal{H}_s$, for every s , we may talk about smoothness of $A_{z, \zeta}$ of (2.1.1) as maps $\mathcal{H}_s \rightarrow \mathcal{H}_{s-m}$ for some fixed $s \in \mathbb{R}^2$, whenever an initial $A \in L(\mathcal{H}_s, \mathcal{H}_{s-m})$, is given. Again, by ‘smoothness’ we mean smoothness in the parameters z, ζ , and in operator norm topology of $L(\mathcal{H}_s, \mathcal{H}_{s-m})$. We then have

Theorem 2.3.4 *The family $A_{z, \zeta}$ of an operator $A \in L(\mathcal{H}_s, \mathcal{H}_{s-m})$ is smooth in $L(\mathcal{H}_s, \mathcal{H}_{s-m})$ if and only if $A = a(x, D)$ is a pseudodifferential operator of order m with symbol in ψt_m .*

Proof. Assume first that $s = (m_1, 0)$, as specified above. We can assume the above prop.2.3.2 valid also for the case of an $A \in L(\mathcal{H}_s, \mathcal{H}_{s-m})$, simply, since the partial derivatives of $A_{z, \zeta}$ at $z = \zeta = 0$ are given as the iterated commutators $ad_x^\iota ad_D^\theta A$. Now, for $A = \langle x \rangle^{m_2} A_0 \langle D \rangle^{m_1}$ we calculate that

$$(2.3.6) \quad [D_j, A] = -im_2 \frac{x_j}{\langle x \rangle^2} A + \langle x \rangle^{m_2} [D_j, A_0] \langle D \rangle^{m_1},$$

$$(2.3.7) \quad [x_j, A] = \langle x \rangle^{m_2} [x_j, A_0] \langle D \rangle^{m_1} + im_1 A \frac{D_j}{\langle D \rangle^2},$$

as well as

$$(2.3.8) \quad [D_j, A_0] = im_2 \frac{x_j}{\langle x \rangle^2} A_0 + \langle x \rangle^{-m_2} [D_j, A] \langle D \rangle^{-m_1},$$

$$(2.3.9) \quad [x_j, A_0] = \langle x \rangle^{-m_2} [x_j, A] \langle D \rangle^{-m_1} - im_1 A_0 \frac{D_j}{\langle D \rangle^2}.$$

The 4 equations tell us that existence of $A, [D_j, A], [x_j, A]$ in $L(\mathcal{H}_s, \mathcal{H}_{s-m})$ is equivalent to existence of $A_0, [D_j, A_0], [x_j, A_0]$ in $L(\mathcal{H})$. Clearly this may be iterated to show that existence of $ad_D^\iota ad_x^\theta A$ in $L(\mathcal{H}_s, \mathcal{H}_{s-m})$ for all ι, θ is equivalent to existence of $ad_D^\iota ad_x^\theta A_0$ for all ι, θ .

Actually, this conclusion applies for all s , not only for $s = (m_1, 0)$, but we then must look at A_0 in $L(\mathcal{H}_{s-(m_1, 0)})$ rather than in $L(\mathcal{H})$. At any rate, we find that theorem 2.3.4 is an immediate consequence of theorem 2.3.3. Q.E.D.

Finally let us also look at the classes $Op\psi s_m$ and ask whether they may be characterized by a similar smoothness as in thm.2.2.1. Indeed, there is no trouble

repeating the above arguments. We get the operators S_o and R_τ well defined as bounded operators in every \mathcal{H}_s . In fact, S_o even remains unitary in every \mathcal{H}_S while R_τ sends $\langle x \rangle$ into $\langle \tau x \rangle$ and $\langle D \rangle$ into $\langle D/\tau \rangle$. Differentiating $\langle x \rangle^m$ for τ gets us

$$(2.3.10) \quad \partial_\tau \langle \tau x \rangle^m = \tau m \frac{x^2}{1 + \tau^2 x^2} \langle \tau x \rangle^m$$

where the factor $\frac{x^2}{\langle \tau x \rangle^2}$ is a bounded operator. So, for dilations, we get formulas similar to (2.3.6)-(2.3.9). For rotations we get such formulas without the additional terms. We summarize this:

Theorem 2.3.5 *Let $s, m \in \mathbb{R}^2$ be given. The 4 groups $\{e^{-izD}\}$ and $\{e^{i\zeta x}\}$ and $\{S_o\}$ and $\{R_\tau\}$ act smoothly on an operator $A \in L(\mathcal{H}_s, \mathcal{H}_{s-m})$, in the sense of strong operator convergence of $L(\mathcal{H}_s, \mathcal{H}_{s-m})$, if and only if $A = a(x, D)$ with symbol $a(x, \xi) \in \psi t_m$ satisfying the following condition ψs_m :*

Every finite application of the η_{jl} to the symbol $a(x, \xi)$ must belong to ψt_m , where

$$(2.3.11) \quad \eta_{jl} = \varepsilon_{jl} - \varepsilon_{lj} \text{ as } j \neq l, \quad \eta_{00} = \sum_1^3 \varepsilon_{jj},$$

where

$$(2.3.12) \quad \varepsilon_{jl} = \xi_j \partial_{\xi_l} - x_l \partial_{x_j}, \quad j, l = 1, 2, 3.$$

2.4 A Useful Result on L^2 -Inverses and Square Roots

In this section we want to discuss some simple but useful applications of thm.2.3.4. With a slightly different argument prop.2.4.1, below, was already proven by R.Beals [Be2].

Proposition 2.4.1 *For any $s, m \in \mathbb{R}^2$ if a ψ do $A \in Op\psi c_m$ [which naturally extends to a bounded operator $\mathcal{H}_s \rightarrow \mathcal{H}_{s-m}$] possesses a bounded inverse $B = A^{-1} : \mathcal{H}_{s-m} \rightarrow \mathcal{H}_s$ then B must be a ψ do in $Op\psi c_{-m}$.*

We first make some simple reformulations.

Proposition 2.4.2 *We have*

$$(2.4.1) \quad \psi c_m = \{a \in \psi t_m : a_{(\iota)}^{(\theta)} \in \psi t_{(m_1 - |\theta|, m_2 - |\iota|)} \quad \forall \theta, \iota\}.$$

The proof is evident - just by looking at (1.2.2).

Applying thm.2.3.4 and fla. (2.1.2) we then get this:

Proposition 2.4.3 *For any fixed $s, m \in \mathbb{R}^2$ the class $Op\psi c_m$ consists precisely of all $A \in L(\mathcal{H}_s, \mathcal{H}_{s-m})$ such that (i) $A_{z,\zeta}$ of (2.1.1) is smooth in $L(\mathcal{H}_s, \mathcal{H}_{s-m})$, and (ii) each family $\partial_z^t \partial_\zeta^\theta A_{z,\zeta}$ is smooth in $L(\mathcal{H}_s, \mathcal{H}_{(s_1-m_1+|\theta|, s_2-m_2+|\iota|)})$. Or, equivalently, each family $\langle x \rangle^{|\iota|} \langle D \rangle^{|\theta|} \partial_z^t \partial_\zeta^\theta A_{z,\zeta}$ is smooth as a map $\mathcal{H}_s \rightarrow \mathcal{H}_{s-m}$.*

Moreover, the cdn. (ii), above, may be replaced by (ii'): each family $\partial_z^t \partial_\zeta^\theta A_{z,\zeta}$ is smooth in $L(\mathcal{H}_{s_1-|\theta|, s_2-|\iota|}, \mathcal{H}_{s-m})$, equivalent to requiring each $\partial_z^t \partial_\zeta^\theta A_{z,\zeta} \langle x \rangle^{|\iota|} \langle D \rangle^{|\theta|}$ to be smooth as a map $\mathcal{H}_s \rightarrow \mathcal{H}_{s-m}$.

Now the proof of prop.2.4.1 is immediate: Let $A = a(x, D) \in \psi c_m$ have a bounded inverse $B = A^{-1} \in L(\mathcal{H}_{s-m}, \mathcal{H}_s)$. Then we get $B_{z,\zeta} = (A_{z,\zeta})^{-1}$, and find that

$$(2.4.2) \quad B_{z,\zeta|z} = -B_{z,\zeta} A_{z,\zeta|z} B_{z,\zeta} ,$$

first as a map $\mathcal{H}_{s-m} \rightarrow \mathcal{H}_s$, using that $B_{z,\zeta} \in L(\mathcal{H}_{s-m}, \mathcal{H}_s)$, and $A_{z,\zeta|z} \in Op\psi t_m \subset L(\mathcal{H}_s, \mathcal{H}_{s-m})$ only (a weaker condition). The derivative exists in norm of $L(\mathcal{H}_{s-m}, \mathcal{H}_s)$. Similarly for higher derivatives and for ζ -derivatives. From thm.2.3.4 it then follows that $B = b(x, D) \in Op\psi t_{-m} \subset L(\mathcal{H}_t, \mathcal{H}_{t+m})$ for all $t \in \mathbb{R}^2$. With that information we may go back to fla. (2.4.2) and conclude that $B_{z,\zeta|z} \in L(\mathcal{H}_t, \mathcal{H}_{t+m+e^1})$ for all t . Iteration and application for ζ -derivatives then confirms the cdn. of prop.2.4.3 (with m replaced by $-m$), completing the proof.

Proposition 2.4.4 *Assume that $m_j \geq 0$, $j = 1, 2$, and that an md -elliptic ψ do $A = a(x, D) \in Op\psi c_m$ (with scalar (complex-valued) symbol) is self-adjoint and positive definite in \mathcal{H} , in the sense that¹³*

$$(2.4.3) \quad \langle u, Au \rangle \geq a_0 \langle u, u \rangle \text{ for all } u \in \mathcal{H}_s$$

with some $a_0 > 0$. Then the positive square root \sqrt{A} and its inverse \sqrt{A}^{-1} belong to $Op\psi c_{m/2}$ and $Op\psi c_{-m/2}$, respectively.

Proof: Under the assumptions it follows that the Hilbert space inverse $B = A^{-1} \in L(\mathcal{H})$ of the unbounded operator A with domain \mathcal{H}_s exists, and that we have $\|B\| \leq \frac{1}{a_0}$. This also implies that B is an inverse of A in $L(\mathcal{H}_s, \mathcal{H}_0)$. Hence, by prop.4.1, we also get $B \in Op\psi c_{-m}$.

¹³What we mean, more precisely, is that the unbounded operator A with domain $\mathcal{H}_s \subset \mathcal{H}$ coincides with its Hilbert space adjoint so that there exists a spectral resolution of A in the Hilbert space \mathcal{H} .

The positive square root C of the bounded self-adjoint operator B of \mathcal{H} exists by standard arguments. Moreover, we have

$$(2.4.4) \quad B = \frac{1}{\pi} \int_0^\infty \frac{1}{A + \lambda} \frac{d\lambda}{\sqrt{\lambda}},$$

a well known “resolvent formula” (cf. [Ka1],ch.V,fla.(3.43)). In fact, we might need a more general formula (cf. [Co14],VI,(1.6)):

$$(2.4.5) \quad C^{2j+1} = B^j C = \frac{(-1)^j}{\pi} \frac{1 \cdot 3 \cdots (2j-1)}{2 \cdot 4 \cdots 2j} \int_0^\infty \frac{d\lambda}{\sqrt{\lambda}} \frac{1}{(A + \lambda)^{j+1}}, \quad j = 1, 2, \dots$$

This still is easily derived by a well known complex resolvent integral technique.

First of all we get (with norms and inner product of $\mathcal{H} = \mathcal{H}_0$, and $\Lambda_s = \langle x \rangle^{s_2} \langle D \rangle^{s_1}$ of (1.4.4))

$$(2.4.6) \quad \|Cu\|^2 = \langle u, Bu \rangle = \langle \Lambda_{-m/2} u, \{ \Lambda_{m/2} B \Lambda_{m/2}^* \} \Lambda_{-m/2} u \rangle, \quad u \in \mathcal{S},$$

where the operator $\{\cdot\}$ is in $Op\psi c_0$, hence is L^2 -bounded. Accordingly,

$$(2.4.7) \quad \|Cu\|^2 \leq c^2 \|\Lambda_{-m/2} u\|^2 = \|u\|_{-m/2}^2,$$

and we have $C \in L(\mathcal{H}_{-m/2}, \mathcal{H}_0)$.

In order to apply prop.2.4.3 - to show that $C \in Op\psi c_{-m}$ we next look at the derivative $C_{z,\zeta|z}$. With (2.4.4), also valid for $C_{z,\zeta}$ we get

$$(2.4.8) \quad C_{z,\zeta|z}|_{z=\zeta=0} = \frac{1}{i\pi} \int_0^\infty \frac{d\lambda}{\sqrt{\lambda}} \frac{1}{A + \lambda} [D, A] \frac{1}{A + \lambda}.$$

In order to get control of this look at the commutator

$$(2.4.9) \quad [P, \frac{1}{A + \lambda}] = \frac{1}{A + \lambda} [A, P] \frac{1}{A + \lambda},$$

valid for general operators P . Applying (2.4.9) (and iterating) we get

$$(2.4.10) \quad \frac{1}{A + \lambda} P \frac{1}{A + \lambda} = \sum_{j=0}^N \frac{1}{(A + \lambda)^{j+2}} (ad_A)^j P + \frac{1}{(A + \lambda)^{N+2}} (ad_A)^{N+1} P \frac{1}{A + \lambda}.$$

Here we set $P = [D, A] = -ad_A D$. Clearly then all “coefficients” $ad_A^j P$ are ψ do-s, and they belong to $Op\psi c_{j(m-e)+m-e^2}$. Integrating (2.4.10) (with measure $\frac{d\lambda}{\sqrt{\lambda}}$) from 0 to ∞ , the terms of the sum at right will give (up to a multiplicative constant c_j) the operators $B^{j+1} C (ad_A)^j P = P_j$, by (2.4.5). We have

$$(2.4.11) \quad \|P_j u\|^2 = \langle u, ((ad_A)^j P)^* B^{2j+3} (ad_A)^j P u \rangle,$$

where now all operators are ψ do-s, and the total order of the operator product in (2.4.11) is $-(2j+3)m+2j(m-e)+m-e^2)=-2(m/2+e^2)-2je$. Accordingly, (2.4.12)

$$\|P_j u\|^2 = \langle \Lambda_{-m/2-e^2} u, (\Lambda_{m/2+e^2} \{ \cdot \} \Lambda_{m/2+e^2}) \Lambda_{-m/2-e^2} u \rangle \leq c \|u\|_{-m/2-e^2} ,$$

amounting to $P_j \in L(\mathcal{H}_{m/2-e^2}, \mathcal{H}_0)$. As to the remainder $R_N =$ last term in (2.4.10), note that $\|\frac{1}{(A+\lambda)^l} u\| \leq \|B^l u\|$, as $l, \lambda > 0$. Thus,

$$(2.4.13) \quad \|R_N u\| \leq \|Q_N \frac{1}{A+\lambda} u\|$$

where $Q_N = B^{N+2}(ad_A)^{N+1}P$ is a ψ do of order $-(N+1)e-e^2$. So, if N is sufficiently large, we conclude that the orders of Q_N are less than the orders $-s = (-m_1/2, -m_2/2-1)$, and it follows that $\|Q_N u\| \leq c\|\Lambda_{-s} u\| = c\|u\|_{-s}$. Accordingly,

$$(2.4.14) \quad \|R_N u\| \leq c\|\frac{1}{A+\lambda} u\|_{-s} = \|\frac{1}{A+\lambda+A'} \Lambda_{-s} u\| ,$$

where $A' = \Lambda_{-s} A \Lambda_s^* - A \in Op\psi c_{m-e}$. The point now is that we can show that

$$(2.4.15) \quad \|\frac{1}{A+\lambda+A'} u\| \leq c\frac{1}{1+\lambda} \text{ as } \lambda \geq 0 ,$$

with some constant c . This again relies on the fact that we have

$$(2.4.16) \quad \|A' u\| \leq c\|A^{1-\delta} u\| \leq \frac{1}{2}\|A u\| + c'\|u\| ,$$

with small $\delta > 0$ and with constants c, c' . The latter will need the Heinz inequality¹⁴ for its verification. Details are omitted.

At any rate, we then get the integral $\int_0^\infty \frac{d\lambda}{(1+\lambda)\sqrt{\lambda}} < \infty$. As a consequence we indeed get the desired inequality

$$(2.4.17) \quad \|C_{z,\zeta}|z u\|_0 \leq c\|u\|_{-m/2-e^2} .$$

In a similar way we can derive all the other inequalities for use of prop.2.4.3,(ii'). Q.E.D.

Corollary 2.4.5 *While prop.2.4.4, in its present form, was stated only for an operator A with scalar (complex-valued) symbol, the statement still holds for matrix-valued symbols $a(x, \xi)$ as long as (in addition to assumptions stated) all the commutators of $ad_D^{(l)} ad_x^{(\theta)} a(x, D)$ with A have the order they should have if a were scalar.*

The proof is evident.

¹⁴For self-adjoint positive A, B , if $A \leq B$ then also $A^\tau \leq B^\tau$ for all $0 \leq \tau \leq 1$.

Chapter 3

Decoupling with ψ do-s

3.0 Introduction

Spectral theory of the Dirac Hamiltonian H of (1.0.2) has been vigorously pursued since the early 1930-s. For moderately decent potentials \mathbf{V} and \mathbf{A} it is found that there is a unique self-adjoint realization of H having bands of continuous spectrum along the half-lines $[1, \infty)$ and $(-\infty, -1]$ while the spectrum in the open interval $(-1, 1)$ is discrete, (if any). Particularly, for the hydrogen atom (with no electromagnetic potentials (i.e., $\mathbf{A}_j = 0$) and Coulomb potential $\mathbf{V}(x) = -\frac{c_f}{|x|}$) we get the point-eigenvalues (cf. Sommerfeld [So2], ch.4,§7, or Thaller [Th1],7.4)

$$(3.0.1) \quad \mu_{kl} = \left\{ 1 + \frac{c_f^2}{(k + \sqrt{l^2 - c_f^2})^2} \right\}^{-1/2}, \quad k = 0, 1, \dots, \quad l = \pm 1, \pm 2, \dots$$

It was one of the special features of Dirac's theory that the energy levels represented by (3.0.1) accurately reflect the levels of the hydrogen atom, **including the fine structure** of the hydrogen spectral lines which the Bohr-Sommerfeld planetary model could explain, but the Schrödinger equation could not¹.

On the other hand, the presence of the band $(-\infty, -1]$ was always regarded as a most disturbing fact - due to the tendency of a physical system to sink to lower energy states, one then should conclude that the only stable state would be "energy at $-\infty$ ". The Schrödinger Hamiltonian H_s is semi-bounded below, it does not have the negative continuous spectrum. This seems to give some preference to Schrödinger's model.

Returning to Dirac, the important point is that the operator H really serves as Hamiltonian for **two particles**: We have the *charge conjugation* - an anti-unitary

map, turning equation (1.0.1) into the same equation with H replaced by $-H_-$ with H_- - of the general form (1.0.2) having the same potentials \mathbf{V}, \mathbf{A}_j , but with signs reversed. So, under this transform, the negative energy band becomes the positive band $[1, \infty)$ while the sign of the potential is reversed, as it should be for the positron. So, in view of this ‘‘C-symmetry’’ of the system one wants to conclude that the energy band $(-\infty, -1]$ really belongs to the positron - the ‘‘anti-particle²’’.

¹With our units of time, distance, energy [cf.ch.1,footnote 1] the time dependent Schrödinger equation is of the form

$$(3.0.2) \quad \partial\psi/\partial t + iH_s\psi = 0, \quad H_s = 1 - \frac{1}{2}\Delta + \mathbf{V}(x), \quad \mathbf{V}(x) = -\frac{c_f}{|x|},$$

with the Laplace operator Δ and with ‘‘1’’ representing the rest energy of the electron (usually omitted). Since the field free Dirac Hamiltonian H_0 satisfies $H_0^2 = 1 - \Delta$ - cf.(1.0.3)) - one might just formally write (1.0.2)) (with $\mathbf{A}_j = 0$) as $H = \sqrt{1 - \Delta} + \mathbf{V}$. Compared with (3.0.2) we are reminded of the well known approximation formula $\sqrt{1+x} \approx 1 + \frac{1}{2}x$, valid for small x but not for large x .

The eigenvalues of H_s differ by a relatively small amount from the rest energy 1. They are given by the formula

$$(3.0.3) \quad \lambda_j = 1 - \frac{c_f^2}{2(j+1)^2}, \quad j = 0, 1, 2, \dots$$

The fine structure constant $c_f \approx \frac{1}{137}$ is small, we get $c_f^2 \approx 0.532 \times 10^{-4}$. In (1.0.1) we therefore might approximate

$$(3.0.4) \quad \mu_{kl} \approx 1 - \frac{1}{2} \frac{c_f^2}{(k + \sqrt{l^2 - c_f^2})^2} \approx 1 - \frac{1}{2} \frac{c_f^2}{(k + |l|)^2} = \lambda_{k+|l|-1}.$$

So, clearly, the (multiple) eigenvalues λ_j of H_s split up into a bunch of eigenvalues of H (very close together).

The same splitting (observed as fine structure of the spectral lines) was related to the relativistic degeneration of orbital ellipses within the Bohr Planetary model of the hydrogen atom.

This used to be one feature in favour of Dirac’s theory. The other one, perhaps even more important, is the explanation of the electron spin, to be discussed later on (cf. sec.4.6).

²For the special choice of the matrices α_j, β used in this book (cf. (3.1.6),(3.1.7), below) the charge conjugation map is given by the substitution $\psi = \alpha_1 \bar{\omega}$, with the first Dirac matrix α_1 . [Note, we have $\alpha_1^* = \alpha_1$, and $\alpha_1^2 = 1$, so α_1 is unitary.] Looking at the eigenvalue problem $H\psi = \lambda\psi$ with H of (1.0.2), this substitution will give $H\alpha_1\bar{\omega} = \lambda\alpha_1\bar{\omega} \Leftrightarrow \alpha_1 H\alpha_1\bar{\omega} = \lambda\bar{\omega}$. Now, for our special set of α_j, β , given in (3.1.6), (3.1.7) we get α_1 real, α_2, α_3 pure imaginary, hence $\bar{\alpha}_1 = \alpha_1, \bar{\alpha}_2 = -\alpha_2, \bar{\alpha}_3 = -\alpha_3$, hence $\alpha_1\alpha_1\alpha_1 = \alpha_1 = \bar{\alpha}_1$, $\alpha_1\alpha_2\alpha_1 = i\alpha_3\alpha_1 = -\alpha_2 = \bar{\alpha}_2$, $\alpha_1\alpha_3\alpha_1 = i\alpha_2\alpha_3 = -\alpha_3 = \bar{\alpha}_3$, and also, $\alpha_1\beta\alpha_1 = -\beta\alpha_1^2 = \beta = -\bar{\beta}$, using the relations (1.0.3). Since all potentials are real-valued, we conclude that $\alpha_1 H\alpha_1 = \sum_1^3 \bar{a}_j (D_j - \mathbf{A}_j) - \bar{\beta} + \mathbf{V}$. So, taking a complex conjugate, and using that $D_j = -i\partial_{x_j}$ has $\bar{D}_j = -D_j$, we find that $H\psi = \lambda\psi$ becomes

$$(3.0.7) \quad \sum_{j=1}^3 \alpha_j (D_j + \mathbf{A}_j) + \beta - \mathbf{V} \omega = -\lambda \omega.$$

That is, under this symmetry, we get the same eigenvalue problem back, but with reversed sign

Electrons and positrons, on the other hand, are well distinguished particles; an electron never should become a positron - nor vice versa. So, in the first place now, looking at *physical states* - that is, unit vectors in $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ - we need a rule to decide whether a state ψ represents an electron or a positron.

Thus it might be considered highly desirable to effect a clean split of the Hilbert space \mathcal{H} of physical states into electronic and positronic states, with the general state being a superposition of two such states. That is, one might like an orthogonal direct decomposition

$$(3.0.5) \quad \mathcal{H} = \mathcal{H}_e \oplus \mathcal{H}_p ,$$

where $\psi \in \mathcal{H}_e$ ($\psi \in \mathcal{H}_p$) represents a situation where it is known with certainty that the particle is an electron (a positron).

One would want this decomposition to *reduce* the Dirac operator H - that is, H maps these spaces into themselves - we get

$$(3.0.6) \quad H = H^e + H^p \quad \text{where} \quad H^e : \mathcal{H}_e \rightarrow \mathcal{H}_e , \quad H^p : \mathcal{H}_p \rightarrow \mathcal{H}_p ,$$

(and $H^e = 0$ in \mathcal{H}_p , $H^p = 0$ in \mathcal{H}_e).

Note, the self-adjoint operator H possesses many invariant closed subspaces, and then the orthogonal complement also is invariant, as a consequence of self-adjointness. Accordingly, one will have a very large choice to construct such a split, and, so far, one simply would elect one according to physical convenience or meaningfulness.

In this chapter, we approach this dilemma by offering a decoupling effected by a unitary (strictly classical) **pseudodifferential operator** $U = u(x, D)$ decoupling the Dirac Hamiltonian H , in the sense that

$$(3.0.8) \quad U^*U = UU^* = 1 \quad , \quad U^*HU = \begin{pmatrix} H_e & 0 \\ 0 & H_p \end{pmatrix}$$

where H_e and H_p act on the Hilbert space ${}^3L^2(\mathbb{R}^3, \mathbb{C}^2) = \mathcal{K}$.

To effect this we must impose suitable assumptions on the potentials \mathbf{A}_j, \mathbf{V} to make sure that H is a strictly classical ψ do of order e^1 . We just will require that the potentials are of polynomial growth, and of order -1 , in the sense of ch.1,

of λ and the potentials \mathbf{A} and \mathbf{V} . But \mathbf{A} and \mathbf{V} all have the factor e - hidden by our choice of units. So, if the charge e is replaced by $-e$ then we get the eigenvalue problem (3.0.8). In other words, looking at this symmetry $\psi \leftrightarrow \omega$ we might just as well regard H as Hamiltonian for the positron - an electron with reversed sign of charge. [It is clear, by the way, that $\|\psi\| = \|\omega\|$, and that above correspondence also works for eigenpackets - see our later discussions in ch.7 - .]

footnote 6 - cf. cdn. (X) of sec.3.2, below. And, moreover, we will assume here that \mathbf{A}_j, \mathbf{V} are time-independent.

This restriction to a unitary ψ do is not without merit: It reflects the fact that, mathematically, equation (1.0.1) is a *true wave equation* with a built- in “geometrical optics”. The “light rays”, in this case, are the **orbits of particle propagation**. But, clearly, this particle propagation is two-fold - since electrons and positrons propagate along different orbits.

In pursuit of this two-fold particle propagation the above split (3.0.5) will emerge naturally, together with the unitary map (3.0.8). The geometrical optics just splits the Hilbert space into 2 components, belonging to electron and positron: A particle, known with certainty to be an electron propagates along one of the two kinds of orbit; the positrons use the other kind. Theory of strictly classical ψ do-s is needed to obtain such a split for general potentials.

Clearly one will expect the uncoupling (3.0.8) to be related to the *Foldy-Wouthuysen transform*. Recall, this transform was introduced as an *approximate decoupling* similar to (3.0.8), with an operator U_{FW} composed of explicit expressions related to the entries of the 4×4 -matrix operator H , and error terms going with $\frac{1}{c^2}$ (with $c =$ speed of light) (cf.de Vries [deV1]). Under special assumptions on H this splitting becomes exact, and then coincides with (3.0.8) (cf. sec.3.2 - and, in more detail, [Th1], 5.6).

It is clear that - with (3.0.8) - the two spaces $\mathcal{H}_e, \mathcal{H}_p$ of (3.0.5) are given by

$$(3.0.9) \quad \mathcal{H}_e = U \begin{pmatrix} \mathcal{K} \\ 0 \end{pmatrix} \quad , \quad \mathcal{H}_p = U \begin{pmatrix} 0 \\ \mathcal{K} \end{pmatrix} .$$

In the time-independent case the “precisely predictable observables” of sec.1.0 then simply are the self-adjoint ψ do-s reduced by this split. In particular, a ψ do A will be precisely predictable if and only if we have

$$(3.0.10) \quad U^* A U = \begin{pmatrix} A_e & 0 \\ 0 & A_p \end{pmatrix} ,$$

i.e., the “PP-operators” are uncoupled by U just as H is.

In ch.4 we then will show that there is no “generalized *Zitterbewegung*” for any such precisely predictable observable, in the sense that its Heisenberg transform $A_t = e^{iHt} A e^{-iHt}$ depends smoothly on the parameter t , in a sense to be defined. [And, this will also be discussed for time dependent potentials.]

³Actually, we may have to take away a finite dimensional subspace \mathcal{Z} of \mathcal{K} for the operator H_e and add it to \mathcal{K} for H_p - or vice versa - reflecting the fact that some “positronic” eigenvalues might have wandered into the continuous spectrum of the electron - or vice versa. For details, cf.sec.3.5, below.

3.1 The Foldy-Wouthuysen Transform

Let us come back to the Dirac Hamiltonian of (1.0.2), i.e.,

$$(3.1.1) \quad H = \sum_{j=1}^3 \alpha_j (D_j - \mathbf{A}_j) + \beta + \mathbf{V}(x),$$

where we now assume \mathbf{V} and \mathbf{A}_j time-independent functions of x , and of polynomial growth - order -1 . That is, in detail, as a general assumption, for this chapter,

Condition (X): The function is $C^\infty(\mathbb{R}^3)$; derivatives of order j are $O((1 + |x|)^{-j-1}) = O(\langle x \rangle^{-j-1})$.

With our 4×4 -matrices α_j, β it is clear that H of (3.1.1) acts on vector functions $\psi(t, x)$, taking values in \mathbb{C}^4 , and eq. $\partial\psi/\partial t + iH\psi = 0$ is a first order 4×4 -system of PDE-s.

In the absence of fields, i.e., $\mathbf{V} = \mathbf{A} = 0$, the operator $H = H_0$ has constant coefficients, inviting application of the Fourier transform: We get

$$(3.1.2) \quad F^{-1}H_0F = h_0(\xi) = \alpha \cdot \xi + \beta ,$$

a multiplication operator where $h_0(\xi)$ is a hermitian symmetric 4×4 -matrix function of $\xi = (\xi_1, \xi_2, \xi_3)$. For each $\xi \in \mathbb{R}^3$ the matrix $h_0(\xi)$ has the two distinct real eigenvalues $\lambda_\pm = \pm\sqrt{1 + \xi^2}$, each of multiplicity 2. There exists a unitary 4×4 -matrix function $u(\xi)$ such that $u^*(\xi)h_0(\xi)u(\xi) = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}(\xi)$, where the right hand side stands for the 4×4 -diagonal-matrix with 2×2 -blocks $0 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$, $\lambda = \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix}$. Then, of course, $U = u(D) = F^{-1}u(\xi)F$ defines a unitary operator of the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$, and we get

$$(3.1.3) \quad U^*H_0U = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}(D) = \begin{pmatrix} \Lambda_+ & 0 \\ 0 & \Lambda_- \end{pmatrix}, \quad \Lambda_\pm = \lambda_\pm(D),$$

where again the entries of the matrix are 2×2 -blocks, using $0 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$ and $1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

Note, the right hand side of (3.1.3) no longer contains differential operators, but, rather, singular convolution operators. We may write $\sqrt{1 + \xi^2} = \langle \xi \rangle = \sum \frac{\xi_j}{\langle \xi \rangle} \xi_j + \frac{1}{\langle \xi \rangle}$, then,

$$(3.1.4) \quad \lambda_\pm(D) = \pm \left\{ \sum S_j D_j + S_0 \right\},$$

where $S_j = F^{-1} \frac{\xi_j}{\langle \xi \rangle} F$, $S_0 = F^{-1} \frac{1}{\langle \xi \rangle} F$ are singular convolution operators. S_j , $j > 0$, involves a Cauchy-type singular integral.

In terms of the matrices α, β of (1.0.3), we may write

$$(3.1.5) \quad U = \frac{1}{\sqrt{2+2S_0}}(1 + S_0 - \beta\alpha S) = u(D) ,$$

with $u(\xi) = \frac{1}{\sqrt{1+s_0}}(1 + s_0 - \beta\alpha s)$, where $s_0(\xi) = \frac{1}{\langle \xi \rangle}$, $s(\xi) = \frac{\xi}{\langle \xi \rangle}$, and, as usual, $u(D) = F^{-1}u(\xi)F$. So, clearly, U belongs to an algebra of singular convolution operators generated by the bounded singular integral operators S_j , $j = 1, 2, 3$, and S_0 .

Now let us observe that - formally - a somewhat similar “explicit diagonalization” may be carried out in the case where the operator H has general magnetic potentials \mathbf{A}_j as long as the electrostatic potential \mathbf{V} still vanishes identically. This is called the *Foldy-Wouthuysen transform*⁴ of H . In fact such explicit transform exist whenever the Dirac operator has a “supersymmetry”, as not to be discussed here. Let us use an explicit set of matrices α_j , β : With the “Pauli-matrices”

$$(3.1.6) \quad \sigma_1 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

we set

$$(3.1.7) \quad \alpha = \begin{pmatrix} 0 & i\sigma \\ -i\sigma & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Generally we choose to write our 4×4 -matrices as 2×2 -matrices of 2×2 -blocks. With above α, β and with $\mathbf{V} = 0$, (3.1.1) assumes the “block form”

$$(3.1.8) \quad H = \begin{pmatrix} 1 & i\Xi \\ -i\Xi & -1 \end{pmatrix}, \quad \Xi = \sigma(D - \mathbf{A}) = \sum \sigma_j(D_j - \mathbf{A}_j).$$

All 4 of the 2×2 -blocks of H in (3.1.8) commute, while that matrix is hermitian. One may use ordinary 2×2 -matrix calculus to “diagonalize” this H , in the sense that we get a “block diagonalization” (3.1.3) with suitable 2×2 -matrix operators Λ_{\pm} , and a suitable unitary 4×4 -matrix operator U , but the 2×2 -blocks Λ_{\pm} no longer need to be diagonal. We will call this a “decoupling”. We get $\Lambda_{\pm} = \pm\sqrt{1+\Xi^2}$, and, formula (3.1.5) remains intact, if we just replace S_0 by $\frac{1}{\sqrt{1+\Xi^2}} = \Xi_0$, and (αS) by $\frac{\Xi}{\sqrt{1+\Xi^2}} = \Xi$. Or, in detail, using 2×2 -blocks,

$$(3.1.9) \quad U^* H U = \begin{pmatrix} \Lambda_+ & 0 \\ 0 & \Lambda_- \end{pmatrix}, \quad U = \frac{1}{\sqrt{2+2\Xi_0}} \left\{ (1 + \Xi_0) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - i\Xi \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\} .$$

⁴The Foldy-Wouthuysen transform was introduced in [FW] as an “approximate decoupling”, in connection with the nonrelativistic limit of Dirac theory. $U^* H U$ was decoupled only modulo terms of order $\frac{1}{c^2}$ with c the speed of light - or, in higher approximation of order $\frac{1}{c^4}$, etc.. For the later development, especially the precise decoupling as $\mathbf{V} = 0$ and more generally in the supersymmetric case, we refer to the book of Thaller [Th1], and the review article of deVries [deV1], perhaps also to Grigore, Nenciu, Purice [GNP].

A precise definition of U in the sense of the Hilbert space \mathcal{H} is straight-forward, if we impose $\text{cdn.}(X)$ on the potentials A_j . Especially, the differential operator Ξ has a unique self-adjoint realization; then Ξ_0 and Ξ will be well defined bounded operators of $L^2(\mathbb{R}^3, \mathbb{C}^2)$. But we also wish to emphasize that U as well as $\Lambda = U^*HU$ are (global) pseudodifferential operators on \mathbb{R}^3 . In fact, U belongs to our algebra $Op\psi c_0$ of “strictly classical” ψdo -s of [Co5], discussed in ch.1, assuming that the potentials $\mathbf{A}(x)$ satisfy $\text{cdn.}(X)^5$.

Note the symbol $p(x, \xi) = \sqrt{1 + (\sigma \cdot (\xi - \mathbf{A}))^2}$ is md -elliptic of order e^1 , so that the ψdo $p(x, D)$ has a K -parametrix $Q=q(x, D)$ of order $-e^1$, in the sense of sec.1.3.

In this chapter we want to discuss such a unitary decoupling for cases where also the potential \mathbf{V} no longer vanishes identically - but it also must satisfy $\text{cdn.}(X)$, of course. In that case we cannot expect an explicit formula. However, in sec.3.2 we first will discuss a decoupling modulo a remainder of order $-\infty$ where U has an explicit asymptotic expansion, starting out with (3.1.9) [or (3.1.5)] as the zero order term. Getting a complete decoupling then will be a matter of manipulating remainders in $\mathcal{O}(-\infty)$, as we learned handling them in sec.1.4. This will be discussed in sec’s 3.5 and 3.6.

3.2 Unitary Decoupling Modulo $\mathcal{O}(-\infty)$

In this section we will assume (time-independent) potentials $\mathbf{A}_j, \mathbf{V} \neq 0$, all satisfying $\text{cdn.}(X)$. Similar to our construction of an inverse (mod $\mathcal{O}(-\infty)$) for an md -elliptic ψdo we first shall try to use calculus of ψdo -s to construct a strictly classical 0-order ψdo satisfying the 3 equations (3.0.8) only mod $\mathcal{O}(-\infty)$.

Note, it follows from ψdo -calculus that, with the symbol $u(x, \xi)$ of (3.1.9) - i.e., with⁶

$$(3.2.1) \quad u(x, \xi) = \frac{1}{\sqrt{2 + 2\zeta_0}} \left\{ (1 + \zeta_0) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - i\zeta \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\} ,$$

⁵The differential operator Ξ indeed has a unique self-adjoint realization in \mathcal{H} : It is a sum $\sigma D - \sigma \mathbf{A}$ where $-\sigma \mathbf{A}$ is bounded (under $\text{cdn.}(X)$) while σD is unitarily equivalent to the multiplication $-\sigma \xi$, under the Fourier transform (which maps $\mathcal{S} \leftrightarrow \mathcal{S}$). One thus concludes that $K = 1 + \Xi^2 = 1 + (D - \mathbf{A})^2 - \sigma \text{curl } \mathbf{A} = 1 - \Delta + \mathcal{O}(e^1 - e^2)$ is bounded below by 1, in the Hilbert space \mathcal{H} , hence its inverse and its unique inverse positive square root Ξ_0 are well defined bounded self-adjoint operators of \mathcal{H} . Moreover, $\Xi_j = \Xi_j \Xi_0$ are \mathcal{H} -bounded self-adjoint as well, have bound 1, all as operator $\mathcal{H} \rightarrow \mathcal{H}$, as easily seen. Now, if we use prop.2.4.4 (and its corollary 2.4.5) it follows at once that $\Xi_0 \in Op\psi c_{-e^1}$, hence that $\Xi \in Op\psi c_0$. We again must use prop.2.4.4 to show that also $1/\sqrt{2 + 2\Xi_0} \in Op\psi c_0$. Then, indeed, it follows that U of (3.1.9) belongs to $Op\psi c_0$.

where $\zeta_0 = \frac{1}{\sqrt{1+\Upsilon^2}}$, $\zeta = \frac{\Upsilon}{\sqrt{1+\Upsilon^2}}$, with $\Upsilon(x, \xi) = \sum \sigma_j(\xi_j - A_j(x))$ - we get

$$(3.2.2) \quad u^*(x, D)u(x, D) - 1, \quad u(x, D)u^*(x, D) - 1 \in Op\psi_{c-e},$$

and

$$(3.2.3) \quad u(x, D)^*Hu(x, D) - \begin{pmatrix} \Lambda_+ & 0 \\ 0 & \Lambda_- \end{pmatrix} \in Op\psi_{c-e^2},$$

with $\Lambda_{\pm} = \lambda_{\pm}(x, D)$ $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. Accordingly we may use $u_0(x, \xi) = u(x, \xi)$ as a 0-th approximation for the desired decoupling.

Suppose now, we have found $u_j(x, \xi) \in Op\psi_{c-Ne}$, $j = 0, \dots, N$, such that $U = \sum_{j=0}^N u_j(x, D)$ satisfies

$$(3.2.4) \quad U^*U - 1, \quad UU^* - 1 \in Op\psi_{c-(N+1)e}, \quad U^*HU - \Lambda, \in Op\psi_{c-Ne-e^2},$$

with a ‘‘decoupled’’ $\Lambda = \begin{pmatrix} \Lambda_+ & 0 \\ 0 & \Lambda_- \end{pmatrix}$. Then we shall construct $\omega = u_{N+1} \in \psi_{c-Ne-e}$ such that $V = U + \Omega$ with $\Omega = \omega(x, D)$ satisfies (3.2.4) for $N+1$. By induction we then get an infinite sequence $u_j \in \psi_{c-Ne}$, and the asymptotic sum $u = \sum_0^\infty u_j \in \psi_{c_0}$ will give the desired symbol satisfying (3.2.2),(3.2.3).

We have $V^*V - 1 = (U^*U - 1) + (U^*\Omega + \Omega^*U) + \Omega^*\Omega \in Op\psi_{c-(N+2)e}$, which amounts to the condition

$$(3.2.5) \quad u_0^*\omega + \omega^*u_0 - z_1 \in \psi_{c-(N+2)e} \quad \text{with} \quad z_1(x, D) = 1 - U^*U \in Op\psi_{c-(N+1)e},$$

using that above Ω has $\Omega^*\Omega, \Omega\Omega^* \in Op\psi_{c-2(N+1)e} \subset Op\psi_{c-(N+2)e}$, while (3.2.4) holds [U for N and V for $N+1$]. Similarly $VV^* - 1 \in Op\psi_{c-(N+2)e}$ will hold if we solve

$$(3.2.6) \quad u_0\omega^* + \omega u_0^* - z_2(x, D) \in \psi_{c-(N+2)e} \quad \text{with} \quad z_2(x, D) = 1 - UU^* \in Op\psi_{c-(N+1)e}.$$

Conditions (3.2.5) and (3.2.6) mean that the hermitian symmetric parts of $u_0^*\omega$ and ωu_0^* should be equal to half of z_1 and z_2 , resp. - i.e.

$$(3.2.7) \quad \omega \equiv u_0 \left(\frac{1}{2} z_1 + i\gamma \right) \equiv \left(\frac{1}{2} z_2 + i\delta \right) u_0 \pmod{\psi_{c-(N+2)e}},$$

with hermitian symmetric matrix symbols γ, δ of order $-(N+1)e$. But note that $u_0 z_1 \equiv z_2 u_0 \pmod{\psi_{c-(N+2)e}}$ due to $U(1 - U^*U) = (1 - UU^*)U$. So the two conditions do not contradict. We will treat the first as a sharp equation to determine ω , then the second will hold mod order $-(N+2)e$ with $\delta = u_0^*\gamma u_0$.

⁶We better recall, that $\Upsilon^2 = |\sigma \cdot (\xi - \mathbf{A})|^2 = |\xi - \mathbf{A}|^2$ is a scalar, due to the properties of σ , so also ζ_0 and the square root in (3.2.1) are scalars, while ζ is a 2×2 -matrix. The 2×2 -matrices of (3.2.1) are really 4×4 -matrices - i.e. 2×2 -matrices of 2×2 -blocks.

Next we must satisfy the third condition (3.2.4) with V and $N + 1$ and a new decoupled Λ' . That is, $V^*HV - \Lambda' \equiv (U^*HU - \Lambda) + (\Lambda - \Lambda') + (U^*H\Omega + \Omega^*HU) \in \mathcal{O}p\psi c_{-(N+1)e-e^2}$. For symbols this amounts to $u_0^*h\omega + \omega^*hu_0 \equiv z_3 + z_4$ (with “ \equiv mod order $-(N + 1)e - e^2$ ”, and with the symbols z_3, z_4 of $\Lambda' - \Lambda, \Lambda - U^*HU$. Note that the symbol z_3 of $\Lambda' - \Lambda$ should be “decoupled” and of order $-Ne - e^2$ while z_4 (of order $-Ne - e^2$) is given (but z_3 must be found). Here we substitute $\omega = u_0(\frac{1}{2}z_1 + i\gamma)$, (from (3.2.7)) for

$$(3.2.8) \quad u_0^*hu_0(\frac{1}{2}z_1 + i\gamma) + (\frac{1}{2}z_1 - i\gamma)u_0^*hu_0 = z_3 + z_4 ,$$

where again a hermitian symmetric γ (of order $-(N+1)e$) and a decoupled z_3 (of order $-Ne - e^2$) must be found while z_1 (hermitian, of order $-(N + 1)e$) and z_4 (hermitian, of order $-Ne + e^2$) are given. Note, $u_0^*hu_0 = \lambda = \text{diag}(\lambda_+, \lambda_+, \lambda_-, \lambda_-)$ is the diagonal matrix from (3.1.3),(3.1.4). Therefore the above amounts to

$$(3.2.9) \quad i[\lambda, \gamma] = z_3 + z_4 - \frac{1}{2}\{\lambda z_1 + z_1 \lambda\} = z_5 .$$

Note the right hand side z_5 of (3.2.9) is of order $-Ne - e^2$. That commutator equation can only be solved for γ if z_5 is of the form $\begin{pmatrix} 0 & p \\ p^* & 0 \end{pmatrix}$ (with 2×2 -blocks $0, p$). This determines z_3 as the “decoupled part” of z_5 . Then (3.2.9) has infinitely many solutions, of the form

$$(3.2.10) \quad \gamma = \frac{1}{2i}\zeta_0 \begin{pmatrix} c_1 & p \\ p^* & c_2 \end{pmatrix} ,$$

with general (2×2 -matrix-valued) symbols c_1, c_2 to be chosen such that γ is a symbol of proper order $-(N + 1)e$. So, indeed, the strictly classical ψ do U of order 0 satisfying the 3 equations (3.0.8) modulo $\mathcal{O}(-\infty)$ only exists.

Next, we will remove the “mod $\mathcal{O}(-\infty)$ ” from the first two relations (3.0.8) - so that U indeed becomes a unitary operator of \mathcal{H} . Just as in ch.1 with inverses of ψ do-s this requires some functional analysis.

Note, the operator U thus far constructed is md -elliptic of order 0. Thus we may apply thm.1.4.7 to find that (i) the kernels of U and U^* both are finite dimensional, and they belong to $\mathcal{S} \subset \mathcal{H}$. (ii) The operators U, U^* have closed rank. In other words, U, U^* are *Fredholm operators*.

It is important then to show that their Fredholm index $\text{ind}(U) = \dim \ker U - \dim \ker U^*$ vanishes. To verify this we need some common results of Fredholm theory (cf.[Ka1],ch.4,§5 or [Co11],App A1): The index of a Fredholm operator $A \in L(\mathcal{H})$ does not change if we add a compact operator C or else, a bounded operator B with sufficiently small norm $\|B\|$. To use this, focus on the ψ do $u_0(x, D)$ with $u = u_0$ of (3.2.1). Note that $U - u_0(x, D)$ is of order $-e$, hence it

is a compact operator of \mathcal{H} (rem.1.4.3). Thus $\text{ind}(U) = \text{ind } u_0(x, D)$. Regarding $u_0(x, D)$ we first notice that its Fredholm index is zero if we assume $\mathbf{A}_j = 0$. In that case the symbol is independent of x , so $u_0(x, D) = F^{-1}u_0(\xi)F$ is a unitary operator with $\ker U = \ker U^* = \{0\}$. For potentials $\mathbf{A}_j \not\equiv 0$ form the symbol (3.2.1) with $A_j(x)$ replaced by $s\mathbf{A}_j(x)$, with a constant s , $0 \leq s \leq 1$. This symbol, called $u_0^s(x, \xi)$ satisfies $[u_0^s - u_0^{s_0}]_4 \rightarrow 0$ as $s \rightarrow s_0$ with $[\cdot]_4$ as in thm.1.4.1. By that theorem we thus get $\|u_0^s(x, D) - u_0^{s_0}(x, D)\| \rightarrow 0$ as $s \rightarrow s_0$. In other words the family of operators $u_0^s(x, D)$ is norm continuous in the parameter s . It is md -elliptic for all s , so it is Fredholm for all s . Accordingly the Fredholm index is constant along the interval $[0,1]$. That index is zero for $s = 0$, so also, for $s = 1$. It follows that $u_0(x, D)$ and hence U has index 0.

In other words, $\ker U$ and $\ker U^*$ have the same dimension N . We pick orthonormal bases $\{\varphi_j\}_{j=1\dots N}$ and $\{\omega_j\}_{j=1\dots N}$ of $\ker U$ and $\ker U^*$, resp. and then form the operator $V = U + X$, $X = \sum_1^N \omega_j \langle \varphi_j$. Here we note that $X \in \mathcal{O}(-\infty)$ since $\ker U$ and $\ker U^*$ both are subspaces of \mathcal{S} . Accordingly we still have $1 - V^*V = P \in \mathcal{O}(-\infty)$ and $1 - VV^* = Q \in \mathcal{O}(-\infty)$. In addition we now have $\ker V = \ker V^* = \{0\}$, because the operator X is an isometric map of $\ker U$ onto $\ker U^* = (\text{im } U)^\perp$. So, it just extends the operator as an isometry into its kernel. As a consequence we now have V invertible, as an operator of $L(\mathcal{H})$, and V^* then is invertible as well. So, $V^*V = 1 + C$ is invertible as well, where $C \in \mathcal{O}(-\infty)$.

Lemma 3.2.1 *For a positive definite self-adjoint operator of the form $1 + C$, where $C \in \mathcal{O}(-\infty)$ both the unique positive square root $\sqrt{1 + C}$ and its inverse $(1 + C)^{-1/2}$ are of the form $1 + \mathcal{O}(-\infty)$.*

This is an immediate consequence of cor.2.4.5. A simpler proof will be discussed in sec.3.4, below (cf. prop.3.4.3).

With this lemma we now may define $W = V(V^*V)^{-1/2} = V(1 + C)^{-1/2}$. Clearly then $W = U + \mathcal{O}(-\infty) \in \text{Op}\psi c_0$ is invertible in $L(\mathcal{H})$, and we have $W^*W = 1$, so that W is a unitary operator of \mathcal{H} . Also we have $W^*HW = U^*HU + \mathcal{O}(-\infty)$. So, since U^*HU was decoupled mod($\mathcal{O}(-\infty)$) the same is true for W^*HW . So, we have proven:

Theorem 3.2.2 *Let the C^∞ -potentials \mathbf{A}, \mathbf{V} have the property that derivatives of order k decay like $(1 + |x|)^{-k-1}$. Then there exists a unitary ψ do $U \in \text{Op}\psi c_0$ such that*

$$(3.2.11) \quad U^*HU - \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix} \in \mathcal{O}(-\infty) .$$

Here X, Y are (2×2) -matrices of ψ do-s in $Op\psi c$. In fact we have

$$(3.2.12)$$

$$X = \lambda_+(x, D) + X_0, \quad Y = \lambda_-(x, D) + Y_0, \quad \lambda_{\pm}(x, \xi) = \mathbf{V}(x) \pm \sqrt{1 + (\xi - \mathbf{A}(x))^2},$$

with certain ψ do-s $X_0, Y_0 \in Op\psi c_{-e^2}$, of order $-e^2 = (0, -1)$. Moreover, the operators U, X_0, Y_0 possess asymptotic expansions into an infinite series of terms of lower and lower order, and these terms may be explicitly calculated, by the procedure outlined above⁷. The lowest term of U coincides with the operator of the symbol (3.2.1).

3.3 Relation to Smoothness of the Heisenberg Transform

Before we begin the task of replacing the “ $\in \mathcal{O}(-\infty)$ ” in fla. (3.2.11) by “ $= 0$ ” let us point to the following later result, to be discussed in thm.5.5.1. (The potentials are still time-independent and satisfy cdn.(X)):

Theorem 3.3.1 *An operator $A \in Op\psi c$ (of order m) has a “smooth Heisenberg transform” $A_t = e^{iHt} A e^{-iHt}$ if and only if it also is decoupled mod($\mathcal{O}(-\infty)$), in the sense of (3.2.11) - that is,*

$$(3.3.1) \quad U^* A U - \begin{pmatrix} B & 0 \\ 0 & C \end{pmatrix} \in \mathcal{O}(-\infty),$$

with (blocks of) ψ do-s $B, C \in Op\psi c$ (also of order m), and with U of theorem 3.2.2 - same U as for H .

[Proof see thm.5.7.1.]

Now, for the purpose of building a consistent theory of observables, in the sense of J.v.Neumann [JvN], we will ask for a strict decoupling, not only modulo $\mathcal{O}(-\infty)$. In view of the already achieved decoupling of thm.3.2.2 this reduces to the question whether, after the U of thm.3.2.2 we now can find another *unitary* $V = 1 + Z$, $Z \in \mathcal{O}(-\infty)$ such that

$$(3.3.2) \quad V^* U^* H U V = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix},$$

⁷Note, the final correction of U , to make it a unitary operator, may be ignored, as far as asymptotic expansions of X, Y, U are concerned. They just “redefine” the limit of the infinite sum.

with modified X, Y , but the modification consisting only of additional $\mathcal{O}(-\infty)$ -terms.

In [Co3] we were declaring the “smooth” algebra \mathcal{P} as *algebra of precisely predictable observables*. With an improved unitary $UV = W$, achieving a precise decoupling (3.3.2), we will modify that declaration, and define a new algebra $\mathcal{PX} \subset \mathcal{P}$ of precisely predictable observables, by requesting that

$$(3.3.3) \quad A \in \mathcal{PX} \iff W^*AW = \begin{pmatrix} B & 0 \\ 0 & C \end{pmatrix} .$$

It is evident that (3.3.2) amounts to a *spectral split* of the Hamiltonian H : Defining \mathcal{H}_\pm as the subspaces of \mathcal{H} of all vectors with vanishing last two (first two) of the 4 components, and then $\mathcal{K}_\pm = W\mathcal{H}_\pm$ we get H reduced by the orthogonal direct decomposition

$$(3.3.4) \quad \mathcal{H} = \mathcal{K}_+ \oplus \mathcal{K}_- .$$

The spectrum of the restrictions $H_\pm = H|_{\mathcal{K}_\pm}$ clearly will be that of the self-adjoint operator X resp. Y . In fact we get

$$(3.3.5) \quad W_+^*H_+W_+ = X , \quad W_-^*H_-W_- = Y ,$$

with the restrictions $W_\pm = W|_{\mathcal{K}_\pm}$ (which are unitary maps $W_\pm : \mathcal{K}_\pm \rightarrow \mathcal{H}_\pm$). The spectral theory of X and Y can be readily studied, however, in view of formula (3.2.12): The essential spectra of X and Y coincide with the half-lines $\Sigma_+ = [1, \infty)$ and $\Sigma_- = (-\infty, -1]$, respectively. Outside any neighbourhood of these half-lines there are only finitely many point-eigenvalues of finite multiplicity.

This spectral split we expect to amount to a clean split into an electron and positron part of the Hamiltonian. Accordingly, our above definition of the new algebra \mathcal{PX} of precisely predictable observables amounts to a restriction of observables to those who are also reduced by this split.

Clearly then, referring to our initial discussion, the spaces \mathcal{K}_\pm should be interpreted as spaces of purely electronic and purely positronic physical states - named $\mathcal{K}_+ = \mathcal{H}_e$ and $\mathcal{K}_- = \mathcal{H}_p$. This will convert (3.3.4) into (3.0.5).

We shall discuss a clean decoupling of \mathcal{H} (of the form (3.3.2)) in sec.3.5, below. However, there seems to be an obstruction, at least for our technique, insofar as the split (3.3.2) will have to be made with respect to a decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ where \mathcal{H}_\pm differ from the spaces of 4-vectors with last 2 (first 2) components vanishing, resp. It may be necessary to shift a finite dimensional subspace \mathcal{Z} of rapidly decreasing functions from one of these spaces to the other one.

Instead of directly designing a decoupling of H in the sense of (3.3.2) we will attempt to decouple some special projection of the spectral family of H in the interval between -1 and $+1$ - this automatically also gives a decoupling of H itself. For such decoupling at λ_0 a “deficiency index” ι_{λ_0} must vanish, or else, a space \mathcal{Z} of dimension $|\iota_{\lambda_0}|$ must be shifted. The index ι decreases with λ , so, it may cross 0 for some $\lambda \in (-1, 1)$ and allow decoupling. However, it seems possible that ι does not change sign in $(-1, +1)$. In that case we cannot decouple with respect to the split $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ but first must modify the spaces \mathcal{H}_\pm by adding and subtracting a space \mathcal{Z} . This may result for potentials so strong that some electron eigenvalues wander into the continuous spectrum of the positron, or, vice versa.

For details we refer to sec.3.5, below.

3.4 Some Comments Regarding Spectral Theory

We are departing from thm.3.2.2, and write (3.2.11) in the form

$$(3.4.1) \quad H^\sim = U^* H U = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix} + \begin{pmatrix} 0 & \Gamma^* \\ \Gamma & 0 \end{pmatrix},$$

with self-adjoint 2×2 -blocks X, Y of the form (3.2.12), and a $\Gamma \in \mathcal{O}(-\infty)$. The task then will be, to find a unitary operator

$$(3.4.2) \quad V = \begin{pmatrix} 1 + A & B \\ C & 1 + D \end{pmatrix} = \begin{pmatrix} V_+ & B \\ C & V_- \end{pmatrix}, \quad A, B, C, D \in \mathcal{O}(-\infty),$$

such that $V^* H^\sim V$ is “decoupled” - i.e., has the form (3.3.2), its “ears” (the off diagonal 2×2 -blocks) vanish.

In all of the following we work with potentials satisfying cdn.(X): *Derivatives of order k decay like $(1 + |x|)^{-k-1}$.*

To discuss a complete decoupling of H we now will invoke spectral theory of the self-adjoint partial differential operator system H , in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$. It is known⁸ and easily proven that there is a unique self-adjoint realization of the operator H of (3.1.1). This self-adjoint operator H has essential spectrum consisting of the half-lines $(-\infty, -1] = \Sigma_-$ and $[1, \infty) = \Sigma_+$. The spectrum in $(-1, 1)$ is discrete, with at most countably many eigenvalues of finite multiplicity clustering at ± 1 only. The unitary transform H^\sim of H is self-adjoint too, with the same spectrum. Let $\{E_\lambda : \lambda \in \mathbb{R}\}$ be the spectral family of H^\sim .

⁸To investigate the spectral theory of H of (3.1.1) one might look at H as an H_0 -compact

The operators X and Y of (3.4.1) (or (3.2.11)) have essential spectrum Σ_+ and Σ_- , respectively. Again, their spectrum is discrete outside of these half-lines. Verification of this requires some simple arguments of ψ do-theory⁹.

We will require the following result:

Lemma 3.4.1 *Let $P_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, with 2×2 -blocks again. Then $E_\lambda = 1 - P_0 - e_\lambda$, where $e_\lambda \in \mathcal{O}(-\infty)$, for all $\lambda \in (-1, 1)$.*

Proof. We must examine the difference between the spectral family E_λ of the operator H^\sim of (3.4.1), and that of $H^\Delta = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix}$ there, in order to prove lemma 3.1.1. Assume $-1 < \lambda < 1$, and first assume that λ is not an eigenvalue, not of H^\sim , nor of H^Δ . For simplicity, write $M = H^\sim$, $N = H^\Delta$, for a moment. For simplicity let $\lambda = 0$, noting that a general λ (as above) may be treated similarly.

The integral $\int_{-i\eta}^{i\eta} (M - \lambda)^{-1} d\lambda = I_\eta(M)$ (along part of the imaginary axis) exists under norm convergence of \mathcal{H} , as a Riemann integral, because the integrand

perturbation of $H_0 = \alpha \cdot D + \beta$, writing $H = H_0 + \{\mathbf{V} - \sum \alpha_j \mathbf{A}_j\} = H_0 + Z$. Note, H_0 is diagonalized by the Fourier transform (cf. (3.1.2)), and its spectrum is readily confirmed as the union $\Sigma_+ \cup \Sigma_-$ with both these half-lines giving absolutely continuous spectrum (of infinite multiplicity). There are no point-eigenvalues of H_0 . We have $H_0^2 = 1 - \Delta$, and H_0^{-1} exists as a ψ do in $Op\psi_{c_{-e^1}}$ - symbol independent of x . H itself is md -elliptic of order e^1 hence its null space is finite dimensional and belongs to \mathcal{S} , by thm.1.4.7. It must be self-adjoint in the domain of H_0 (i.e., the Sobolev space \mathcal{H}_{e^1} , $e^1 = (1, 0)$), since the potentials are bounded, so that $Z \in L(\mathcal{H})$. If $\ker H \neq \{0\}$ we consider $H' = H + \sum \varphi_j \langle \varphi_j$ with an orthonormal base $\{\varphi_j\}$ of $\ker H$. Clearly H and H' have the same spectral theory, except that H' no longer has the eigenvalue 0 (and is invertible). We also may write $H' = H_0 + Z$ where now Z has an additional term of order $-\infty$. So, WLOG, we assume $\ker H = \{0\}$, and then work with H instead of H' . Since the potentials all are of order $-e^2$ - by $\text{cdn}(X)$ - we find that $C = H_0^{-1}Z \in Op\psi_{c_{-e}}$ is compact, by rem.1.4.3. We may write $H = H_0(1 + C) = (1 + C^*)H_0$, hence $H^{-1} = (1 + C)^{-1}H_0^{-1} = H_0^{-1}(1 + C^*)^{-1}$. We get $(1 + C)^{-1} = 1 - C(1 + C)^{-1}$, hence $H^{-1} = H_0^{-1} - C(1 + C)^{-1}H_0^{-1}$, where the last term is compact - since products of compact and bounded operators are compact.

Now, it follows that the essential spectrum of any operator - that is, all points of the spectrum except isolated point-eigenvalues of finite multiplicity does not change, if one adds a compact operator (cf.[Ka1],or,[Col1]). Hence H^{-1} and H_0^{-1} have the same essential spectrum - and so have H and H_0 . Thus, indeed, the essential spectrum of H must consist precisely of the union $\Sigma_+ \cup \Sigma_-$. [But we have no statement, of course, about the more precise nature of $\text{Sp}(H)$. Under special condition - such as for potentials depending on $r = |x|$ only one knows much more, such as absolute continuity, etc.]

⁹For this we use a similar argument as for H : One will compare the operators $\lambda_\pm(x, D)$ with the operator $\pm\langle D \rangle$, noting that the further perturbations X_0 and Y_0 again do not influence the essential spectrum. Get $\langle \xi - \mathbf{A}(x) \rangle - \langle \xi \rangle = (\mathbf{A}(x)^2 - 2\xi \cdot \mathbf{A}(x)) / \{\langle \xi - \mathbf{A}(x) \rangle + \langle \xi \rangle\} \in \psi_{c_{-e^2}}$, as well as $\mathbf{V}(x) \in \psi_{c_{-e^2}}$. So, we get $X = \langle D \rangle + Z'$, $Y = -\langle D \rangle + Z''$ with $Z', Z'' \in \psi_{c_{-e^2}}$. Again $\langle D \rangle$ is md -elliptic of order e^1 - as are X, Y , and $\langle D \rangle^{-1}$ exists - a ψ do in $Op\psi_{c_{-e^1}}$ with symbol independent of x . The spectrum of $\langle D \rangle$ equals Σ_+ . We may exactly repeat the argument of the preceding footnote to also show that Σ_\pm is the essential spectrum of X (Y). [Again, the study of more detailed properties of these spectra requires a more delicate analysis.]

is (norm-) smooth (even analytic). We may write $\int_{-i\eta}^{i\eta} = \int_0^{i\eta} + \int_{-i\eta}^0$, and set $\lambda = i\mu$ in the first, $\lambda = -i\mu$ in the second integral, with $0 \leq \mu \leq \eta$. A calculation then gives

$$(3.4.3) \quad M^{-1}I_\eta(M) = 2i \int_0^\eta (M^2 + \mu^2)^{-1} .$$

Here the integrand is $O(\mu^{-2})$, as $\mu \rightarrow \infty$. Hence the improper Riemann integral $\int_0^\infty = \lim_{\eta \rightarrow \infty} \int_0^\eta$ again exists in norm convergence of \mathcal{H} .

For a real number $a \neq 0$ we have $\int_0^\infty \frac{d\mu}{a^2 + \mu^2} = \frac{1}{|a|} \int_0^\infty \frac{d\mu}{1 + \mu^2} = \frac{\pi}{2|a|}$. Using the spectral theorem we thus confirm that

$$(3.4.4) \quad I(M) = \lim_{\mu \rightarrow \infty} I_\eta(M) = i\pi \operatorname{sgn}(M) = i\pi(1 - 2E_0) ,$$

noting that $\int_{-\infty}^{+\infty} \operatorname{sgn}(\lambda) dE_\lambda = -E_0 + (1 - E_0) = 1 - 2E_0$. Note that $\int_{-i\infty}^{i\infty}$ in (3.4.3) exists only as a Cauchy principal value, and only pointwise, for $u \in \operatorname{dom}(M)$.

The corresponding formula holds for $N = H^\Delta$, where we observe that (i) the domains $\operatorname{dom}(N), \operatorname{dom}(M)$ are equal, and (ii) the spectral projection F_0 at 0, for the operator N must be of the form $\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + S$ with an operator $S \in \mathcal{O}(-\infty)$. So, in order to show that $E_0 - 1 + P_0$ is $\mathcal{O}(-\infty)$, it suffices to look at the difference

$$(3.4.5) \quad R = I(N) - I(M) = \int_{-i\infty}^{i\infty} (M - \lambda)^{-1} \Lambda (N - \lambda)^{-1} d\lambda$$

with $\Lambda = M - N = \begin{pmatrix} 0 & \Gamma^* \\ \Gamma & 0 \end{pmatrix}$ of (3.4.1), $\Lambda \in \mathcal{O}(-\infty)$.

We claim that this difference R is of order $-\infty$. To see this, let again $\Lambda_s = \langle x \rangle^{s_1} \langle D \rangle^{s_2}$, for $s = (s_1, s_2)$. This operator Λ_s is an isometry $\mathcal{H}_s \rightarrow \mathcal{H}$, with the weighted Sobolev spaces \mathcal{H}_s of sec.1.4. To show that $R \in \mathcal{O}(-\infty)$ we must confirm that $\Lambda_s R \Lambda_t \in \mathbf{L}(\mathcal{H})$ for all $s, t \in \mathbb{R}^2$. But we have

$$(3.4.6) \quad \Lambda_s (M - \lambda) \Lambda_s^{-1} = M + B_s - \lambda = (M - \lambda)(1 + (M - \lambda)^{-1} B_s) ,$$

where $B_s = \Lambda_s M \Lambda_s^{-1} - M \in \operatorname{Op}\psi c_{(0,-1)} \subset \mathcal{H}$ by the commutator rules and L^2 -boundedness for pseudodifferential operators. M and $\Lambda_s M \Lambda_s^{-1}$ have the same spectrum, since their resolvents also are K -parametrics. On the other hand, for large $|\lambda|$ the operator $(M - \lambda)^{-1}$ becomes small, on the integration path, so that $(1 + (M - \lambda)^{-1} B_s) - 1 = K_{s,\lambda}$ exist and is uniformly bounded. A similar argument holds for the operator N (instead of M). Since we must have $\Lambda_s \Lambda \Lambda_t \in \mathbf{L}(\mathcal{H})$ for all s, t , we may pull Π_s and Π_t through the resolvents. to get a smooth integrand, bounded by $|\lambda|^{-2}$ for large $|\lambda|$. Thus the integral exists as improper Riemann integral, in norm convergence of \mathcal{H} . It follows that indeed R is of order $-\infty$. Q.E.D.

Remark 3.4.2 E_λ increases and is piecewise constant, in that interval, and jumps only by a projection onto a finite dimensional subspace of \mathcal{S} , at the eigenvalues. Thus the eigenvalues of M (and those of N) need no longer be excluded.

Proposition 3.4.3 For $A \in \mathcal{O}(-\infty)$, if $(1 + A)^{-1}$ exists, it is of the form $1 + B$, $B \in \mathcal{O}(-\infty)$. For a self-adjoint $A \in \mathcal{O}(-\infty)$ all eigen functions to an eigenvalue $\neq 0$ belong to $\mathcal{S} = \mathcal{S}(\mathbb{R}^3)$. If, in addition, $1 + A \geq 0$, then we have $\sqrt{1 + A} = 1 + B$ where $B \in \mathcal{O}(-\infty)$.

Proof, (We base this on facts discussed in sec.1.4.) First of all, $1 + A$, for $A \in \mathcal{O}(-\infty)$ is an md-elliptic ψ do of order 0. Thus it has a K-parametrix, unique up to an additional term in $\mathcal{O}(-\infty)$. Clearly a special K-parametrix is given by 1. An L^2 -inverse C of $1 + A$, if it exists, must also be a ψ do in $Op\psi_{C_0}$, hence a parametrix. Hence it differs from 1 only by an operator in $\mathcal{O}(-\infty)$.

A selfadjoint $A \in \mathcal{O}(-\infty)$ is a compact operator, hence has discrete spectrum (except at 0). If $\lambda \neq 0$ is an eigenvalue, then $A - \lambda$ is Fredholm in $L^2 = \mathcal{H}_0$, hence Fredholm in every polynomially weighted Sobolev space $\mathcal{H}_s = \mathcal{H}_{(s_1, s_2)}$, and its null space is independent of $s = (s_1, s_2)$, so, must be a subspace of $\cap \mathcal{H}_s = \mathcal{S}$, by thm.1.4.7. Hence all eigenvectors to $\lambda \neq 0$ must belong to \mathcal{S} .

For A as above let $1 + A \geq 0$. For $\sqrt{1 + A} = 1 + B$, $B \in \mathcal{O}(-\infty)$ it suffices to show that $(1 + A)^{-\frac{1}{2}} = 1 + C$, $C \in \mathcal{O}(-\infty)$, assuming $(1 + A)^{-1}$ to exist. For, if that inverse does not exist, then let P be the orthogonal projection onto $\ker(1 + A) \subset \mathcal{S}$. We get $P \in \mathcal{O}(-\infty)$, since $\ker(1 + A)$ is finite dimensional. Then $(1 + A + P)^{-1}$ exists, and we may write $\sqrt{1 + A} - 1 = (1 + A)(1 + A + P)^{-\frac{1}{2}} - 1 \in \mathcal{O}(-\infty)$. Using a well known formula for the inverse square root, write

$$(3.4.7) \quad (1 + A)^{-\frac{1}{2}} = \frac{1}{\pi} \int_0^\infty \frac{d\lambda}{\sqrt{\lambda}} (A + 1 + \lambda)^{-1} .$$

Taking the difference between (3.4.7) and the same formula for $A = 0$ we get

$$(3.4.8) \quad 1 - (1 + A)^{-\frac{1}{2}} = \frac{1}{\pi} \int_0^\infty \frac{d\lambda}{\sqrt{\lambda}} \frac{A}{(1 + \lambda)(A + 1 + \lambda)} .$$

Here the integral at right belongs to every \mathcal{H}_s , hence to \mathcal{S} . This follows, using the same technique as for R of (3.4.5). Q.E.D.

3.5 Complete Decoupling for $V(x) \not\equiv 0$

After above preparations we now will discuss a complete decoupling of H (or, of H^\sim by an operator of the form $1 + \mathcal{O}(-\infty)$). Our discussion here can be strictly

confined to the class $\mathcal{O}(-\infty)$ of integral operators. It was noted that $\mathcal{O}(-\infty)$ is an (adjoint invariant) subalgebra of $L(\mathcal{H})$.

Let us fix some point $\lambda_0 \in (-1, 1)$, not an eigenvalue of H^\sim . By lemma 3.4.1 above we have

$$(3.5.1) \quad P = 1 - E_{\lambda_0} = P_0 + Z, \quad Z = \begin{pmatrix} F & G \\ G^* & H \end{pmatrix}, \quad F, G, H \in \mathcal{O}(-\infty), \quad F^* = F, \quad H^* = H.$$

Instead of directly looking for a V satisfying (3.3.2) we try to find a unitary V such that

$$(3.5.2) \quad V^*PV = P_0.$$

Such V also must satisfy $V^*(1 - P)V = 1 - P_0 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$. But we have $H^\sim = PH^\sim P + (1 - P)H^\sim(1 - P)$, since P and H^\sim commute. Thus it follows that also $V^*H^\sim V$ is ψ -diagonal¹⁰.

Vice versa, if (3.3.2) holds, we need not to have $V^*PV = P_0$. Rather, it follows that

$$(3.5.3) \quad V^*PV - P_0 = \begin{pmatrix} M & 0 \\ 0 & N \end{pmatrix}.$$

with finite dimensional projections $-M, N$. Indeed, if $H^\diamond = V^*H^\sim V = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix}$ is ψ -diagonal then $P_0H^\diamond(1 - P_0) = (1 - P_0)H^\diamond P_0 = 0$. Especially, P_0 commutes with H^\diamond , hence also commutes with the spectral projection $P^\diamond = V^*PV$. That is, $P^\diamond P_0 = P_0 P^\diamond \Rightarrow P_0 P^\diamond(1 - P_0) = (1 - P_0)P^\diamond P_0 = 0$, i.e., P^\diamond is ψ -diagonal. But the operator Y has its essential spectrum in the interval Σ_- only, so, there are at most finitely many point eigenvalues above λ_0 . This implies that the LR-corner N of P^\diamond (which counts the spectrum above λ_0) must be an orthogonal projection of finite rank. Similarly, Y has its essential spectrum in Σ_+ , so that again only finitely many point eigenvalues are below λ_0 . That is, the UL-corner $-M$ of $1 - P^\diamond$ must be a projection of finite rank. So, indeed, $P^\diamond - P_0$ is a symmetry as in (3.5.3).

Given P of the form (3.4.2) (which must satisfy $P^2 = P$) we now look for V , as in (3.5.1), satisfying

$$(3.5.4) \quad V^*V = 1, \quad PV = VP_0.$$

[Note, the additional condition $VV^* = 1$ is implied: $V = 1 + Z$, with Z of order $-\infty$ is a compact perturbation of 1, hence is Fredholm, with index 0. If $V^*V = 1$

¹⁰An operator A in 2×2 -block-diagonal form with respect to a given direct decomposition $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ will be called “ ψ -diagonal”, in this section. [That is, A leaves both spaces $\mathcal{H}_{1,2}$ invariant.] We also may say that such operator has “its ears” equal to 0.

then $\ker V = \{0\}$, hence $\dim \ker V^* = \dim \ker V = 0 \Rightarrow \ker V^* = \{0\} \Rightarrow V$ is invertible, and $VV^* = 1$ follows as well.] Evaluating (3.5.4) in 2×2 -block-matrix form, get

$$(3.5.5)$$

$$(1+A^*)(1+A)+C^*C = 1, (1+D^*)(1+D)+B^*B = 1, (1+A^*)B+C^*(1+D) = 0,$$

using $V^*V = 1$, and, from the second relation (3.5.4),

$$(3.5.6)$$

$$FU_+ + GC = 0, G^*U_+ + (H-1)C = 0, (1+F)B + GU_- = 0, G^*B + HU_- = 0.$$

From $P^2 = P$ we get

$$(3.5.7) \quad F(1+F) + GG^* = 0, G^*G + H(H-1) = 0, FG + GH = 0.$$

These are satisfied a priori for F, G, H .

We must have $0 \leq 1+F \leq 1$, $0 \leq H \leq 1$, since the projections $P, 1-P$ are self-adjoint positive.

The (self-adjoint) operators $1+F$ and $1-H$ are compact perturbations of 1, hence they are Fredholm. Their null spaces are finite dimensional, and their inverses exist in the ortho-complements $\ker(1+F)^\perp$, $\ker(1-H)^\perp$, resp., mapping these spaces to themselves.

Assume first $\ker(1+F) = \ker(1-H) = \{0\}$, so that the two inverses exist in the entire space. Then the second and third relations (3.5.6) may be solved for C, B . We get

$$(3.5.8) \quad C = (1-H)^{-1}G^*V_+, \quad B = -(1+F)^{-1}GV_-.$$

Substitute this into the first and 4-th relation (3.5.6) for

$$(3.5.9) \quad FV_+ + G(1-H)^{-1}G^*V_+ = 0, \quad -G^*(1+F)^{-1}GV_- + HV_- = 0.$$

This looks like a serious restriction of V_\pm . However, as a consequence of (3.5.7) it is found that the coefficients $F + G(1-H)^{-1}G^* = 0$, and $F - G^*(1+F)^{-1}G = 0$ both vanish, so that the choice of V_\pm still is completely free. Indeed, $FG + GH = 0$ of (3.1.7) implies $(1+F)G = G(1-H)$, or, $G(1-H)^{-1} = (1+F)^{-1}G$, and $(1-H)^{-1}G^* = G^*(1+F)^{-1}$. Thus $F + G(1-H)^{-1}G^* = F + (1+F)^{-1}GG^* = (1+F)^{-1}\{F(1+F) + GG^*\} = 0$, using the first of (3.5.7). Similarly for the other coefficient.

We conclude that $PV = VP_0$ of (3.5.6) holds for any matrix V of the form (3.4.2), for an arbitrary choice of V_\pm , with C, B of (3.5.8). Then, to make V unitary, we must substitute (3.5.8) into (3.5.5), and solve these equations for A and D . Substituting C from (3.5.8) into the first of (3.5.5) get

$$(3.5.10) \quad (1+A^*)(1+A) + (1+A)^*\{(1+F)^{-1}GG^*(1+F)^{-1}\}(1+A) = 1.$$

Using (3.5.7) to express GG^* we get

$$(3.5.11) \quad R = (1 + F)^{-1}GG^*(1 + F)^{-1} = -F(F + 1)^{-1}.$$

With this (3.5.10) assumes the form $(1 + A)^*(1 + R)(1 + A) = 1$. This is solved by setting

$$(3.5.12) \quad V_+ = (1 + A) = (1 + A)^* = (1 + R)^{-1/2} = (1 + F)^{1/2}.$$

Similarly, the second equation (3.5.5) is solved by

$$(3.5.13) \quad V_- = (1 + D) = (1 - H)^{1/2}.$$

The third relation (3.5.5) is also satisfied with such choice of A, B . We have proven:

Proposition 3.5.1 *For an orthogonal projection P as in (3.5.1) assume that $(1 + F)^{-1}$ and $(1 - H)^{-1}$ exist. Then the matrix (3.4.2) with*

$$(3.5.14) \quad A = \sqrt{1 + F} - 1, \quad B = -G\sqrt{1 - H}^{-1}, \quad C = G^*\sqrt{1 + F}^{-1}, \quad D = \sqrt{1 - H} - 1.$$

provides a solution of (3.5.2) (with V of the form (3.4.2)). In particular, $V - 1$ belongs to $\mathcal{O}(-\infty)$, in view of prop.3.4.2.

In general, while we cannot expect the inverses of $1 + F$ and $1 - H$ to exist in all of $L^2(\mathbb{R}^3, \mathbb{C}^2)$, they certainly will exist in closed subspaces of finite codimension, as already mentioned. We have the orthogonal direct decompositions of $\mathcal{H}_+ = \mathcal{H}_- = L^2(\mathbb{R}^3, \mathbb{C}^2)$:

$$(3.5.15) \quad \mathcal{H}_+ = \ker(1 + F) \oplus \mathcal{H}_+^\circ, \quad \mathcal{H}_- = \mathcal{H}_-^\circ \oplus \ker(1 - H),$$

with $\mathcal{H}_+^\circ = \text{im}(1 + F)$, $\mathcal{H}_-^\circ = \text{im}(1 - H)$.

Examining (3.5.7) we note that $GG^*u = 0$ on $\ker(1 + F)$, and $G^*Gu = 0$ on $\ker(1 - H)$. This implies $G^*u = 0$ on $\ker(1 + F)$, and $Gu = 0$ on $\ker(1 - H)$. Note, we must regard $G : \mathcal{H}_- \rightarrow \mathcal{H}_+$, and $G^* : \mathcal{H}_+ \rightarrow \mathcal{H}_-$. So, G and G^* are represented by a pair of 2×2 -block-matrices, with respect to the decompositions (3.5.15). The above then means that $G \sim \begin{pmatrix} 0 & 0 \\ G^\circ & 0 \end{pmatrix}$, $G^* \sim \begin{pmatrix} 0 & G^{\circ*} \\ 0 & 0 \end{pmatrix}$. Or, if we now write

$$(3.5.16) \quad \mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$$

in the form of a 4-fold direct sum

$$(3.5.17) \quad \mathcal{H} = \mathcal{H}_+^\circ \oplus \mathcal{H}_-^\circ \oplus \ker(1 + F) \oplus \ker(1 - H),$$

then the projection P assumes the form

$$(3.5.18) \quad P = \begin{pmatrix} P^\circ & 0 \\ 0 & Q \end{pmatrix}, \text{ with } P^\circ = \begin{pmatrix} F^\circ & G^\circ \\ G^{\circ*} & H^\circ \end{pmatrix}, \quad Q = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$

where, of course, the matrix elements are ordered according to (3.5.17), with Q projecting onto $\ker(1 + F) \oplus \ker(1 - H)$. In order to bring this matrix onto the form $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, we will no longer insist on the direct decomposition (3.5.16). Rather, we will write

$$(3.5.19) \quad \mathcal{H} = \mathcal{H}_+^\circ \oplus \mathcal{H}_-^\circ, \text{ with } \mathcal{H}_+^\circ = \mathcal{H}_+^\circ \oplus \ker(1 - H), \quad \mathcal{H}_-^\circ = \mathcal{H}_-^\circ \oplus \ker(1 + F).$$

Then, with respect to the new decomposition (3.5.19), we just have to ψ -diagonalize the operator P° of (3.5.18), by a unitary V° of the form (3.4.2), with respect to $\mathcal{H}^\circ = \mathcal{H}_+^\circ \oplus \mathcal{H}_-^\circ$, and then define $V^\circ = \begin{pmatrix} V^\circ & 0 \\ 0 & 1 \end{pmatrix}$. The latter task, however, may be solved by application of proposition 3.5.1 to the operator $P^\circ : \mathcal{H}^\circ \rightarrow \mathcal{H}^\circ$. Or, rather, we must repeat the abstract construction leading to V of prop.3.5.1 now for the restrictions of A, B, C, D to \mathcal{H}_\pm° , respectively, where assumptions of prop.3.5.1 hold. Using the fact that the projections onto the finite dimensional subspaces $\ker(1 - H) = \mathcal{N}$, $\ker(1 + F) = \mathcal{M}$ of \mathcal{S} belong to $\mathcal{O}(-\infty)$ we indeed then get a $V^\circ - 1 \in \mathcal{O}(-\infty)$, and this even remains true if we replace 1 in the LR-corner of V° by any other linear operator of $\mathcal{M} \oplus \mathcal{N}$. Note that \mathcal{N} , \mathcal{M} are eigenspaces of H , F , hence belong to \mathcal{S} , by prop.3.4.2.

Returning to our old direct decomposition (3.5.16), we may express this result in the form (3.5.3), i.e.,

$$(3.5.20) \quad V^{\circ*} P V^\circ - P_0 = \begin{pmatrix} M & 0 \\ 0 & N \end{pmatrix},$$

where now $-M, N$ are the orthogonal projections onto the spaces \mathcal{M} , \mathcal{N} . However, the operator $V^{\circ*} H^\circ V^\circ$ needs not to be ψ -diagonal with respect to (3.5.16), while it will be ψ -diagonal with respect to (3.5.19).

Now if we assume $\dim(\mathcal{M}) = \dim(\mathcal{N})$ then this “deficiency” is easily corrected by involving any unitary map $\mathcal{M} \rightarrow \mathcal{N}$, to switch the two spaces, thus returning from the decomposition (3.5.19) to (3.5.16), as we should like. If these dimensions are not equal, then such a unitary map does not exist, of course. However, if, for example, we have “ $<$ ”, instead of “ $=$ ”, then \mathcal{M} will be unitarily equivalent to a subspace $\mathcal{N} \ominus \mathcal{Z}$, with a proper subspace \mathcal{Z} of \mathcal{N} . If we then make the above “unitary switch of spaces” we will convert (3.5.19) into $\mathcal{H} = \{\mathcal{H}_+^\circ \oplus \ker(1 + F) \oplus \mathcal{Z}\} \oplus \{\mathcal{H}_-^\circ \oplus \ker(1 - H) \ominus \mathcal{Z}\}$. With definition of \mathcal{H}_\pm° by (3.5.17) this yields

$$(3.5.21a) \quad \mathcal{H} = \{\mathcal{H}_+ \oplus \mathcal{Z}\} \oplus \{\mathcal{H}_- \ominus \mathcal{Z}\},$$

where we recall that \mathcal{Z} , as a subspace of $\ker(1-H)$, must be a subspace of $\mathcal{H}_- \cap \mathcal{S}$. Similarly, if we have “ $>$ ”, then we will get

$$(3.5.21b) \quad \mathcal{H} = \{\mathcal{H}_+ \oplus \mathcal{Z}\} \oplus \{\mathcal{H}_- \oplus \mathcal{Z}\} ,$$

with a finite dimensional subspace \mathcal{Z} of $\mathcal{H}_+ \cap \mathcal{S}$.

This suggests introducing a “deficiency index”

$$(3.5.22) \quad \iota = \iota(\lambda_0) = \dim \ker(1+F) - \dim \ker(1-H) .$$

If ι vanishes then we succeeded in constructing the desired operator \mathbf{V} -i.e., then our ψ do $W = UV$ decouples the Dirac Hamiltonian. For negative ι then we constructed a decoupling with respect to a split of the form (3.5.21a). For positive, with respect to (3.5.21b). In either case, by the way, we have

$$(3.5.23) \quad \dim \mathcal{Z} = |\iota| .$$

Note that, of course, our index ι depends on the choice of the point $\lambda_0 \in (-1, 1)$ we made initially. Observe here that

$$(3.5.24) \quad \ker(1+F) = \ker P_\lambda \cap \mathcal{H}_+ , \quad \ker(1-H) = \ker E_\lambda \cap \mathcal{H}_- .$$

In particular this implies that $\ker(1+F)$ decreases, while $\ker(1-H)$ increases, as λ increases from -1 to $+1$. There will be limits of $\{\ker(1+F)\}$ and $\{\ker(1-H)\}$ as $\lambda \rightarrow \pm 1$, and those spaces are piecewise constant in λ , jumping only at the eigenvalues of H^\sim , (and there only if the corresponding eigenspace contains a nonvanishing function in \mathcal{H}_\pm , respectively).

It follows that our index function ι_λ is piecewise constant and non-increasing, as λ increases from -1 to $+1$, assuming only integer values. If it becomes 0 for some λ_0 , then above construction will work, for that λ_0 , and we will get the decoupling (3.3.2), with the split between electron and positron state occurring at λ_0 : All the spectrum above (below) λ_0 generates electron (positron) states, respectively. If ι_λ assumes both positive and negative values, then it either will also assume 0, or else jump - at some eigenvalue λ_0 from “+” to “-”. But even if it does that, without assuming 0, then we still will get our decoupling at that λ_0 by properly splitting the eigenspace at λ_0 .

The monotone function ι_λ has limits $\iota_{\pm 1}$ as $\lambda \rightarrow \pm 1$ (where $\pm\infty$ is allowed). Assume then, that $\iota_1 > 0$, for example. Clearly the limit of $\mathcal{M} = \mathcal{M}_\lambda \rightarrow \mathcal{M}_1$ is a finite dimensional subspace of \mathcal{S} . We get $\dim \mathcal{N}_\lambda = \dim \mathcal{M}_\lambda - \iota_\lambda \leq \dim \mathcal{M}_0$, as $\lambda > 0$, since $\iota_\lambda > 0$ and \mathcal{M}_λ decreases. Hence the \mathcal{N}_λ have bounded dimension and must also converge towards a finite dimensional subspace \mathcal{M}_1 of \mathcal{S} as $\lambda \rightarrow 1$.

Looking at the above space $\mathcal{Z} = \mathcal{Z}_\lambda$ of (3.5.21b), here a subspace of $\mathcal{H}_+ \cap \mathcal{S}$, its dimension $|\iota_\lambda|$ decreases to the limit $|\iota_1|$, and we may choose it to decrease with λ to a limit \mathcal{Z}_1 . Since ι_λ is a step function, assuming integer values, it must be constant near 1. Hence $\mathcal{Z}_\lambda = \mathcal{Z}_1$ is constant near 1.

Similarly, if we assume that $\iota_{-1} < 0$ (i.e., that ι_λ assumes only negative values), then we obtain a “mimimal” finite dimensional subspace $\mathcal{Z} \in \mathcal{H}_- \cap \mathcal{S}$ and a decoupling of the form (3.5.21a), with that space \mathcal{Z} . The space \mathcal{Z} is minimal in the sense that our technique does not supply any such space of smaller dimension. Again the splitting (3.5.21a) may be obtained by using any $\lambda > -1$, sufficiently close to -1 .

Let us finally note, that our space \mathcal{Z} might be made smaller still if we could secure some point-eigenvalues within the continuous spectrum Σ_+ (or Σ_-), with the property that a subspace $\mathcal{T} \neq \{0\}$ of the corresponding eigenspace belongs to \mathcal{S} . In that case we could work with the spectral projection $P_\lambda + T \supset P_\lambda$, λ close to ± 1 , T =projection onto \mathcal{T} , which possibly might give a smaller space \mathcal{Z} (or even $\mathcal{Z} = 0$). However, while isolated point-eigenvalues necessarily have their eigenspaces in \mathcal{S} , this is not proven for points within the continuous spectrum.

3.6 Split and Decoupling are not unique - Summary

Let us shortly address the questions around the *distinction* of the ψ do-decoupling we have achieved. First of all, it is clear that there are other unitary ψ do-s achieving a decoupling. For example, we may conjugate the decoupled $H^\Delta = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix}$ by a unitary ψ do of the form $K = \begin{pmatrix} K_e & 0 \\ 0 & K_p \end{pmatrix}$ with unitary ψ do-s K_e, K_p acting on \mathcal{H}_\pm (properly modified by adding and subtracting that space \mathcal{Z}). This amounts to replacing V by VK . It will leave the two spaces \mathcal{H}_e and \mathcal{H}_p unchanged. If we insist on the condition $K - 1 \in \mathcal{O}(-\infty)$ then it also will leave the asymptotic expansions of thm.3.2.2 unchanged. Otherwise these expansions will look different, but we still have a unitary operator $UVK \in \text{Op}\psi c_0$ decoupling the Hamiltonian H . In this case we might just speak about changing the representation of the decoupled Hamiltonian H .

On the other hand, it might be important to notice that our split does not create a precise ordering of discrete “energy levels” into two categories, one containing electron- the other one positron-energy levels. Any two eigenvectors $\begin{pmatrix} \psi \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ \omega \end{pmatrix}$ of $\begin{pmatrix} X & 0 \\ 0 & 0 \end{pmatrix}$ and $\begin{pmatrix} 0 & 0 \\ 0 & Y \end{pmatrix}$, resp., belong to \mathcal{S} , assuming their eigenvalues λ and μ are not in the continuous spectrum of X or Y , resp.. Then let $\chi = \begin{pmatrix} \psi \\ -\omega \end{pmatrix}$, and define $Z = \chi \langle \chi \in \mathcal{O}(-\infty)$, assuming that $\|\psi\| = \|\omega\| = 1$. Confirm that $1 - Z$

is unitary, equal to 1 at $\{(\begin{smallmatrix} \psi \\ 0 \end{smallmatrix}), (\begin{smallmatrix} 0 \\ \omega \end{smallmatrix})\}^\perp$, but it exchanges $(\begin{smallmatrix} \psi \\ 0 \end{smallmatrix})$ and $(\begin{smallmatrix} 0 \\ \omega \end{smallmatrix})$. The operator $UV(1 - Z)$ (with U of thm.3.2.2 and V of thm.3.5.2) also is a unitary ψ do $\in Op\psi c_0$ decoupling H , with X and Y of (3.3.2) changed by an additional term of order $-\infty$. However, for this decoupling, the energy level λ - formerly belonging to $(\begin{smallmatrix} \psi \\ 0 \end{smallmatrix}) \in \mathcal{H}_+$ - now belongs to $(\begin{smallmatrix} 0 \\ \omega \end{smallmatrix}) \in \mathcal{H}_-$. Also, the level μ now belongs to \mathcal{H}_+ . In other words, the level λ now is positronic, but the level μ is electronic.

Note also, this construction is possible only if both electronic and positronic bound states exist. Somehow, the construction seems to keep track of the total number of electronic and positronic bound states each.

On the other hand the question arises whether our construction also might reach others of the many splits of \mathcal{H} into two orthogonal subspaces left invariant by \mathcal{H} . To illuminate this, let us look at the potential free case and the spectral family of the operator $H_0 = \alpha \cdot D + \beta$. This operator is unitary equivalent to the matrix-multiplication $u(\xi) \rightarrow h_0(\xi)u(\xi) = v(\xi)$, via the Fourier transform. Here $h_0(\xi) = \alpha \cdot \xi + \beta$ has eigenvalues $\pm\langle\xi\rangle$. We need the eigen-projections $p_\pm(\xi) = \frac{1}{2}(1 \pm h_0(\xi)/\langle\xi\rangle)$ of $h_0(\xi)$. The spectral family $\{F(\lambda) : \lambda \in \mathbb{R}\}$ of the multiplication operator $h_0(\xi)$, acting on a subspace of \mathcal{H} , is a matrix-multiplication again. For any $\lambda < -1$ the projection F_λ is given by

$$(3.6.1) \quad u(\xi) \rightarrow p_-(\xi)u(\xi) \text{ as } \langle\xi\rangle > -\lambda, = 0 \text{ as } \langle\xi\rangle \leq -\lambda.$$

In other words, if $\chi_\lambda(\xi)$ denotes the characteristic function of the set $\{|\xi|^2 > \lambda^2 - 1\}$, then the projection F_λ is given by the multiplication $u(\xi) \rightarrow p_-(\xi)\chi_\lambda(\xi)u(\xi)$, where the function $p_-(\xi)\chi_\lambda(\xi)$ has a jump-discontinuity along the sphere $|\xi|^2 = \lambda^2 - 1$, so neither the multiplication operator nor its Fourier transform belong to $Op\psi c_0$. A similar argument shows that the same holds, if $\lambda > 1$. In other words, the partition

$$(3.6.2) \quad \mathcal{H} = F_\lambda(D)\mathcal{H} \oplus (1 - F_\lambda(D))\mathcal{H}$$

(reducing H_0) is not generated by projections which belong to $Op\psi c_0$. However, if a decoupling by a $U \in Op\psi c_0$ were possible, giving the split (3.6.2) as split (3.3.4) then we would arrive at $F_\lambda(D) = U\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}U^* \in Op\psi c_0$ -i.e., a contradiction.

This seems to show that our ψ do-technique above aims at the right kind of split.

Let us summarize:

Theorem 3.6.1 *Let the potentials of H be time-independent and satisfy cdn.(X). Then any λ in the interval $\{|\lambda|, 1\}$ may be regarded as **limit between electronic and positronic states**, in the sense that \mathcal{H}_e and \mathcal{H}_p may be defined as images*

of the spectral projections of H above and below λ , respectively [with a possible eigen-space at λ split arbitrarily].

Any such split may be decoupled by a unitary ψ do $U_\lambda \in Op\psi c_0$, in the sense that

$$(3.6.3) \quad U_\lambda^* H U_\lambda = H^\lambda = \begin{pmatrix} X^\lambda & 0 \\ 0 & Y^\lambda \end{pmatrix},$$

where $U_\lambda, X^\lambda, Y^\lambda$ satisfy the asymptotic expansions of thm.3.2.2, with terms independent of λ - so, differ only by an operator in $\mathcal{O}(-\infty)$.

Here the matrix at right of (3.6.3) is with respect to a split

$$(3.6.4) \quad \mathcal{H} = \mathcal{H}_+^\lambda \oplus \mathcal{H}_-^\lambda,$$

where, in essence, \mathcal{H}_+^λ and \mathcal{H}_-^λ are the spaces $\{(u) \}$ and $\{(v) \}$ with $u, v \in L^2(\mathbb{R}^3, \mathbb{C}^2)$, resp., except that an arbitrary subspace $\mathcal{Z}_\lambda \subset \mathcal{S}(\mathbb{R}^3, \mathbb{C}^2)$ of dimension $|\iota_\lambda|$ must be shifted from one of these spaces to the other one.

The integers-valued function ι_λ is non-increasing. If $\iota_\lambda > 0$ then

$$(3.6.5b) \quad \mathcal{H}_+^\lambda = \{(u) : u \in \mathcal{Z}_\lambda^\perp\}, \quad \mathcal{H}_-^\lambda = \{(v) : v \in L^2(\mathbb{R}^3, \mathbb{C}^3), v \in \mathcal{Z}_\lambda\}.$$

If $\iota_\lambda < 0$ then

$$(3.6.5a) \quad \mathcal{H}_-^\lambda = \{(v) : v \in L^2(\mathbb{R}^3, \mathbb{C}^3), v \in \mathcal{Z}_\lambda\}, \quad \mathcal{H}_+^\lambda = \{(u) : u \in \mathcal{Z}_\lambda^\perp\}.$$

If $\iota_\lambda = 0$ then no correction by shifting a space \mathcal{Z}_λ is necessary.

One might add to thm.3.6.1 that a split $\mathcal{H} = \mathcal{H}_e \oplus \mathcal{H}_p$ in the sense of the theorem might be designed in such a way that any finite orthonormal set of eigenvectors belonging to the interval $|\lambda| < 1$ may be shifted from \mathcal{H}_e to \mathcal{H}_p , or, vice versa.

3.7 Decoupling for Time Dependent Potentials

In chapter 6 we will obtain a complete decoupling of the Dirac operator for a special class of time-dependent potentials - those obtained from a time-independent Hamiltonian by introducing new space-time coordinates, using a Lorentz transform.

In general, if potentials depend on time - so that also $H = H(t)$ is time-dependent, then the Dirac equation will be decoupled by a (time-dependent) unitary ψ do $U(t) \in Op\psi c_0$ such that (not (3.0.8) holds, but, rather)

$$(3.7.1)$$

$$U^*(t)U(t) = U(t)U^*(t) = 1, \quad U^*(t)H(t)U(t) - iU^*(t)\dot{U}(t) = \begin{pmatrix} H_e & 0 \\ 0 & H_p \end{pmatrix} = H^\sim(t),$$

for all t . Indeed, if we then set $u(t) = U(t)v(t)$ into $\dot{u} + H(t)u = 0$ we get $0 = \partial_t(Uv) + iHUv = U\dot{v} + \dot{U}v + iHUv$ i.e., the decoupled equation

$$(3.7.2) \quad \dot{v} + iH\tilde{v} = 0 .$$

Assuming then that we have general time-dependent potentials $\mathbf{V}(t, x), \mathbf{A}(t, x)$ with properties similar to those derivable for Lorentz-transformed time-independent ones, it turns out that a construction similar to that of sec.3.2 will be successful at least in obtaining a decoupling mod $\mathcal{O}(-\infty)$ again. The key to this will be the fact, that the extra term $U^*(t)\dot{U}(t)$ appearing in (3.7.1) can be expected to be of order $-e^2 = e^1 - e$. In other words, the third relation (3.7.1) appears as a perturbation of (3.2.3) by a term of “lower order”, since the main term U^*HU will be of order e^1 . In effect, then, the iteration of sec.3.2 must be modified, but it still will work.

We will require the following assumptions on $\mathbf{V}(t, x), \mathbf{A}(t, x)$:

Condition (XT): \mathbf{V} and \mathbf{A} are C^∞ in t and x , and the time-derivatives $\partial_t^j \mathbf{V}, \partial_t^j \mathbf{A}$ are of polynomial growth in x , of order $-1 - j$, for $j = 0, 1, \dots$. That is, x -derivatives of order l of $\partial_t^j \mathbf{V}$ and $\partial_t^j \mathbf{A}$ are $O((1 + |x|)^{-1-j-l})$, for $j, l = 0, 1, \dots$.

As in sec.3.2 we start with a first approximation, setting $U_0(t) = u_0(t; x, D)$ with $u_0(t; x, \xi) = u(t; x, \xi)$, with the symbol u of (3.2.1), (now also depending on t , since it involves $\mathbf{A} = \mathbf{A}(t, x)$). But the dependence on t is only through $\mathbf{A}(t, x)$, so that \dot{u}_0 is a product¹¹ of $\dot{\mathbf{A}}$ with $\text{grad}_\xi u_0$: This is a symbol in ψ_{c-e^2} , even in ψ_{c-e} , under *cdn.*(X).

Now the equivalent of (3.2.3) may be written as

$$(3.7.3) \quad U_0^*(t)H(t)U_0(t) - iU_0^*\dot{U}_0 - \begin{pmatrix} \Lambda_+ & 0 \\ 0 & \Lambda_- \end{pmatrix} \in \text{Op}\psi_{c-e^2} .$$

However, in (3.7.3), the term $-iU^*\dot{U}$ is of order $-e^2 - e$, so that it just may be omitted: that is, we land at the same (3.2.3) again, with the perturbation just being absorbed by the lower order terms. Since (3.2.2) remains unchanged, we then again may use $u_0 = u$ of (3.2.1) as a 0-th approximation.

As to the induction argument, following (3.2.3), let us just look at the first step: We must construct $V(t) = U_0(t) + \Omega(t)$ with suitable $\Omega(t) = \omega(t; x, D) \in \text{Op}\psi_{c-e}$ such that

$$(3.7.4) \quad V^*V - 1, VV^* - 1 \in \text{Op}\psi_{c-2e}, V^*HV - \Lambda - iV^*\dot{V} \in \text{Op}\psi_{c-e-e^2},$$

with a decoupled Λ .

¹¹ $u_0(x, \xi) = u(x, \xi)$ with $u(x, \xi)$ of (3.2.1) depends only on $\Upsilon = \sigma(\xi - \mathbf{A}(t, x))$ [with $\Upsilon^2 = (\xi - \mathbf{A}(t, x))^2$ a scalar]. Clearly, a time differentiation will produce a symbol of order $-e^2$.

Here the first two conditions (3.7.4) do not differ from those imposed in (3.2.4). So the symbol ω should be chosen according to (3.2.7) again- except that we may add a hermitian symmetric matrix symbol of order $-2e$ to z_1 , since such addition cannot change the first two relations (3.7.4). This is useful, indeed, because for the third (3.7.4) we'd better choose z_1 not as the precise symbol of $1 - U^*U$ [that time-derivative might be difficult to control], but as the first term of the Leibniz expansion (1.0.9) of $\text{symb}(1 - U^*U)$ - i.e., $z_1 = 1 - u_0^*u_0$. That, indeed will make \dot{z}_1 controllable - [in fact, for our present first step we even have $z_1 = \dot{z}_1 = 0$].

Looking at the third (3.7.4), we get

$$\begin{aligned} V^*HV - \Lambda' - iV^*\dot{V} &\equiv \\ (U_0^*HU_0 - \Lambda) + (\Lambda - \Lambda') + (\Omega^*HU_0 + U_0^*H\Omega) - iU_0^*\dot{U}_0 - iU_0^*\dot{\Omega} - i\Omega^*\dot{\Omega} & \pmod{Op\psi c_{-2e}} \\ = \text{I} + \text{II} + \text{III} + \text{IV} + \text{V} + \text{VI} & . \text{ We have set } \Lambda = \lambda(x, D) \text{ with} \\ \lambda = \text{diag}(\lambda_+, \lambda_+, \lambda_-, \lambda_-), \lambda_{\pm} = \mathbf{V} \pm \langle \xi - \mathbf{A} \rangle. & \end{aligned}$$

Here we ignore the terms V and VI, and try determining our Ω by decoupling the symbol of the remaining sum I+II+III+IV, hoping that this will give an Ω with $\dot{\Omega} \in Op\psi c_{-e-e^2}$, so that the terms IV, V terms are $Op\psi c_{-e-e^2}$.

Since we have $z_1 = 0$ in (3.2.7) we must set $\Omega = \omega(t, x, D)$ with $\omega = iu_0\gamma$, where $\gamma \in \psi c_{-e}$ is a hermitian symmetric symbol to be determined.

Now, indeed, the symbol of $\Lambda - \Lambda'$ already is decoupled, by construction. Regarding I: Using Leibniz formulas we will get the leading symbol a finite sum

$-i(u_0^*h_{|\xi}u_0|_x + u_{0|x\xi}^*hu_0 + u_{0|\xi}^*(hu)|_x) \in \psi c_{-e}$, where we note that the time-derivative of this term again belongs to ψc_{-e-e^2} [and one gains another $-e$ for each further “()”]. This follows simply because time dependence is through the variable $\xi - \mathbf{A}(t, x)$ only, and since \mathbf{A} satisfies $\text{cdn.}(XT)$.

Regarding III: Taking again only the leading terms of the Leibniz expansions the symbol of this will be $-i[\lambda, \gamma]$ with above diagonal matrix λ . Setting $\gamma = \begin{pmatrix} \gamma_1 & \gamma_2 \\ \gamma_3 & \gamma_4 \end{pmatrix}$, for a moment we will get $i(\lambda_+ - \lambda_-) \begin{pmatrix} 0 & -\gamma_2 \\ \gamma_3 & 0 \end{pmatrix}$.

Regarding IV: The leading symbol will be $u_0^*\dot{u}_0$. Again any further time-differentiation will generate another “ $-e$ ”.

Setting the sum of the leading symbols of I,II,III,IV equal to 0 then indeed will determine γ - or, rather γ_2 and γ_3 only - while γ_1 and γ_4 are left arbitrary, and we will set them = 0 - in such a way that time-derivatives of order j are of je orders lower.

This is exactly what we need for our iteration. We will not follow through all details of further iterations, which now should be clear in principle.

It also is clear that the removal of $\mathcal{O}(-\infty)$ in the first two relations (3.7.4) - i.e., replacing “ $\in \mathcal{O}(-\infty)$ ” by “= 0” there, to make $U(t)$ unitary will work exactly

as in the proof of thm.3.2.2. We have proven:

Theorem 3.7.1 *Let the potentials \mathbf{V}, \mathbf{A}_j be time-dependent, and assume that $\text{cdn.}(XT)$ holds. Then there exists a unitary ψ do $U(t) = u(t, x, D) \in \text{Op}\psi c_0$ such that the substitution $\psi(t, x) = (U(t)\chi(t))(x, \xi)$ transforms the Dirac equation $\dot{\psi} + H(t)\psi = 0$ into the form*

$$(3.7.5) \quad \dot{\chi} + iH^\Delta(t)\chi = 0 \text{ with } H^\Delta(t) = \begin{pmatrix} \Lambda_+ & 0 \\ 0 & \Lambda_- \end{pmatrix} + \mathcal{O}(-\infty),$$

a decoupling with respect to the split $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ where \mathcal{H}_\pm consist of the 4-vector-valued functions with last two (first two) components equal to 0, respectively.

The two operators $\Lambda_+ = X(t)$ and $\Lambda_- = Y(t)$ possess asymptotic expansions of the form (3.2.12), i.e.,

$$(3.7.6) \quad X(t) = \lambda_+(t, x, D) + X_0(t) , \quad Y(t) = \lambda_-(t, x, D) + Y_0(t) ,$$

with

$$(3.7.7) \quad \lambda_\pm(t, x, \xi) = \mathbf{V}(t, x) \pm \sqrt{1 + (\xi - \mathbf{A}(t, x))^2} ,$$

where now $X_0(t), Y_0(t)$ depend on t , and the expansions may be arbitrarily differentiated for t .

All t -derivatives of the symbol $u(t, x, \xi)$ exist, and are symbols again. Moreover, we have

$$(3.7.8) \quad \partial_t^j u(t, x, \xi) \in \psi c_{-je} \text{ for } j = 0, 1, \dots .$$

Moreover, we have

$$(3.7.9) \quad \partial_t^j X(t) , \partial_t^j Y(t) \in \text{Op}\psi c_{e^1 - je^2} , \quad j = 0, 1, \dots .$$

Chapter 4

Smooth Pseudodifferential Heisenberg Representation

4.0 Introduction

In this and the following chapter we will investigate time-dependence of ψ do-observables when physical states are kept constant in time. In particular we look for “smooth” dependence on t in uniform operators norms (of our weighted Sobolev spaces). Clearly the exponential operator e^{-iHt} - for time-independent H - or, more generally, the evolution operator $U(\tau, t)$ of $H(t)$, are not even continuous in strong operator topology, they are only (what functional analysts call) “strongly continuous”. We shall see that our smoothness translates into a powerful condition on the symbol $a(x, \xi)$ of a ψ do, which is not passed by many observables. In a sense, the rejected observables experience some kind of “Zitterbewegung”.

This investigation raises a variety of formal questions, possibly of strong physical interest. These are studied in the present chapter, while in ch.5 we will attempt a mathematically rigorous discussion.

We already pointed to the fact that the observables with smooth Heisenberg representation are closely related to the “precisely predictable observables”, i.e., the operators splitting under our rigorous decoupling of ch.3 (cf. thm.3.3.1). In fact, we will find that **all** precisely predictable observables may be found by departing from a symbol $q(x, \xi)$ commuting with the symbol $h(x, \xi)$ of the Hamiltonian H , for all x, ξ , and going through an iterative construction of lower and lower order corrections $z_1(x, \xi), z_2(x, \xi), \dots$, to be added to $q(x, D)$. Then, finally, we still must add a correction $z_\infty(x, \xi)$ of order $-\infty$ to the asymptotic sum $q + \sum_1^\infty z_j$, to

arrive at a symbol $a(x, \xi) = q + \sum_1^\infty z_j + z_\infty$ such that the self-adjoint operator $A = \frac{1}{2}\{a(x, D) + a(x, D)\}$ gives a precisely predictable observable.

This procedure is mathematically correct, but, in general, will supply a practically inaccessible symbol $a(x, \xi)$. Normally it will be possible to obtain only the first correction $z_1(x, \xi)$, in some special cases we also control the second (or even the third). To attempt some Physics, we thus will work with $a(x, \xi) = q(x, \xi) + z(x, \xi)$ where we set $z = z_1$ (or, perhaps, $z = z_1 + z_2$, if z_2 is explicitly available).

With this principle in mind we will lay out the construction of (the first corrections) z_1, z_2 only, in this chapter, and investigate standard dynamical observables, like location, momentum, etc. In many cases we may choose the initial symbol $q(x, \xi)$ as the symbol of the (not precisely predictable) observable in question - for location, we use $q(x, \xi) = x_1$ - the symbol of the multiplication operator $u(x) \rightarrow x_1 u(x)$, with the first location coordinate x_1 . This works because the scalar function x_1 trivially commutes with the matrix $h(x, \xi)$.

For other observables - such as the spin - this is not possible. But this only means that we may predict the spin **only** if we know with certainty that the particle is an electron - not a positron (or vice versa). In other words, we must be sure that the corresponding physical state belongs either to \mathcal{H}_e or to \mathcal{H}_p (of the decomposition (3.0.5)).

It turns out, that this smoothness of the Heisenberg representation, and even the construction of only the first correction z_1 will provide a rather perfect connection between classical and quantum physics, insofar as it entails a “geometrical optics”: The smooth propagation of a precisely predictable symbol goes along “light rays”- the classical orbits - and this propagation **also incorporates the propagation of the spin** as a magnetic moment in the electromagnetic field of the given potentials. This we will work out in sec.4.6.

In ch.5, below, we then will focus on a mathematically complete construction of our algebras \mathcal{P} , \mathcal{PA} of precisely predictable observables, proving a variety of theorems.

Finally, at this place, we perhaps might point to a logical complication showing up only if potentials depend on time - so, it never appeared in our previous presentations of this material: “Prediction of an observable” usually means that we focus on a given observable A valid for all times - such as the location coordinates x . For a given physical state ψ at time $t = 0$ we want to predict location at some (or at every) later time t - this would be the quantum mechanical equivalent of predicting the orbit of the particle. Using Heisenberg representation this means that we want to look at the expectation value \check{A}_t of the operator $A_t = U(t, 0)AU(0, t)$ - with $A = x$ and the evolution operator $U(\tau, t)$ of the Dirac equation - in the state

ψ . But our above “smoothness condition” addresses itself not to above A_t but to (smoothness in t of) the map $A \rightarrow U(0, t)AU(t, 0)$, we shall call the “inverse Heisenberg transform”. If potentials are time-independent then the two above transforms are just given by $e^{iHt}Ae^{-iHt}$ and $e^{-iHt}Ae^{iHt}$ – involving just a change from t to $-t$, not affecting differentiability. But, if potentials depend on time then it is convenient for us to use the inverse Heisenberg transform.

4.1 Dirac Evolution with Time-Dependent Potentials

Note that the Dirac Hamiltonian H of (1.0.2) belongs to $Op\psi c$ if we assume that the potentials \mathbf{V}, \mathbf{A}_j are of polynomial growth¹ in x , for every fixed time t . In fact, we get $H = H(t) \in Op\psi c_m$ with $m = (1, N) = e^1 + Ne^2$ with the N mentioned there. Clearly $H(t)$ is formally self-adjoint. As in ch.3 we generally assume $\text{cdn.}(X)$, i.e., that $N = -1$:

The potentials \mathbf{V}, \mathbf{A}_j of H are $C^\infty(\mathbb{R}^3)$, and their derivatives of order k are $O((1 + |x|)^{-1-k})$ for all $k = 0, 1, \dots$

Recall, the operators $H(t)$ then are md-elliptic of order $e^1 = (1, 0)$. Indeed, the symbol of $K = H\langle D \rangle^{-1}$ will be $k = \sum \alpha_j s_j(\xi) + (\beta + \gamma(x))\langle \xi \rangle^{-1}$ with $\gamma(x) = \mathbf{V}(x) - \sum \alpha_j \mathbf{A}_j(x)$. For $|\xi| = \infty$ we have $\langle \xi \rangle^{-1} = 0$ and $\sum s_j^2(\xi) = \frac{\xi^2}{1+\xi^2} = 1$, so that $k^2(x, \xi) = 1 \Rightarrow k(x, \xi)$ is invertible with bounded inverse. For $|x| = \infty$ we have $\gamma(x) = 0$, hence $h(x, \xi) = h_0(x, \xi) \Rightarrow k^2 = k^*k = 1 \Rightarrow |k^{-1}| = 1$. Thus $h(x, \xi)\langle \xi \rangle^{-1}$ is md-elliptic of order 0 $\Rightarrow H$ and h are md-elliptic of order e^1 . The same may be stated for the operators $H \pm i$ - For $(h \pm i)\langle \xi \rangle^{-1}$ there is no change, as $|\xi| = \infty$, while for $|x| = \infty$ we get $h_0(x, \xi) \pm i$ nonsingular, since the matrix h_0 is hermitian. One concludes that $H(t)$ has a unique self-adjoint realization² with domain $\text{dom } H(t) = \mathcal{H}_{e^1}$.

Assume first that $H(t) = H$ is independent of t . We then conclude existence of the (unitary) group e^{-iHt} (cf. [Ka1], ch.9 for example, or just apply the spectral decomposition theorem for the self-adjoint H) as evolution operator of the Dirac

¹Recall, this means that x -derivatives of order j are $O((1 + |x|)^{(N-j)})$ for some N , called the order.

²We know that $(H \pm i) : \mathcal{H}_{e^1} \rightarrow \mathcal{H}$ while $\|(H \pm i)u\|^2 = \|Hu\|^2 + \|u\|^2 \geq \|u\|^2 \Rightarrow H \pm i$ is 1 to 1. Let $f \in \mathcal{H}$ and $\langle f, (H + i)u \rangle = 0$ for all $u \in \mathcal{H}_{e^1}$. But $H + i$ has a K-parametrix $E \in Op\psi c_{-e^1}$ with $(H + i)E = 1 + K$, $K \in \mathcal{O}(-\infty)$. Substitute $u = Ev$, $v \in \mathcal{S}$, for $\langle f, v + Kv \rangle = 0$ valid for all $v \in \mathcal{S}$. This yields $f = -k^*f \in \mathcal{S} \subset \mathcal{H}_{e^1} = \text{dom}(H)$. But then get $(H - i)f = 0 \Rightarrow f = 0$. Thus the image of $H + i$ is dense in \mathcal{H} , hence $= \mathcal{H}$. Similarly for $H - i$ which implies H self-adjoint. [For another proof cf. ch.3, footnote 5.]

equation (1.0.1) in the Hilbert space \mathcal{H} . In particular, for $u(t) = e^{-iHt}u_0$, $u_0 \in \text{dom}(H) = \mathcal{H}_{e^1}$ the derivative $\partial_t u(t)$ exists in \mathcal{H} and $u(t)$ solves (1.0.1), and e^{-iHt} is strongly (but not uniformly) continuous in t .

Now, we may use the same argument to also conclude that the group e^{-iHt} is well defined (strongly continuous) in every \mathcal{H}_s , with $\text{dom}_s(H) = \mathcal{H}_{s+e^1}$ - $u(t) = e^{-iHt}u_0$ differentiable in \mathcal{H}_s for $u_0 \in \mathcal{H}_{s-e^1}$. The point is that, with $\Lambda_s = \langle x \rangle^{s_2} \langle D \rangle^{s_1}$ of (1.4.2), (1.4.3) and $H_s = \Lambda_s H \Lambda_s^{-1}$, and $u(t)$ solving (1.0.1) in \mathcal{H}_s we get $u_s(t)$ to solve $\partial_t u_s(t) + iH_s u_s(t) = 0$ in \mathcal{H} . Clearly $H_s = H + P_s$ where $P_s \in \text{Op}sc_{-e^2} \subset \text{Op}\psi c_0$ is bounded in \mathcal{H} . We again get $H_s + \lambda$ md-elliptic of order e^1 , for all $\Im(\lambda) \neq 0$, while $\|(H_s + \lambda)u\| \geq \|(H + \lambda)u\| - \|P_s u\| \geq (|\Im(\lambda)| - \|P_s\|)\|u\|$, for $u \in \mathcal{S}$ and $|\Im(\lambda)| > \|P_s\|$. The latter implies that $H_s + \lambda$ is 1 to 1 in \mathcal{S} while md-ellipticity implies that the orthocomplement of the range belongs to \mathcal{S} , so that it must be 0, i.e. the resolvent $(H_s + \lambda)^{-1}$ exists for $|\Im(\lambda)| > \|P_s\|$, and this gives existence of $e^{-iH_s t}$. In turn we thus get existence of e^{iHt} as strongly continuous group on \mathcal{H}_s , for every s . [But, of course, e^{-iHt} no longer is unitary there. Rather, we get an estimate $\|e^{-iHt}\| = O(e^{c_s|t|})$ with some constant c_s .] Conclude thus that e^{-iHt} is defined as an operator acting on all temperate distributions $u \in \mathcal{S}' = \cup \mathcal{H}_s$, as an operator³ of order 0.

With time-dependent potentials we no longer may think of a group e^{-iHt} but, instead, will get an “evolution operator” $U(\tau, t)$ such that $u_\tau(t) = U(\tau, t)u_0$ solves the initial-value problem

$$(4.1.1) \quad \partial_t u_\tau(t) + iH(t)u_\tau(t) = 0, \quad t \in \mathbb{R}, \quad u_\tau(\tau) = u_0.$$

We quote the result below - as special case of [Co5], ch.6, thm.3.1. Its proof uses a different technique: First use a Friedrich’s-type “mollifier” to “regularize” the symbol $h(t)$ of $H(t)$ to get an operator $H_\varepsilon(t)$ of order 0, allowing Picard’s theorem for solving the formal ODE (1.0.1). Then pass to the limit $\varepsilon \rightarrow 0$, using the Arzela-Ascoli theorem, where it is essential that commutators with Λ_s of matrix-valued operators of order m are of order $s + m - e$ while Λ_{-e} is compact, giving the necessary compactness for Arzela-Ascoli.

³Recall from sec.1.4, a continuous operator $A : \mathcal{S}' \rightarrow \mathcal{S}'$ will be said to be “of order $m = (m_1, m_2)$ ” if its restriction to \mathcal{H}_s is continuous as a map $\mathcal{H}_s \rightarrow \mathcal{H}_{s-m}$ for all s . Note then that the ψ do-s in $\text{Op}\psi c_m$ all are of order m . Vice versa, of course, an operator $\mathcal{S}' \rightarrow \mathcal{S}'$ of order m does not have to be a strictly classical ψ do. For example, let $A = e^{i\langle D \rangle}$. We may think of A as a ψ do with symbol $a(x, \xi) = e^{i\langle \xi \rangle}$. But this symbol clearly does not belong to ψc . On the other hand, the family $A_t = e^{i\langle D \rangle t}$ solves the differential equation $\dot{A}_t - i\langle D \rangle t A_t = 0$. An argument as above shows that $\|A_t\|_s = O(e^{c_s|t|})$ for all s , so that, indeed, A is of order 0. Similarly, it is easily verified that $e^{-iH_0 t}$ is not a ψ do in $\text{Op}\psi c$, while, of course, it may be written formally as a ψ do. Such operators may be elegantly treated replacing $e^{ix\xi}$ by $e^{i\varphi(x, \xi)}$ with a different “phase function” $\varphi(x, \xi)$. They are called “Fourier integral operators” (FIO-s) (cf. [Ta1], [Tr1]). In general, the operators e^{-iH} , under our cnd.(X) on potentials, will be FIO-s.

Theorem 4.1.1 *Let us assume that the potentials \mathbf{V}, \mathbf{A}_j and their time-derivatives $\partial_t^l \mathbf{V}, \partial_t^l \mathbf{A}_j$, $l = 1, 2, \dots$, all satisfy *cdn.*(X) - x -derivatives of order k decay like $(1 + |x|)^{-1-k}$, for all k .*

Then there exists a unique “evolution operator” $U(\tau, t) \in \mathcal{O}(0)$ [of order 0], defined for all $\tau, t \in \mathbb{R}$, and such that

$$(4.1.2) \quad U(\tau, \tau) = 1, \quad U(t, \kappa)U(\tau, t) = U(\tau, \kappa), \quad U(t, \tau)U(\tau, t) = 1,$$

for all $\kappa, \tau, t \in \mathbb{R}$, and such that $U(\tau, t)$ satisfies the two abstract ODE-s

$$(4.1.3) \quad \partial_t U(\tau, t) + iH(t)U(\tau, t) = 0, \quad \partial_\tau U(\tau, t) - iU(\tau, t)H(\tau) = 0,$$

for all τ, t . In particular, the function $U(\tau, t)$ is strongly continuous in $L(\mathcal{H}_s)$ for all $s \in \mathbb{R}^2$, and its derivatives $\partial_\tau^j \partial_t^l U(\tau, t)$ exist in strong convergence of $L(\mathcal{H}_s, \mathcal{H}_{s-(j+l)e^1})$, and they are strongly continuous as operators $\mathcal{H}_s \rightarrow \mathcal{H}_{s-(j+l)e^1}$ for all $s \in \mathbb{R}^2$. In particular, these derivatives are operators of order $(j + l)e^1$.

Note: *Even though the evolution operator $U(\tau, t)$ (or, for time-independent H the operator e^{-iHt}) are operators of order 0 they are **not** ψ do-s in $Op\psi c_0$. Already for vanishing potentials we may formally write $P = e^{-iHt}$ as a ψ do $P = p(x, D)$ with symbol $p(x, \xi) = e^{-ith_0(\xi)}$ (with the matrix $h_0(\xi)$ of (3.1.2)) independent of x . However, this symbol does not belong to ψc_0 - although it indeed belongs to the algebra ψt_0 of thm.2.1.1. Especially, our Leibniz formulas (1.0.8),(1.0.9) are not valid for such operators - i.e. the asymptotic convergence fails. One may find a more complicated calculus of symbols for similar operators in [Hoe3],[Ta1],[Tr1]. But we will not require this here.*

Returning to quantum mechanics, in the “Heisenberg representation” we assume that physical states - the unit vectors ψ of \mathcal{H} - are constant in time, while observables - the unbounded self-adjoint operators A acting on a dense subspace of \mathcal{H} - propagate by the formula⁴

$$(4.1.4) \quad A \rightarrow A_t = U(\tau, t)AU(t, \tau)$$

while t propagates from τ to t .

⁴With “Schrödinger’s representation” the observables stay constant in time while the physical states propagate, in the sense that $\psi_0 \in \mathcal{H}$ at $t = 0$ propagates into $\psi(t)$ at time t , where $\psi(t)$ is the solution of $\dot{\psi} + iH\psi = 0$ satisfying $\psi(0) = \psi_0$. That is, we have $\psi(t) = U(0, t)\psi_0$ (that is, $\psi(t) = e^{-iHt}\psi_0$ for time-independent H).

Now, either we are given a state ψ_0 at $t = 0$ and want to predict a given observable A at some later time t . [This might be the normal situation: Certain well known “dynamical observables” are given as well defined operators at any time - such as location, momentum,..., and one might want to predict their propagation in time.] At time t the expectation value \check{A}_t of A in the (thus

In the following we now will not admit the most general self-adjoint operator A as observable, but assume that, in addition, A must be (represented by) a self-adjoint pseudodifferential operator⁵ in $Op\psi c_m$, for some m .

Such restriction seems natural, in view of our discussion in ch.2, noting that an observable should be “insensitive” against translations, dilations, rotations, both in configuration space and in momentum space.

The selection of “useful” observables will be further restricted by asking for “smooth” dependence of the function $A \rightarrow A_t$ with respect to the variable t . While this might be felt to be a natural condition, we also might point to the fact that just the “Zitterbewegung” experienced by observables like ‘location’ might be interpreted as “non-smoothness” of that observable.

So, this seems to point at one of the most important obstacles to Dirac’s theory. More precisely we have in mind asking for two further restrictions:

Starting with a ψ do $A \in Op\psi c_m$ the (inverse) Heisenberg transform A_t of (4.1.4) should again be a ψ do in ψc_m .

And, A_t should depend smoothly on t - in a sense to be specified.

[In particular, its symbol $a_t(x, \xi)$ should be smooth in t .]

4.2 Observables with Smooth Heisenberg Representation

In this section we will allow time-dependent potentials satisfying *cdn.*(X) with all their time-derivatives, for all $t \in \mathbb{R}$. Mainly we focus on the Hamiltonian $H(t)$ of (1.0.2) again⁶.

propagated) state $\psi(t)$ will be $\check{A}_t = \langle \psi(t), A\psi(t) \rangle = \langle \psi_0, A_t\psi_0 \rangle$ with $A_t = U(t, 0)AU(0, t)$ (i.e., $A_t = e^{iHt}Ae^{-iHt}$, for time-independent H).

Or else, the state $\psi(t) = \psi_t$ at time t might be given, and one might want to get information on A in the original state ψ_0 . Then we get $\check{A}_0 = \langle \psi_t, U(0, t)AU(t, 0)\psi_t \rangle$, (i.e., $e^{-iHt}Ae^{iHt}$ for time-independent H).

If we now work with general time-dependent $H(t)$ then we must use (4.1.4) as propagation formula for observables, while the “other” map $A \rightarrow U(t, 0)AU(0, t)$ really gives the “Heisenberg representation”. For time-independent H this just is a matter of sign reversal of t . But for general $H(t)$ dependence of U on t and τ is slightly different, because we no longer have $H(t)$ commuting with $H(\tau)$ as $\tau \neq t$.

⁵There is the question of uniqueness of self-adjoint realizations of such an operator [For example the scalar operator $L = \partial_x^2 + x^4$ (in one x -variable will have many self-adjoint realizations (cf. [Ti1], thm.5.11 - there is limit circle case then), but only one of them would qualify as a strictly classical ψ do. as an investigation shows.] We leave this point without a general answer, noting that our ψ do-s have their natural extension to S' which also should specify their self-adjoint extension under consideration. In particular, this question seems trivially answered for the standard dynamical observables.

By thm.4.1.1 the differential equation (1.0.1) - i.e. $\dot{u}(t) + iH(t)u(t) = 0$, has an evolution operator $U(\tau, t)$ of order 0, where $U|_t, U|_\tau$ are of order e^1 , assuming only that also the differentiated potentials $\partial_t^j V, \partial_t^j A_j$, $j = 0, 1, \dots$, all satisfy cdn.(X) The operator $U(\tau, t)$ satisfies

$$(4.2.1) \quad \partial_t U(\tau, t) + iH(t)U(\tau, t) = 0, \text{ and } , \partial_\tau U(\tau, t) - iU(\tau, t)H(\tau) = 0,$$

and,

$$(4.2.2) \quad U(\tau, \tau) = 1, \quad U(\kappa, t)U(\tau, \kappa) = U(\tau, t), \quad U(t, \tau)U(\tau, t) = 1, \quad t, \tau, \kappa \in \mathbb{R}.$$

In the special case of time-independence we just have $U(\tau, t) = e^{-i(t-\tau)H}$.

For a first approach, look at the “propagation”

$$(4.2.3) \quad A_{\tau t} = U(\tau, t)AU(t, \tau)$$

of some linear operator A . [The physical state u is transformed back from time t to time τ , then the observable A is applied, and then we transform forward again, from τ to t (see also footnote 4) - this is what we called the inverse Heisenberg representation] A formal differentiation of (4.2.3) produces

$$(4.2.4) \quad \partial_t A_{\tau t} = -i[H(t), A_{\tau t}], \quad A_{\tau \tau} = A.$$

Under our present assumptions we may translate τ into 0. We thus will keep $\tau = 0$ fixed and write $A_{0t} = A_t$ and $\partial_t a = \dot{a}$, to simplify notation. Recall, $U(\tau, t)$ normally will not be a ψ do in $Op\psi c$. Thus we cannot normally expect A_t to be in $Op\psi c$, even if we assume $A \in Op\psi c$. However, there will be a special class of operators $A \in Op\psi c$ with the property that also $A_t \in Op\psi c$ for all t . Assuming that A belongs to that class, we may approach (4.2.4) symbol-wise: Let $A = a(x, D)$ with $a(x, \xi) \in \psi c_m$, and then assume $A_t = a_t(x, \xi)$ with $a_t \in \psi c_m$. Using calculus of ψ do-s we may express the symbol of the commutator $[H(t), A_t]$ by an asymptotic series

$$(4.2.5) \quad \text{symb}([H(t), A_t]) = [h, a_t] + \sum_{j=1}^{\infty} \frac{(-i)^j}{j!} \{h, a_t\}_j,$$

with the “Poisson brackets”

$$(4.2.6) \quad \{a, b\}_1 = \{a, b\} = a|_\xi b|_x - b|_\xi a|_x, \quad \{a, b\}_2 = a|_{\xi\xi} b|_{xx} - b|_{\xi\xi} a|_{xx}, \text{ etc.}, \dots$$

⁶However, (with proper modification) this just as well applies to the case where H is replaced by a more general self-adjoint ψ do K of order e^1 - such as the FW-transformed H (i.e., $K = U^*HU$) of (3.0.7). Existence of the evolution operator (or of e^{-iKt} , for time-independent K) again follows with the techniques of sec.4.1, under proper assumptions on the time-derivatives of the symbol.

Thus (4.2.4) may be stated by writing

$$(4.2.7) \quad \partial_t a_t = -i[h(t), a_t] - \{h(t), a_t\} + \frac{i}{2}\{h(t), a_t\}_2 + \dots$$

where the first term at right tends to be of order higher than m , unless we assume some kind of commutativity between $h(t)$ and a_t . Our assumption of “smoothness” of the (inverse) Heisenberg representation will include that (i) a and a_t are symbols of (strictly classical) ψ do-s of the same order m , and that, moreover, (ii) \dot{a}_t even is a symbol of order $m - e^2$. With this, (4.2.7) implies that the commutator $[h(t), a_t]$ must be of order $m - e^2$ as well. Especially, the terms of the asymptotic sum, at right, are of order $m - e^2, m - e^2 - e, m - e^2 - 2e, \dots$, so the sum also is of order $m - e^2$.

The above implies that there is a clean split of a_t into a sum

$$(4.2.8) \quad a_t = q_t + z_t, \text{ with } q_t = p_+ a_t p_+ + p_- a_t p_-, \quad z_t = p_+ a_t p_- + p_- a_t p_+,$$

where q_t commutes with $h(t)$ while z_t is of order $m - e$.

In (4.2.8) we have used the projections $p_{\pm} = p_{\pm}(t)$ of the spectral decomposition of (the 4×4 -matrices) $h(t)$. In particular we have

$$(4.2.9) \quad h = \lambda_+ p_+ + \lambda_- p_- \quad \text{where} \quad p_{\pm} = \frac{1}{2} \left(1 \pm \frac{h_0(\zeta)}{\langle \zeta \rangle} \right),$$

with $\zeta = \xi - A(t, x)$, $h_0(\zeta) = \alpha\zeta + \beta$. Note p_{\pm} are orthogonal 4×4 -projection matrices of rank 2 commuting with $h(t)$, for all t, x, ξ and with

$$(4.2.10) \quad p_{\pm}^* = p_{\pm}, \quad p_{\pm}^2 = p_{\pm}, \quad p_+ p_- = p_- p_+ = 0, \quad p_+ + p_- = 1, \quad x, \xi \in \mathbb{R}^3, \quad t \in \mathbb{R}.$$

One should keep in mind that p_{\pm} depend on t if the potentials are time-dependent.

Clearly the p_{\pm} are symbols in ψc_0 , so q_t of (4.2.8) belongs to ψc_m while evidently $[h(t), q_t] = 0$ for all t, x, ξ . On the other hand one confirms⁷ that $z_t \in \psi c_{m-e}$.

With the split (4.2.8) eq. (4.2.7) (and the initial condition $A_0 = A$) assume the form

$$(4.2.11) \quad \dot{q}_t + \dot{z}_t \equiv -i[h(t), z_t] - \{h(t), q_t\} \pmod{\psi c_{m-e^2-e}}, \quad q_0 = q, \quad z_0 = z,$$

noting that the terms at right of (4.2.7) are of order $m + e^1, m - e^2, m - e^2 - e, m - e_2 - 2e, \dots$, and with $q = p_+ a p_+ + p_- a p_-$, $z = p_+ a p_- + p_- a p_+$. Then we treat

⁷The eigenvalues of $h = \alpha \cdot (\xi - \mathbf{A}) + \beta + \mathbf{V}$ are $\lambda_{\pm} = \pm \langle \xi - \mathbf{A} \rangle + \mathbf{V}$. Hence $\lambda_+ - \lambda_- = 2\langle \xi - \mathbf{A} \rangle$, and one computes that $z_t = \frac{1}{2} \{ p_+ [h, a_t] p_- - p_- [h, a_t] p_+ \} / \langle \xi - \mathbf{A} \rangle$. Since we know that $[h(t), a_t] \in \psi c_{m-e^2}$, it indeed follows that $z_t \in \psi c_{m-e}$.

(4.2.11) as a sharp (commutator) equation for the symbol $z(x, \xi)$ - still dropping \dot{z} as to be of lower order (which has to be checked, after solving), In other words, we try to determine an approximate q_t and z_t as solutions of the (sharp) equation

$$(4.2.12) \quad [h(t), z_t] = i(\dot{q}_t + \{h(t), q_t\}) = w_t \quad , \quad q_0 = q \quad , \quad z_0 = z \quad .$$

It will be found that the symbol q_t is *uniquely determined* just by its initial value $q_0 = q$ and the conditions to be imposed to make (4.2.12) solvable with some z_t . The initial value q may be *any* symbol in ψc_m (for some given m) commuting with the symbol $h(0)$ for all x, ξ . Once q_t is found, we then get a formula for the possible symbols z_t , where one confirms that $z_t \in \psi c_{m-e}$ and even $\dot{z} \in \psi c_{m-e-e^2}$, so that indeed $q_t + z_t$ satisfies (4.2.11), as a first approximation of (4.2.7). Then we will seek the next approximation by going with the Ansatz $a_t = q_t + z_t + w_t$ into eq. (4.2.7) where now the symbol $w_t \in \psi c_{m-2e}$ is to be found. Again some approximative commutator equation similar to (4.2.11) will have to be solved, Some further condition on z_t will have to be imposed to make that equation solvable. In this way, iterating the procedure, we will get an infinite number of corrections, of lower and lower order. Their asymptotic sum will satisfy (4.2.8) mod $\psi c_{-\infty}$ - that is, mod $\mathcal{O}(-\infty)$. But *every* operator in $\mathcal{O}(-\infty)$ is a strictly classical ψ do, and $\mathcal{O}(-\infty)$ is an ideal of $\mathcal{O}(0)$. Since $U(\tau, t) \in \mathcal{O}(0)$ one then concludes that (4.2.4) and (4.2.3) hold sharply.

All of the discussion of higher order approximations will be postponed to ch.5, however. Here we only look at the construction of q_t and z_t as solutions of the sharp equation (4.2.12), starting with some arbitrary q commuting with $h(0)$.

Since $q_t(x, \xi)$ commutes with $h(t)$, it leaves the eigenspaces $S_{\pm} = \text{im}(p_{\pm}(t, x, \xi))$ invariant, and we must be able to write

$$(4.2.13) \quad q_t = q_t^+ p_+ + q_t^- p_-$$

with linear maps $q_t^{\pm} : S_{\pm} \rightarrow S_{\pm}$.

First assume (as additional condition) that these $q_t^{\pm}(x, \xi)$ are multiples of the 4×4 -identity matrix. [We shall find that this Ansatz leads to a solution if only the initial value q_0 has that property. All scalar dynamical observables (with symbol a multiple of the 4×4 -identity) have this property, so it might be worthwhile to look at it.]

Given a symbol $q_t \in \psi c_m$ with $[h(t), q_t] = 0$ the commutator equation (4.2.12) will be solvable with some $z(x, \xi)$ if and only if we have the conditions

$$(4.2.14) \quad p_+(t)(\dot{q}_t + \{h(t), q_t\})p_+(t) = 0 \quad , \quad p_-(t)(\dot{q}_t + \{h(t), q_t\})p_-(t) = 0 \quad ,$$

for all x, ξ, t . Assuming (4.2.14) we get all solutions of eq. (4.2.12) in the form

$$(4.2.15) \quad z_t = c_+ + c_- + \frac{1}{\lambda_+ - \lambda_-} \{p_+ w_t p_- - p_- w_t p_+\}, \quad \lambda_+ - \lambda_- = 2\langle \xi - A(t, x) \rangle .$$

with w_t of (4.2.12), and arbitrary matrices $c_{\pm} = c_{\pm}^t(x, \xi)$ satisfying $c_{\pm} = p_{\pm} c_{\pm} p_{\pm}$. It turns out, looking at higher iterations, that the c^t are arbitrary for $t = 0$ but they have to satisfy some conditions for $t \neq 0$. Now we have

Proposition 4.2.1 *Assume that above q_t^{\pm} are scalar multiples of the 2×2 -identity. Then the conditions (4.2.14) just mean that the two (complex-valued) symbols $q_t^{\pm}(x, \xi)$ satisfy the equations*

$$(4.2.16) \quad \dot{q}_t^+ + \{\lambda_+, q_t^+\} = 0 \quad , \quad \dot{q}_t^- + \{\lambda_-, q_t^-\} = 0 \quad ,$$

with Poisson brackets $\{\cdot, \cdot\} = \{\cdot, \cdot\}_1$ of (4.2.6.).

Note that eq.s (4.2.16)) give two scalar first order PDE-s (with real coefficients) for the two complex-valued functions $q_t^{\pm}(x, \xi)$ of 7 variables t, x, ξ . Each involves only one of the functions q_t^{\pm} ; they are independent of each other. Together with the initial conditions $q_0^{\pm}(x, \xi) = q^{\pm}(x, \xi)$ they will determine unique solutions $q_t^{\pm}(x, \xi)$, defined for all t, x, ξ .

This kind of initial-value problem will be shortly discussed at the end of this section (together with a proof for prop.4.2.1). But a detailed study will be found in sec.5.5. As a consequence of the discussion there we have

Proposition 4.2.2 *Each of the two (scalar first order) PDE-s (4.2.16) has a unique solution $q_t^{\pm}(x, \xi)$ assuming the initial value $q_t^{\pm}(x, \xi) = q^{\pm}(x, \xi)$ at $t = 0$. They are smooth functions of all variables x, ξ, t if they are smooth in x, ξ initially - for $t = 0$. Moreover, an initial symbol $q^{\pm}(x, \xi) \in \psi c_m$ generates a solution q_t^{\pm} which remains in ψc_m for all t .*

Let us assume this proposition for now.

Note, it is an automatic consequence of the DE (4.2.16) that we have $\dot{q}_t^{\pm} \in \psi c_{m-e^2}$ if $q_t^{\pm} \in \psi c_m$, as asserted by prop.4.2.2. This is, because the operation $\{\lambda_{\pm}, \cdot\}$ lowers the order of a symbol by e^2 . Moreover, differentiating (4.2.16) for t we get $\ddot{q}_t = -\{\dot{\lambda}, q_t\} - \{\lambda, \dot{q}_t\} \in \psi c_{m-2e^2}$. And this may be iterated for

$$(4.2.17) \quad \partial_t^j q_t^{\pm}(x, \xi) \in \psi c_{m-je^2} \quad , \quad j = 0, 1, \dots .$$

Notice that prop.4.2.2 and (4.2.17) and the formula (4.2.15) for z_t imply that q_t and z_t constructed from fla-s (4.2.16) with initial value $q = q^+ p_+ + q^- p_-$ (where q^{\pm} are scalar symbols in ψc_m) define a $q_t \in \psi c_m$ with $\dot{q}_t \in \psi c_{m-e^2}$, while we

indeed also get $z_t \in \psi c_{m-e}$ and $\dot{z}_t \in \psi c_{m-e-e^2}$, assuming that the c_{\pm}^t are properly selected. Later analysis of further corrections (in ch.5) will show that selection of c_{\pm}^0 is free (and we usually will set $c_{\pm}^0 = 0$, since we want a correction of a given commuting symbol). However, for $t \neq 0$ the c_{\pm}^t will have to satisfy a condition, to be discussed in thm.5.1.1.

Apart from this “open end”, however, it is clear that we get a well defined q_t and z_t with $z_t \in \psi c_{m-e}$, $\dot{z}_t \in \psi c_{m-e-e^2}$ such that eq. (4.2.7) holds mod(ψc_{m-e-e^2}) for $a_t = q_t + z_t$. [Later construction of further corrections may fix the choice of c_{\pm}^t but within ψc_{m-e-e^2} , and not for $t = 0$.]

In this way we have constructed a *first order corrected symbol* $a_t^{\sim} = q_t + z_t$ - and, in particular, an “initial correction” $z = z_0$ to any symbol $q \in \psi c_m$ commuting with $h(0)$ for every x, ξ , and which is scalar in the two spaces $S_{\pm}(0, x, \xi)$. Moreover the propagated symbol still has the same property - it splits into a sum $q_t + z_t$ where q_t commutes with $h(t)$, and is scalar in $S_{\pm}(t, x, \xi)$ while z_t is of lower order $m - e$.

But the correction is *not complete* insofar as (4.2.4) is valid only mod ($Op\psi c_{m-e-e^2}$).

In sec.4.3, below, we shall apply this result to construct first order corrections for a variety of well known dynamical observables, all with the property that (i) they belong to $Op\psi c_m$, for some m , and (ii) their symbol is scalar in the two eigenspaces of the symbol of the Hamiltonian.

Proof of prop.4.2.1. Using the indices j, l, r to indicate either “+” or “-” we get

$$(4.2.18) \quad p_j \dot{p}_l = -\dot{p}_j p_l + \dot{p}_j \delta_{jl} ,$$

by differentiating (4.2.10), and corresponding formulas for x - (or ξ -) derivatives. This implies

$$(4.2.19) \quad p_l \dot{p}_r p_l = -\dot{p}_l p_r p_l + \dot{p}_l p_l \delta_{lr} = 0 ,$$

and, similarly,

$$(4.2.20) \quad p_j p_r |x p_j = p_j p_r | \xi p_j = 0 .$$

Also,

$$(4.2.21) \quad p_l \dot{q} p_l = \sum_r p_l \dot{q}_r p_r p_l + \sum_r q_r p_l \dot{p}_r p_l = \dot{q} p_l .$$

Next, we also find that

$$(4.2.22) \quad p_l \{p_j, p_r\} p_l = 0 ,$$

because the left hand side equals equals

$$\begin{aligned} &= p_l p_j |_{\xi} p_r |_x - p_l p_r |_{\xi} p_j |_x p_l \\ &= -p_l |_{\xi} p_j p_r |_x p_l + \delta_{jl} p_l |_{\xi} p_r |_x p_l + p_l |_{\xi} p_r p_j |_x p_l - \delta_{lr} p_l |_{\xi} p_j |_x p_l \\ &= p_l |_{\xi} p_j |_x p_r p_l - p_l |_{\xi} p_r |_x p_l \delta_{jr} + \delta_{jl} p_l |_{\xi} p_r |_x p_l \\ &\quad - p_l |_{\xi} p_r |_x p_j p_l + p_l |_{\xi} p_r |_x p_l \delta_{rj} - \delta_{lr} p_l |_{\xi} p_j |_x p_l = 0 . \end{aligned}$$

Accordingly,

$$\begin{aligned} &p_l \{h, q\} p_l \\ &= \sum_{j,r} p_l \{(\lambda_j |_{\xi} p_j + \lambda_j p_j |_{\xi})(q^r |_x p_r + q^r p_r |_x) - (q^r |_{\xi} p_r + q^r p_r |_{\xi})(\lambda_j |_x p_j + \lambda_j p_j |_x)\} p_l \\ &= \{\lambda_l, q^l\} p_l + \sum_{j,r} q^r \lambda_j p_l \{p_j, p_r\} p_l = \{\lambda_l, q^l\} p_l , \text{ because, in each term, the} \\ &\text{two differentiations “}\partial_{\xi}\text{” and “}\partial_x\text{” will either both go onto projections - then the} \\ &\text{corresponding sum will be } \sum \lambda_j q^r p_l \{p_j, p_r\} p_l = 0, \text{ by (4.2.22)) - or, only one will go} \\ &\text{onto a projection, the other onto a scalar - then there will be a factor } p_l \partial p_j p_l = 0, \\ &\text{by (4.2.20). Or, finally, both will land on scalars - then we will get } \{\lambda_l, q^l\} p_l, \text{ as} \\ &\text{stated.} \end{aligned}$$

Substituting this and (4.2.19) into (4.2.14) we indeed get (4.2.16), q.e.d.

Finally some comments about solving the PDE-s (4.2.16). Focus on the first,

$$(4.2.23) \quad \partial_t q + \lambda_{|\xi} q |_x - \lambda_{|x} q |_{\xi} = 0 ,$$

where we drop “+”, for a moment. The general solution of this equation consists of all functions which are constant along all solution curves of the system (of 6 ODE-s in 6 unknown functions)

$$(4.2.24) \quad \dot{x} = \lambda_{|\xi}(t; x, \xi) , \quad \dot{\xi} = -\lambda_{|x}(t; x, \xi) .$$

Indeed, for any $(x(t), \xi(t))$ solving (4.2.24) get

$$\begin{aligned} \frac{\partial}{\partial t} q(t; x(t), \xi(t)) &= \dot{q} + q_{|x} \dot{x} + q_{|\xi} \dot{\xi} = \dot{q} + \lambda_{|\xi} q_{|x} - \lambda_{|x} q_{|\xi} = 0 - \text{that is,} \\ q(t; x(t), \xi(t)) &= \text{const.} \end{aligned}$$

Note, the initial-value problem of the (Hamiltonian) system (4.2.24) is (locally) uniquely solvable, and we shall show in sec.5.5 that, under our present assumptions on the function $\lambda(x, \xi)$, the solution $(x_t(x^0, \xi^0), \xi_t(x^0, \xi^0))$ through the point (x^0, ξ^0) , at $t = 0$, extends infinitely, for all $t \in \mathbb{R}$. This defines⁸ a “flow” - that

⁸Generally, the flow $\nu_{\tau t} : \mathbb{R}^6 \rightarrow \mathbb{R}^6$ is defined for any pair of reals τ, t by following the solution curve from (x^0, ξ^0) at $t = \tau$ to (x, ξ) at t . This map will depend smoothly on τ and t , and there will be the “group property” $\nu_{t\kappa} \circ \nu_{\tau t} = \nu_{\tau\kappa}$ for all τ, t, κ . In sec.5.5 we shall show that composition $a(x, \xi) \rightarrow a \circ \nu_{\tau t}$ maps $\psi_{c_m} \rightarrow \psi_{c_m}$. In particular the inverse map of ν_{0t} is given by ν_{t0} , just be using above group property (together with the fact that $\nu_{tt} = 1$ for all t).

is, a family $\nu_{0t} : \mathbb{R}^6 \rightarrow \mathbb{R}^6$ of diffeomorphisms $(x^0, \xi^0) \rightarrow (x_{0t}(x^0, \xi^0), \xi_{0t}(x^0, \xi^0))$ mapping \mathbb{R}^6 onto \mathbb{R}^6 . To solve the initial-value problem for the PDE (4.2.23) - getting the unique solution satisfying our given initial value $q^+(x^0, \xi^0)$ at $t = 0$ - we must use the inverse of the above map: For any (x, ξ) we follow the solution curve of (4.2.24) backward from (x, ξ) to its intersection with $t = 0$, at some point (x_0, ξ^0) . Then, since q was seen constant along that curve, we define the value of $q_t(x, \xi)$ as the value of $q(x^0, \xi^0)$.

In this way we arrive at a well defined function $q_t(x, \xi)$ which is smooth in t, x, ξ and represents a symbol in ψc_m for every t , as shall be seen in sec.5.5.

Clearly the above, carried out for “+”, may just as well be done for “-”. So, all together, we have this:

Theorem 4.2.3 *The “commuting part” $q = q_0$ of our (first-approximated) symbol $a^\sim(x, \xi)$ propagates as $q_{0t} = q \circ \nu_{t0}$ along the Hamiltonian flow ν_{t0} of the system (4.2.24). Then the (first) correction z_{0t} is given by fla.(4.2.15), with symbols c_{\pm}^{0t} of order $m - e$, left arbitrary for $t = 0$ but needing further restraint for $t \neq 0$ - to be discussed later on. [But “ $c_{\pm}^{\tau t} \equiv 0$ in t will give a valid first correction with $A_{\tau t}^\sim = a_{\tau t}^\sim(x, D)$ satisfying (4.2.4) mod($Op\psi c_{m-e-e_2}$).]*

Now, at the end of this section we emphasize again that the symbol propagation of thm.4.2.3 is not leading to “prediction of observables”: The expectation value $\langle \psi, A_t \psi \rangle$ (with $A_t = A_{0t}$ of (4.2.3)) represents the observable A applied to the state ψ at time t transformed backward to time $t = 0$. For example, if $A = x = \text{location}$ and $\psi = \delta(x - x^0)$ [the particle is located at x^0 (at time t)] then the spectral properties of A_{0t} reflect the possible statements about location the particle might have assumed at time $t = 0$ (in the past).

What we must answer, to *predict* A is just the inverse problem: We need $A_{t0} = U(t, 0)AU(0, t)$ which does not satisfy a formula like (4.2.4) [This means that we are given an observable $A = A_{tt}$ at time t ; we transform it back to 0, apply it to our state ψ_0 there, and then transform it back to t - indeed, this means that we now are predicting measurement of the observable A at time t , given a state at 0.].

However, what we practiced above for the initial time $t = 0$, may be repeated for a general initial time $t = \tau$, resulting in a general symbol flow $\nu_{\tau t}$, defined for all $\tau, t \in \mathbb{R}$. We discussed the symbol propagation $q = q_\tau \rightarrow q_{\tau t} = q \circ \nu_{t\tau}$ for fixed τ and varying t as a first approximation, but now will use the formula

$$(4.2.25) \quad q_{t0} = q \circ \nu_{0t}$$

to describe the (approximate) symbol propagation of the (forward) Heisenberg representation. Otherwise there is no change.

Remark 4.2.4 *The reader may guess that the flow $\nu_{\tau t}$ just reflects the classical motion of the particle underlying this problem. Indeed this will be confirmed, but only after we also discuss the case of a symbol (4.2.13) where the q_{ξ}^{\pm} need not be multiples of 1, but may be hermitian symmetric operators of the two-dimensional spaces S_{\pm} . Interestingly, this also will bring the spin propagation - as a magnetic moment moving in the given field - into the picture. For details cf. sec.4.6, below.*

4.3 Dynamical Observables with Scalar Symbol

The tools developed in the preceding section are sufficient for an application to some - even though not all - of the standard dynamical observables.

Let us return to the case of time-independent potentials. Then H is constant in time and we get $U(\tau, t) = e^{-i(t-\tau)H}$. Accordingly, the operators $U(0, t)AU(t, 0)$ and $U(t, 0)AU(0, t)$ assume the form $e^{-iHt}Ae^{iHt}$ and $e^{iHt}Ae^{-iHt}$, the latter giving the Heisenberg representation, the first just the same, but with time reversal. It may be useful to summarize the results of sec.4.2 for the time-independent case.

Theorem 4.3.1 *For time-independent potentials \mathbf{A}, \mathbf{V} consider any symbol $q \in \psi_{C_m}$ with the property that $[q(x, \xi), h(x, \xi)] = 0$ with $h(x, \xi) = \alpha(\xi - \mathbf{A}(x)) + \beta + \mathbf{V}(x)$, for all x, ξ , and that, moreover, $q(x, \xi)$ is a scalar multiple of 1 in the two (2-dimensional) eigenspaces $S_{\pm}(x, \xi)$ of the 4×4 -matrix $h(x, \xi)$. Then, let $(x_{0t}^{\pm}(x, \xi), \xi_{0t}^{\pm}(x, \xi))$ denote the (unique) solution of the system (of 6 ODE-s in 6 unknown functions)*

$$\dot{x}(t) = \lambda_{\pm|\xi}(x(t), \xi(t)) , \quad \dot{\xi}(t) = -\lambda_{\pm|x}(x(t), \xi(t))$$

through the point $(x, \xi) \in \mathbb{R}^6$, with the eigenvalues $\lambda_{\pm}(x, \xi) = \mathbf{V}(x) \pm \langle \xi - \mathbf{A}(x) \rangle$ of $h(x, \xi)$, and let $\nu_{0t}^{\pm} : \mathbb{R}^6 \rightarrow \mathbb{R}^6$ be the diffeomorphisms $(x, \xi) \rightarrow (x_{0t}^{\pm}(x, \xi), \xi_{0t}^{\pm}(x, \xi))$.

Using the two eigenprojections

$$p_{\pm}(x, \xi) = \frac{1}{2}(1 \pm (\alpha(\xi - \mathbf{A}(x)) + \beta)/\langle \xi - \mathbf{A}(x) \rangle) \text{ of } h(x, \xi) \text{ we must have}$$

$$q(x, \xi) = q^+(x, \xi)p_+(x, \xi) + q^-(x, \xi)p_-(x, \xi) , \text{ with scalar symbols } q^{\pm}(x, \xi).$$

Then define

$$(4.3.1)$$

$$q_t(x, \xi) = q_t^+(x, \xi)p_+(x, \xi) + q_t^-(x, \xi)p_-(x, \xi) \text{ with } q_t^{\pm}(x, \xi) = (q^{\pm} \circ \nu_{0t}^{\pm})(x, \xi) ,$$

and

$$(4.3.2) \quad z_t = \frac{i}{2\langle \xi - \mathbf{A}(x) \rangle} (p_+ \{h, q_t\} p_- - p_- \{h, q_t\} p_+) .$$

[Specifically, $z = z_0$ does not require knowledge of q_t , and just needs the Poisson bracket $\{h, q\} = h_{|\xi}q_{|x} - q_{|\xi}h_{|x}$ of $q(x, \xi)$ initially given. Also note, the term of (4.2.15) generated by \dot{q}_t in (4.2.12) vanishes if potentials are time-independent.]

Then the operator $Q_{corr} = q(x, D) + z(x, D)$ differs from an operator with smooth Heisenberg representation (i.e., in the algebra \mathcal{P} of sec.3.3 or sec.'s 5.1. , 5.2) only by a ψ do in $Op\psi c_{m-2e}$.

As already mentioned, total energy is represented by the Hamiltonian H itself. It is clear that - for time-independent potentials⁹ - we have $H_t = e^{iHt} H e^{-iHt} = H$ independent of t . So, the Heisenberg transform is not only smooth, but is even constant. The same is true for the total angular momentum $J = x \times D + \frac{1}{2} \begin{pmatrix} \sigma^0 \\ 0 \sigma \end{pmatrix}$ if $\mathbf{A} \equiv 0$ and \mathbf{V} is rotationally symmetric, because this differential operator J is known to commute with H (cf. footnote 11 of ch.7.), so that again $J_t = e^{iHt} J e^{-iHt} = J$ for all t .

Looking for applications of thm.4.3.1 we notice that certainly its assumptions are satisfied for any “scalar” observable - i.e., whenever the symbol of an observable is a multiple of the 4×4 -identity matrix. Evidently this is the case for most standard dynamical observables. So, we now can calculate *first order corrections* $z(x, \xi)$ for many standard dynamical observables, starting with the symbol q of such observable. For calculation of $z(x, \xi)$ write (setting $h^0 = \alpha \cdot (\xi - \mathbf{A}(x)) + \beta$)

$$(4.3.3) \quad q = q^+ p_+ + q^- p_- = r + s h^0, \text{ with } r = q^+ + q^-, \quad s = (q^+ - q^-) / \langle \xi - \mathbf{A}(x) \rangle .$$

Clearly this decomposition for H itself gives $h(x, \xi) = \mathbf{V}(x) + h^0(x, \xi)$. Generally, $r(x, \xi)$ and $s(x, \xi)$ are scalars, under the assumptions of the theorem. And, vice versa, if r and s are scalars then q^\pm are scalars as well. For an observable with scalar symbol q we get $s = 0, r = q$, so that

$$(4.3.4) \quad \{h, q\} = \{\mathbf{V}, q\} + \{h^0, q\} = \{\mathbf{V}, q\} + \alpha \cdot \langle \xi - \mathbf{A}(x), q \rangle .$$

⁹If potentials depend on time then we must be aware that the operators $H(t)$ and $H(\tau)$ no longer need to commute, as $t \neq \tau$. Not even symbol-wise we need to have $[h(t), h(\tau)] = 0$, although under our assumptions (of cdn.(X)) we still have $h(t) - h(\tau) \in \psi c_{-e^2} = \psi c_{e^1 - e}$, so, $[h(t), h(\tau)]$ is a symbol of lower order, with respect to $h(t)$.

Still, since $q = h(0)$ commutes with $h(0)$, and since $h(0; x, \xi)$ is scalar in each of the two spaces $S_\pm(x, \xi)$ a (first order) correction symbol $z_t(x, \xi) \in \psi c_{-e^2}$ may be calculated [although in the time-dependent case this correction does not vanish anymore]. Accordingly, the total energy observable $H(0)$ then possesses a precisely predictable approximation, but it is no longer precisely predictable itself.

Incidentally, the self-adjoint operators $H(\tau)$, for $\tau \neq t$ do not have their individual precisely predictable corrections - except that they differ from $H(0)$ (which has such correction) by an operator of order $e^1 - e$. We shall see in ch.5 that the precisely predictable observables form an algebra \mathcal{P} - subalgebra of $Op\psi c$. But this algebra depends on t , for time-dependent potentials. Then $H(t)$ has an $H(t)_{corr}$ in $\mathcal{P}(t)$, for every t , but (generally) not in $\mathcal{P}(\tau)$ for $t \neq \tau$. [Note, if the potentials \mathbf{V}, \mathbf{A} are periodic in t , then $H(t)$ will have a precisely predictable approximation in $\mathcal{P}(\tau)$ periodically - for $\tau = t + j\pi$, with some period π , but not for other values of τ .]

Then $z(x, \xi)$ requires calculation of¹⁰

$$(4.3.5) \quad p_+ \alpha p_- - p_- \alpha p_+ = \frac{i}{\langle \xi - \mathbf{A} \rangle} (\mu + \rho \times (\xi - \mathbf{A})) .$$

For a scalar symbol $q(x, \xi)$ we then get the correction symbol

$$(4.3.6) \quad z(x, \xi) = \{ \mathbf{V}(x), q(x, \xi) \} - \lambda_c(x, \xi) \cdot \{ \xi - \mathbf{A}(x), q(x, \xi) \} ,$$

with the formal 3-vector

$$(4.3.7) \quad \lambda_c = \frac{1}{2\langle \xi - \mathbf{A}(x) \rangle^2} (\mu + \rho \times (\xi - \mathbf{A}(x))) ,$$

using the constant (3-vectors of) matrices $\mu = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}$ and $\rho = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}$, and the vector product “ \times ”.

If q is scalar only in each of the spaces S_{\pm} , so that s in (4.3.3) does not vanish identically, then fla. (4.3.6) gets the additional terms¹¹

$$(4.3.8) \quad -\lambda_c \cdot \{ \mathbf{V}, s(\xi - \mathbf{A}) \} + \{ \mathbf{V}, s \} \mu \cdot \frac{\xi - \mathbf{A}}{\langle \xi - \mathbf{A} \rangle} - \langle \xi - \mathbf{A} \rangle v \cdot \alpha + h^0 v \cdot \frac{\xi - \mathbf{A}}{\langle \xi - \mathbf{A} \rangle} ,$$

with λ_c of (4.3.7) and $v_j = s|_{x_j} + \sum_l \mathbf{A}_{j|x_l} s|_{\xi_l}$.

The above may be applied to observables like location, momentum, angular momentum: Location coordinates are given as the multiplication operators $u(x) \rightarrow x_j u(x)$, $j = 1, 2, 3$. These are self-adjoint operators of \mathcal{H} with symbol $a^j(x, \xi) = x_j$ independent of ξ . Clearly a^j belongs to ψc_{e^2} and it commutes with $h(x)$. Applying fla. (4.3.6) to the symbol $q = a^j$ - with $m = e^2$ to determine a (first) correction symbol $z(x, \xi) \in \psi c_{-e^1}$ we get

$$(4.3.9) \quad x_{corr} = x - \lambda_c , \quad \lambda_c(x, \xi) = \frac{1}{2\langle \xi - \mathbf{A} \rangle^2} \{ \mu + \rho \times (\xi - \mathbf{A}) \} .$$

We are aware that further corrections are needed to get an operator with a smooth Heisenberg transform. However, it might be interesting then to obtain the explicit z , in this case. Note - the location coordinates themselves do not have this smoothness property; they need these corrections.

Note, the above symbol x_{corr} is a self-adjoint 4×4 -matrix. However, the corresponding ψ do $x_{corr}(x, D)$ is not self-adjoint, so cannot represent an observable.

¹⁰cf. also [Co5], p.331, fla.(4.7).

¹¹To include the case of time-dependent potentials here: Assuming q^{\pm} scalar in S_{\pm} , we also have to add just one more term to (4.3.6) or (4.3.8) - the expression $-s(x, \xi) \lambda_c(0; x, \xi) \cdot \dot{\mathbf{A}}(0, x)$, with λ_c of (4.3.7) and $s(x, \xi) = (q^+(x, \xi) - q^-(x, \xi)) / \langle \xi - \mathbf{A}(0, x) \rangle$ of (4.3.3). Especially, if $q(x, \xi)$ is scalar in \mathbb{C}^4 this correction vanishes.

This, however, is easily cured by defining the (first-)corrected location observable as¹²

$$(4.3.10) \quad X_{corr} = \frac{1}{2}(x_{corr}(x, D) + x_{corr}(x, D)^*) = x + \frac{1}{2}(\lambda_c(x, D) + \lambda_c(x, D)^*) .$$

[In particular, note that the symbol $\lambda_c(x, \xi)$ is of order $-e^1$, i.e., its order is $e = (1, 1)$ units lower than that of the location operator x .] Let us state our interpretation again, at this point:

The location observable x we would like to predict. However, x is not precisely predictable while X_{corr} (nearly) is. So, we may predict X_{corr} , in the sense of v. Neumann's rules, but then must be aware of a possible error of our expectation value of magnitude $|\Re(\langle u, \lambda_c(x, D)u \rangle)|$ in the physical state u - the difference between \check{x} and \check{X} .

Incidentally, this error is easily estimated: For vanishing potentials the operator norm of (the components of) $\lambda_c(x, D)$ is not larger than 1, as easily seen. For non-vanishing potentials this should not change much (even though we did not check details).

The location variable has the physical dimension of a length. But our unit length is the Compton wave length of the electron, as mentioned initially (ch.1, footnote 1.) So, this inaccuracy of our prediction of location seems perfectly natural¹³.

The above construction of a corrected observable may be repeated (so far) for every observable $A = a(x, D)$ where the symbol $a \in \psi_{c_m}$ commutes with $h(x, \xi)$, and may be written as $a = a^+p_+ + a^-p_-$ with scalar symbols $a^\pm(x, \xi)$. Apart from location, this is true for the following dynamical observables. In the list, below, we are giving the symbols of the (first order) corrections with some discussion, but without derivation¹⁴. We may come back later on, to study their spectral theory, etc. In each case, as for location x above, the corrected symbol is a self-adjoint matrix, but the corresponding ψ do still must be "symmetrized" - using the (self-adjoint) symbol a_{corr} we take the (self-adjoint) operator $A_{corr} = \frac{1}{2}(a_{corr}(x, D) + a_{corr}(x, D)^*)$ as (first order) corrected observable.

¹²This formal difficulty often is avoided by using a slightly amended definition of a ψ do A represented by a given symbol a , called the Weyl-representation (cf. sec.1.6). While the Weyl representation offers this (and certain other) advantage(s), it also brings forth some further complications of certain formulas, notably the Leibniz formulas (1.0.8),(1.0.9). This is why we are avoiding it here.

¹³Recall our correction recognizes only the first of infinitely many others we cannot analyze.

¹⁴The derivation, in each case, will be a matter of applying fla. (4.3.6) (or (4.3.8)) for the symbol q of the (uncorrected) observable in question.

Momentum:

$$(4.3.11) \quad p = (p_1, p_2, p_3) , \quad p_j = D_j = -i \frac{\partial}{\partial x_j} : \quad p_{corr} = \xi - \sum \lambda_{cl}(x, \xi) A_{l|x(x)} ,$$

with the components λ_{cl} of the formal 3-vector λ_c of (4.3.7).

But note that the correction of the symbol $\xi \in \psi_{c_e^1}$ is of order $-e^1 - 2e^2 = e^1 - 2e$, due to our cdn.(X) imposed on the A_j . This means that the first order correction of the momentum p is zero. Only a second order correction is listed in (4.3.11) while other second order terms were ignored. In other words, we rather should write (4.3.11) as

$$(4.3.11') \quad p = (p_1, p_2, p_3) , \quad p_j = D_j = -i \frac{\partial}{\partial x_j} : \quad p_{corr} = \xi ,$$

i.e., there is *no* first order correction to be added to the symbol of p .

(Orbital) Angular momentum:

$$(4.3.12) \quad L = x \times p : L_{corr}(x, \xi) = x \times \xi - \lambda_c(x, \xi) \times \xi - \sum \lambda_{cl}(x \times A_{l|x}) .$$

Again, with λ_c of (4.3.7), and, again, the last term is of order $-e$ - two units e lower than the corrected symbol $x \times \xi$, so it should be omitted, since other corrections of that order will come forth: We should write (4.3.12) as

$$(4.3.12') \quad L = x \times p : L_{corr}(x, \xi) = x \times \xi - \lambda_c(x, \xi) \times \xi .$$

Electrostatic potential:

$$(4.3.13) \quad \mathbf{V}(x) : \quad \mathbf{V}_{corr}(x, \xi) = \mathbf{V} + \mathcal{E}(x) \cdot \lambda_c(x, \xi) , \quad \mathcal{E} = -\text{grad } \mathbf{V} .$$

We will discuss the spectral theory of this operator¹⁵ in sec.7.3f .

Mechanical momentum:

$$(4.3.14) \quad \pi = p - \mathbf{A} : \quad \pi_{corr}(x, \xi) = \xi - \mathbf{A}(x) - \mathcal{B} \times \lambda_c , \quad \mathcal{B} = \text{curl } \mathbf{A} .$$

Relativistic mass:

$$(4.3.15) \quad M = H - V : \quad M_{corr} = h(x, \xi) - \mathbf{V}(x) - \mathcal{E}(x) \cdot \lambda_c(x, \xi) .$$

Again, the correction of $h(x, \xi) - \mathbf{V}(x) \in \psi_{c_{e^1}}$ listed is of order $-e^1 - 2e^2$ - i.e., $2e$ units lower. However, in this case we cannot expect any other correction of

¹⁵Actually, we went through the calculations for obtaining a second order correction for this observable (cf. sec.5.6.).

that order¹⁶ , so, the symbol M_{corr} of (4.3.15) already has the first and second corrections represented.

Note that the formal 3-vector $\lambda_c(x, \xi)$ seems to govern every correction above.

Clearly some dynamical observables are missing in above list, such as spin and current. These have symbols not commuting with $h(x, \xi)$ - or else, their symbol does commute with $h(x, \xi)$ but it is not a multiple of 1 in the two eigenspaces of h . This latter type will be discussed in the next section, below.

4.4 Symbols Non-Scalar on S_{\pm}

In this section we will continue the discussion of sec.4.2, and construct a first order correction z_t also for the case of a symbol for a $q \in \psi_{c_m}$ still commuting with $h(t, x, \xi)$ but without the property that $q(x, \xi)|S_{\pm}(x, \xi)$ are multiples of the identity. We return to time-dependent potentials for this.

Things are quite similar as in sec.4.2, except that we do not have the result of prop.4.2.1, used to translate conditions (4.2.14) into a useful form. For this we will have to analyze the two linear maps $q_t^{\pm}(x, \xi) : S_{\pm}^t(x, \xi) \rightarrow S_{\pm}^t(x, \xi)$ of the (2-dimensional) $S_{\pm}^t(x, \xi)$ with respect to *suitable bases* of these spaces.

Note, we already have a unitary map $u(t; x, \xi)$, taking the symbol $h(t; x, \xi)$ onto the diagonal form $\text{diag}\{\lambda_+, \lambda_+, \lambda_-, \lambda_-\}$, given explicitly¹⁷ by (3.2.1). Moreover, $u(t; x, \xi)$ is a symbol in ψ_{c_0} for every t . It is clear that the first two (last two) columns of $u(t; x, \xi)$ supply orthonormal bases of $S_+^t(x, \xi)$ (of $S_-^t(x, \xi)$). However, to simplify some calculations, we will expand arbitrary vectors, using the two pairs of bi-orthogonal systems, obtained by avoiding the factor $\frac{1}{\sqrt{2+2\zeta_0}}$ in the first system - called φ_j - and applying its square for the second - called ψ_j . That is, we set (for S_+):

$$(4.4.1) \quad (\varphi_1, \varphi_2) = \begin{pmatrix} 1+v_0 \\ -i\sigma v \end{pmatrix}, \quad \psi_j = \frac{1}{2+2v_0} \varphi_j, \quad j = 1, 2,$$

and, (for S_-):

$$(4.4.2) \quad (\varphi_3, \varphi_4) = \begin{pmatrix} -i\sigma v \\ 1+\zeta_0 \end{pmatrix}, \quad \psi_j = \frac{1}{2+2v_0} \varphi_j, \quad j = 3, 4,$$

with $v_0 = 1/\langle \zeta \rangle$, $v = \zeta/\langle \zeta \rangle$, $\zeta = \xi - A$. Clearly the linear maps $q_t^{\pm}(x, \xi)$ are represented by 2×2 -matrices $\kappa_t^{\pm} = ((\kappa_{tj}^{\pm}))$ with respect to the bases (4.4.1) (or

¹⁶Actually, since $H = M + \mathbf{V}(x)$ commutes with H the symbol of H needs no corrections - it has the first correction as well as all the others equal to zero. It follows that corrections for M (of any order) must equal the negative of the corresponding correction for $\mathbf{V}(x)$. Accordingly, the first correction for M vanishes; the second is listed in (4.3.15). As mentioned we even calculated a second correction for $\mathbf{V}(x)$. This must give the third correction of M .

¹⁷Our potentials are time-dependent here, but the formula (3.2.1) remains intact.

(4.4.2)) of S_{\pm}^t . We express this by writing

$$(4.4.3) \quad q_t^{\pm} = \sum_{j,l=1}^2 \kappa_{tjl}^{\pm} p_{tjl}^{\pm},$$

with $p_{tjl}^+ = \psi_j \langle \varphi_l$ and $p_{tjl}^- = \psi_{j+2} \langle \varphi_{l+2}$. It is clear also that

$$(4.4.4) \quad p_{\pm} = p_{t11}^{\pm} + p_{t22}^{\pm}.$$

With such preparation we may look at cdn.'s (4.2.14) again. Note, we had $p_{\pm} \dot{p} p_{\pm} = 0$, but it is no longer true that also $p_{\pm} \dot{p}_{jl}^{\pm} p_{\pm} = 0$, although we still have $p_{\mp} p_{jl}^{\pm} = 0 \Rightarrow p_{\mp} \dot{p}_{jl}^{\pm} = -\dot{p}_{\mp} p_{jl}^{\pm}$, hence

$$(4.4.5) \quad p_{\mp} \dot{p}_{jl}^{\pm} p_{\mp} = -\dot{p}_{\mp} p_{jl}^{\pm} p_{\mp} = 0, \quad p_{\mp} p_{jl|\xi}^{\pm} p_{\mp} = p_{\mp} p_{jl|x}^{\pm} p_{\mp} = 0.$$

Inspecting the other formulas [(4.2.21)-(4.2.22)] used in the proof of the proposition in sec.4.2 we find a similar effect: Looking at $p_+ \dot{q} p_+$, for example, we get

$$(4.4.6) \quad p_+ \dot{q} p_+ = p_+ \dot{q}_+ p_+ = \sum \kappa_{jl}^+ p_+ \dot{p}_{jl}^+ p_+ + \sum \dot{\kappa}_{jl}^+ p_{jl}^+,$$

where the first term at right no longer needs to vanish, although all terms involving $q_t^-(x, \xi)$ have disappeared.

Similarly, looking at

$$(4.4.7) \quad p_+ \{h, q\} p_+ = p_+ \{\lambda_+ p_+, q\} p_+ + p_+ \{\lambda_- p_-, q\} p_+ = (I) + (II)$$

we get

(I) = $p_+ \{\lambda_+, q\} p_+ + \lambda_+ p_+ \{p_+, q\} p_+$, while

(II) = $\lambda_{-|\xi} p_+ p_- q_{|x} p_+ + \lambda_{-|x} p_+ q_{|\xi} p_- p_+ + \lambda_- p_+ \{p_-, q\} p_+ = \lambda_- p_+ \{p_-, q\} p_+$, since $p_+ p_- = p_- p_+ = 0$. Also, $p_+ + p_- = 1$ implies $p_{-|x} = -p_{+|x}$ and $p_{-|\xi} = -p_{+|\xi}$, hence, $\{p_-, q\} = -\{p_+, q\}$, so that, (II) = $-\lambda_- p_+ \{p_+, q\} p_+$. Together we get

$$(4.4.8) \quad p_+ \{h, q\} p_+ = p_+ \{\lambda_+, q\} p_+ + (\lambda_+ - \lambda_-) p_+ \{p_+, q\} p_+.$$

For further simplifications note that $\lambda_+ - \lambda_- = 2\langle \zeta \rangle = 2(\xi - A)$. Also, $q = q^+ + q^-$, where $p_+ \{\lambda_+, q^-\} p_+ = 0$, by (4.4.5), since λ_+ is a scalar. Furthermore, $p_+ \{p_+, q^-\} p_+ = p_+ p_{+|\xi} q_{|x}^- p_+ - p_+ q_{|\xi}^- p_{+|x} p_+ = -p_+ p_{+|\xi} q_{|x}^- p_+ + p_+ p_{+|\xi} q_{|x}^- p_+ = 0$, where we used that $p_+ q^- = q^- p_+ = 0$ implies $p_+ q_{|\xi}^- = -p_{+|\xi} q^-$, $q_{|x}^- p_+ = q^- p_{+|x}$. With these simplifications we get

$$(4.4.9+) \quad p_+ \{h, q\} p_+ = p_+ \{\lambda_+, q_+\} p_+ + 2\langle \zeta \rangle p_+ \{p_+, q_+\} p_+.$$

Repeating the above for “-” we get

$$(4.4.9-) \quad p_- \{h, q\} p_- = p_- \{\lambda_-, q_-\} p_- - 2\langle \zeta \rangle p_- \{p_-, q_-\} p_- .$$

After this, it is clear that we again have split the two conditions (4.2.14) into separate systems for q_{\pm} : The first cdn. involves only q_+ , the second only q_- . We may rewrite (4.2.14) as

$$(4.4.10) \quad p_{\pm} q'_{\pm} p_{\pm} \pm 2\langle \zeta \rangle p_{\pm} \{p_{\pm}, q_{\pm}\} p_{\pm} = 0 ,$$

where again “'” means differentiation along the flow - i.e., $\partial_t + \lambda_{\pm|\xi} \partial_x - \lambda_{\pm|x} \partial_{\xi}$ - different for the two flows.

For a full evaluation of (4.4.10) we now will translate it into a matrix form. Using (4.4.6) and (4.2.20) (i.e., $p_{\pm} p'_{\pm} p_{\pm} = 0$ for any directional derivative “'”) we translate (4.4.10) into

$$(4.4.11) \quad \sum_{jl} p_{jl} \kappa'_{jl} + \sum_{jl} \kappa_{jl} (pp'_{jl} p) + 2\langle \zeta \rangle \sum_{jl} \kappa_{jl} p \{p, p_{jl}\} p = 0 ,$$

where we again restricted to “+” and dropped the “+”. Evidently, the first term of (4.4.11) has the matrix $((\kappa'_{jl}))$. The matrices of the other two terms may be written as $W\kappa$ with a linear map W acting on 2×2 -matrices. Thus (4.4.11) may be written as

$$(4.4.12) \quad (\kappa_t^{\pm})' + W_t^{\pm} \kappa_t^{\pm} = 0$$

with

$$(4.4.13) \quad \kappa' = \dot{\kappa} + \lambda_{\pm|\xi} \partial_x \kappa - \lambda_{\pm|x} \partial_{\xi} \kappa .$$

So, again, this will be 4×4 -systems of (linear homogeneous) ODE-s along the particle flows.

In fact we can improve on the term $W^{\pm} \kappa^{\pm}$, insofar as it turns out that we may write

$$(4.4.14) \quad W^{\pm} \kappa^{\pm} = [\Theta^{\pm}, \kappa^{\pm}]$$

with certain 2×2 -matrix-valued symbols Θ^{\pm} at right and the matrix-commutator $[\Theta^{\pm}, \kappa^{\pm}]$. Indeed, (dropping “+”, and with “'” = any directional derivative) we have $pp_{jl} = p_{jl}$, hence $pp'_{jl} + p'p_{jl} = p'_{jl} \Rightarrow (1 - p)p'_{jl} = p'p_{jl}$. Thus $pp_{|\xi} p_{jl|x} p = pp_{|\xi} (1 - p)p_{jl|x} p = (pp_{|\xi} p_{|x}) p_{jl}$, and, similarly, $pp_{jl|x} p = p_{jl} (pp_{|\xi} p_{|x} p)$. Using (4.4.4) and $p_{jl} = \psi_j \rangle \langle \varphi_l$ (for “+”) we may write

$$(4.4.15) \quad pp_{|\xi} p_{|x} p = \sum_{kr} \langle \varphi_k, p_{|\xi} p_{|x} \psi_r \rangle p_{kr} .$$

Thus we get - with $p_{jl}p_{kr} = \psi_j \langle \varphi_l, \psi_k \rangle \langle \varphi_r = \delta_{lk} p_{jr}$ - that

$$(4.4.16) \quad p\{p, p_{jl}\}p = \sum_{kr} \langle \varphi_k, p_{|\xi} p_{|x} \psi_r \rangle (p_{kl} \delta_{rj} - p_{jr} \delta_{kl}) ,$$

hence - with $\Theta_{jl}^1 = \langle \varphi_j, p_{|\xi} p_{|x} \psi_l \rangle$ - the last term in (4.4.11) will be

$$(4.4.17) \quad = 2\langle \zeta \rangle \sum_{jlk r} \kappa_{jl} \Theta_{kr}^1 (p_{kl} \delta_{rj} - p_{jr} \delta_{lk}) = 2\langle \zeta \rangle \sum_{jl} ([\Theta^1, \kappa^+])_{jl} p_{jl}^+ .$$

In a similar way one finds that the second term of (4.4.11) - and, generally, a term of the form $\sum_{jl} \kappa_{jl} p(p_{jl})'p$, with any directional derivative “ \prime ” - may be written as $\sum_{jl} [\Theta^\sim, \kappa] p_{jl}$ with $\Theta^\sim = (\langle \varphi_j, \psi_l' \rangle)$. Indeed, get $p(p_{jl})'p = \sum_{kr} p_{kr} (\langle \varphi_k, \psi_j' \rangle \langle \varphi_l, \psi_r \rangle + \langle \varphi_k, \psi_j \rangle \langle \varphi_l', \psi_r \rangle)$. Differentiating $\langle \varphi_k, \psi_j \rangle = \delta_{kj}$ we get $\langle \varphi_k', \psi_j \rangle + \langle \varphi_k, \psi_j' \rangle = 0$. It follows that

$$(4.4.18) \quad pp'_{jl}p = \sum_{kr} p_{kr} (\Theta_{kj}^\sim \delta_{lr} - \delta_{kj} \Theta_{lr}^\sim) .$$

So,

$$(4.4.19) \quad \sum_{jl} \kappa_{jl}^+ pp'_{jl}p = \sum_{jl} [\Theta^\sim, \kappa^+]_{jl} p_{jl} .$$

All in all then the sum of the two last terms at left of (4.4.11) assumes the form

$$(4.4.20) \quad \sum_{jl} p_{jl}^+ [\Theta^+, \kappa^+] , \quad \Theta_{jl}^+ = \langle \varphi_j, \psi_j' \rangle + 2\langle \zeta \rangle \langle \varphi_j, p_{|\xi} p_{|x} \psi_l \rangle ,$$

where now “ \prime ” means the special directional derivative along the flow of (4.2.24), as defined by (4.4.13). There is an analogous consideration for “ $-$ ” which will be left to the reader.

In other words, (4.4.11) (or (4.4.12)) now assumes the form

$$(4.4.21) \quad (\kappa_t^\pm)' + [\Theta_t^\pm, \kappa_t^\pm] = 0 , \quad (\Theta_t^\pm)_{jl} = \langle \varphi_j^\pm, (\psi_l^\pm)' \rangle + 2\langle \zeta \rangle \langle \varphi_j^\pm, p_{\pm|\xi} p_{\pm|x} \psi_l^\pm \rangle ,$$

where we have introduced the new notation $\varphi_j^+ = \varphi_j, \psi_j^+ = \psi_j, \varphi_j^- = \varphi_{j+2}, \psi_j^- = \psi_{j+2}$, for $j = 1, 2$.

Clearly, the above should be further evaluated, using details of our bi-orthogonal systems of (4.4.1) and (4.4.2). This will be done in sec.4.6, below, where we will look at “geometrical optics” by studying the “particle flow” under physical aspects. We shall find that not only the classical orbits of electron and positron, but also the propagation of spin is reflected in this kind of symbol propagation.

For our present purpose, it will be important to observe that there will be a complete analogue to prop.4.2.2, asserting a unique solution - now of the system

(4.4.21) - with κ_t^{\pm} providing a symbol q_t in ψc_m if the initial-value q is such a symbol, by way of (4.2.13) and (4.4.3). This will be discussed in sec.5.5. With that, fla.(4.2.15) with w_t of (4.2.12) automatically will give the necessary correction symbol z_t in ψc_{m-e} , and (4.4.21) automatically will give $\dot{q}_t \in \psi c_{m-e^2}$, implying that $z_t \in \psi c_{m-e-e^2}$ may be neglected. Then, of course, the machinery of sec.4.2 also applies to initial symbols not scalar in the two spaces S_{\pm} , as we shall require in sec.4.5, below.

Note, by the way, the symbols Θ_{jl}^{\pm} belong to ψc_{-e^2} .

Looking at eqn. (4.4.21) [for “+” again, dropping “t” and “+”]: For a constant 2×2 -matrix Θ the system $\kappa' + [\Theta, \kappa] = 0$ (of 4 ODE-s in 4 unknown functions $\kappa(t)$) is solved by $\kappa(t) = e^{-\Theta t} \kappa(0) e^{\Theta t}$, this giving the unique solution of the initial-value problem, fixing $\kappa(0) = \kappa^0$. Here $Q(t) = e^{-\Theta t}$ solves $Q' + \Theta Q = 0$ with initial value $Q(0) = 1$ - it represents the evolution operator of that constant coefficient system.

Our Θ of (4.4.21) depends on t , but one finds the same relation between the two ODE-s $\kappa' + [\Theta(t), \kappa] = 0$ and $Q' + \Theta(t)Q = 0$: Let $Q(\tau, t)$ denotes the evolution operator of the 2×2 -ODE $\dot{q} + X(t)q = 0$ with an $X = X(t)$ depending on t , i.e.,

$$(4.4.22) \quad \partial_t Q(\tau, t) + X(t)Q(\tau, t) = 0, \quad Q(\tau, \tau) = 1,$$

equipped with the usual “group property” $Q(\tau, t) = Q(\tau_1, t)Q(\tau, \tau_1)$ for all τ, τ_1, t . Then the unique solution of the ODE $\dot{U} + [X(t), U] = 0$ with initial value $U(0)$ is given by $U(t) = Q(0, t)U(0)Q(t, 0)$. In the case of (4.4.21) we have the derivative “’” along the particle flow. That is, we must set

$$(4.4.23) \quad X(t) = \Theta(t, x(t), \xi(t))$$

with any solution curve $x(t), \xi(t)$ of the Hamiltonian system (4.2.24). With such $X(t)$ we then define

$$(4.4.24) \quad \kappa(t, x(t), \xi(t)) = Q(0, t)\kappa(0, x_0, \xi_0)Q(t, 0).$$

Clearly we get $\kappa(0, x(0), \xi(0)) = \kappa(0, x_0, \xi_0)$, assuming our curve starts at (x_0, ξ_0) for $t = 0$. A differentiation at once confirms that

$$(4.4.25) \quad \partial_t \kappa(t, x(t), \xi(t)) = [X(t), \kappa(t, x(t), \xi(t))] = -[\Theta(t, x(t), \xi(t)), \kappa(t, x(t), \xi(t))].$$

We have proven:

Theorem 4.4.1 *For time-dependent potentials satisfying cdn.(X) with all their time-derivatives, and an initial symbol $q_0(x, \xi) \in \psi c_m$ commuting with $h(0, x, \xi)$ for*

all x, ξ (but without the condition that $q_0(x, \xi)$ is scalar in the two spaces $S_{\pm}(x, \xi)$) a continuation symbol $q_t(x, \xi)$ (commuting with $h(t, x, \xi)$ for all t) is given by writing

$$(4.4.26) \quad q_t^{\pm} = \sum_{j,l=1}^2 \kappa_{tjl}^+ p_{tjl}^+ + \sum_{j,l=1}^2 \kappa_{tjl}^- p_{tjl}^- ,$$

where the dyads p_{tjl}^{\pm} are defined as in (4.4.3), while the 2×2 -matrices $\kappa_t^{\pm} = ((\kappa_{tjl}^{\pm}))$ are determined by fla. (4.4.24) with the evolution operator $Q = Q^{\pm}(\tau, t)$ of the problem (4.4.22) with $X(t)$ of (4.4.23), where $\Theta = \Theta^{\pm}$ is given by (4.4.21) and $x(t), \xi(t)$ are the solutions of (4.2.24) - again for \pm , respectively, and with initial conditions $x^{\pm}(0) = x_0$, $\xi^{\pm}(0) = \xi_0$.

Then the first correction symbol $z_t \in \psi_{c_{m-e}}$ is given as in thm.4.2.3 - using fla. (4.2.15) with above redefined q_t . Again the symbols c_t of (4.2.15) are free at $t = 0$, but they need further restraint for general t (cf. proof of thm.5.1.1.(ii)).

4.5 Spin and Current

The spin-observable usually is defined as the (formal 3-vector of) matrices

$$(4.5.1) \quad S = \frac{1}{2}\rho, \quad \rho_j = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}_j ,$$

motivated by the fact that - for rotationally symmetric potentials - the total angular momentum

$$(4.5.2) \quad J = x \times D + \frac{1}{2}\rho = L + S$$

commutes with H , so can be predicted independently of any energy observations¹⁸.

Now, it is clear that the multiplication operator $S_j = \frac{1}{2}\rho_j$ belongs to $Op\psi_{c_0}$, and has symbol $a(x, \xi) = \frac{1}{2}\rho_j$ independent of x and ξ . Evidently, this symbol does **not** commute with the symbol $h(x, \xi)$ of H , so that the constructions of sec.4.2 and sec.4.4 both do not apply.

In such a case, however, one may argue as follows: This observable S can be *meaningfully predicted* only if it is known in advance (with certainty - i.e., probability 1) that the particle is an electron (a positron). Recall our split $\mathcal{H} = \mathcal{H}_e \oplus \mathcal{H}_p$ of (3.0.5), realized in sec.3.5, and the corresponding partition of unity

¹⁸cf. footnote 11 of ch.7.

$1 = P_e + P_p$, where P_e and P_p are ψ do-s in $Op\psi c_0$ with symbol p_{\pm} (modulo $\mathcal{O}(-\infty)$).

If the physical state u belongs to \mathcal{H}_e then we have $u = P_e u$, hence for the expectation value \check{S} we get

$$(4.5.3) \quad \check{S} = \langle u, Su \rangle = \langle u, P_e S P_e u \rangle .$$

Note, the operator $S_e = P_e S P_e$ is a ψ do with symbol

$$(4.5.4) \quad s_e(x, \xi) = \frac{1}{2} p_+ \rho p_+ \pmod{\psi c_{-e}} ,$$

and the symbol $s_e \in \psi c_0$ commutes with $h(x, \xi)$, for all x, ξ . So, it could well be used as a symbol q of sec.4.2 to construct a correction with smooth Heisenberg transform, which would be precisely predictable. But it could be used as approximation for the spin-observable only for physical states where the particle is an electron - for sure. To get such symbol working for both spaces \mathcal{H}_e **and** \mathcal{H}_p one might take the sum

$$(4.5.5) \quad \tilde{S} = P_e S P_e + P_p S P_p ,$$

with symbol $\pmod{\psi c_{-e}}$

$$(4.5.6) \quad \tilde{s}(x, \xi) = \frac{1}{2} (p_+ \rho p_+ + p_- \rho p_-) .$$

Clearly, with p_{\pm} of (4.2.9) , we get

$$(4.5.7) \quad \tilde{s} = \frac{1}{4} \left\{ \rho + \frac{1}{\langle \zeta \rangle^2} (\alpha \zeta + \beta) \rho (\alpha \zeta + \beta) \right\} .$$

We get $\beta \rho \beta = \rho$, and, $\alpha_1 \rho_1 \beta + \beta \rho_1 \alpha_1 = 0$ while $\alpha_2 \rho_1 \beta = \beta \rho_1 \alpha_2 = -\mu_3$ and $\alpha_3 \rho_1 \beta = \beta \rho_1 \alpha_3 = \mu_2$. This gives

$$(4.5.8) \quad (\alpha \zeta) \rho_1 \beta + \beta \rho_1 (\alpha \zeta) = -2\zeta_2 \mu_3 + 2\zeta_3 \mu_2 = 2(\mu \times \zeta)_1 .$$

Furthermore,

$$(4.5.9) \quad (\alpha \zeta) \rho_1 (\alpha \zeta) = 2\zeta_1 (\rho \zeta) - \zeta^2 \rho_1 ,$$

hence,

$$(\alpha \zeta + \beta) \rho (\alpha \zeta + \beta) = 2\rho + 2\mu \times \zeta + 2\zeta(\rho \zeta) - \langle \zeta \rangle^2 \rho , \text{ so that,}$$

$$(4.5.10) \quad \tilde{s} = \frac{1}{2\langle \zeta \rangle^2} \left\{ \rho + \mu \times \zeta + \zeta(\rho \zeta) \right\} .$$

We then might offer the operator $\tilde{S} = \tilde{s}(x, D)$ for the approximation procedure of sec.4.2, to construct \tilde{S}_{corr} as precisely predictable approximation. However, it is clear then that this will work only for physical states in \mathcal{H}_e or \mathcal{H}_p .

As another approach to the same problem we might look at the decomposition

$$(4.5.11) \quad J = L + S = x \times D + \frac{1}{2}\rho .$$

of the total angular momentum into spin and orbital contributions. We constructed the symbol of a precisely predictable approximation of the observable L (or only its first installment) in (4.3.12'), as

$$(4.5.12) \quad l_{corr} = x \times \xi - \lambda_C \times \xi , L_{corr} = \frac{1}{2}(l_{corr}(x, D) + l_{corr}(x, D)^*) .$$

For $A = 0$ and rotationally symmetric $V(x)$ we know that $[H, J] = 0$. Assuming this we get λ_C independent of x ; we then might write (4.5.11) in the form

$$(4.5.13) \quad J = J_{corr} = L_{corr} + (S + \lambda_C(D) \times D) .$$

Both terms of the last sum are of the same order 0. Moreover,

$\lambda_C \times \xi = \frac{1}{2\langle \xi \rangle^2} \{ \mu \times \xi - \xi \times (\rho \times \xi) \} = \frac{1}{2\langle \xi \rangle^2} \{ \mu \times \xi + (\rho \xi) \xi - \xi^2 \rho \}$. Thus the symbol of that sum is

$$(4.5.14) \quad \frac{1}{2}\rho + \frac{1}{2\langle \xi \rangle^2} \{ \mu \times \xi + (\rho \xi) \xi - \xi^2 \rho \} = \frac{1}{2\langle \xi \rangle^2} \{ \rho + \mu \times \xi + (\rho \xi) \xi \} = \tilde{s}(x, \xi) .$$

In other words, (4.5.13) assumes the form

$$(4.5.15) \quad J = L_{corr} + \tilde{S} ,$$

where now the *naturally corrected spin* \tilde{S} does have its symbol $\tilde{s} = \frac{1}{2}(p_+ \rho p_+ + p_- \rho p_-)$, (by (4.5.6)) indeed *commuting with* $h(x, \xi)$.

In other words,

Proposition 4.5.1 *For $\mathbf{A}_j = 0$ and rotationally symmetric \mathbf{V} there is a corrected decomposition (4.5.15) of the total angular momentum into a precisely predictable orbital component and a spin component where now the (uncorrected) symbol of the spin commutes with $h(x, \xi)$, so that it may be entered into the correction procedure¹⁹ of thm.4.2.3 or thm.4.4.1. This (uncorrected) new spin symbol $\tilde{s}(x, \xi)$ coincides with the symbol of (4.5.6) in the general case, useful for the expectation value of S only in the case where the precise nature of the particle - either electron or positron - is known with certainty.*

We will not calculate any further correction of the spin-observable, after having achieved a "0-th correction" making our procedure of sec's 4.2 and 4.4 applicable. However, let us get the linear maps q^\pm explicitly, used to correct the symbol

¹⁹and, more precisely into that of thm.5.1.1.

$\tilde{s}(x, \xi)$ of our natural spin \tilde{S} . That is, we should obtain explicitly the matrices κ^\pm of (4.4.3). Using (4.4.4) we have

$$(4.5.16) \quad p_+ \rho p_+ = \sum_{j,l} p_{jj}^+ \rho p_{ll}^+ = \frac{1}{2 + 2/\langle \zeta \rangle} \sum_{j,l} \langle \varphi_j, \rho \varphi_l \rangle p_{jl}^+ .$$

So, for κ^+ we must calculate the matrix (with $v_0 = 1/\langle \zeta \rangle$, $v = \zeta/\langle \zeta \rangle$)

$$(\varphi_1, \varphi_2)^* \rho (\varphi_1, \varphi_2) = \begin{pmatrix} 1+v_0 \\ -i\sigma v \end{pmatrix}^* \begin{pmatrix} \sigma^0 \\ 0 \end{pmatrix} \begin{pmatrix} 1+v_0 \\ -i\sigma v \end{pmatrix} = (1 + 1/\langle \zeta \rangle)^2 \sigma + \frac{1}{1+\zeta^2} (\sigma \zeta) \sigma (\sigma \zeta) .$$

One find that $(\sigma \zeta) \sigma (\sigma \zeta) = 2(\sigma \zeta) \zeta - \zeta^2 \sigma$, hence

$$(4.5.17) \quad \kappa^+ = \frac{1}{\langle \zeta \rangle} \sigma + \frac{1}{\langle \zeta \rangle (1 + \langle \zeta \rangle)} (\sigma \zeta) \zeta$$

Evidently this is not a multiple of 1, so, we must apply the theory of sec.4.4. For the matrix κ^- we get exactly the same formula, i.e.,

$$(4.5.18) \quad \kappa^- = \frac{1}{\langle \zeta \rangle} \sigma + \frac{1}{\langle \zeta \rangle (1 + \langle \zeta \rangle)} (\sigma \zeta) \zeta .$$

As another observable, frequently used, but wit symbol non-commuting with $h(x, \xi)$, let us mention the *current*. The 3 components C_j of the current usually are given to coincide with the 3 Dirac matrices α_j of (1.0.2) - for us given by (3.1.7). But we must remember here that this describes the *current density*. The corresponding observable then would be the (matrix-) multiplication operator $\psi(y) \rightarrow \alpha_j \delta(x - y) \psi(y)$ (with the delta-function $\delta(x - y)$), describing current density at the point x . Again, while this is a linear operator $\mathcal{S} \rightarrow \mathcal{S}$ it does not define a preclosed operator of \mathcal{H} , and hence, does not qualify as an observable. What one must take instead is the (distribution) limit (as $\varepsilon \rightarrow 0$) of $c_j^\varepsilon = \alpha_j \delta_\varepsilon(x - y)$ with $\delta_\varepsilon(x) = \delta_1(x/\varepsilon)$ where $\delta_1 \in \mathcal{S}$, $\int \delta_1 dx = 1$. These $c_j^\varepsilon(x)$ are well defined multiplication operators (and ψ -do-s in $Op\psi_{C(0,-\infty)}$), as $\varepsilon > 0$.

We remind of the *continuity equation*

$$(4.5.19) \quad \partial_t \rho^0(x) + \text{div } c^0(x) = 0 ,$$

linking²⁰ the current density to the particle density $\rho^0(x)$, given as observable by $\rho^0(x) = \delta(x - y)$ - involving the same limit $\rho^0(x) = \lim_{\varepsilon \rightarrow 0} \delta^\varepsilon(x)$.

²⁰The expectation value of $\rho^0(x)$ at a state ψ will be $\check{\rho} = \int \psi^*(y) \delta(x - y) \psi(y) dy = |\psi(x)|^2$. Similarly, the expectation value of $c_j^0(x)$ will be $\check{c}_j^0(x) = \psi(x)^* \alpha_j \psi_j(x)$. Assuming that $\psi(t, x)$ is a solution of the Dirac equation we then indeed get (4.5.19) for the expectation values, since a_j are hermitian, while D_j are skew-hermitian, and all potentials are real. In fact we then even get the continuity relation (4.5.19) not only for $\rho^0(x)$ and $c^0(x)$ but even for (the expectation values of) $\rho^\varepsilon(x)$ and $c^\varepsilon(x)$.

We can only work with the (smeared out) current and particle density $c^\varepsilon(x)$ and $\rho^\varepsilon(x)$, and notice that both belong to $Op\psi c_{(0,-\infty)}$. The symbol of ρ^ε commutes with h but the symbol of c^ε does not.

We then repeat the argument given for the spin observable: Assuming that the nature of the particle is known with certainty - either it is an electron or a positron, then we work with the symbol

$$(4.5.20) \quad \tilde{c}^\varepsilon(x^0) = \{p_+ \alpha p_+ + p_- \alpha p_-\} \delta^\varepsilon(x^0 - x) ,$$

i.e., the principal part of an operator giving the same expectation value as $c_j^\varepsilon(x)$ for such physical states. A calculation shows that

$$(4.5.21) \quad \tilde{c}^\varepsilon(x^0) = (h(x, \xi) - \mathbf{V}(x)) \frac{\xi - \mathbf{A}}{\langle \xi - \mathbf{A} \rangle^2} \delta^\varepsilon(x^0 - x) .$$

Clearly, this symbol is scalar in each of the two spaces S_\pm , since all terms are scalar, except $h(x, \xi)$. Thus we may use the calculus of sec.4.2 to determine the first correction. Details are left to the reader.

4.6 Classical Orbits for Particle and Spin

In this section we want to look at the Hamiltonian flow in (x, ξ) -space (i.e., phase space) induced by the “equations of motion” (4.2.24) - a system of 6 ODE-s in the 6 unknown functions $x(t), \xi(t)$ -, and, more generally, the propagation of the matrix $\kappa^\pm(x, \xi)$ along these orbits, described by eqn.s (4.4.21). We shall see that there indeed is a propagation of a point charge in the given electromagnetic field (induced by \mathbf{V} and \mathbf{A}), and also a propagation of a magnetic moment vector (of Bohr strength) sitting on that point charge.

Explicitly, the system (4.2.24) for $\lambda_+ = \langle \xi - \mathbf{A} \rangle + \mathbf{V}$ looks like this:

$$(4.6.1) \quad \dot{x} = \frac{1}{\langle \xi - \mathbf{A}(t, x) \rangle} (\xi - \mathbf{A}(t, x)) , \quad \dot{\xi} = \frac{1}{\langle \xi - \mathbf{A}(t, x) \rangle} \sum_j (\xi_j - \mathbf{A}_j(t, x)) \mathbf{A}_{j|x} - \mathbf{V}_{|x} .$$

The first equation may be solved for $\xi - \mathbf{A}$: We get

$$(4.6.2) \quad \xi - A = \frac{\dot{x}}{\sqrt{1 - \dot{x}^2}} , \quad \langle \xi - \mathbf{A} \rangle = \frac{1}{\sqrt{1 - \dot{x}^2}} .$$

Equating the derivative $\dot{\xi}$ of (4.6.2) with the second (4.6.1) gives

$$(4.6.3) \quad \left(\frac{\dot{x}}{\sqrt{1 - \dot{x}^2}} \right)' + \partial_t \mathbf{A}(t, x(t)) = -\mathbf{V}_{|x} + \sum_j \dot{x}_j \mathbf{A}_{j|x} .$$

In (4.6.3) we get $\partial_t \mathbf{A}(t, x(t)) = \mathbf{A}_{|t}(t, x(t)) + \sum_l \dot{x}_l(t) \mathbf{A}_{|x_l}(t, x(t))$. Now we use the relation

$$(4.6.4) \quad \dot{x} \times \text{curl } \mathbf{A} = \sum_l (\dot{x}_l \mathbf{A}_{l|x} - \dot{x}_l \mathbf{A}_{|x_l}) .$$

As a consequence (4.6.3) assumes the form

$$(4.6.5) \quad \left(\frac{\dot{x}}{\sqrt{1-\dot{x}^2}} \right)' = -\mathbf{A}_{|t}(t, x(t)) - \mathbf{V}_{|x}(t, x(t)) + \dot{x} \times \text{curl } \mathbf{A}(t, x(t)).$$

According to ch.1, footnote 1 we have the electric and magnetic field \mathcal{E} and \mathcal{H} given by

$$(4.6.6) \quad \mathcal{E} = -\mathbf{A}_{|t} - \text{grad } \mathbf{V} , \quad \mathcal{B} = \text{curl } \mathbf{A} ,$$

and the relativistic mass will be $\frac{1}{\sqrt{1-\dot{x}^2}}$, in the physical units we employ here. Accordingly (4.6.5) reads

$$(4.6.7) \quad \left(\frac{\dot{x}}{\sqrt{1-\dot{x}^2}} \right)' = \mathcal{E} + \dot{x} \times \mathcal{B} .$$

Clearly this exactly describes the acceleration of the charged particle under the force of the (time-dependent) electromagnetic field acting on it.

The above was evaluated for λ_+ . For λ_- we get the same equation (4.6.7), except that left hand side bears a minus sign - in accordance with the fact that, for a positron, all forces act in the opposite direction.

But now let us also try to interpret the propagation of (4.4.21), coming into play only for observables with symbols inducing a nontrivial map of the two eigenspaces S_{\pm} . It will be necessary then to evaluate the matrices Θ^{\pm} of (4.4.21).

Two things are important: First - (4.4.21) again is an ODE for the 2×2 -matrix - say, $\kappa = \kappa^+$, - again along the particle orbits - solutions of (4.2.24), with differentiation “ $'$ ” = $\partial_t + \lambda_{|\xi} \partial_x - \lambda_{|x} \partial_{\xi}$. Arguments similar to those in sec.4.2 apply, concerning the two propagations $A \rightarrow U(0, t)AU(t, 0)$ and (the Heisenberg representation) $A \rightarrow U(t, 0)AU(0, t)$, with the difference that q_t now does not propagate constant along the flow, but rather, as a solution of an initial-value problem of a first order linear homogeneous ODE.

Second, to simplify calculations, we note that the matrices Θ occur only in a commutator of the “equations of motion”. When we evaluate it we may omit any additive term giving a scalar multiple of the 2×2 - identity matrix, because its contribution to the commutator will vanish. We shall write “ $a = b(\text{mod } 1)$ ” if $b - a$ is a scalar multiple of the identity matrix

Again we focus on “+” and drop the +-sign in notation.

First we look at (the 2×2 -matrix)

$$(4.6.8) \quad \Theta^\sim = ((\langle \varphi_j, \psi'_i \rangle)) = (\varphi_1, \varphi_2)^* (\psi'_1, \psi'_2) .$$

From (4.4.1) we get

$$(4.6.9) \quad (\varphi_1, \varphi_2) = (1 + v_0)(-i\sigma\gamma) , \quad (\psi_1, \psi_2) = \frac{1}{2}(-i\sigma\gamma) , \quad \text{with } g = \frac{v}{1 + v_0} = \frac{\zeta}{1 + \langle \zeta \rangle} ,$$

hence $(\psi'_1, \psi'_2) = \frac{1}{2}(\frac{0}{-i\sigma\gamma'})$, and,

$$(4.6.10) \quad \Theta^\sim = \frac{1}{2}(1 + v_0)(\sigma\gamma)(\sigma\gamma') = \frac{1}{2}(1 + v_0)i\sigma.(\gamma \times \gamma') \pmod{1} .$$

Here we used the well known formula

$$(4.6.11) \quad (\sigma\xi)(\sigma\eta) = \xi.\eta + i\sigma.(\xi \times \eta) , \quad \xi, \eta \in \mathbb{R}^3 .$$

Note, $\gamma = \zeta/(1 + \langle \zeta \rangle)$ is a scalar multiple of $\zeta = \xi - \mathbf{A}$, hence $\gamma \times \gamma' = \frac{1}{(1 + \langle \zeta \rangle)^2} \zeta \times \zeta'$, since $\zeta \times \zeta = 0$. Thus we get - all $\pmod{1}$ -

$$(4.6.12) \quad \Theta^\sim = \frac{i}{2} \frac{1}{\langle \xi - \mathbf{A} \rangle (1 + \langle \xi - \mathbf{A} \rangle)} \sigma.((\xi - \mathbf{A}) \times (\xi - \mathbf{A})') .$$

Next we calculate

$$(4.6.13) \quad (\xi - \mathbf{A})' = \{ \partial_t + \sum_j \lambda_{|\xi_j} \partial_{x_j} - \sum_j \lambda_{|x_j} \partial_{\xi_j} \} (\xi - \mathbf{A}) ,$$

where $\lambda_{|\xi_j} = (\xi_j - \mathbf{A}_j)/\langle \xi - \mathbf{A} \rangle$ and $\lambda_{|x_j} = \mathbf{V}_{|x_j} - \sum_l \mathbf{A}_l |_{x_j} (\xi_l - \mathbf{A}_l)/\langle \xi - \mathbf{A} \rangle$.
The result is this:

$$(4.6.14) \quad (\xi_k - \mathbf{A}_k)' = -\mathbf{A}_{k|t} - \mathbf{V}_{|x_k} - \sum_j \frac{\xi_j - \mathbf{A}_j}{\langle \xi - \mathbf{A} \rangle} (\mathbf{A}_{k|x_j} - \mathbf{A}_{j|x_k}) , \quad k = 1, 2, 3.$$

The last term equals $+\frac{1}{\langle \xi - \mathbf{A} \rangle} (\text{curl } \mathbf{A} \times (\xi - \mathbf{A}))_k$. Thus we have

$$(4.6.15) \quad \zeta' = (\xi - \mathbf{A})' = -\mathbf{A}_{|t} - \mathbf{V}_{|x} + \frac{1}{\langle \xi - \mathbf{A} \rangle} \text{curl } \mathbf{A} \times (\xi - \mathbf{A}) ,$$

and we get

$$(4.6.16) \quad (\xi - \mathbf{A}) \times (\xi - \mathbf{A})' = \zeta \times \zeta' = \zeta \times (-\mathbf{V}_{|x} - \mathbf{A}_{|t}) - \frac{1}{\langle \zeta \rangle} (|\zeta|^2 \mathcal{B} - (\zeta.\mathcal{B})\zeta) .$$

All together we get

$$(4.6.17) \quad \Theta^\sim = -\frac{i}{2} \frac{1}{\langle \zeta \rangle (1 + \langle \zeta \rangle)} \sigma.(\zeta \times \mathcal{E} + \frac{1}{\langle \zeta \rangle} (|\zeta|^2 \mathcal{B} - (\zeta.\mathcal{B})\zeta)) .$$

Next we set out to calculate the other part $2\langle\zeta\rangle\Theta^1$ of the matrix Θ of (4.4.20). Here it might be some help to go back and write

$$(4.6.18) \quad 2\langle\zeta\rangle pp|_{\xi} p|_x p = pp_{\xi} h|_x p ,$$

noting that $2\langle\zeta\rangle pp|_{\xi} p|_x p = \lambda_+ pp|_{\xi} p|_x p + \lambda_- pp|_{\xi} p|_{-x} p$ while $pp|_{\xi} p = 0$.

We get

$$(4.6.19) \quad 2\langle\zeta\rangle\Theta^1 = \frac{1}{2}(1 + v_0)(1, i\sigma\gamma)p|_{\xi} h_0(\zeta)|_x (-\frac{1}{i\sigma\gamma}) \pmod{1}$$

with $h^0(\zeta) = \alpha\zeta + \beta$, since the term $\mathbf{V}|_x(1, i\sigma\gamma)(-\frac{1}{i\sigma\gamma}) = \mathbf{V}|_x(1 + |\gamma|^2)$ is scalar, using (4.6.11).

Now we get $p = \frac{1}{2}(1 + \frac{h_0(\zeta)}{\langle\zeta\rangle}) = \frac{1}{2}(1 + v_0 h_0(\zeta))$, hence $p|_{\xi_k} = \frac{1}{2}(v_0|_{\xi_k}/v_0)h_0(\zeta) + \frac{1}{2}v_0\alpha_k$ where the first term at right will generate a scalar multiple of 1, hence may be ignored. Also, $h_0(\zeta)|_{x_k} = (\sum \alpha_j(\xi_j - A_j) + \beta)|_{x_k} = -(\alpha.A)|_{x_k}$. Substituting into (4.6.19) we get

$$(4.6.20) \quad 2\langle\zeta\rangle\Theta^1 = -\frac{v_0}{4}(1 + v_0)(1, i\sigma\gamma)\left(\sum_{j'l} \mathbf{A}_{j|x_l} \alpha_j \alpha_l\right)(-\frac{1}{i\sigma\gamma}) .$$

But we have

$$(4.6.21) \quad \sum_{j'l} \mathbf{A}_{j|x_l} \alpha_j \alpha_l = \text{div } \mathbf{A} - i\rho \cdot \text{curl } \mathbf{A} ,$$

with $\rho = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}$, where again the first term may be ignored, when we substitute this into (4.6.20). We get

$$(4.6.22) \quad 2\langle\zeta\rangle\Theta^1 = -\frac{i}{4}v_0(1 + v_0)(1, i\sigma\gamma)\rho \cdot \mathcal{B}(-\frac{1}{i\sigma\gamma}) .$$

A matrix calculation then gives

$$(4.6.23) \quad (1, i\sigma\gamma) \begin{pmatrix} \sigma\mathcal{B} & 0 \\ 0 & \sigma\mathcal{B} \end{pmatrix} (-\frac{1}{i\sigma\gamma}) = (\sigma\mathcal{B}) + (\sigma\gamma)(\sigma\mathcal{B})(\sigma\gamma) = \sigma((1 - |\gamma|^2)\mathcal{B} + 2(\gamma\mathcal{B}\gamma)) .$$

We have $1 - |\gamma|^2 = \frac{2}{1 + \langle\zeta\rangle}$ so (4.6.23) equals

$$(4.6.24) \quad \frac{2}{1 + \langle\zeta\rangle}(\mathcal{B} + \frac{1}{1 + \langle\zeta\rangle}(\zeta\mathcal{B})\zeta) .$$

All together we then get

$$(4.6.25) \quad 2\langle\zeta\rangle\Theta^1 = -\frac{i}{2} \frac{1}{\langle\zeta\rangle^2} \sigma \cdot (\mathcal{B} + \frac{1}{1 + \langle\zeta\rangle}(\zeta\mathcal{B})\zeta) .$$

Collecting things, up to here: We have

$$(4.6.26) \quad \Theta = \Theta^\sim + 2\langle \zeta \rangle \Theta^1$$

with Θ^1 of (4.6.25) and

$$(4.6.27) \quad \Theta^\sim = -\frac{i}{2} \frac{1}{\langle \zeta \rangle (1 + \langle \zeta \rangle)} \sigma \cdot (\zeta \times \mathcal{E} + \frac{1}{\langle \zeta \rangle} (|\zeta|^2 \mathcal{B} - (\zeta \cdot \mathcal{B}) \zeta)) .$$

We may write $\Theta = -\frac{i}{2} \sigma \cdot \Upsilon$ with

$$(4.6.28) \quad \Upsilon = \frac{1}{\langle \zeta \rangle (1 + \langle \zeta \rangle)} (\zeta \times \mathcal{E} - \frac{1}{\langle \zeta \rangle} (|\zeta|^2 \mathcal{B} - (\zeta \cdot \mathcal{B}) \zeta)) + \frac{1}{\langle \zeta \rangle^2} (\mathcal{B} + \frac{1}{1 + \langle \zeta \rangle} (\zeta \cdot \mathcal{B}) \zeta) .$$

Any (hermitian symmetric) 2×2 -matrix κ may be (uniquely) written as $\kappa = \kappa^0 + \sigma \cdot \vec{\kappa}$, (often called the Garding-Wightman representation). In this form the DE (4.4.21) reads like this:

$$(4.6.29) \quad (\kappa^0)' = 0 , \quad \vec{\kappa}' + \Upsilon \times \vec{\kappa} = 0 .$$

The first equ. (4.6.29) coincides with (4.2.16), or its translation (4.6.7), using standard physical terms - this happens if q_t is a multiple of the identity. In order to evaluate the second (4.6.29) we must simplify Υ of (4.6.28).

Notice the terms with $(\zeta \cdot \mathcal{B}) \zeta$ cancel while \mathcal{B} carries the factor $\frac{1}{\langle \zeta \rangle^2} (1 + \frac{\zeta^2}{1 + \langle \zeta \rangle}) = \frac{1}{\langle \zeta \rangle^2 (1 + \langle \zeta \rangle)} (1 + \zeta^2 + \langle \zeta \rangle) = \frac{1}{\langle \zeta \rangle}$.

Thus we get

$$(4.6.30) \quad \Upsilon = \frac{1}{\langle \zeta \rangle (1 + \langle \zeta \rangle)} \zeta \times \mathcal{E} + \frac{1}{\langle \zeta \rangle} \mathcal{B} .$$

We still must use (4.6.1) and (4.6.2) to introduce visible physical quantities. We get

$$(4.6.31) \quad \Upsilon = \frac{\sqrt{1 - \dot{x}^2}}{1 + \sqrt{1 - \dot{x}^2}} \dot{x} \times \mathcal{E} + \sqrt{1 - \dot{x}^2} \mathcal{B} .$$

All in all then, our equations (4.2.14) have assumed a form characterized as follows:

Theorem 4.6.1 *We consider time-dependent potentials \mathbf{V}, \mathbf{A} satisfying $cdn.(X)$ with all their time-derivatives.*

Under the Heisenberg transform $A \rightarrow A_t = U(t, 0)AU(0, t)$ the “commutative part” q of the symbol $a = q + z \in \psi c_m$ of a “precisely predictable” observable $A = a(x, D)$ propagates as $q \rightarrow q_t = q_t^+ + q_t^-$ where $q_t^\pm(x, \xi)$ leave the eigenspaces $S_\pm(t, x, \xi)$ of the Hamiltonian symbol $h(t, x, \xi)$ (to $\lambda_\pm = \mathbf{V} \pm \langle \xi - \mathbf{A}(t, x) \rangle$) invariant.

Specifically, the map $q_t^+(x, \xi) : S_+(t, x, \xi) \rightarrow S_+(t, x, \xi)$ has a matrix $\kappa_t^+ = \kappa_t(x, \xi)$ (with respect to the bi-orthonormal system (4.4.1)) which decomposes as $\kappa = \kappa^0 + \sigma \cdot \vec{\kappa}$, and with κ^0 propagating as a constant along the “electron particle flow” determined by the “classical equations of motion” (4.6.7) - i.e.,

$$(4.6.32) \quad \left(\frac{\dot{x}}{\sqrt{1-\dot{x}^2}} \right)' = \mathcal{E} + \dot{x} \times \mathcal{B} .$$

On the other hand, the 3-vector $\vec{\kappa}_t$ propagates along the same classical electron flow, obeying an equation of motion of a magnetic moment vector (the spin-vector), of the form

$$(4.6.33) \quad \frac{1}{\sqrt{1-\dot{x}^2}} \vec{\kappa}' = \mathcal{B}^\sim , \text{ where } \mathcal{B}^\sim = \mathcal{B} + \frac{1}{1+\sqrt{1-\dot{x}^2}} \dot{x} \times \mathcal{E} ,$$

with the electric and magnetic field strength \mathcal{E} and \mathcal{B} of (4.6.6), where “ $'$ ” denotes the directional derivative along the flow, given by (4.4.13).

Similarly, the other part q^- of the symbol q will propagate with a matrix κ_- (with respect to the system (4.4.2)) for S_- and “classical orbits” of the positron and the positron spin, described by equations corresponding to (4.6.31)-(4.6.33).

Remark 4.6.2 Looking at thm.4.6.1 one observes that the value of the right hand side at a given t, x, ξ represents the magnetic field strength \mathcal{B}^\sim an electron, located at x with momentum ξ , moving at velocity \dot{x} - effected by the field of \mathbf{A}, \mathbf{V} - should experience at time t . If we interpret the vector $\vec{\kappa}(t, x, \xi)$ as the **magnetic moment** of the electron at (t, x, ξ) - which moves with the particle along the orbit through (t, x, ξ) - then $\vec{\kappa}'(t, x, \xi)$ should be the rate of change of that magnetic moment.

The factor $\frac{1}{\sqrt{1-\dot{x}^2}} \approx 1$ for relativistically small velocities should be regarded as a relativistic correction. So then, eqn. (4.6.33) just states that the magnetic moment approximately has the absolute value 1 - that is, it is of “Bohr-strength” (cf.[So1]) as it should be.

Remark 4.6.3 According to the “Stern-Gerlach effect” the orbit of an electron should also depend on the direction of its spin. But, in the above, such effect is not evident. Rather we get just the classically determined orbits of electron and positron without influence of the spin.

Note, however, this Stern-Gerlach effect is quantum mechanical, insofar as in all experiments proving it, there are only 2 spin-directions observed, not a continuous distribution - as it seems to us. So, since we are only looking at a first approximation, in this chapter, it may not be astonishing that this effect escapes our observation.

The (only) two-fold orbits of our theory arise from the fact that the Dirac Hamiltonian's symbol $h(t, x, \xi)$ - as 4×4 -matrix, has only two distinct eigenvalues $\lambda_{\pm} = \mathbf{V} \pm \langle \xi - \mathbf{A} \rangle$, each one of multiplicity 2. If we look closely at the decoupled Hamiltonian of sec.3.5 then it appears that a split of λ_+ into 2 distinct eigenvalues - both differing from λ_+ only by a symbol of order $-e^2$ - might be more natural to use for obtaining orbits of the electron. However, such split is not strong enough to be incorporated into our theory of observables, since it will disappear as $|x| + |\xi| \rightarrow \infty$.

Also, the construction of higher order corrections of observables, we will discuss in ch.V, will give us additional "decoupled symbols" - the matrices c_{\pm} of (4.2.15) (propagating in time) - to be considered while determining classical orbits.

Chapter 5

The Algebra of Precisely Predictable Observables

5.0 Introduction

In this chapter we will start by discussing a precise theorem giving a necessary and sufficient condition for smoothness of the (inverse) Heisenberg transform, with some “framing conditions” added. Note, the symbol classes ψc_m carry a “topology” (in fact, a Frechet topology), defined by the sup norms¹

$$(5.0.1) \quad \|a\|_{jl} = \sum_{|\theta|=j, |\iota|=l} \|\langle x \rangle^{-m_2+j} \langle \xi \rangle^{-m_1+l} a_{(\theta)}^{(\iota)}(x, \xi)\|_{L^\infty(\mathbb{R}^6)}, \quad j, l = 0, 1, 2, \dots,$$

where, as usual $\|b(x, \xi)\|_{\mathbb{R}^6} = \sup_{x, \xi \in \mathbb{R}^3} |b(x, \xi)|$. This allows a definition of differentiability of a symbol $a_t(x, \xi)$ for a parameter t : We shall say that

$a_t = a_t(x, \xi)$ belongs to $C^\infty(\mathbb{R}, \psi c_m)$ (or that the symbol a_t depends smoothly on t) if $a_t(x, \xi) \in C^\infty(\mathbb{R} \times \mathbb{R}^6)$ and if, in addition, the time-derivatives $\dot{a}_t, \ddot{a}_t, \dots, \partial_t^j a_t, \dots$ all exists in all of the above norms (5.0.1). Then also the ψ do $A_t = a_t(x, D)$ will be called a *smooth* functions of t (within the space $Op\psi c_m$).

We return to sec.4.2, and its assumptions there: time-dependent potentials \mathbf{A}_j, \mathbf{V} satisfying cnd.(X) with all their time-derivatives, for all t . We have the

¹In view of the results presented in ch.2 it is possible to carry over this Frechet topology to the operator class $Op\psi c_m$ by using the (countably many) norms $\|\langle x \rangle^{m_2-|\iota|} ad_x^\theta ad_D^\iota A \langle D \rangle^{m_1-|\theta|}\|_{\mathcal{H}}$. In view of (2.1.7) [which expresses the symbol as a trace of the product of a fixed trace class operator and an operator of the form (2.1.5)] we then get an equivalent topology on $Op\psi c_m$.

evolution operator $U(\tau, t)$ of the Dirac equation, an operator of order 0, - for time-independent \mathbf{A}_j, \mathbf{V} coinciding with $e^{-i(t-\tau)H}$ - and consider the (inverse) Heisenberg representation $A \rightarrow A_t = U(0, t)AU(t, 0)$, for an unbounded operator A acting on a dense subdomain of \mathcal{H} . We still assume $A \in Op\psi_{c_m}$ to be a strictly classical ψ do, and set $\tau = 0$.

In ch.4 - centering around relation (4.2.7) - we were developing a procedure to determine A_t for a given A - assuming that (i) $A_t = a_t(x, D)$ still belongs to $Op\psi_{c_m}$, while (ii) even $a_t \in \psi_{c_{m-e^1}}$. Actually, it was seen that these two conditions alone imply that the symbol $a(x, \xi)$ of such an operator must “nearly” commute with the symbol $h(0; x, \xi)$ of the Hamiltonian $H(t)$ at $t = 0$. More precisely, there must be a decomposition $a = q + z$ - and, generally, $a_t = q_t + z_t$, where $q_t(x, \xi)$ commutes with $h(t; x, \xi)$ [so, $q(x, \xi) = q(0, x, \xi)$ commutes with $h(0; x, \xi)$], for all x, ξ while $z = z_0$, $z_t \in \psi_{c_{m-e}}$.

Also, starting with an arbitrary given symbol $q \in \psi_{c_m}$ with $[h(0; x, \xi), q(x, \xi)] = 0$ for all x, ξ , we were attempting to construct a “correction symbol” $z(x, \xi) \in \psi_{c_{m-e}}$ - and, more generally, continuations q_t with $[q_t, h(t)] = 0$ and $z_t(x, \xi) \in \psi_{c_{m-e}}$ with $z_0 = z$ such that $A = a(x, D)$ with $a = q + z$ has a smooth (inverse) Heisenberg representation, given by $a_t(x, D)$ with $a_t = q_t + z_t$.

Our construction - so far - was not carried out completely, insofar as only q_t and an approximative z and z_t were obtained. This approximation was seen to be useful, however, insofar as it was correct “modulo lower order” - that is, its error tends to get negligibly small as $|x| + |\xi| \rightarrow \infty$. And the usefulness of this was confirmed, perhaps, since, among other facts, we were able to derive the classical equations of motion from it - including motion of the spin as a classical magnetic moment vector.

In the present chapter we will offer a mathematically complete theory, showing that an iteration of our procedure can be designed which indeed will supply a precise correction symbol $z \in \psi_{c_{m-e}}$ for every symbol $q \in \psi_{c_m}$ commuting with the Hamiltonian symbol $h(t, x, \xi)$ at $t = 0$ such that indeed (1) q and z both will have “extensions” $q_t \in \psi_{c_m}$ and $z_t \in \psi_{c_{m-e}}$, for all $t \in \mathbb{R}$, where $q_0 = q$, $z_0 = z$, while $[h(t; x, \xi), q_t(x, \xi)] = 0 \forall x, \xi \in \mathbb{R}^3, t \in \mathbb{R}$; (2) $q_t \in C^\infty(\mathbb{R}, \psi_{c_m})$ and $z_t \in C^\infty(\mathbb{R}, \psi_{c_{m-e}})$; (3) $A = q(x, D) + z(x, D)$ and $A_t = q_t(x, D) + z_t(x, D)$ satisfy $A_t = U(0, t)AU(t, 0)$ - that is, A_t is the (inverse) Heisenberg representation of A .

In sec.5.1, below, we will set up the precise class of operators for the above, and then will state and prove the corresponding theorem. The main ingredient of the proof will just be an iteration of the procedure in sec’s 4.2 and 4.4. But we again will need detailed facts about symbol propagation. These will be discussed

in sec.'s 5.4 and 5.5 together with those postponed in our discussions of sec's 4.2 and 4.4.

Our discussion in sec.5.1 will get us an algebra $\mathcal{P}(0)$ of precisely predictable observables at the initial point $\tau = 0$, but the procedure will work for any given initial τ , of course. Moreover, the operators of $\mathcal{P}(0)$ will propagate – with their inverse Heisenberg transform, creating the algebra $\mathcal{P}(\tau)$ at some arbitrary τ . These facts will be discussed in sec. 5.2. In sec.5.3 we return to the discussion of physical consequences surrounding this kind of “prediction”.

In sec.5.6 we will obtain an explicit second correction, at least for two dynamical observables - the energy split into potential and relativistic mass. [Here we assume time-independence and vanishing magnetic potentials \mathbf{A}_j , but a general $\mathbf{V}(x)$.]

In earlier publications [Co3],[Co4] we proposed the concept of precisely predictable observable as that of a self-adjoint operator $A \in Op\psi c$ with smooth Heisenberg representation, in the above sense. Such observables thus may be constructed from any given $q(x, \xi) \in \psi c$ commuting with $h(0; x, \xi)$ by constructing above correction symbol z , then defining $B = q(x, D) + z(x, D)$ and finally choosing $A = \frac{1}{2}(B + B^*)$, to obtain a self-adjoint operator (and a precisely predictable observable).

In the case of time-independent symbols this choice may be refined, by bringing into play the Dirac decoupling of ch.3. Namely, after proving thm.3.3.1 \equiv thm.5.5.1 we may use the precisely decoupling unitary operator U of sec.3.5 and declare only those self-adjoint ψ do-s precisely predictable which decouple precisely by that U . For precisely predictable approximations - in the sense of ch.4 or ,rather, of sec.5.1 - this means that we still must add a correction of order $-\infty$ after carrying out the iteration constructed in sec.5.1. This will be discussed in sec.5.8, after first discussing a proof of thm.3.3.1 in sec.5.7.

In the details of proofs, given in this chapter we will be partly dependent on certain results discussed in detail in [Co5], ch.VI, but too lengthy to be taken into the present book. Mostly they are straight-forward but more complicated extensions of theorems discussed here under restricted assumptions - for easier access.

5.1 A Precise Result on ψ do-Heisenberg Transforms

For every $m \in \mathbb{R}^2$ let us introduce the class $\mathcal{P}_m \subset Op\psi c_m$ of all (strictly classical) pseudodifferential operators $A = a(x, D) \in Op\psi c_m$ with the following property:

The (inverse) Heisenberg transform $A_t = U(0, t)AU(t, 0)$ (with the evolution operator $U(\tau, t)$ of the Dirac equation (1.0.1),(1.0.2) - with time-dependent potentials), belongs to $Op\psi_{c_m}$ again, for every $t \in \mathbb{R}$. Moreover, we have $A_t = a_t(x, D)$ with a symbol $a_t \in C^\infty(\mathbb{R}, \psi_{c_m})$, and, moreover, we have

$$(5.1.1) \quad \partial_t^j a_t(x, \xi) \in \psi_{c_{m-je^2}} \text{ , } j = 0, 1, 2, \dots \text{ .}$$

The class \mathcal{P} - evidently an (L^2 -adjoint invariant) algebra²- then is defined as union of all \mathcal{P}_m :

$$(5.1.2) \quad \mathcal{P} = \bigcup_{m \in \mathbb{R}^2} \mathcal{P}_m \text{ .}$$

General assumptions³ on the potentials of H : For $a(t, x) = \mathbf{V}(t, \mathbf{x}), \mathbf{A}_j(t, \mathbf{x})$ and also for all time-derivatives $\partial_t^j a(t, x)$, $j = 0, 1, 2, \dots$ require cdn.(X) of sec.3.1:

$$(5.1.3) \quad \partial_t^j \partial_x^\theta a(t, x) = O((1 + |x|)^{-1-|\theta|}) \text{ , } x \in \mathbb{R}^3 \text{ ,}$$

for each compact t -interval, and for each multi-index θ .

Theorem 5.1.1 (i) For each $A = a(x, D) \in \mathcal{P}_m$ the symbol allows a decomposition

$$(5.1.4) \quad a = q + z \text{ , with } z \in \psi_{c_{m-e}} \text{ , } [h(0; x, \xi), q(x, \xi)] = 0 \text{ , } x, \xi \in \mathbb{R}^3 \text{ .}$$

(ii) Vice versa, if a symbol $q \in \psi_{c_m}$ commutes with $h(0)$ for all $x, \xi \in \mathbb{R}^3$, there exists $z \in \psi_{c_{m-e}}$ with $A = a(x, D) \in \mathcal{P}_m$, for $a = q + z$. Here the “correction symbol” is an asymptotic sum $z = \Sigma z_j \pmod{\mathcal{O}(-\infty)}$, with solutions z_j of first order commutator equations, recursively, where z_{j-1} must be adjusted to insure solvability for z_j .

(iii) Suppose $A_1, A_2 \in \mathcal{P}_m$ (both must have a decomposition (5.1.4)) have the same q . Then $b = z_1 - z_2$ is symbol of $b(x, D) \in \mathcal{P}_{m-e}$; it allows (5.1.4) with $m - e$ instead of m .

²Regarding the algebra properties: Note that asymptotic sums (in the sense of prop.1.2.2) are finite sums near any finite x, ξ , hence may be differentiated term by term. This shows that cdn. (5.1.1) remains valid for products and adjoints of operators. It is evident that the algebra \mathcal{P} and its graded subspaces \mathcal{P}_m depend on the choice of the “initial point” - in our case $\tau = 0$, except if potentials are time-independent. So, we should refer to $\mathcal{P}(0)$, or, in general, $\mathcal{P}(\tau)$. Later it will be seen that $A \rightarrow A_t$ provides an algebra isomorphism $\mathcal{P}(0) \rightarrow \mathcal{P}(t)$.

³Then the (4×4 -matrix-valued) symbol $h(x, \xi)$ and the eigenvalues $\lambda_\pm(x, \xi)$ all belong to $\psi_{c_{e1}}$, while the unitary $u(x, \xi)$ of (3.2.1), the projections p_\pm of (4.2.9), and the dyads p_{tj}^\pm of (4.4.3) all belong to ψ_{c_0} .

Proof. We postpone the proof⁴ of (iii) to sec.5.7. [While we wanted to state this here - since it is a kind of uniqueness statement, linking (i) and (ii) - it is easier to verify (and perhaps more transparent) after we learn about the unitary decoupling of our algebra \mathcal{P} in sec.5.7.]

In essence, we will have to refine and continue the argument of sec.4.2. Let $A \in \mathcal{P}_m$. Note, the derivatives $\partial_t U(0, t)$ and $\partial_t U(t, \tau)$ exist in $L(\mathcal{H}_s, \mathcal{H}_{s-e^1})$ for every s , and $\partial_t U(0, t) = -iH(t)U(0, t)$, $\partial_t U(t, 0) = iU(t, 0)H(t)$ are operators of order e^1 - not ψ do-s, but they map $\mathcal{H}_s \rightarrow \mathcal{H}_{s-e^1}$, continuously⁵. Thus it follows that (4.2.4)) holds - i.e.

$$(5.1.5) \quad \dot{A}_t = -i[H(t), A_t] \quad , \quad t \in \mathbb{R} \quad , \quad A_0 = A \quad ,$$

holds, where again $A_t = a_t(x, D) \in Op\psi c_m$, by assumption. Using (5.1.1) and ψ do-calculus (1.2.3)-(1.2.6) we then get (4.2.7), i.e.,

$$(5.1.10) \quad \dot{a}_t = -i[h(t), a_t] - \{h(t), a_t\} + \frac{i}{2}\{h(t), a_t\}_2 + \dots \pmod{\mathcal{O}(-\infty)} \quad , \quad a_0 = a \quad .$$

By (5.1.1) we also have $\dot{a}_t \in \psi c_{m-e^2}$ while all other terms except the first at right are in ψc_{m-e^2} . It follows that the commutator $[h(t), a_t](x, \xi)$ belongs to ψc_{m-e^2} .

⁴The point is that cdn. (5.1.1) may not be needed for a study of a “local algebra” corresponding to \mathcal{P} . Note, if in (5.1.10) we ignore all Poisson brackets at right as terms of lower order [they are ψc_{m-e^2}] then we get

$$(5.1.6) \quad \dot{a} = i[h, a_t] \pmod{\psi c_{m-e^2}} \quad .$$

With the projections $p_{\pm} = \frac{1}{2}(1 \pm h(\xi)/\langle \xi - \mathbf{A} \rangle)$ - assuming \mathbf{A} time-independent, for a moment - and $X_{\varepsilon\delta} = p_{\varepsilon}Xp_{\delta}$, $\varepsilon, \delta = \pm$, it follows that

$$(5.1.7) \quad [h, a_t]_{++} = [h, a_t]_{--} = 0 \quad , \quad [h, a_t]_{+-} = 2\langle \xi - \mathbf{A} \rangle a_{t+-} \quad , \quad [h, a_t]_{-+} = -2\langle \xi - \mathbf{A} \rangle a_{t-+} \quad .$$

Accordingly, we conclude that (modulo ψc_{m-e^2}) we have

$$(5.1.8) \quad \dot{a}_{t++} = \dot{a}_{t--} = 0 \quad , \quad \dot{a}_{t+-} = 2i\langle \xi - \mathbf{A} \rangle a_{t+-} \quad , \quad \dot{a}_{t-+} = -2i\langle \xi - \mathbf{A} \rangle a_{t-+} \quad .$$

If this were sharp equations - not only mod $(\psi c_m - e^2)$ - then this at once implies that a_{t++} and a_{t--} would be independent of t - so equal to their value at $t = 0$, while we get

$$(5.1.9) \quad a_{t+-} = a_{+-}(x, \xi)e^{2it\langle \xi - \mathbf{A} \rangle} \quad , \quad a_{t-+} = a_{-+}(x, \xi)e^{-2it\langle \xi - \mathbf{A} \rangle} \quad .$$

Here it is easily verified that the functions a_{t+-} and a_{t-+} can be (strictly classical) symbols only if the “starting symbol” $a(x, \xi)$ has order $m_1 = -\infty$ - that is it belongs to $\psi c_{-\infty, m_2} = \cap\{\psi c_{m_1, m_2} : m_1 \in \mathbb{R}\}$.

Indeed, when taking (multiple) ξ -derivatives of the product (5.1.9) some of them will land on the factor $e^{\pm 2it\langle \xi \rangle}$ which does not produce decay when differentiated for ξ . So, some decay will be lost and must be made up for from the other factor.

So, this explains why our result needs the cdn. (5.1.1) - if we work without that we will get a larger class of ψ do-s: Applying the decoupling operator U to this larger class we will get operators with “ears” in $\psi c_{-\infty, \infty}$.

We will not discuss this in further detail.

⁵cf. thm.4.1.1 - or, more generally [Co5], VI, thm.3.1.

With the eigen-projections $p_{\pm} = p_{\pm}(t)$ of $h(t)$ (of (4.2.9)) write

$$(5.1.11) \quad a_t = a_{t++} + a_{t+-} + a_{t-+} + a_{t--} \text{ with } a_{t\pm\pm} = p_{\pm} a_t p_{\pm} ,$$

to get

$$(5.1.12) \quad [h(t), a_t] = (\lambda_+ - \lambda_-)(a_{t+-} - a_{t-+}) \text{ for all } x, \xi .$$

Thus

$$(5.1.13) \quad a_{t+-} = \frac{1}{2\langle \xi - \mathbf{A} \rangle} p_+ [h(t), a_t] \in \psi c_{m-e} , \quad a_{t-+} = -\frac{1}{2\langle \xi - \mathbf{A} \rangle} p_- [h(t), a_t] \in \psi c_{m-e} .$$

So, just define $q_t = a_{t++} + a_{t--} = p_+ a_t p_+ + p_- a_t p_-$, and $z_t = p_+ a_t p_- + p_- a_t p_+$ to get the decomposition $a = q + z$ as stated - $[h, q] = 0$ for all x, ξ , $q \in \psi c_m$, $z \in \psi c_{m-e}$ (even for all t , not only for $t = 0$), proving (i).

Vice versa - for the proof of (ii), let $q \in \psi c_m$ be given with $[h(0, x, \xi), q(x, \xi)] = 0 \forall x, \xi$. In sec.4.2 and sec.4.4 we already constructed symbols⁶ $q_t \in \psi c_m$ and $z_t \in \psi c_{m-e}$ solving eq. (5.1.10) modulo ψc_{m-e-e^2} . As next step we will go into (5.1.10) with $a_t = q_t + z_t + w_t$, $w_t \in \psi c_{m-2e}$, $\dot{w}_t \in \psi c_{m-2e-e^2}$ (seeking an improvement w_t for our first correction z_t), in the attempt to improve our approximation. Using that z_t satisfies (4.2.16), and that $[h(t), q_t] = 0$ we conclude from (5.1.10) that

$$(5.1.14) \quad i[h(t), w_t] + \{h(t), z_t\} - \frac{i}{2}\{h(t), q_t\}_2 + \dot{z}_t \in \psi c_{m-2e-e^2} .$$

In particular, note that $\{h, q_t\}_j \in \psi c_{m+e^1-j_e}$ and $\{h, z_t\}_j \in \psi c_{m+e^1-(j+1)_e}$, so that only the Poisson brackets listed in (5.1.14) appear. But we must assume, for now, that also $\dot{w}_t \in \psi c_{m-2e-e^2}$, for the w_t we will construct. This indeed will be verified later on for the w_t we now attempt to construct by setting the left hand side of (5.1.14) equal to 0. In other words, we try to solve the commutator equation

$$(5.1.15) \quad [h(t), w_t] = i(\{h(t), z_t\} + \dot{z}_t - \frac{i}{2}\{h(t), q_t\}_2) = x_t ,$$

where the right hand side is in ψc_{m-e-e^2} . Again a solution w_t of (5.1.15) exists if and only if we have

$$(5.1.16) \quad p_+ x_t p_+ = p_- x_t p_- = 0 .$$

⁶Recall that q_t was constructed using the Hamiltonian flow induced by $h(t; x, \xi)$. It will be essential that this flow has the following property: Write it as $(f_t, \varphi_t) = (f_t(x, \xi), \varphi_t(x, \xi))$, so that $\dot{f}_t = h_{|\xi}(t, f_t, \varphi_t)$, $\dot{\varphi}_t = -h_{|x}(t, x, \xi)$ and $f_0(x, \xi) = x$, $\varphi_0(x, \xi) = \xi$. For any symbol $a \in \psi c_m$ (and any m , any t) we then must have $a_t(x, \xi) = a(f_t(x, \xi), \varphi_t(x, \xi)) \in \psi c_m$. This is the statement of thm.5.4.3, below. Note, this automatically also implies that $\dot{a}_t = (a_{|x})_t(h_{|\xi})_t - (a_{|\xi})_t(h_{|x})_t \in \psi c_{m-e^2}$ -etc. [With cor.5.4.4 we also get the required cnd. (5.1.1) for $a_t = q_t + z_t$.]

This will *not* automatically be true. However, we recall that the symbol z_t we constructed in sec.4.2, explicitly given by (4.2.15), was not uniquely determined. Rather, z_t of sec.4.2 was given by (4.2.15) with w_t of (4.2.12) as soon as we have determined q_t . Recall, q_t was obtained by letting the components q^\pm float along the particle flow, as described in sec.4.2 and sec.4.4. But in (4.2.15) there are those functions c_\pm with $c_\pm = p_\pm c_\pm p_\pm$, so far left quite arbitrary except for assuming that they are symbols in ψc_{m-e} with $\dot{c}_\pm \in \psi c_{m-e-e^2}$. Replacing z_t in (5.1.15) with $z_t + c_t$, where z_t is given by (4.2.15) with $c_\pm = 0$ and $c_t = c_+ + c_-$ we may write (5.1.16) as

$$(5.1.17) \quad p_\pm(t)(\dot{c}_t + \{h(t), c_t\} + (\dot{z}_t + \{h(t), z_t\} - \frac{i}{2}\{h(t), q_t\}_2))p_\pm(t) = 0 ,$$

where now the symbol $y_t = \dot{z}_t + \{h(t), z_t\} - \frac{i}{2}\{h(t), q_t\}_2 \in \psi c_{m-e-e^2}$ is completely determined by our preceding operations. So, again, first we must determine c_t by solving the two equations (5.1.17). Once c_t solving (5.1.17) is found we have (5.1.16) with

$$(5.1.18) \quad x_t = i(\{h(t), z_t + c_t\} + \dot{z}_t + \dot{c}_t - \frac{i}{2}\{h(t), q_t\}_2) ,$$

and then simply have

$$(5.1.19) \quad w_t = d_{t+} + d_{t-} + \frac{1}{2\langle \xi - A(t, x) \rangle} (p_+ x_t p_- - p_- x_t p_+) ,$$

verified just as (4.2.15). Again $d_{t\pm}$ are arbitrary symbols in ψc_{m-2e} satisfying $d_\pm = p_\pm d_\pm p_\pm$, and we may impose the additional condition that $\dot{d}_\pm \in \psi c_{m-2e-e^2}$. Then we get $\dot{w}_t \in \psi c_{m-2e-e^2}$ as required for our Ansatz $a_t = q_t + z_t + w_t$.

Now we must solve the problem of finding a solution c_t of (5.1.17). Observe that c_t commutes with $h(t)$, by construction, just as q_t did, in our first construction. Moreover, the two matrices $c_{t\pm}$ of (4.2.15) correspond to (what we called) q_t^\pm in (4.2.13). Moreover, the conditions (5.1.17) for c_t - i.e., $p_\pm(\dot{c}_t + \{h(t), c_t\} + y_t)p_\pm = 0$ look exactly like eq.'s (4.2.14) on q_t , except that we now have an additional "inhomogeneous" term $p_\pm y_t p_\pm$ which was 0 in (4.2.15).

We may apply the technique of sec.4.4 again to convert (5.1.17) into a pair of first order PDE-s for the matrices γ_t^\pm of $c_{t\pm}$ with respect to the bi-orthogonal systems (4.4.1)-(4.4.2): With the matrices p_{jl}^\pm defined there we have $c_{t\pm} = \sum \gamma_{jl}^\pm p_{jl}^\pm$, and let also $p_\pm y_t p_\pm = \sum v_{jl}^\pm p_{jl}^\pm$. Then the same calculation performed in sec.4.4 transforms (5.1.17) into two 2×2 -matrix systems of the form

$$(5.1.20) \quad (\gamma_t^\pm)' + [\Theta_t^\pm, \gamma_t^\pm] + v_t^\pm = 0 , \quad (\Theta_t^\pm)_{jl} = \langle \varphi_j^\pm, (\psi_l^\pm)' \rangle + 2\langle \zeta \rangle \langle \varphi_j^\pm, p_{\pm|\xi} p_{\pm|x} \psi_l^\pm \rangle ,$$

with notations as in (4.4.21). The first system (for "+") contains only the unknown 2×2 -matrix function γ^+ , the other one only γ^- . There is the directional derivative

“” along the Hamiltonian flow of the system (4.2.24) again, for the two cases “+” and “-”, and the first (5.1.20) translates into the (system of) first order inhomogeneous ODE-s

$$(5.1.21) \quad \gamma'_t + [\Theta, \gamma_t] + v_t, \quad t \in \mathbb{R},$$

for the 2×2 -matrix function $\gamma_t(x, \xi)$, assuming “+” (and omitting “+”). The system (5.1.21) is uniquely solvable, given an initial matrix γ_0 . In sec.5.5 we will show that the solution γ_t extends uniquely for all $t \in \mathbb{R}$, and defines a symbol in ψc_{m-e} , given that $\gamma_0 \in \psi c_{m-e}$, [and, of course, using that $y_t \in \psi c_{m-e-e^2}$ implies $v_t \in \psi c_{m-e-e^2}$]. Normally we will assume that $\gamma_0 = 0$ to get $c_0 = 0$, so that the “commuting part” of our symbol a equals q . It also will follow that $\dot{\gamma}_t \in \psi c_{m-e-e^2}$. With this all, we then are assured that the condition for solvability of the commutator equation (5.1.15) is satisfied, so that then we may write down its solution in the form (5.1.19).

Note then, that, indeed, $\dot{w}_t \in \psi c_{m-2e-e^2}$, due to $y_t = -ix_t \in \psi c_{m-e-e^2}$, as we requested, when setting up (5.1.15). [And, moreover, cor.5.4.4 will give the required cdn. (5.1.1) for $a_t = q_t + z_t + w_t$.]

Note also, that we now have uniquely⁷defined functions $c_{t\pm}$ in (4.2.15), assuming that $c_{0\pm} = 0$.

It now should be clear that we may repeat this process of correction arbitrarily, to get a sequence $z_t, w_t, s_t, r_t, \dots$ of corrections of lower and lower order. To indicate just the next step: we will go with the Ansatz $a_t = q_t + z_t + w_t + s_t$ into equ. (5.1.5) and use that $[h(t), q_t] = 0$ and that (4.2.12) and (5.1.15) are valid. This will give yet another commutator equation

$$(5.1.22) \quad [h(t), s_t] = i(\{h(t), w_t\} + \dot{w}_t - \frac{i}{2}\{h(t), z_t\}_2 - \frac{1}{6}\{h(t), q_t\}_3) = \omega_t,$$

modulo ψc_{m-3e-e^2} , assuming that also $\dot{s}_t \in \psi c_{m-3e-e^2}$. We then solve the sharp equation (5.1.22), and again get a condition $p_{\pm}\omega_t p_{\pm} = 0$ for the right hand side of (5.1.22). This last condition translates into an ODE along the particle flows, for the matrices of $d_{t\pm}$ just like (5.1.21) for the γ_t or (4.4.21) for the κ_t . Again we must invoke thm.5.4.3 to verify that the d_t obtained are symbols of proper order, and that also $\dot{s}_t \in \psi c_{m-3e-e^2}$, as needed for the Ansatz. Furthermore, again, cor.5.4.4

⁷Note that our initial split $a_t = q_t + z_t$, obtained while proving statement (i) of our theorem, - i.e. (5.1.11),(5.1.12),(5.1.13), above - will bring forth different q_t and z_t , as we have constructed now: We will get the split $a_t = (q_t + c_t) + z_t$, with z_t of (4.2.15), setting $c_{\pm} = 0$ there. In other words, our q_t there no longer will be the initial q flowing along the particle flow. Rather, there will be a lower order perturbation c_t of q_t also commuting with $h(t)$ but propagating differently. One might try to relate this to the Stern-Gerlach correction of particle orbits, for different spins.

will bring the required cdn.(5.1.1) for the “partial sum” $a_t = q_t + z_t + w_t + s_t$. The new correction s_t then will be given by a formula like (5.1.19) with x_t replaced by ω_t and new arbitrary symbols d_t .

In this way we end up with a sequence $z_t^1 = z_t \in \psi c_{m-e}, z_t^2 = w_t \in \psi c_{m-2e}, z_t^3 = s_t \in \psi c_{m-3e}, \dots, z_t^j \in \psi c_{m-je}, \dots$, such that the “partial sum”

$A_t^N = q_t(x, D) + \sum_{j=1}^N z_t^j(x, D) \in Op\psi c_m$ satisfies (5.1.5) modulo a term of order $m - Ne - e^2$, for all $N = 1, 2, 3, \dots$. The asymptotic sum $z_t^\infty = \sum_1^\infty z_t^j$, in the sense of prop.1.2.2, then will give an operator $A_t = q_t(x, D) + z_t^\infty(x, D)$ satisfying⁸ (5.1.5) mod $\mathcal{O}(-\infty)$. Then form

$$(5.1.23) \quad B_t = U(t, 0)A_t^\infty U(0, t) - A_0^\infty .$$

Note we have $B_0 = 0$ and $\dot{B}_t = iU(t, 0)[H(t), A_t^\infty]U(0, t) + U(t, 0)\dot{A}_t^\infty U(0, t)$, where $U(0, t)$ and $U(t, 0) = U^*(0, t)$ are of order 0 (as evolution operators of a semi-strictly hyperbolic system of ψ do-s) while $\dot{A}_t^\infty + i[H(t), A] \in \mathcal{O}(-\infty)$, as just derived (cdn.(5.1.5)). It follows that $\dot{B}_t \in c^\infty(\mathbb{R}, \mathcal{O}(-\infty))$ as well. Integrating from 0 to t it follows that $B_t \in C^\infty(\mathbb{R}, \mathcal{O}(-\infty))$. In other words, we get

$$(5.1.24) \quad U(0, t)A_t^\infty U(t, 0) = A_t^\infty + U(0, t)B_t U(t, 0) ,$$

where again the last term belongs to $C^\infty(\mathbb{R}, \mathcal{O}(-\infty))$. But $\mathcal{O}(-\infty) = Op\psi c_{-\infty}$, by prop.1.4.6. Hence $U(0, t)B_t U(t, 0) = \check{z}_t^\infty(x, D)$ is a ψ do with some symbol $\check{z}_t \in \psi c_{-\infty}$. In particular, the right hand side of (5.1.24) is a ψ do of the form $q_t(x, D) + (z_t^\infty + \check{z}_t^\infty)(x, D)$ where the symbol $a_t = q_t + (z_t + \check{z}_t)$ satisfies cdn.(5.1.1), while $z_t^\infty + \check{z}_t^\infty$ is a symbol in ψc_{m-e} .

Conclusion: For the given symbol q commuting with $h(0)$ and $a = q + z_0^\infty$ with z_0^∞ , as defined above, we have $U(0, t)A^\infty U(t, 0) = A_t^\infty + \check{Z}_t^\infty = (q_t + z_t^\infty + \check{z}_0^\infty)(x, D)$.

This completes the proof of (ii).

5.2 Relations between the Algebras $\mathcal{P}(t)$

It might be useful now to reformulate our results of sec.5.1, by removing the special emphasis we put onto the point $\tau = 0$ as the “initial point” for the start of the smooth-inverse Heisenberg transform.

Looking at the definition of \mathcal{P}_m and \mathcal{P} around fla. (5.1.1), and at the group property

$$(5.2.1) \quad U(\tau, t) = U(\kappa, \tau)U(\tau, \kappa)$$

⁸That asymptotic sum is a finite sum near every finite t, x, ξ - even in compact t -intervals. Hence it may be t -differentiated term by term, and we get cdn.(5.1.1) for it.

of the evolution operator $U(\tau, t)$ - valid for *all* $\tau, \kappa, t \in \mathbb{R}$ - it will be clear that, with $\mathcal{P}(0) := \mathcal{P}$, defined as in sec.5.1, and

$$(5.2.2) \quad \mathcal{P}_m(\tau) = \{A_\tau = U(0, \tau)AU(\tau, 0) : A \in \mathcal{P}_m\}, \quad \mathcal{P}(\tau) = \cup \mathcal{P}_m(\tau),$$

we have defined a graded algebra for every $\tau \in \mathbb{R}$, just as for $\tau = 0$.

In particular, we note that $\mathcal{P}(\tau)$ may be redefined exactly parallel to the definition of $\mathcal{P} = \mathcal{P}(0)$ in sec.5.1:

$\mathcal{P}_m(\tau)$ consists precisely of all (strictly classical) ψ do-s $A = a(x, D) \in \text{Op}\psi c_m$ such that $A_{\tau t} = U(\tau, t)AU(t, \tau)$ belongs to $\text{Op}\psi c_m$ again, for all $t \in \mathbb{R}$, and that, moreover, $A_{\tau t} = a_{\tau t}(x, D)$ with symbol $a_{\tau t}$ satisfying

$$(5.2.3) \quad \partial_t^j a_{\tau t}(x, \xi) \in \psi c_{m-je^2}, \quad j = 0, 1, 2, \dots$$

In fact, let $A = a(x, D) \in \mathcal{P}(\tau)$. Such A is of the form $A = U(0, \tau)A^0U(\tau, 0)$ with some $A^0 = a^0(x, D) \in \mathcal{P} = \mathcal{P}(0)$, by our definition of $\mathcal{P}(\tau)$, and then we have $a(x, \xi) = a_\tau^0(x, \xi)$ with a_τ^0 defined as in (5.1.1). Using (5.2.1) we then get

$$(5.2.4) \quad A_{\tau t} = U(\tau, t)AU(t, \tau) = U(\tau, t)U(0, \tau)A^0U(\tau, 0)U(t, \tau) = U(0, t)A^0U(t, 0) = A_t^0.$$

Thus,

$$(5.2.5) \quad a_{\tau t}(x, \xi) = a_t^0(x, \xi).$$

This shows at once that we have (5.2.3) if and only if we have (5.1.1).

Similarly we conclude that

$$(5.2.6) \quad U(\tau, t)\mathcal{P}_m(\tau)U(t, \tau) = U(\tau, t)U(0, \tau)\mathcal{P}_mU(\tau, 0)U(t, \tau) = U(0, t)\mathcal{P}_mU(t, 0) = \mathcal{P}_m(t),$$

so that we have an algebra isomorphism $\mathcal{P}(\tau) \rightarrow \mathcal{P}(t)$ given by the map

$$(5.2.7) \quad \mathcal{P}(\tau) \rightarrow U(\tau, t)\mathcal{P}(\tau)U(t, \tau) = \mathcal{P}(t).$$

It might be important here to point to an inherent **unsymmetry** between the parameters t and τ here: For a given $A \in \text{Op}\psi c_m$ the two-parameter family $\{A_{\tau t} = U(\tau, t)AU(t, \tau) : \tau, t \in \mathbb{R}\}$ is well defined, taking values in the class of operators of order m . If $A \in \mathcal{P}(\tau)$ for some specific τ then we know that $A_{\tau t} \in \mathcal{P}(t) \subset \text{Op}\psi c_m$ again is a ψ do for all t . But this needs not to be true for other τ , specifically we expect it to be false in a neighbourhood of such τ .

On the other hand, if potentials are time-independent, then, of course, we get $U(\tau, t) = e^{-i(t-\tau)H}$ with the (time-independent) H . In that case we clearly have

$$(5.2.8) \quad A_{\tau t} = e^{-i(t-\tau)H} A e^{i(t-\tau)H} = A_{0, t-\tau} ,$$

which shows that, in this case, we have $\mathcal{P}(\tau) = \mathcal{P}$ independent of t . Moreover, the algebra isomorphism (5.2.7) then becomes an automorphism of \mathcal{P} . We then may say that \mathcal{P} is an invariant algebra of the Dirac equation - conjugation with the evolution operator leaves \mathcal{P} invariant.

Note, in the time-independent case, we may use the “forward Heisenberg transform” to define the algebra \mathcal{P} - this then only amounts to a time-reversal.

To repeat this again: The total-energy observable H is precisely predictable - it belongs to the algebra \mathcal{P} - in the case of time-independence. **But this is not so, if potentials depend on time**, although in that case still there exists the lower order correction symbol of thm.5.1.1. for the total energy $H(\tau)$ at time τ .

5.3 About Prediction of Observables again

To clarify our approach regarding Heisenberg transform and precise (or approximate) prediction of observables let us here discuss a comparison of classical and quantum mechanics, looking at - say - the orbit of our particle, as a classical prediction of future behaviour of the mechanical system - electron or positron in a given electro-magnetic field - we are studying.

Classically, at time $t = 0$, we are given the space-momentum coordinates - perhaps also the magnetic moment - of the particle. So, we are given the space and momentum coordinates x and ξ (and, perhaps, also the initial vectors $\vec{\kappa}^{\pm}$ of sec.4.6) at time $t = 0$. We then have the equations of motion (derived for us in sec.4.6) - a system of first order ODE-s determining the propagation of $x, \xi, \vec{\kappa}^{\pm}$ giving us an initial-value problem (for ODE-s) with completely determined initial data. From these data we can derive a unique orbit of the particle, predicting $x(t), \xi(t), \vec{\kappa}^{\pm}(t)$ with infinite accuracy - theoretical error = 0.

In quantum mechanics - with our special interpretation of v.Neumann’s rules - we have given corresponding observables x_j, D_j as linear operators on the Hilbert space \mathcal{H} , postponing discussion of the spin for now. These observables work at any time t . With the Schrödinger representation, for a moment, we have not an initial x or an initial momentum ξ given, at time $t = 0$, but, rather, an initial *physical state* $\psi_0(x) \in \mathcal{H}$ with $\|\psi_0\| = 1$. This may be a (near) eigen-state of x - i.e. a $\delta_\varepsilon(x - x^0)$ - certifying location of the particle near x^0 , or similarly a (near) eigenstate of D - but not both. With Schrödinger location and momentum are given by x and D

for all t , but the state ψ_0 propagates as a solution of $\dot{\psi} + iH(t)\psi = 0$ from ψ_0 into $\psi(t) = U(0,t)\psi_0$. An attempt to predict x or D at time t then amounts to studying the observable $A = x$ or $A = D$ in the state $\psi(t)$ - or, equivalently, with Heisenberg, the observable $U(t,0)AU(0,t) = A_{t0}$ in the state ψ_0 .

Now, since neither x nor D belongs to the algebra $\mathcal{P}(t)$ containing the precisely predictable observables at time t , the expectation value of A in the state $\psi(t)$ cannot be predicted with infinite accuracy in the sense of v.Neumann. Rather, we must hope to find a precisely predictable approximation A_∞ of A . In that respect we note that $A \in \mathcal{P}(t)$ is equivalent to $A_{t0} \in \mathcal{P}(0)$, by fla. (5.2.7). So we now may try to apply thm.5.1.1(ii) - either on the operator A for $\mathcal{P}(t)$ or also on A_{t0} for $\mathcal{P}(0)$ to construct an approximation of A from the algebra $\mathcal{P}(t)$. Of course, this works only if the symbol of A commutes with the symbol $h(t,x,\xi)$ of $H(t)$ - which is true for $A = x$ and $A = D$.

Nevertheless, we should make the point that **this - precisely - is the replacement, Quantum Mechanics makes for our observation of the orbit of the particle.**

Or, with some weaker attempt, one may only construct the first iteration, as we did in ch.4.

Even if we would succeed in constructing such $A_\infty \in \mathcal{P}(t)$, we might still have to refine this by adding yet another correction of order $-\infty$ to get into the still smaller algebra \mathcal{PX} of sec.5.8.

5.4 Symbol Propagation along Flows

In this section we finally attack the problem of symbol propagation under the Hamiltonian flows $\nu_{\tau t}$ used repeatedly in sec.'s 4.2, 4.4, 4.6, and sec.5.1. Generally we assume given a (real-valued) symbol $\lambda_t = \lambda(t;x,\xi) \in \psi c_{e^1}$, $t \in \mathbb{R}$. Moreover, we assume $\lambda_t \in C^\infty(\mathbb{R}, \psi c_{e^1})$ using the norms (5.0.1) for $m = e^1$. Clearly this may be verified for the two symbol eigenvalues $\lambda_t^\pm = \mathbf{V}(t,x) \pm \langle \xi - \mathbf{A}(t,x) \rangle$ of our Dirac Hamiltonian H , if the potentials $\mathbf{V}(t,x)$, $\mathbf{A}_j(t,x)$ satisfy cdn.(X) with all their time derivatives.

Repeatedly, in the preceding sections, we were facing a problem of investigating symbol properties of solutions of an initial-value problem of a first order PDE of the form

$$(5.4.1) \quad \partial_t u + \lambda_{|\xi} \cdot \partial_x u - \lambda_{|x} \cdot \partial_\xi u + ku - l = 0, \quad u(0) = u_0,$$

where $k = k(t) = k(t;x,\xi)$, $l = l(t) = l(t;x,\xi)$, $u_0 = u_0(x,\xi)$ are given symbols. In the simplest case we had $k = l = 0$, and the solution $u(t;x,\xi)$ a scalar. Then it

was found that the general solution of equ. (5.4.1) consists of all functions constant along the flow generated by the system of 6 ODE-s in 6 unknown functions $x(t), \xi(t)$

$$(5.4.2) \quad \dot{x} = \lambda|_{\xi}(t; x, \xi) , \quad \dot{\xi} = -\lambda|_x(t; x, \xi) .$$

But we also needed to look at problems of the form (5.4.1) with non-vanishing k or l , and even with matrix-valued solutions $u(t; x, \xi)$ - such as equ. (4.4.21), or equ. (5.1.15).

In the latter case, (5.1.1) turns into an ODE along the flow, of the form

$$(5.4.1') \quad \tilde{u}' + \tilde{k}\tilde{u} = \tilde{l} , \quad \tilde{u}(0) = u_0 ,$$

where we set $\tilde{g}(\tau) = g \circ \nu_{0\tau} = g(\tau; x_{0\tau}(x, \xi), \xi_{0,\tau}(x, \xi))$, and with “ $'$ ” = ∂_{τ} . Again $\nu_{0\tau}$ denotes the flow $(x, \xi) \rightarrow (x_{0\tau}(x, \xi), \xi_{0,\tau}(x, \xi))$ generated by the Hamiltonian system (5.4.2).

We shall provide answers to questions around symbol properties of solutions $u(t; x, \xi)$ of (5.4.1) in 3 steps:

(i) The components $f(x, \xi) = x_{0\tau}(x, \xi)$ and $\varphi(x, \xi) = \xi_{0\tau}(x, \xi)$ of the flow $\nu_{0\tau}$ are symbols. Specifically, we get $f = x_{0\tau} \in \psi c_{e^2}$ and $\varphi = \xi_{0\tau} \in \psi c_{e^1}$. Moreover, we have f, φ of the same order than x, ξ , respectively. That is, $c\langle x \rangle \leq \langle f \rangle \leq C\langle x \rangle$ and $c\langle \xi \rangle \leq \langle \varphi \rangle \leq C\langle \xi \rangle$ with positive constants c, C , in compact τ -intervals.

(ii) The substitution $g \rightarrow g \circ \nu_{0\tau}$ preserves the symbol property of the function g - in the sense that $g \in \psi c_m$ if and only if $g \circ \nu_{0\tau} \in \psi c_m$.

(iii) The solution of (the ODE-initial value problem) (5.4.1') possesses the same symbol properties as its initial-value u_0 and its un-homogeneous term \tilde{b} , assuming that the (matrix-) function \tilde{k} is ψc_0 . That is - assuming that $\tilde{k} \in \psi c_0$ and that $u_0, \tilde{l}(\tau) \in \psi c_m$ we will get $\tilde{u}(\tau) \in \psi c_m$ as well. Moreover⁹, if even $\tilde{k} \in \psi c_{-e^2}$ and $\tilde{l}(\tau) \in \psi c_{m-e^2}$, then it also follows that $\tilde{u}' \in \psi c_{m-e^2}$. [This latter fact is an immediate consequence of equ.(5.4.1'), once we have that $\tilde{u}(\tau) \in \psi c_m$. It is of crucial importance for our results, because it will guarantee that $\dot{q} \in \psi c_{m-e^2} \cdot \dot{z}_t \in \psi c_{m-e-e^2} , \dot{w}_t \in \psi c_{m-2e-e^2}$, etc.]

In this section we focus on verifying (ii) and (iii), above. Note that (ii) is a consequence of (i), with some calculations, while (iii) is an extension of some

⁹Actually, to verify (5.1.1) for the symbol constructed in step (ii) of thm.5.1.1, we must verify that also a j -fold time derivative applied to the unknown symbol u in (5.5.1) will give a je^2 -fold improvement in the order of u - i.e., that $\partial_t^j u \in \psi c_{m-je^2}$ for $j=1,2,\dots$. This, however, follows automatically, once we impose proper conditions on the coefficient symbols (cf. corollary 5.4.4).

facts already developed in sec.1.5 for scalar equations. Clearly (ii) means that, regarding symbol properties of solutions of the PDE (5.4.1) we may safely focus on the ODE (5.4.1'): A coefficient of (5.4.1) belongs to a ψc_s if and only if the corresponding coefficient $\tilde{\cdot}$ belongs to ψc_s , and the same holds also for the solutions u and \tilde{u} . We shall discuss (i) in sec.5.5, below - this involves a somewhat more delicate procedure (cf. prop.5.5.1 and thm.5.5.2).

Proposition 5.4.1 *We have $g(x, \xi) \in \psi c_m$ if and only if*

$$(g \circ \nu_{0\tau})(x, \xi) = g(f(x, \xi), \varphi(x, \xi)) \in \psi c_m.$$

Proof. In view of the inversion property of the flow $\nu_{\tau\tau'}$ it suffices to prove the “if”. Let $v(x, \xi) = g(f(x, \xi), \varphi(x, \xi))$. Looking at (1.2.2) we get

$$(5.4.3) \quad |v(x, \xi)| = |g(f, \varphi)| \leq c \langle f \rangle^{m_2} \langle \varphi \rangle^{m_1} \leq c' \langle x \rangle^{m_2} \langle \xi \rangle^{m_1},$$

using that x, f and ξ, φ are of the same order, respectively (cf.(i) above, or, prop.5.5.1). This confirms the first estimate (1.2.2) for v .

Next, we get

$$(5.4.4) \quad v_{|x} = g_{|x} f_{|x} + g_{|\xi} \varphi_{|\xi}.$$

Here $g_{|x} = O(\langle f \rangle^{m_2-1} \langle \varphi \rangle^{m_1})$ and $g_{|\xi} = O(\langle f \rangle^{m_2} \langle \varphi \rangle^{m_1-1})$, using (1.2.2) for g . Also, $f_x = O(1)$, but $\varphi_x = O(\langle \xi \rangle / \langle x \rangle)$, using (1.2.2) for $f \in \psi c_{e_2}$ and $\varphi \in \psi c_{e_1}$ (as stated in (i) again - or, look at thm.5.5.2). Since f, x and φ, ξ are of the same order, we then indeed get $v_{|x} = O(\langle x \rangle^{m_2-1} \langle \xi \rangle^{m_1})$. This is one of the two estimates (1.2.2) involving derivatives of order $|\iota| + |\theta| = 1$, and the other one follows similarly. In fact this outline should be sufficient to explain the induction argument completing the proof.

Next, to discuss (iii) above - which involves only an ODE - we need¹⁰ the explicit form of the evolution operator for a system of first order ODE-s, in terms of a fundamental system of solutions of the “corresponding homogeneous equation” $\tilde{u}' + \tilde{k}\tilde{u} = 0$:

This evolution operator $E(\tau, t)$ just equals the $N \times N$ -matrix solution of the equation satisfying the initial condition $E(\tau, \tau) = 1$. In other words, $E(\tau, t)$ is the unique $N \times N$ -matrix-function solving

$$(5.4.5) \quad \partial_t E(\tau, t) + \tilde{k}(t; x, \xi) E(\tau, t) = 0, \quad E(\tau, \tau) = 1.$$

¹⁰It may help to note that, already in sec.1.5 - fla. (1.5.4),(1.5.5) - we discussed the fact that the function $u_0 = e^{-ikt}$, for a symbol $k \in \psi c_0$, belongs to ψc_0 . Observe that u_0 is the evolution operator of the ODE $\dot{u} + ik u = 0$, i.e., we have our problem here for the scalar case, of a 1-vector u . Similarly we now must prove the same symbol property for the general case, involving N -vectors.

We may use E to solve the problem (5.4.1') - we get¹¹

$$(5.4.6) \quad \tilde{u}(t) = E(0, t)u_0 + \int_0^t E(\tau, t)\tilde{l}(\tau)d\tau .$$

From (5.4.6) we may directly read off the symbol property of \tilde{u} , once we have the proposition, below.

Proposition 5.4.2 *The function $E(\tau, t) = E(\tau, t; x, \xi)$ belongs to ψc_0 for any fixed choice of τ, t .*

Proof. This proof follows some very technical but standard arguments in theory of ODE's, concerning dependence of solutions on initial values. We present only a discussion showing that the very first two symbol estimates (1.2.2) hold. This should give a hint how it may be extended to obtain all other such estimates.

Differentiating (5.4.5) for x we get

$$(5.4.7) \quad (\langle x \rangle \tilde{u})' + \tilde{k}(\langle x \rangle \tilde{u}) + (\langle x \rangle \tilde{k}|_x) \tilde{u} = 0 .$$

Write (5.4.5) and (5.4.7) together in matrix form:

$$(5.4.8) \quad v' + \begin{pmatrix} k & 0 \\ \langle x \rangle k|_x & 0 \end{pmatrix} v = 0 , \quad v(0) = \begin{pmatrix} u_0 \\ \langle x \rangle u_{0|x} \end{pmatrix} = v_0 ,$$

where we dropped “ $\tilde{\cdot}$ ”, for a moment, and introduced the vector $v = \begin{pmatrix} u \\ \langle x \rangle u|_x \end{pmatrix}$.

Important to note then: The matrix in (5.4.8) is bounded in x, ξ [for a compact τ, t -interval], in view of estimates (1.2.2) for $k \in \psi c_0$. So, we may use (5.4.8) for the estimate

$$(5.4.9) \quad |v'| \leq c|v| ,$$

with a constant c independent of x, ξ, τ, t . Then (5.4.9) gives $|(|v|^2)'| \leq 2c|v|^2$ which may be integrated for

$$(5.4.10) \quad |v| \leq |v_0|e^{c|t-\tau|} .$$

Clearly this implies the first two estimates (5.4.2) for the evolution matrix $E(\tau, t)$ and for order $m = 0$. Q.E.D.

We summarize our results - anticipating the results, concerning remark (i) above, to be discussed in sec 5.4, below.

¹¹To confirm (5.4.5) just left-multiply by $E(t, 0)$, use the “group property” $E(t, \kappa)E(\tau, t) = E(\tau, \kappa)$ [which follows from definition of E] and differentiate, obtaining equal left and right hand sides. We have equality in (5.4.6) at $t = 0$, so equality holds everywhere.

Theorem 5.4.3 *Let the real-valued $\lambda = \lambda(t; x, \xi)$ belong to $C^\infty(\mathbb{R}, \psi_{c_{e^1}})$. Then the (unique) solution $u(t, x, \xi)$ of the first order initial value problem (5.4.1) with given ($N \times N$ -matrix-valued) symbols $k(t; x, \xi) \in C^\infty(\mathbb{R}, \psi_{c_0})$ and $l(t) = l(t; x, \xi) \in C^\infty(\mathbb{R}, \psi_{c_m})$ - for some $m = (m_1, m_2)$, and with $u_0 \in \psi_{c_m}$, exists for all times t , and it belongs to $C^\infty(\mathbb{R}, \psi_{c_m})$.*

If, in addition, we have $k \in C^\infty(\mathbb{R}, \psi_{c_{-e^2}})$ and $l \in C^\infty(\mathbb{R}, \psi_{c_{m-e^2}})$, then it also follows that $\dot{u} = \partial_t u \in C^\infty(\mathbb{R}, \psi_{c_{m-e^2}})$.

The last statement of the theorem still requires the observation that, once we have shown that $u \in C^\infty(\mathbb{R}, \psi_{c_m})$, every term of equ. (5.4.1), except the first one, will be in $\psi_{c_{m-e^2}}$ so that this also follows for the first term \dot{u} . Moreover, an induction argument shows that we have

Corollary 5.4.4 *Under the assumptions of thm.5.4.3, if in addition we have*

$$(5.4.11) \quad \partial_t^j \lambda \in \psi_{c_{-je^2}}, \quad \partial_t^j \in \psi_{c_{-(j+1)e^2}}, \quad \partial_t^j l \in \psi_{c_{m-(j+1)e^2}}, \quad \text{for } j \geq 1,$$

then it also follows that $\partial_t^j u \in \psi_{c_{m-je^2}}$ for all $j=1, 2, \dots$.

Indeed, this follows for j by differentiating (5.4.1) for t and using that it is true for $j-1$.

We then may go back to (5.1.16), (5.1.17), for example and note that indeed there $\Theta \in \psi_{c_{-e^2}}$, while v_t also is of e^2 orders lower, so that the last sentence of thm.5.4.3 applies. Also, we may use cor. 5.4.4, looking at higher t -derivatives.

5.5 The Particle Flows Components are Symbols

Let us now fill in the missing link of sec.5.4 - discussing (i) there. Generally we assume given a symbol $\lambda_t = \lambda(t; x, \xi) \in \psi_{c_{e^1}}$, $t \in \mathbb{R}$. Moreover, we assume $\lambda_t \in C^\infty(\mathbb{R}, \psi_{c_{e^1}})$ using the norms (5.0.1) for $m = e^1$. Clearly this may be verified for the two symbol eigenvalues $\lambda_t^\pm = V(t, x) \pm \langle \xi - A(t, x) \rangle$ of our Dirac Hamiltonian H , if the potentials $V(t, x), A_j(t, x)$ satisfy cdn.(X) with all their time derivatives. Then consider the system of 6 ODE-s in 6 unknown functions $x(t), \xi(t)$

$$(5.5.1) \quad \dot{x} = \lambda_{|\xi}(t; x, \xi), \quad \dot{\xi} = -\lambda_{|x}(t; x, \xi),$$

with initial conditions

$$(5.5.2) \quad x(\tau) = x^0, \quad \xi(\tau) = \xi^0,$$

where $x^0, \xi^0 \in \mathbb{R}^3$ are given 3-vectors.

Differentiability for t implies Lipschitz continuity in t , hence a local unique solution of (5.5.1),(5.5.2) exists in some interval $|t - \tau| \leq \varepsilon > 0$, by Picard's theorem. For an ODE of this kind the problem of extending that solution into a larger t -interval is just a matter of deriving *apriori estimates*¹². Here is such an apriori estimate:

Let us write $f = f(t, \tau; x, \xi) = f(x, \xi) = x_{\tau t}(x, \xi)$, $\varphi = \varphi(t, \tau; x, \xi) = \varphi(x, \xi) = \xi_{\tau t}(c, \xi)$, so that (5.5.1),(5.5.2) assume the form

$$(5.5.3) \quad \dot{f} = \lambda_{|\xi}(t; f, \varphi), \quad \dot{\varphi} = -\lambda_{|x}(t; f, \varphi), \quad f = x, \varphi = \xi \text{ at } t = \tau.$$

Proposition 5.5.1 *For any given finite interval $|t - \tau| \leq \eta_0$ (any $0 < \eta_0 < \infty$) we have the apriori estimates*

$$(5.5.4) \quad c\langle x \rangle \leq \langle f \rangle \leq C\langle x \rangle, \quad c\langle \xi \rangle \leq \langle \varphi \rangle \leq C\langle \xi \rangle, \text{ for all } |t - \tau| \leq \eta_0,$$

with constants $c, C > 0$ independent of t, x, ξ (but possibly depending on η_0).

Proof. We have

$$(5.5.5) \quad \langle f \rangle \cdot = \frac{f \dot{f}}{\langle f \rangle} = \lambda_{|\xi} \frac{f}{\langle f \rangle} = O(\langle f \rangle), \quad \langle \varphi \rangle \cdot = -\frac{\lambda_{|x} \varphi}{\langle \varphi \rangle} = O(\langle \varphi \rangle).$$

Integrating this, under the initial conditions $\langle f \rangle = \langle x \rangle$, $\langle \varphi \rangle = \langle \xi \rangle$ at $t = \tau$ we get

$$(5.5.6) \quad \left| \log \frac{\langle f \rangle}{\langle x \rangle} \right| \leq c_0, \quad \left| \log \frac{\langle \varphi \rangle}{\langle \xi \rangle} \right| \leq c_0$$

with constant $c_0 = \eta_0 \sup\{|\lambda_{|\xi}|, |\lambda_{|x}|/\langle \xi \rangle\} : x, \xi \in \mathbb{R}^3, |t - \tau| \leq \eta_0\}$. The logarithm is an increasing function, so (5.5.6) implies (5.5.4) with constants $c = e^{-c_0}, C = e^{c_0}$, q.e.d.

As a consequence of the proposition the flow $\nu_{\tau t} : \mathbb{R}^6 \rightarrow \mathbb{R}^6$ indeed exists for all τ, t . It is given by the map $(x, \xi) \rightarrow (f(x, \xi), \varphi(x, \xi))$. Using well known differentiability properties of solutions of ODE-s, derivatives $\partial_t^j \partial_\tau^l \partial_x^\theta \partial_\xi^\iota f$, $\partial_t^j \partial_\tau^l \partial_x^\theta \partial_\xi^\iota \varphi$ of any order j, l, θ, ι exist and are continuous - and they satisfy all equations obtained

¹²This means the following: Assuming the local solution may be extended into $|t - \tau| \leq \eta_0$ then one must use the equation and initial conditions only to derive boundedness of that solution (in that interval). If one succeeds in doing so, then the local solution indeed extends into that interval (and satisfies that "apriori estimate"). This is true because the estimate provides a "box" the solution cannot leave, and where the derivatives also stay bounded, so that the solution cannot oscillate either, while a local solution (for continuation) exists wherever it goes.

by formally differentiating (5.5.1) or (5.5.2) with respect to any of the variables t, τ, x, ξ .

We want to show that $f(x, \xi) \in \psi_{c_{e^2}}$, $\varphi(x, \xi) \in \psi_{c_{e^1}}$ for every t, τ , i.e., that $f_{(\theta)}^{(\iota)}$, $\varphi_{(\theta)}^{(\iota)}$ satisfy the estimates (1.2.2), for their orders $m = e^2, e^1$, respectively. Clearly for $\theta = \iota = 0$ this is implied by (5.5.4). We prepare for an induction proof by considering next the case $|\iota| + |\theta| = 1$ (i.e., by differentiating (5.5.3) once - for one of the x, ξ (occurring in the initial conditions only)). Write $f_{(\theta)}^{(\iota)} = v$, $\varphi_{(\theta)}^{(\iota)} = w$, for a moment, and get

$$(5.5.7) \quad \begin{aligned} \dot{v} &= \lambda_{|\xi x} v + \lambda_{|\xi \xi} w, \quad v = x_{(\theta)}^{(\iota)} \quad \text{as } t = \tau, \\ \dot{w} &= -\lambda_{|xx} v - \lambda_{|x\xi} w, \quad w = \xi_{(\theta)}^{(\iota)} \quad \text{as } t = \tau, \end{aligned}$$

with the 3×3 -matrices

$$(5.5.8) \quad \lambda_{|\xi x} = ((\lambda_{|\xi_j x_i}(t; f, \varphi))), \quad \lambda_{|x\xi} = ((\lambda_{|x_j \xi_i}(t; f, \varphi))), \quad \text{etc.}$$

Under our assumptions we get $\lambda_{|\xi x}, \lambda_{|x\xi} \in \psi_{c_{-e^2}}$ and $\lambda_{|xx} \in \psi_{c_{e^1-2e^2}}$, $\lambda_{|\xi\xi} \in \psi_{c_{-e^1}}$, implying corresponding estimates for the coefficients of the system (5.5.7). Let us multiply the first equation (5.5.7) by $\frac{1}{\langle f \rangle}$, and the second equation by $\frac{1}{\langle \varphi \rangle}$, and regard (5.5.7) as a system

$$(5.5.9) \quad \dot{p} = Pp, \quad p = p^0 \quad \text{at } t = \tau,$$

of first order ODE-s for the vector $p = \begin{pmatrix} p_1 \\ p_2 \end{pmatrix}$, with $p_1 = \frac{v}{\langle f \rangle}$, $p_2 = \frac{w}{\langle \varphi \rangle}$, and with the matrix

$$(5.5.10) \quad P = \begin{pmatrix} \lambda_{|\xi x}(f, \varphi) & \frac{\langle \varphi \rangle}{\langle f \rangle} \lambda_{|\xi \xi}(f, \varphi) \\ -\frac{\langle f \rangle}{\langle \varphi \rangle} \lambda_{|xx}(f, \varphi) & -\lambda_{|x\xi}(f, \varphi) \end{pmatrix} + \begin{pmatrix} -\frac{f \lambda_{|\xi}}{\langle f \rangle^2} & 0 \\ 0 & \frac{\varphi \lambda_{|x}}{\langle \varphi \rangle^2} \end{pmatrix},$$

where the second matrix at right is generated by the conversion of the vector $\begin{pmatrix} \dot{v}/\langle f \rangle \\ \dot{w}/\langle \varphi \rangle \end{pmatrix}$ into \dot{p} . Both matrices clearly are $O(\frac{1}{f})$, using that the symbols $\lambda_{|\xi x}(t; f, \varphi) = O(\frac{1}{\langle f \rangle})$, etc., and also using (a slight improvement of) (5.5.4). Note that (5.5.9) implies

$$(5.5.11) \quad |p|^2 = 2\Re(p \cdot \dot{p}) = 2\Re(p \cdot Pp) = O(|p|^2), \quad |p|^2 = |p(\tau)|^2 \quad \text{at } t = \tau.$$

Integrating this we get

$$(5.5.12) \quad \left| \log \frac{|p(t)|}{|p(\tau)|} \right| \leq c|t - \tau| \frac{1}{\langle f \rangle}.$$

That is,

$$(5.5.13) \quad |p(\tau)| e^{-c|t-\tau|/\langle f \rangle} \leq |p(t)| \leq |p(\tau)| e^{c|t-\tau|/\langle f \rangle},$$

with some constant c , depending on the t -interval chosen.

Finally, we must distinguish between the cases where an x - (or ξ -) derivative was taken. If $|\iota| = 1, \theta = 0$ then we have $v = 0, |w| = 1$ at $t = \tau$, so that $p^0 = (\delta_{ji}^0 / \langle \varphi \rangle) = c^0 / \langle \varphi \rangle$, for some constant 6-vector c^0 , $|c^0| = 1$. Then (5.5.13) amounts to

$$(5.5.14) \quad f_{|\xi} = O\left(\frac{\langle f \rangle}{\langle \varphi \rangle}\right) \quad , \quad \varphi_{|\xi} = O(1) \quad .$$

In view of (5.5.4) this gives the desired symbol estimates (1.2.2) for one ξ -derivative. Similarly one derives that estimate for one x -derivative. Substituting this back into the ODE (5.5.9) we also get estimates for the derivatives \dot{v} and \dot{w} - namely,

$$(5.5.15) \quad \dot{f}_{|\xi} = O\left(\frac{1}{\langle \xi \rangle}\right) \quad , \quad \dot{f}_{|x} = O\left(\frac{1}{\langle x \rangle}\right) \quad , \quad \dot{\varphi}_{|\xi} = O\left(\frac{1}{\langle x \rangle}\right) \quad , \quad \dot{\varphi}_{|x} = O\left(\frac{\langle \xi \rangle}{\langle x \rangle^2}\right) \quad ,$$

valid in any finite t -interval.

Note, that (5.5.15) are exactly the first estimates needed to show that

$$(5.5.16) \quad \dot{f} \in \psi c_0 \quad , \quad \dot{\varphi} \in \psi c_{e^1 - e^2}$$

as we shall proceed to show, in the following.

To continue this iteration differentiate (5.5.7) again - for some x_j or ξ_l , to get some $f_{(\theta)}^{(\iota)}, \varphi_{(\theta)}^{(\iota)}$ with $|\iota| + |\theta| = 2$, now called v', w' . That derivative - for the moment denoted by "'' - may land on the old u, v , or else on the coefficients $\lambda_{|\xi x}, \dots$. Also, on the initial conditions, where we now will get $v = w = 0$ since $x_{(\theta)}^{(\iota)} = \xi_{(\theta)}^{(\iota)} = 0$ for such ι, θ . We shall get

$$(5.5.17) \quad \begin{aligned} \dot{v}' &= \lambda_{|\xi x} v' + \lambda_{|\xi \xi} w' + q_1 \quad , \quad v' = 0 \text{ as } t = \tau \quad , \\ \dot{w}' &= -\lambda_{|xx} v' - \lambda_{|x\xi} w' + q_2 \quad , \quad w' = 0 \text{ as } t = \tau \quad , \end{aligned}$$

with

$$(5.5.18) \quad q_1 = \lambda'_{|\xi x} v + \lambda'_{|\xi \xi} w \quad , \quad q_2 = -\lambda'_{|xx} v - \lambda'_{|x\xi} w \quad .$$

We make the same transformations, defining now $p_1 = \frac{v'}{\langle f \rangle}$, $p_2 = \frac{w'}{\langle \varphi \rangle}$, and $r_1 = \frac{q_1}{\langle f \rangle}$, $r_2 = \frac{q_2}{\langle \varphi \rangle}$, $r = \begin{pmatrix} r_1 \\ r_2 \end{pmatrix}$, for

$$(5.5.19) \quad \dot{p} = Pp + r \quad , \quad p = 0 \text{ at } t = \tau \quad ,$$

with the matrix P of (5.5.10) again. Eq. (5.5.19) will lead to an estimate, similar as (5.5.9) was implying (5.5.11). But, before we do this let us investigate the properties of the 2-vector $r = \begin{pmatrix} r_1 \\ r_2 \end{pmatrix}$. And, in fact, we want to prepare our induction

proof, so, we better examine the rules used to estimate such r after repeated differentiations. For example, we have

$$(5.5.20) \quad \lambda'_{|\xi x} = \lambda_{|\xi x x}(t, f, \varphi) f' + \lambda_{|\xi x \xi}(t, f, \varphi) \varphi' ,$$

and similar formulas for $\lambda'_{|\xi \xi}, \lambda'_{|x x}, \lambda'_{x \xi}$, where, in each case, as a rule, we always convolve the last mentioned differentiation with the vector f' or φ' , etc. Thus r_1 (and r_2 as well) appear as a sum of terms which are products of a (3-fold (x, ξ) -) derivative of λ and two first derivatives of f or φ , and a factor $\frac{1}{\langle f \rangle}$ or $\frac{1}{\langle \varphi \rangle}$. [Write $v = f', w = \varphi'$, for a moment, to emphasize this, then

$r_1 = \frac{1}{\langle f \rangle} \{ \lambda_{|\xi x x} f' f' + \lambda_{|\xi x \xi} \varphi' f' + \lambda_{|\xi \xi x} f' \varphi' + \lambda_{\xi \xi \xi} \varphi' \varphi' \}$, and similarly for r_2 .] While the first (x, ξ) -derivative of λ is coupled to the factor $\frac{1}{\langle f \rangle}$ (for “ $|x$ ”) or $\frac{1}{\langle \varphi \rangle}$ (for “ $|\xi$ ”) the second and third are linked to “ f' ” (for “ $|x$ ”) and “ φ' ” (for “ $|\xi$ ”).

Since (x, ξ) -differentiation of λ always generates a factor $\frac{1}{\langle f \rangle}$ or $\frac{1}{\langle \varphi \rangle}$, resp., in the estimate, the products mentioned (making q_j) always obey the estimate

$$(5.5.21) \quad r_j = O\left(\frac{|f'| |f'|}{\langle f \rangle^3} + \frac{|f'| |\varphi'|}{\langle f \rangle^2 \langle \varphi \rangle} + \frac{|\varphi'| |f'|}{\langle f \rangle^2 \langle \varphi \rangle} + \frac{|\varphi'| |\varphi'|}{\langle f \rangle \langle \varphi \rangle^2} \right) .$$

Recall we are aiming at the derivatives $f_{(\theta)}^{(\iota)}$, so that we must have “ $\iota + \iota = \binom{\iota}{\theta}$ ”. Accordingly, each fraction at right of (5.5.20) must be $O(\frac{1}{\langle f \rangle} \langle f \rangle^{-|\theta|} \langle \varphi \rangle^{-|\iota|})$. Similarly, for r_2 , so, we get

$$(5.5.22) \quad r = O(\langle x \rangle^{-1-|\theta|} \langle \xi \rangle^{-|\iota|}) .$$

Using (5.5.22) in (5.5.19) we then arrive at

$$(5.5.23) \quad p = O(\langle x \rangle^{-1-|\theta|} \langle \xi \rangle^{-|\iota|}) ,$$

and this supplies the estimates for (5.5.24), below, for all $|\iota| + |\theta| \leq 2$.

Theorem 5.5.2 *The two functions $f(x, \xi) = f_{\tau t}(x, \xi) = x_{\tau t}(x, \xi)$ and $\varphi(x, \xi) = \varphi_{\tau t}(x, \xi) = \xi_{\tau t}(x, \xi)$ are (strictly classical) symbols, together with all their t -derivatives. In fact we have*

$$(5.5.24) \quad f \in \psi c_{e^2} , \dot{f} \in \psi c_0 , \varphi \in \psi c_{e^1} , \dot{\varphi} \in \psi c_{e^1 - e^2} ,$$

Going ahead in our induction proof, let us next examine what happens if we keep on differentiating (5.5.7) (or (5.5.17)) again and again for an (x, ξ) -variable: If all these derivatives land on the v, w of (5.5.7) or the v', w' of (5.5.17) we will get the expression of (5.5.7), now with $v = f_{(\theta)}^{(\iota)}$, $w = \varphi_{(\theta)}^{(\iota)}$. But there also will

be other terms, generated whenever not all additional derivatives land on u, v of (5.5.7). So, in the new equations there will be a linear combination of terms

$$(5.5.25) \quad (\nabla_x^{j+\varepsilon_1} \nabla_\xi^{l+\varepsilon_2} \lambda) \prod_{\sum \nu_r=j} f_{(\theta_r)}^{(\nu_r)} \prod_{\sum \mu_s=l} \varphi_{(\mu_s)}^{(\nu_s)},$$

where $e_j = 0, 1$, $\varepsilon_1 + \varepsilon_2 = 1$, and where all $|\nu_r| + |\theta_r|$ and $|\nu_s| + |\mu_s|$ are $< |l| + |\theta|$, so that their corresponding estimates (1.2.2) are already known. We then will define $p_1 = \frac{v}{\langle f \rangle}$, $p_2 = \frac{w}{\langle \varphi \rangle}$, and divide the combination of terms (5.5.25) by $\langle f \rangle$ and $\langle \varphi \rangle$, respectively, to get a new r_1, r_2 , to finally obtain a new (5.5.19) again, with the same matrix P of (5.5.10).

An examination of the terms (5.5.25) then will give estimates similar to (5.5.21), and, finally (5.5.22) and (5.5.23), and the next estimate (5.5.24), which then is proven by induction.

This completes the induction proof of thm.5.5.2.

5.6 A Secondary Correction for the Electrostatic Potential

Let us here go through the details of a secondary correction, for the special dynamical observable $\mathbf{V}(x)$ - i.e., the electrostatic potential. Recall, that infinitely many corrections may be constructed whenever the symbol of an observable commutes with $h(x, \xi)$. Here we have such a symbol $\mathbf{V}(x)$. Perhaps it will help to get familiar with this construction.

In this section we assume the magnetic potentials $\equiv 0$, so that the Dirac Hamiltonian is given by $H = \sum \alpha_j D_j + \beta + \mathbf{V}(x)$. Applying thm.5.1.1(ii) to the multiplication operator $u(x) \rightarrow V(x)u(x)$ with symbol $q(x, \xi) = \mathbf{V}(x) \in \text{Op}\psi c_{-e^2}$ [assuming $\mathbf{V}(x)$ satisfies cdn.(X)] we obtain an operator $A = a(x, D) \in \mathcal{P}_{-e^2}$ with symbol given by an asymptotic expansion $a(x, \xi) = \mathbf{V}(x) + z(x, \xi) + \dots$. Moreover, this asymptotic expansion extends to $A_t = e^{iHt} A e^{-iHt} \in \mathcal{P}_{-e^2}$; we have $a_t(x, \xi) = q_t(x, \xi) + z_t(x, \xi) + w_t(x, \xi) + s_t(x, \xi) + \dots$, where $q_0(x, \xi) = \mathbf{V}(x)$, $z_0(x, \xi) = z(x, \xi)$, \dots

We must have $\dot{A}_t = i[H, A_t]$, or, in terms of symbols,

$$(5.6.1) \quad \dot{a}_t = i[h, a_t] + \{h, a_t\} - \frac{i}{2}\{h, a_t\}_2 - \frac{1}{6}\{h, a_t\}_3 + \frac{i}{24}\{h, a_t\}_4 + \dots$$

The “first correction symbol” $z_0(x, \xi)$ (for $t = 0$) already was explicitly constructed in sec.4.2. In our present setting it is given as

$$(5.6.2) \quad z(x, \xi) = z_0(x, \xi) = \mathcal{E} \cdot \lambda_c(x, \xi), \quad \mathcal{E} = -\text{grad } \mathbf{V}, \quad \lambda_c = \frac{1}{2\langle \xi \rangle^2} \{ \mu + \rho \times \xi \},$$

with the matrices μ, ρ of (4.3.7).

But we also need z_t for $t \neq 0$ for our construction of the next correction $w_t(x, \xi)$. In that respect, we recall the construction of sec.4.2: We explicitly obtained

$$(5.6.3) \quad q_t(x, \xi) = p_+(\xi)\mathbf{V}(x_t^+(x, \xi)) + p_-(\xi)\mathbf{V}(x_t^-(x, \xi)) ,$$

$$z_t = \frac{1}{2\langle \xi \rangle} \{p_+\omega_t p_- - p_-\omega_t p_+\} + c_{t+} + c_{t-} ,$$

where (i) $x_t^\pm(x, \xi)$ denotes the x -component of the solution (x_t, ξ_t) of the Hamiltonian system (4.2.24), given for us as

$$(5.6.4) \quad \dot{x} = \pm \xi / \langle \xi \rangle , \quad \dot{\xi} = \mathcal{E}(x) ,$$

through the point (x, ξ) , while (ii) $\omega_t = i(\{h, q_t\} - \dot{q}_t)$, and, $p_\pm = \frac{1}{2}(1 \pm (\alpha\xi + \beta)/\langle \xi \rangle)$ are the eigenprojections of the symbol $h(x, \xi)$. Furthermore, (iii) $c_{t\pm} = p_\pm c_{t\pm} p_\pm$ may be arbitrarily chosen (as symbols in ψc_{-e-e^2}) at $t = 0$. but they still must be properly determined for $t \neq 0$ - as to solve a certain differential equation, namely, eq. (5.6.7), below - that reduces to a set of ODE-s along the flow of (5.6.4).

Here we are looking for the second correction $w_t(x, \xi) \in \psi c_{-e^2-2e}$, while we had $z_t \in \psi c_{-e^2-e}$. In sec.5.1 we derived a commutator equation for w_t :

$$(5.6.5) \quad [h, w_t] = i(\{h, z_t\} - \dot{z}_t - \frac{i}{2}\{h, q_t\}_2) = \chi_t ,$$

where the right hand side is in ψc_{m-e-e^2} . Again a solution w_t of (5.6.5) exists if and only if we have

$$(5.6.6) \quad p_+\chi_t p_+ = p_-\chi_t p_- = 0 .$$

This will *not* automatically be true. Rather, to satisfy (5.6.6) we interpret it as a differential equation for the - so far undetermined - symbols $c_{t\pm}$ of (5.6.3): Changing notations, let z_t be the (well determined) symbol of (5.6.3) setting $c_{t\pm} \equiv 0$ there, and replace z_t in (5.6.5) by $z_t + c_t$ with $c_t = c_{t+} + c_{t-}$, interpreting (5.6.6) as equations for c_t :

$$(5.6.7) \quad p_\pm(\dot{c}_t - \{h, c_t\} + (\dot{z}_t - \{h, z_t\} + \frac{i}{2}\{h, q_t\}_2))p_\pm = 0 .$$

Also, χ_t in equ. (5.6.5) will assume the new form

$$(5.6.8) \quad \chi_t = i(\{h, z_t\} - \dot{z}_t - \frac{i}{2}\{h, q_t\}_2 + \{h, c_t\} - \dot{c}_t) .$$

After getting the solvability straight, the solution of (5.6.5) will be

$$(5.6.9) \quad w_t = \frac{1}{2\langle \xi \rangle} (p_+\chi_t p_- - p_-\chi_t p_+) + d_{t+} + d_{t-} .$$

We are only interested in w_0 here, where we may set $d_{0\pm} = 0$. Also we will assume $c_{0\pm} = 0$. This sets the stage for our calculation: the projections p_{\pm} are independent of t ; from (5.6.3) - using (5.6.4) - we get

$$(5.6.10) \quad \dot{q}_t = -p_+(\xi)\mathcal{E}(x_t^+(x, \xi)) \cdot \frac{\xi_t^+(x, \xi)}{\langle \xi_t^+(x, \xi) \rangle} - p_-(\xi)\mathcal{E}(x_t^-(x, \xi)) \cdot \frac{\xi_t^-(x, \xi)}{\langle \xi_t^-(x, \xi) \rangle} .$$

Inserting (5.6.10) into $\omega_t = i(\{h, q_t\} - \dot{q}_t)$, and the result into $z_t = \frac{1}{2\langle \xi \rangle} \{p_+\omega_t p_- - p_-\omega_t p_+\}$ we will get an explicit formula for z_t (strongly simplifying) for $t = 0$. However, we also need $\dot{z}_0 = \frac{1}{2\langle \xi \rangle} (p_+\dot{\omega}_0 p_- - p_-\dot{\omega}_0 p_+)$, with $\dot{\omega}_0 = i(\{h, \dot{q}_0\} - \ddot{q}_0)$, in the sequel. After calculating \ddot{q} we then may set $t = 0$, henceforth, with strong simplifications. We get

$$(5.6.11) \quad p_+\ddot{q}_0 = p_+(\mathbf{V}_{|x_j x_l} \dot{x}_{0j}^+ \dot{x}_{0l}^+ - \mathcal{E} \cdot \ddot{x}_0^+) ,$$

where $\dot{x}_t^+ = \lambda_{+|\xi}(\xi_t)$, hence, $\ddot{x}_t^+ = \lambda_{+|\xi\xi} \cdot \dot{\xi}_t = -\lambda_{+|\xi\xi}(\xi_t) \cdot \lambda_{+|x}(x_t)$.

Recall, we have $\lambda_{\pm}(x, \xi) = \mathbf{V}(x) \pm \langle \xi \rangle$, hence, $\lambda_{+|x}(x, \xi) = -\mathcal{E}(x)$, $\lambda_{+|\xi} = \xi/\langle \xi \rangle$, and $\lambda_{+|\xi_j \xi_l} = \delta_{jl}/\langle \xi \rangle - \xi_j \xi_l / \langle \xi \rangle^3$. Therefore, $\dot{x}_0^+ = \xi/\langle \xi \rangle$ and $\ddot{x}_0^+ = \mathcal{E}_j/\langle \xi \rangle - (\mathcal{E}\xi)_j/\langle \xi \rangle^3$. This gives

$$(5.6.12) \quad (p_+\ddot{q}_0)(x, \xi) = p_+(\xi) \left\{ \mathbf{V}_{x_j x_l}(x) \frac{\xi_j \xi_l}{\langle \xi \rangle^2} + \frac{(\mathcal{E}(x)\xi)^2}{\langle \xi \rangle^3} - \frac{\mathcal{E}^2(x)}{\langle \xi \rangle} \right\} .$$

Similarly, for “-”, we have $\lambda_{-|x} = \lambda_{+|x}$, but $\lambda_{-|\xi} = -\lambda_{+|\xi}$, etc., giving a corresponding formula for $p_-\ddot{q}_0$. Adding both formulas we get

$$(5.6.13) \quad \ddot{q}_0(x, \xi) = \mathbf{V}_{|x_j x_l}(x) s_j(\xi) s_l(\xi) - h_0(\xi) s_0^2(\xi) \{ \mathcal{E}^2(x) - (\mathcal{E}(x) s(\xi))^2 \} ,$$

where we still have used that $p_+ + p_- = 1$, $p_+ - p_- = h_0(\xi)/\langle \xi \rangle$ with $h_0 = \alpha\xi + \beta$, and also have introduced $s_0(\xi) = 1/\langle \xi \rangle$, $s(\xi) = \xi/\langle \xi \rangle$.

Moreover, note that

$$(5.6.14) \quad q_0 = \mathbf{V}(x) , \quad \dot{q}_0 = -\mathcal{E}(x) s(\xi) ,$$

the latter from (5.6.10) for $t = 0$.

From (5.6.14) we get

$$(5.6.15) \quad \omega_0(x, \xi) = -i\mathcal{E}(x)(\alpha - s(\xi)) ,$$

and $\dot{\omega}_t = i(\{h, \dot{q}_t\} - \ddot{q}_t)$, hence $\dot{\omega}_0 = i(\{h, \dot{q}_0\} - \ddot{q}_0)$, where we get \dot{q}_0 and \ddot{q}_0 from (5.6.14) and (5.6.13). We get

$$(5.6.16) \quad \{h, \dot{q}_0\} = -\{h, (\mathcal{E}(x) s(\xi))\} = \mathbf{V}_{|x_j x_l}(x) \alpha_j s_l(\xi) - s_0(\xi) (\mathcal{E}^2 - (\mathcal{E}(x) s(\xi))^2) ,$$

hence

$$(5.6.17) \quad \dot{\omega}_0 = i\{\mathbf{V}_{|x_j x_l}(x)(\alpha_j - s_j(\xi))s_l(\xi) - Z(x, \xi)s_0(\xi)(1 - h_0(\xi)s_0(\xi))\},$$

setting $Z(x, \xi) = \mathcal{E}^2(x) - (\mathcal{E}(x)s(\xi))^2$, for a moment.

Next, calculating $\dot{z}_0 = \frac{1}{2}s_0(p_+\dot{\omega}_0p_- - p_-\dot{\omega}_0p_+)$ we notice that the term with factor Z cancels out, when we substitute $\dot{\omega}_0$ from (5.6.17), because Z is 4×4 -scalar while its factor $1 - h_0s_0$ equals $2p_-$. It follows that

$$(5.6.18) \quad \dot{z}_0 = \frac{i}{2}s_0(\xi)V_{|x_j x_l} s_l(\xi)(p_+\alpha_j p_- - p_-\alpha_j p_+),$$

since also the remaining term is scalar and cancels, due to $p_+ \cdot p_- - p_- \cdot p_+ = 0$. In (5.6.18) we use that

$$(5.6.19) \quad p_+\alpha p_- - p_-\alpha p_+ = s_0(\xi)(h_0(\xi)\alpha - \xi) = is_0(\xi)(\mu + \rho \times \xi) = 2i\langle \xi \rangle \lambda_c(\xi),$$

so that we get

$$(5.6.20) \quad \dot{z}_0 = -\mathbf{V}_{|x_j x_l}(x)s_j(\xi)\lambda_{Cl}(\xi),$$

with λ_c of (5.6.2).

Next we turn to the calculation of $\chi_0 = i(\{h, z_0\} - \dot{z}_0 - \frac{i}{2}\{h, \mathbf{V}\}_2)$, as in (5.6.5), for $t = 0$. Note, the last term vanishes; we have $\{h, \mathbf{V}\}_2 = h_{|\xi\xi}\mathbf{V}_{|xx} - \mathbf{V}_{|\xi\xi}h_{|xx} = 0$. Furthermore,

$$(5.6.21) \quad \{h, z_0\} = \{h, \mathcal{E}(x)\lambda_c(\xi)\} = -\alpha_j \mathbf{V}_{|x_j x_l}(x)\lambda_{Cl}(\xi) + \lambda_{c_j|\xi_l}(\xi)\mathcal{E}_j(x)\mathcal{E}_l(x).$$

For calculation of $\lambda_{c_j|\xi_l}$ we note that (5.6.19) implies

$$(5.6.22) \quad \lambda_{c_j} = \frac{i}{2}s_0^2(\xi)(\xi_j - h_0(\xi)\alpha_j),$$

so that

$$(5.6.23) \quad \lambda_{c_j|\xi_l} = -2s_0(\xi)s_l(\xi)\lambda_{c_j}(\xi) + \frac{i}{2}s_0^2(\xi)(\delta_{jl} - \alpha_l\alpha_j).$$

The second term at the right in (5.6.21) equals $2s_0(\xi)(s(\xi)\mathcal{E}(x))(-\lambda_c(\xi)\mathcal{E}(x)) + \frac{i}{2}s_0(\xi)(\mathcal{E}^2(x) - (\alpha\mathcal{E}(x))^2)$. We need $\theta_0 = \dot{z}_0 - \{h, z_0\}$, i.e.,

$$(5.6.24) \quad \begin{aligned} \theta_0 &= \mathbf{V}_{|x_j x_l}(x)(\alpha_j - s_j(\xi))\lambda_{Cl}(\xi) \\ &\quad + 2s_0(\xi)(s(\xi)\mathcal{E}(x))(\lambda_c(\xi)\mathcal{E}(x)) - \frac{i}{2}s_0^2(\xi)(\mathcal{E}^2(x) - (\alpha\mathcal{E})^2). \end{aligned}$$

With this θ_0 (and, more generally, $\theta_t = \dot{z}_t - \{h, z_t\} + \frac{i}{2}\{h, q_t\}_2$) cdn. (5.6.7) for the functions c_t reads

$$(5.6.25) \quad p_{\pm}\chi_t p_{\pm} = 0 \text{ for } \chi_t = i(\theta_t + \{h, c_t\} - \dot{c}_t),$$

and then we have the desired w_0 given as $w_0 = \frac{1}{2}s_0(p_+\chi_0p_- - p_-\chi_0p_+)$, according to (5.6.9). But we imposed the condition $c_0 \equiv 0$, so that $\{h, c_0\} = 0$. Moreover, the matrix function c_t was always satisfying $p_+c_t p_- = p_-c_t p_+ = 0$. This implies $p_+\dot{c}_t p_- = p_-\dot{c}_t p_+ = 0$, since the projections p_\pm are independent of t . Thus it follows that $p_\pm\chi_0p_\mp = ip_\pm\theta_0p_\mp$. Or, in other words, the special form of the “diagonal blocks” $c_{0\pm}$ is irrelevant for our next correction w_0 - we get

$$(5.6.26) \quad w_0 = \frac{i}{2}s_0(\xi)(p_+\theta_0p_- - p_-\theta_0p_+) ,$$

with θ_0 of (5.6.24). For the calculation write $\theta_0 = \theta^1 + \theta^2 + \theta^3$ with the 3 terms at right of (5.6.24). We claim that $p_+\theta^1p_- - p_-\theta^1p_+ = 0$. Indeed, this is a matter of handling $(\alpha - s)\lambda_c$, since other factors are 4×4 -scalars. From (5.6.19) we derive $2i\langle\xi\rangle\lambda_c = (p_+\alpha p_- - p_-\alpha p_+)$. This implies $p_-\lambda_c p_- = 0$. Using $p_+ + p_- = 1$ get $2i\langle\xi\rangle p_+(\alpha - s)\lambda_c p_- = p_+(\alpha - s)p_+(p_+\alpha p_-) + p_+(\alpha - s)p_-(p_-\lambda_c p_-)$, where the last term at right vanishes. But the first term vanishes too. Here is the calculation: $4p_+\alpha_j p_+ = (1 + \alpha s + \beta s_0)\alpha_j(1 + \alpha s + \beta s_0) = \alpha_j + (\alpha s)\alpha_j(\alpha s) + (\beta s_0)\alpha_j(\beta s_0) + (\alpha_j(\alpha s) + (\alpha s)\alpha_j) + (\alpha_j(\beta s_0)(\beta s_0)\alpha_j) + ((\alpha s)\alpha_j(\beta s_0) + (\beta s_0)\alpha_j(\alpha s)) = [1] + [2] + [3] + [4] + [5] + [6]$. Here $[3] = -s_0^2\alpha_j$; $[4] = 2s_j$; $[5] = 0$; $[6] = 2\beta s_0 s_j$. Also, $[2] = \sum_{kl} s_k s_l \alpha_k \alpha_j \alpha_l = -\sum_{kl} s_k s_l \alpha_k \alpha_l \alpha_j + 2\sum_{kl} s_k s_l \alpha_k \delta_{lj} = -|s|^2\alpha_j + 2(\alpha s)s_j$. Using that $s_0^2 + |s|^2 = 1$ we then get $[1] + \dots + [6] = \alpha_j(1 - s_0^2 - |s|^2) + 2s_j(\alpha s + \beta s_0 + 1) = 4s_j(\xi)p_+$. That is,

$$(5.6.27) \quad p_+(\alpha_j - s_j)p_+ = 0 , \quad p_-(\alpha_j + s_j)p_- = 0 ,$$

where the second relation is derived similarly. Accordingly we indeed get

$$(5.6.28) \quad p_+(\alpha - s)\lambda_c p_- = 0 , \quad p_-(\alpha - s)\lambda_c p_+ = 0 ,$$

where again the second relation follows similarly. Accordingly the term θ^1 makes no contribution to our w_0 .

For the term θ^2 we must focus on

$$(5.6.29) \quad p_+\lambda_c p_- - p_-\lambda_c p_+ = -\frac{i}{2}s_0(p_+\alpha p_- + p_-\alpha p_+) ,$$

as follows from (5.6.19) and a little calculation. Now, $2(p_+\alpha_j p_- + p_-\alpha_j p_+) = \frac{1}{2}((1 + h_0 s_0)\alpha_j(1 - h_0 s_0) + (1 - h_0 s_0)\alpha_j(1 + h_0 s_0)) = \alpha_j - h_0 s_0 \alpha_j h_0 s_0 = \alpha_j - (\alpha s)\alpha_j(\alpha s) - (\beta s_0)\alpha_j(\beta s_0) - ((\alpha s)\alpha_j(\beta s_0) + (\beta s_0)\alpha_j(\alpha s)) = [1] - [2] - [3] - [6]$, with above notation. So, we continue $= \alpha_j + |s|^2\alpha_j - 2(\alpha s)s_j + s_0^2\alpha_j - 2\beta s_0 s_j = 2\alpha_j - 2h_0 s_0 s_j$. That is,

$$(5.6.30) \quad p_+\alpha p_- + p_-\alpha p_+ = \alpha - h_0(\xi)s_0(\xi)s(\xi) ,$$

and

$$(5.6.31) \quad p_- \lambda_c p_- - p_- \lambda_c p_+ = -\frac{i}{2} s_0(\xi) (\alpha - h_0(\xi) s_0(\xi) s(\xi)) .$$

It follows that θ^2 supplies the term

$$(5.6.32) \quad w_0(x, \xi) = \frac{1}{2} s_0^3(\xi) (s(\xi) \mathcal{E}(x)) (\mathcal{E}(x) (\alpha - h_0(\xi) s_0(\xi) s(\xi)) ,$$

as follows since the third term θ^3 again will make no contribution to w_0 . For the latter we look at $p_+ \alpha_j \alpha_l p_- - p_- \alpha_j \alpha_l p_+ = (p_+ \alpha_j p_+) (p_+ \alpha_l p_-) + (p_+ \alpha_j p_-) (p_- \alpha_l p_-) - (p_- \alpha_j p_+) (p_+ \alpha_l p_+) - (p_- \alpha_j p_-) (p_- \alpha_l p_+) = s_j (p_+ \alpha_l p_- + p_- \alpha_l p_+) - s_l (p_+ \alpha_j p_- + p_- \alpha_j p_+)$, where we used (5.6.27) and $1 = p_+ + p_-$. With (5.6.30) we get

$$(5.6.33) \quad p_+ \alpha_j \alpha_l p_- - p_- \alpha_j \alpha_l p_+ = s_j \alpha_l - s_l \alpha_j .$$

Then it is evident that $p_+ \theta^3 p_- - p_- \theta^3 p_+ = 0$ follows, so that, indeed, fla. (5.6.32) gives the complete second correction symbol.

As to the secondary corrected operator, note that we may arrange the various factors at right of (5.6.32) in any convenient order, since any commutators generated would be one order e lower than the order of $w(x, \xi)$, so would not count. So, we state:

Proposition 5.6.1 *We have*

$$(5.6.34) \quad \begin{aligned} (\mathbf{V}(x))_2^{\sim} &= \mathbf{V}(x) + \frac{1}{2} \{ (\mathcal{E}(x) \lambda_c(D)) + (\lambda_c(D) \mathcal{E}(x)) \} \\ &+ \frac{1}{4} \{ (\mathcal{E}(x) s(D)) (\mathcal{E}(x) (\alpha - h_0(D) s_0(D) s(D))) s_0^3(D) \\ &+ s_0^3(D) ((\alpha - h_0(D) s_0(D) s(D)) \mathcal{E}(x)) (s(D) \mathcal{E}(x)) \} , \end{aligned}$$

this giving a self-adjoint operator $(\mathbf{V}(x))_2^{\sim}$.

5.7 Smoothness and FW-Decoupling

In this section we consider a Dirac Hamiltonian $H = \alpha(D - \mathbf{A})\beta + \mathbf{V}$ with time-dependent potentials \mathbf{A}_j, \mathbf{V} satisfying cdn.(XT) of sec.3.7. We then want to establish the following result.

Theorem 5.7.1 *Let $U(t) = u((t, x, D) \in Op\psi c_0$ be any unitary operator decoupling of the Dirac equation $\dot{\psi} + H(t)\psi = 0 \text{ mod } \mathcal{O}(-\infty)$, in the sense of sec.3.7. That is, we have*

$$(5.7.1) \quad U^* H U - i U^* \dot{U} = H^\Delta(t) = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix} + \begin{pmatrix} 0 & \Gamma^* \\ \Gamma & 0 \end{pmatrix} , \quad \Gamma \in \mathcal{O}(-\infty) ,$$

with respect to the split $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4) = \mathcal{H}_+ \oplus \mathcal{H}_-$, with $\mathcal{H}_\pm = L^2(\mathbb{R}^3, \mathbb{C}^2)$.

Then a strictly classical ψ do $A \in Op\psi c_m$ has a smooth (inverse) Heisenberg representation $A \rightarrow A_t = U(\tau, t)AU(t, \tau)$ at τ , in the sense of (5.1.1) if and only if

$$(5.7.2) \quad U^*(\tau)AU(\tau) - \begin{pmatrix} B & 0 \\ 0 & C \end{pmatrix} \in \mathcal{O}(-\infty)$$

with some (2×2 -blocks) $B, C \in Op\psi c_m$.

That is, $A \in Op\psi c_m$ belongs to the class $\mathcal{P}_m(\tau)$ if and only if (5.7.2) holds.

The proof of thm.5.7.1 requires some preparations. Let us first go and transform the evolution operator $U(\tau, t) = U_H(\tau, t)$ of our Dirac equation $\dot{u} + iH(t)u = 0$, setting $u(t) = U(t)v(t)$ with the decoupling unitary operator $U(t)$ of the theorem. We get $\dot{v} + iH^\Delta(t)v = 0$, i.e., $v(t) = U_{H^\Delta}(\tau, t)v(\tau)$, with the evolution operator $U_{H^\Delta}(\tau, t)$ of the transformed equation, while, of course, we also have $u(t) = U(t)v(t) = U_H(\tau, t)u(\tau) = U_H(\tau, t)U(\tau)v(\tau)$. It follows that

$$(5.7.3) \quad U_{H^\Delta}(\tau, t) = U^*(t)U_H(\tau, t)U(\tau) \ , \ \tau, t \in \mathbb{R} \ .$$

Now, given any ψ do $A = a(x, D) \in Op\psi c_m$, let $A_{\tau t} = U_H(\tau, t)AU_H(t, \tau)$ be its inverse Heisenberg transform, taken at an initial point τ . We clearly get

$$(5.7.4) \quad U^*(t)A_{\tau t}U(t) = (U^*(t)U_H(\tau, t)U(\tau))(U^*(\tau)AU(\tau))(U^*(\tau)U_H(t, \tau)U(t)) \ .$$

Defining $A^\Delta = U^*(\tau)AU(\tau)$ we thus get

$$(5.7.5) \quad A_{\tau t}^\Delta = U^*(t)A_{\tau t}U(t) = U_{H^\Delta}(\tau, t)A^\Delta U_{H^\Delta}(t, \tau) \ .$$

The point then is that we want to show that $A_{\tau t}^\Delta$ is a ψ do in $Op\psi c_m$ with symbol $a_{\tau t}^\Delta(x, \xi)$ satisfying a condition like (5.1.1) (or, rather, (5.2.3)) - i.e.,

$$(5.7.6) \quad \partial_t^j a_{\tau t}^\Delta(x, \xi) \in \psi c_{m-je^2} \ , \ j = 0, 1, 2, \dots \ ,$$

if and only if $A^\Delta - \begin{pmatrix} B & 0 \\ 0 & C \end{pmatrix} \in \mathcal{O}(-\infty)$, with some 2×2 - ψ do-s $B, C \in Op\psi c_m$. Then we must compare smoothness of $A_{\tau t}^\Delta$ with smoothness of $A_{\tau t}$ and show that they mean the same.

Proposition 5.7.2 *Let $X^\Delta(t) = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix}$ with $X = X(t)$, $Y = Y(t)$ of (5.7.1), and let $U_{X^\Delta}(\tau, t)$ be the evolution operator of the equation $u + iX^\Delta(t)u = 0$. Then we have*

$$(5.7.7) \quad \mathcal{O}(\tau, t) = U_{H^\Delta}(\tau, t)U_{X^\Delta}(t, \tau) - 1 \in C^\infty(\mathbb{R}^2, \mathcal{O}(-\infty)) \ .$$

Proof. Using [Co5],VI, cor.3.3 we know that both operators, U_{H^Δ} , U_{X^Δ} are of order 0 while their partial derivatives for t and τ are of order $j e^1$ with the combined order j of t - and τ -differentiation. We get

$$(5.7.8) \quad \begin{aligned} \partial_\tau O(\tau, t) &= iU_{H^\Delta}(\tau, t)H^\Delta(\tau)U_{X^\Delta}(t, \tau) - iU_{H^\Delta}(\tau, t)X^\Delta(\tau)U_{X^\Delta}(t, \tau) \\ &= iU_{H^\Delta}(\tau, t)\Gamma^\Delta(\tau)U_{X^\Delta}(t, \tau) , \end{aligned}$$

where $\Gamma^\Delta = H^\Delta - X^\Delta \in \mathcal{O}(-\infty)$. It follows that $\partial_\tau O(\tau, t) \in \mathcal{O}(-\infty)$. Similarly for all higher τ, t -derivatives. Integrating from τ to t we conclude that (5.7.7) holds, q.e.d.

Proposition 5.7.3 *Let $\check{a}_{\tau t}(x, \xi)$ be the symbol of $\check{A}_{\tau t} = U_{X^\Delta}(\tau, t)AU_{X^\Delta}(t, \tau)$. Then $A_{\tau t}^\Delta$ is a ψ do with symbol $a_{\tau t}^\Delta(x, \xi)$ satisfying (5.7.6) if and only if $\check{A}_{\tau t}$ is a ψ do with symbol $\check{a}_{\tau t}(x, \xi)$ satisfying (5.7.6).*

The proof is evident, in view of (5.7.7).

Proposition 5.7.4 *The operator $\check{A}_{\tau t}$ is a ψ do in $Op\psi c_m$ with symbol $\check{a}_{\tau t}(x, \xi)$ satisfying (5.7.6) if and only if $\check{A} - \begin{pmatrix} B^0 \\ 0 C \end{pmatrix} \in \mathcal{O}(-\infty)$, with some 2×2 - ψ do-s $B, C \in Op\psi c_m$.*

Proof. Clearly the system of equations $\dot{u} + iX^\Delta(t)u = 0$ is fully decoupled: we may write $u = \begin{pmatrix} v \\ w \end{pmatrix}$ where then the 2-vectors v and w satisfy

$$(5.7.9) \quad \dot{v} + iX(t)v = 0 , \quad \dot{w} + iY(t)w = 0 .$$

It follows that $U_{X^\Delta} = \begin{pmatrix} V^0 \\ 0 W \end{pmatrix}$ also is fully decoupled, so that

$$(5.7.10) \quad \check{A}_{\tau t} = \begin{pmatrix} B_{\tau t} & G_{\tau t} \\ G_{\tau t}^* & C_{\tau t} \end{pmatrix} ,$$

where

$$(5.7.11) \quad B_{\tau t} = V(\tau, t)BV(t, \tau) , \quad C_{\tau t} = W(\tau, t)CW(t, \tau) ,$$

and

$$(5.7.12) \quad G_{\tau t} = V(\tau, t)GW(t, \tau) ,$$

setting $A = \begin{pmatrix} B & G \\ G^* & C \end{pmatrix}$.

Using (3.2.12) - or, rather, its generalization¹³ to time-dependent potentials in thm.3.7.1 - we have

$$(5.7.13) \quad X = \langle D \rangle + X_1 , \quad Y = -\langle D \rangle + Y_1 , \quad \text{with } X_1, Y_1 \in Op\psi c_{-e^2} .$$

As a consequence we have

¹³Note, we have $\lambda_\pm(x, \xi) \mp \langle \xi \rangle \in \psi c_{-e^2}$, so that, indeed, (3.2.12) implies (5.2.13).

Proposition 5.7.5 *The entire graded algebra of all 2×2 -matrix-valued ψ do-s in $Op\psi c$ is left invariant under the conjugations $B \rightarrow \check{B}_{\tau t}$ and $C \rightarrow \check{C}_{\tau t}$. And, moreover, the symbols $\check{B}_{\tau t}(x, \xi)$ and $\check{C}_{\tau t}(x, \xi)$ both satisfy the cdn.(5.7.6) for each $B, C \in Op\psi c_m$.*

We will not discuss the details of the proof of prop.5.7.5 here, but refer the reader to [Co5],VI, thm.5.1 - or else, one may go through the details of our proof of thm.5.5.1 (ii) under the present slightly different assumptions¹⁴. The point is that the operator $X(t)$ or $Y(t)$ substituting for $H(t)$ in thm.5.5.1 equals the scalar term $\pm \langle D \rangle \in \psi c_{e^1}$ modulo a lower order matrix-valued term $X_1(t)$ or $Y_1(t)$ This has the effect that just any symbol $q(x, \xi) \in \psi c_m$ commutes with the symbol of X (or Y) mod lower order, so that we may construct a lower order correction $z(x, D) \in Op\psi c_{m-e}$ for any $q(x, D) \in Op\psi c_m$. Moreover, this may be iterated: we'll get a correction $w \in \psi c_{m-2e}$ for z and find that $q - w = (q + z) - (z + w)$ is a symbol of the invariant algebra, etc.,... So, finally, taking an asymptotic sum, we will obtain a correction $z_\infty \in \mathcal{O}(-\infty)$ such that $q(x, D) + z_\infty(x, D)$ belongs to the invariant algebra. Since that algebra contains $\mathcal{O}(-\infty)$ it follows that it also contains the entire $Op\psi c$.

Especially it also is confirmed that we get (5.7.6) as stated, just in the same way as we obtained it for thm.5.1.1.

The proof of prop.5.7.4. then hinges on the following

Proposition 5.7.6 *For any ψ do $G \in Op\psi c$ we have $G_{\tau t}$ of (5.7.12) a ψ do with symbol $g_{\tau t}(x, \xi)$ satisfying (5.7.6) if and only if $G \in \mathcal{O}(-\infty)$.*

Proof. For a $G \in \mathcal{O}(-\infty)$ we trivially have $G_{\tau t} \in \mathcal{O}(-\infty)$, together with all its τt -derivatives, simply because the two evolution operators $V(\tau, t)$ and $W(\tau, t)$ are of order 0 and their t, τ -derivatives of total order j also are of order je^1 . Thus we then indeed have G a ψ do of any order m and cdn.'s (5.7.6) also hold for any m .

¹⁴Our present equation $\dot{u} + i(H^\Delta + \Gamma^\Delta)u = 0$ is semi-strictly hyperbolic of type e^1 because the operator H^Δ belongs to $Op\psi c_{e^1}$, and, moreover, the symbol - modulo lower order terms - equals the block-matrix $\begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}$ with $\lambda_\pm = \mathbf{V} \pm \langle \xi \rangle$. This 4×4 -matrix-valued function has 2 eigenvalues $\lambda_\pm(\xi)$ of constant rank 2 for all x, ξ , and we have $|\lambda_+(\xi) - \lambda_-(\xi)| \geq 2\langle \xi \rangle$ (actually “=”, for all x, ξ . For any such semi-strictly hyperbolic system $\dot{u} + iKu = 0$ of type e^1 we have a complete analogon of thm.5.1.1 - one defines an algebra \mathcal{P}_K of operators $A \in Op\psi c_m$ (for some m) with $A_t = U_K(0, t)AU_K(t, 0)$ (with the evolution operator U_K of K) satisfying (5.1.1), (5.1.2). Then the 3 statements of thm.5.1.1 hold literally, but we may split $K = K_0 + K_1$ where $K_1 \in Op\psi c_{-e^2}$, and then replace H in thm.5.1.1 by K_0 , instead of using the entire K instead of H . The proofs also run exactly parallel. We will not discuss this thm. in more detail, but refer to [Co5] (or, more compactly, [Co3], thm.5.1).

Vice versa, assume that $Q \in \text{Op}\psi c_m$ satisfies $G_{\tau t} = g_{\tau t}(x, D)$ with $\gamma_{\tau t}$ satisfying (5.7.6). Differentiating for t and setting $t = \tau$ we get

$$(5.7.14) \quad \dot{G}_{\tau\tau} = -i(X(\tau)G - GY(\tau)) .$$

Using (5.7.13) and the fact that the commutator $[\langle D \rangle, Q]$ is of order $m - e^2$, since $\langle D \rangle$ is scalar, and that $\dot{G} \in \text{Op}\psi c_{m-e^2}$, by (5.7.6), we conclude that

$$(5.7.15) \quad 2i\langle D \rangle Q \in \text{Op}\psi c_{m-e^2} \Rightarrow Q \in \text{Op}\psi c_{m-e} .$$

Now, this procedure may be iterated. Differentiating twice for t we get

$$(5.7.16) \quad \ddot{G}_{\tau t} = -i(\dot{X}(t)G_{\tau t} - G_{\tau t}\dot{Y}(t)) - \Omega_t^2(G_{\tau t}) ,$$

where we define $\Omega_t^j(G)$ iteratively, setting $\Omega_t^0(G) = G$ and $\Omega_t^{j+1} = -i(X(t)\Omega_t^j(G) - \Omega_t^j(G)X(t))$. Setting $t = \tau$ we then get

$$(5.7.17) \quad \ddot{G}_{\tau\tau} = -i(\dot{X}(\tau)G - G\dot{Y}(\tau)) + \Omega_\tau^2(G) .$$

Now we use (5.7.6),(3.7.6) and (3.7.9) to find that (5.7.17) implies $\Omega_\tau^2(G) \in \text{Op}\psi c_{m-2e^2}$. On the other hand, using that we already know that $G \in \text{Op}\psi c_{m-e}$, by the above (and again using (5.7.13)) and the fact that commutators with (the scalar operator) $\langle D \rangle^j$ add the term $je^1 - e = -e^2$ to the order of the commutant) one finds that $\Omega_\tau^2(G) = 4\langle D \rangle^2 G \pmod{\text{Op}\psi c_{m-2e^2}}$. It follows that $G \in \text{Op}\psi c_{m-2e}$. With further iterations, using the expression $\Omega_\tau^j(G)$ for larger j and (5.7.6) for higher derivatives, one indeed confirms that G must be of order $m - je$ for all $j = 1, 2, \dots$. Thus we get $G \in \mathcal{O}(-\infty)$, q.e.d.

Finally, for the proof of thm.5.7.1, we still need to verify equivalence between (5.1.1) and (5.7.6).

Proposition 5.7.7 *We have a_t satisfying (5.1.1) if and only if a_t^Δ satisfies (5.7.6).*

Proof. Assume that a_t satisfies (5.1.1) - for a given $A = a(x, D) \in \text{Op}\psi c_m$, and $A_{\tau t} = a_{\tau t}(x, \xi) = U_H(\tau, t)AU_H(t, \tau)$. With our Leibniz formulas we get

$$(5.7.18) \quad a_{\tau t}^\Delta(x, \xi) = \sum_{\nu, \iota, \theta} \frac{(-i)^{\nu+\iota+\theta}}{\nu! \iota! \theta!} (((u_{(\theta)}^{*(\theta+\iota)})_{a_{t(\iota)}})^{(\nu)} u_{(\nu)})(x, \xi) = (u^* a_t u)(x, \xi) + \dots ,$$

where this may be considered reordered into an asymptotic sum of (finite sums of) terms of order $m, m - e, m - 2e, \dots$. We have

$$(5.7.19) \quad \frac{1}{\varepsilon}(a_{\tau t+\varepsilon}(x, \xi) - a_{\tau t}(x, \xi)) - \dot{a}_{\tau t}(x, \xi) = \int_0^1 d\kappa(\dot{a}_{\tau t+\varepsilon\kappa} - \dot{a}_{\tau t})(x, \xi) .$$

Under assumptions (5.1.1) it is clear that the right hand side converges¹⁵ to 0 (in all the Fréchet norms of ψc_{m-e^2}). In particular also the t -derivative $\dot{A}_{\tau t}$ exists in operator norm of every $L(\mathcal{H}_s, \mathcal{H}_{s-m+e^2})$, and we get

$$(5.7.20) \quad \dot{A}_{\tau t} = \dot{a}_{\tau t}(x, D) , \quad \ddot{A}_{\tau t} = \ddot{a}_{\tau t}(x, D) , \quad \dots .$$

But the operators $U = u(t, x, D)$ and U^* are of order 0, and their t -derivatives of order j are of order $-je$ (by (3.7.6)), hence $A_{\tau t}^\Delta = U^*(t)A_{\tau t}U(t)$ has the same property : Its t -derivative of order j exists in every $L(\mathcal{H}_s, \mathcal{H}_{s-m+je^2})$, and we get

$$(5.7.21) \quad \dot{A}_{\tau t}^\Delta = \dot{a}_{\tau t}^\Delta(x, D) , \quad \ddot{A}_{\tau t}^\Delta = \ddot{a}_{\tau t}^\Delta(x, D) , \quad \dots .$$

In particular, to show differentiability of an asymptotically convergent sum one will only need to verify that the formally differentiated terms still satisfy the required estimates (1.2.2). Q.E.D.

The proof of thm.5.7.1 then also is complete.

Finally, we now come back to an old-postponed problem: the proof of (iii) in thm.5.1.1.

Suppose an operator A belongs to \mathcal{P}_m , but we also know that $A \in \psi c_{m-e}$. Applying thm.5.7.1 above, we then conclude that $A^\Delta = U^*(0)AU(0)$ is of the form $A^\Delta = \begin{pmatrix} B & 0 \\ 0 & C \end{pmatrix} + \Gamma$ with $B, C \in Op\psi c_m$ and $\Gamma \in \mathcal{O}(-\infty)$. But we must also have $B, C \in Op\psi c_{m-e}$ since $A \in Op\psi c_{m-e}$ while $U, U^* \in Op\psi c_0$. Applying prop.5.7.5 for $m - e$ it then follows that also B, C satisfy cdn.'s (5.7.6) for $m - e$, not only for m . But then thm.5.7.1 implies that $A \in \mathcal{P}_{m-e}$, as stated in thm.5.1.1 (iii). Q.E.D.

5.8 The Final Algebra of Precisely Predictables

We are returning to time-independent potentials here, just because the decoupling of sec.3.5 has not been worked out for general potentials depending on time. [But we will allow the special time dependent case of ch.6, obtained by Lorentz-transforming a time-independent H .]

The result of section 5.7 was linking the algebra \mathcal{P} of observables with smooth time-propagation to the class of strictly classical ψ do-s which can be decoupled mod($\mathcal{O}(-\infty)$) under the Foldy-Wouthuysen transform of ch.3. But we noticed before that a “non-penetrable” barrier is needed between “electron states” and “positron states”, and that *no observation should mix up these two spaces* - that

¹⁵The difference under the integral at right may be written as $\varepsilon\kappa \int_0^1 d\lambda \ddot{a}_{\tau t+\lambda}(x, \xi)$, where $\ddot{a}_{\tau t+\lambda}$ and its (x, ξ) -derivatives satisfy estimates (1.2.2) even for $m - 2e^2$, not only for $m - e^2$. Thus it indeed follows that the t -derivative exists in all the Fréchet-norms induced by (1.2.2) for $m - e_2$.

is, a *precisely predictable observable* A should preserve these spaces: We should require that such A also is strictly decoupled by the transform U strictly decoupling H .

Thus we now introduce the sub-algebra $\mathcal{PX} \subset \mathcal{P}$ of all strictly classical ψ do-s $A \in \text{Op}\psi c$ such that

$$(5.8.1) \quad U^*AU = \begin{pmatrix} B & 0 \\ 0 & C \end{pmatrix},$$

where $U \in \text{Op}\psi c_0$ denotes the strictly decoupling unitary ψ do of sec.3.5.

This decoupling is with respect to the split $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ where \mathcal{H}_\pm equal $L^2(\mathbb{R}^3, \mathbb{C}^2)$, slightly corrected by (possibly) moving a finite dimensional space of rapidly decreasing functions from “+” to “-” (or “-” to “+”).

The spaces \mathcal{H}_e and \mathcal{H}_p (of electronic and positronic states, resp.) then will be defined as

$$(5.8.2) \quad \mathcal{H}_e = U\mathcal{H}_+, \quad \mathcal{H}_p = U\mathcal{H}_-.$$

And we then finally propose the self-adjoint operators of \mathcal{PX} as *precisely predictable observables*. These operators indeed have the needed property:

Starting with an electronic state $\psi \in \mathcal{H}_e$ we get as expectation value for the prediction the number $\check{A} = \langle \psi, A\psi \rangle = \langle \psi, B\psi \rangle$, not influenced by the positronic part C of A - referring to (5.8.1).

In particular, if the measurement results in an eigenvalue λ of A , this will be an eigenvalue of B , belonging to an eigen function of B - a function again belonging to \mathcal{H}_e . So, indeed, an electron never turns into a positron, due to a measurement.

Chapter 6

Lorentz Covariance of Precise Predictability

6.0 Introduction

It is known and very essential to Dirac's theory that it is compatible with a transformation of coordinates under the laws of special relativity. In other words, if we change the (space-time) coordinate system by a Lorentz transform then Dirac's equation remains intact - except for the physically significant changes of potentials - for example, a moving electrostatic field will also generate a magnetic field, under Faraday's laws¹.

Recall, that a Lorentz transform is defined as any invertible linear transformation $\begin{pmatrix} t' \\ x' \end{pmatrix} = L \begin{pmatrix} t \\ x \end{pmatrix}$ (with a constant real 4×4 -matrix L) under which the wave operator $\square = \partial_t^2 - \Delta$ does not change. This is true if and only if the matrix L satisfies the condition

$$(6.0.1) \quad L^T J L = J \text{ with the diagonal matrix } J = \text{diag}(1, -1, -1, -1) .$$

The linear maps L satisfying (6.0.1) form a group - the Lorentz-group. Actually one also should include the *translations* $\begin{pmatrix} t \\ x \end{pmatrix} \rightarrow \begin{pmatrix} t \\ x \end{pmatrix} + c$, with a constant 4-vector b , to then obtain the *Poincaré group* of transformations $\begin{pmatrix} t' \\ x' \end{pmatrix} = L \begin{pmatrix} t \\ x \end{pmatrix} + c$.

We are only interested in the "proper groups" (of Lorentz or Poincaré transforms not reversing time (and with determinant 1)). That is we will assume the component l_{00} of the matrix $L = \begin{pmatrix} l_{00} & l_{01} \\ l_{10} & l_{11} \end{pmatrix}$ to be positive, so that we get t' increasing

¹Also, the Dirac- 4×4 -matrices a_j, β might change, but in such a way that the crucial condition (1.0.3) remains intact.

whenever t increases. The classes of these (Lorentz or Poincaré) transforms form groups as well. We then will address the question about behaviour of precisely predictable observables under proper Lorentz (or Poincaré) coordinate transforms.

Using the group property it seems practical to approach this question looking at a suitable set of generators of the groups. The proper Lorentz group \mathcal{L}_p is generated by the maps² $L_o = \begin{pmatrix} 1 & 0 \\ 0 & o \end{pmatrix}$ [with any 3×3 -rotation matrix o] and the special Lorentz transforms $(t, x) \rightarrow (t', x')$, where, with fixed $\theta \in \mathbb{R}$,

$$(6.0.2) \quad t' = t \cosh \theta - x_1 \sinh \theta, \quad x'_1 = x_1 \cosh \theta - t \sinh \theta, \quad x'_2 = x_2, \quad x'_3 = x_3.$$

leaving the coordinates $\tilde{x} = (x_2, x_3)$ unchanged and involving only t and x_1 .

We tend to regard the action of translations or (time-independent) rotations L_o as (more or less) trivial³ but, still, these cases perhaps may serve as examples

²Clearly the transforms L_o are proper Lorentz transforms. For a general proper Lorentz transform L we may multiply left and right by an L_o such that the two 3-vectors l_{10} and l_{01}^T point into the positive x_1 -direction. From $L^T J L = J$ (and $L J L^T = J$ - verified from (6.0.1)) we conclude that $l_{11}^T l_{10} = l_{00} l_{01}^T$ and also $l_{11} l_{01}^T = l_{00} l_{10}$. If both l_{10} and l_{01}^T point into the x_1 -direction then this means that $(1, 0, 0)^T$ is an eigenvector of both l_{11} and l_{11}^T , so that $l_{11} = \begin{pmatrix} l_{111} & l_{112} \\ l_{121} & l_{122} \end{pmatrix}$ with vanishing 2-vectors $l_{112}^T = l_{121} = 0$. Thus, a Lorentz matrix L of this form splits into a map $\tilde{x} \rightarrow \tilde{x}$ (which must be an L_o) and a map $\begin{pmatrix} t \\ x_1 \end{pmatrix} \rightarrow \begin{pmatrix} t' \\ x'_1 \end{pmatrix}$. The latter then is easily seen to be of the form (6.0.2).

³Looking at a translation $\begin{pmatrix} t \\ x \end{pmatrix} \rightarrow \begin{pmatrix} t \\ x \end{pmatrix} + c$ and a map L_o first, we note that either coordinate transform leaves the algebra $Op\psi c$ and all its subspaces $Op\psi c_m$ invariant: The operator $a(x, D)$ goes into $a(x - b, D)$ and $a(ox, D)$, respectively, where $c = \begin{pmatrix} t \\ \tau \end{pmatrix}$. Moreover, a translation $t' = t + \tau, x' = x + b$ sends the Dirac equation (1.0.1) into $\partial\psi/\partial t' + iH'\psi = 0$ with H' exactly of the form (1.0.2), with the same matrices α_j, β but the potentials \mathbf{A}, \mathbf{V} replaced by $\mathbf{A}' = \mathbf{A}(t + \tau, x + b), \mathbf{V}' = \mathbf{V}(t + \tau, x + b)$. Since α, β remain the same, the split $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ also remains the same. Going through all the operations, it becomes clear that the two unitary decouplings ψ do-s U and U' of ch.III constructed for H and H' may be related by $U' = T_b U T_{-b}$ with $T_b u(x) = u(x + b)$. [There is no uniqueness in the construction of sec.3.5, but the above U' works. For time dependent potentials we should use $U'(t) = T_b U(t + \tau) T_{-b}$.]

For an L_o with an orthogonal map $o = (o_{jl})$ the Dirac Hamiltonian H of (1.0.2) will change into $H' = \sum \alpha'_j (D'_j - \mathbf{A}'_j) + \beta + \mathbf{V}'$, with unchanged β but $\alpha'_j = \sum_l o_{jl} \alpha_l$, and $\mathbf{V}'(t, x) = \mathbf{V}(t, ox)$. A calculation confirms that (i) the matrices $\alpha'_j, \beta' = \beta$ still satisfy relations (1.0.3). Moreover, (ii) with our choice of α, β (cf.(3.1.7)) the α' still are of the form (3.1.7) with σ_j replaced by $\sigma'_j = \sum o_{jl} \sigma_l$. Furthermore (iii) we still have $\sigma'_1 \sigma'_2 = i\sigma'_3, \sigma'_2 \sigma'_3 = i\sigma'_1, \sigma'_3 \sigma'_1 = i\sigma'_2$, just as for the σ_j . Finally (iv) there exists a constant unitary 2×2 -matrix $\varphi = \varphi(o)$ of determinant 1 such that $\varphi^* \sigma'_j \varphi = \sigma_j$. [Such a matrix φ must diagonalize σ'_3 since $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. Its columns will be the two normalized eigenvectors of σ'_3 each carrying an arbitrary factor $e^{i\lambda}, e^{i\mu}$, where λ, μ may be adjusted to obtain precisely $\varphi^* \sigma'_j \varphi = \sigma_j$, for $j = 1, 2$. This fixes only $\lambda - \mu$, but φ becomes unique up to a free choice of sign \pm if we also request that $\det \varphi = 1$. This fact addresses a well known relation between the Lie groups $SU(2)$ and $SO(3)$. The inverse of above map $SO(3) \rightarrow SU(2)$ describes a Lie-group homomorphism covering $SU(2)$ twice.] So, with the 4×4 -matrix $\check{\varphi} = \begin{pmatrix} \varphi & 0 \\ 0 & \varphi \end{pmatrix}$, we have $\check{H} = \check{\varphi}^* H' \check{\varphi} = \alpha(D' - A') + \beta + V'$, and then should compare the unitary ψ do-s U and $\check{U} = \check{\varphi}^* U' \check{\varphi}$, using the same α, β , with different potentials.

to outline our task: Of course, we will ask the question whether our concept of precisely predictable observables (and its surrounding facts) depend on the choice of coordinate system. Under any of above transforms the Dirac equation will remain intact, with covariantly changed potentials - perhaps with different Dirac matrices α, β , but still a Dirac equation. Generally, in this chapter, we will get restricted to **time-independent potentials**. After a boost the time-independent potentials may become time-dependent though, (with a rather special time-dependence), but they still will satisfy *cdn.(X)*. There will be algebras \mathcal{P} and $\mathcal{P}\mathcal{X}$ (independent of the initial point τ), before and after the change of coordinates. Now, as it comes to the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ of physical states, this space should remain the same, if we deal with an L_o or with a translation by $\begin{pmatrix} 0 \\ b \end{pmatrix}$, since the locus “ $t = 0$ ” in Minkowsky space \mathbb{R}^4 does not change. In the new coordinates $x' = ox$ (or $x' = x + b$) a state $\psi(x)$ will assume the form $\psi'(x') = \psi(x' - b) = (T_{-b}\psi)(x')$ (or $\psi'(x') = \psi(o^T x') = (S_{o^T}\psi)(x')$). An observable A then will go into the observable $A' = T_b A T_{-b}$ (or, $A' = S_o A S_{o^T}$). Note, T_b and S_o are unitary maps $\mathcal{H} \leftrightarrow \mathcal{H}$ inverted by T_{-b} and S_{o^T} . So, in the Hilbert space \mathcal{H} of physical states our coordinate transform just corresponds to the unitary map $\psi \rightarrow Z^*\psi$ with $Z = T_b$ (or $Z = S_o$), under which a linear operator $A : \mathcal{H} \rightarrow \mathcal{H}$ transforms into $A' = ZAZ^*$.

We then have the algebras \mathcal{P} and $\mathcal{P}\mathcal{X}$ and their transforms under Z - i.e., $Z\mathcal{P}Z^*$ and $Z\mathcal{P}\mathcal{X}Z^*$ - and we will expect a relation between these algebras and the algebras \mathcal{P}' , $\mathcal{P}\mathcal{X}'$ generated by the transformed Hamiltonian H' .

Now, our split $\mathcal{H} = \mathcal{H}_e \oplus \mathcal{H}_p$ of (3.0.5) is determined by the split $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ with $\mathcal{H}_\pm = L^2(\mathbb{R}^2, \mathbb{C}^3)$ (give or take some subspace \mathcal{Z}), and the unitary map U obtained in sec.3.5. And, the algebras \mathcal{P} , $\mathcal{P}\mathcal{X}$ also depend on the split $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ and the operator $U \in Op\psi c_0$ of sec.3.5. However, if we now examine U , it is clear that $U' = ZUZ^*$ (with $Z = T_b$ (or $Z = S_o$)) belongs to $Op\psi c_0$, again since $Op\psi c_m$ are invariant under linear transformation of variables. Moreover, we get

$$(6.0.3) \quad U'^* H' U' = \begin{pmatrix} X' & 0 \\ 0 & Y' \end{pmatrix} \quad \text{with } X' = ZXZ^*, Y' = ZYZ^*,$$

since evidently the transform Z leaves our split $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ intact [although it might transform the (finite dimensional) space \mathcal{Z} a bit].

It may be important now to recall that there is no uniqueness in the construction of our unitary operator U of sec.3.3 and sec.3.5, nor is the split $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ unique, due to the subspace \mathcal{Z} . But, if we decide to use the above transformed operator U (and the correspondingly transformed space \mathcal{Z}') then, indeed, we get

$$(6.0.4) \quad \mathcal{H} = \mathcal{H}'_e \oplus \mathcal{H}'_p \quad \text{with } \mathcal{H}'_e = U' \mathcal{H}'_+, \mathcal{H}'_p = U' \mathcal{H}'_-.$$

and

$$(6.0.5) \quad U'^* \mathcal{P}' U' = \left\{ \begin{pmatrix} A & B \\ C & D \end{pmatrix} : A, D \in \text{Op}\psi c, B, C \in \mathcal{O}(-\infty) \right\},$$

$$U'^* \mathcal{P}' \mathcal{X}' U' = \left\{ \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} : A, B \in \text{Op}\psi c \right\}.$$

Then we also have

$$(6.0.6) \quad \mathcal{P}' = Z \mathcal{P} Z^*, \quad \mathcal{P}' \mathcal{X}' = Z \mathcal{P}' \mathcal{X}' Z^*.$$

Or, in other words, the concept of precise predictability transforms as it should under this kind of “trivial” Lorentz transformation -

On the other hand, a time-translation $\begin{pmatrix} t \\ x \end{pmatrix} \rightarrow \begin{pmatrix} t+\tau \\ x \end{pmatrix}$ will generate the new observables $A_t = e^{i\tau H} A e^{-i\tau H}$ - i.e., just the Heisenberg transform. We know that this leaves the split (3.0.5) and both algebras $\mathcal{P}, \mathcal{P}' \mathcal{X}'$ invariant.

So, regarding Lorentz-invariance we are left with the special transform (6.0.2) - called “ x_1 -boosts” - or just “boosts”. For such a boost the Dirac equation will keep its general form, as we shall see in sec.6.1. However, since now time is involved, we no longer should keep the initial 3-space $t = 0$ as the location where our physical states are defined. Rather, we should define a new Hilbert space of states along the (also space-like) hyperplane $t' = 0$, and on $t' = 0$ use the new space-coordinates x' . This raises the question of a useful correlation between physical states at $t = 0$, and $t' = 0$, accompanied by the proper change of observables as well. This problem already appeared for the translation, if there is a time-shift - i.e., $\begin{pmatrix} t \\ x \end{pmatrix} \rightarrow \begin{pmatrix} t+\tau \\ x \end{pmatrix}$, for example. In that case we were solving the Dirac equation (1.0.1) with initial condition $\psi(0, x) = \psi_0(x)$, for a given state $\psi_0 \in \mathcal{H}$, getting $\psi(t, x) = e^{-iHt} \psi_0(x)$. Then, choosing $Z = e^{iH\tau}$, we get $A_\tau = Z A Z^* = e^{iH\tau} A e^{-iH\tau}$ as the transformed observable A .

We take this fact as encouragement for seeking the change between the space-like hypersurfaces $t = 0$ and - after a boost (6.0.2) - $t' = 0$ as follows: Again we will extend a given state ψ_0 into 4-space as solution $\psi(t, x) = e^{-itH} \psi_0(x)$ of the Dirac equation (1.1.1). The values of ψ on the plane $t' = 0$ in the proper coordinates x' then should be related to the transformed state.

However the vector of \mathcal{H} (living on \mathbf{S}' of fig.6.0.1) will only be a unit vector if we use a modified inner product $(u, v) = \int u^* \kappa^2 v dx$, with the constant hermitian positive definite 4×4 -matrix $\kappa = \cosh(\theta/2) - \alpha_1 \sinh(\theta/2)$, as will be shown. Thus we will multiply the function $\psi|\mathbf{S}'$ by κ to create the transformed physical state, living on \mathbf{S}' . ψ' then will have norm 1 in \mathcal{H} . The map $R : \psi \rightarrow \psi'$ will be a unitary operator of \mathcal{H} — mapping the physical states on \mathbf{S} onto the physical

states on \mathbf{S}' . (Multiplication by κ should correspond to the well-known relativistic velocity distortion.)

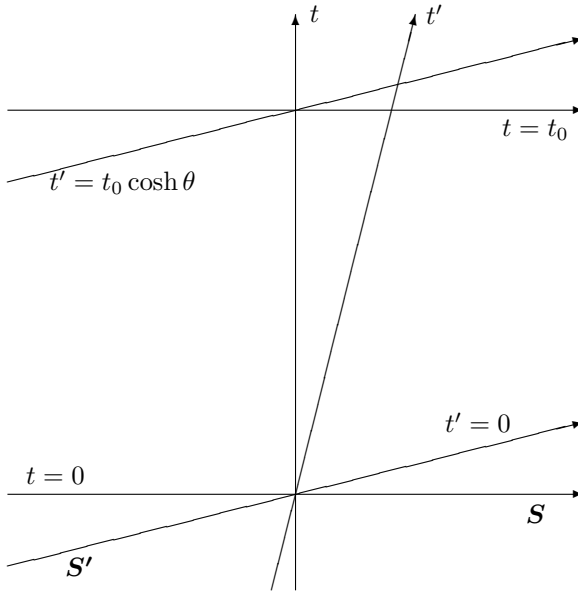


Fig. 6.0.1. The Hilbert space \mathcal{H} is located over the hyperplane $\mathbf{S} = \{t = 0\}$. After the boost (6.0.2) we should work with a Hilbert space over $\mathbf{S}' = \{t' = 0\}$ given as $t = x_1 \tanh \theta$ in the old coordinates. We relate a state ψ_0 on \mathbf{S} to a corresponding state on \mathbf{S}' by restricting the solution of the Dirac equation assuming initial values ψ_0 on \mathbf{S} to \mathbf{S}' , and multiplying it by a “relativistic distortion”. This corresponds to the fact that at the hyperplane $t = t_0$ we traditionally deal with the restriction of the same solution $e^{-iHt}\psi_0$ to $t = t_0$.

The induced transformation of independent and dependent variables will transform the Dirac equation (1.0.1) into the Dirac equation again, with exactly the same α_j, β , but with potentials changed according to the covariant change of electromagnetic field vector (details cf. sec.6.1).

Things are quite different in one respect, however: The transformed potentials now will depend on t as well (except under special assumptions, such as $\mathbf{A}_j = \mathbf{V} \equiv 0$). Still we must ask the question, in general as well as in the special cases, whether or not “precisely predictable” can be defined also in the new coordinates, and whether or not the definitions for both coordinates agree.

Indeed, in sec.6.2 we will show that in the case of vanishing potentials where the unitary map U may be chosen according to (3.1.5), and then there are well defined spaces \mathcal{H}_e and \mathcal{H}_p , we do have

$$(6.0.7) \quad \mathcal{P}' = R\mathcal{P}R^* \text{ and } \mathcal{P}\mathcal{X}' = R\mathcal{P}\mathcal{X}R^* .$$

This fact seems to be nontrivial - To prove it, we had to get some more explicit

representation of the operator R . This happens to be a (global) Fourierintegral operator with rather interesting properties.

On the other hand, for the general case, we find it useful to first investigate another transform of the Dirac equation - namely, the equation

$$(6.0.8) \quad \partial\psi/\partial t + iH'\psi \quad \text{where} \quad H' = RHR^* .$$

Note that H' , the transform of the Hamiltonian H under R still is a “Dirac-type” operator - a first order PDO, not exactly of the form (1.0.2) but similar, and can be explicitly calculated. This is a time-independent operator, not coinciding with the Dirac Hamiltonian obtained by the above coordinate transform - here called $H^\sim(t)$. The Dirac equation $\partial\psi/\partial t + iH^\sim(t)\psi = 0$ possesses an *evolution operator* $U(\tau, t) = U_{H^\sim}(\tau, t)$ as in thm.4.1.1, not of the group form $e^{-iH^\sim(t-\tau)}$. However, one can derive a relation between U_{H^\sim} and $e^{-iH't}$, also involving a translation operator (cf. (6.3.10)) These facts will be helpful for the study of transforming precise predictability.

For $\mathbf{V} = \mathbf{A} = 0$ we can get a direct evaluation of R - in terms of some Fourier transformed nonlinear substitutions, allowing us to directly show (6.0.8). It turns out that R then commutes with the spectral projections of H_0 effecting the split (3.0.5), and the unitary ψ do U of (3.1.5) remains the same.

In the general case we will rely on the fact that the unitary ψ do U constructed in sec.3.5 determines the two projections $P_+ = U \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} U^*$, $P_- = U \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} U^* \in Op\psi c_0$ effecting the split and also the two algebras $\mathcal{P}, \mathcal{P}\mathcal{X}$ of precisely predictables.

We trivially have RU unitary, and

$$(6.0.9) \quad (RU)^* H' (RU) = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix} ,$$

so, RU decouples H' . However, this is **not** a decoupling of H' in our sense, since RU is not a ψ do - the operator R still being a global Fourier integral operator with rather nonlocal properties. But we will try to rectify this by right-multiplying RU with another Fourier integral operator, not disturbing the split (6.0.9), but converting RU into a ψ do. For this construction we will strongly rely on the “formal ψ do ” $E = e(x, D)$ with $e(x, \xi) = e^{i\eta x_1 \langle \xi \rangle}$ [this is not a ψ do in $Op\psi c$, but, rather, a Fourier integral operator]. The U (called U^\diamond) thus constructed will not coincide with U of (3.1.5) if potentials vanish, even though it then has a representation $U^\diamond = u^\diamond(D)$ with some other $u^\diamond(\xi)$ (depending on η) diagonalizing $\text{symp}(H_0)$.

Still, U^\diamond will decouple H' and equ. (6.0.8). And, moreover, **the decoupling achieved by U^\diamond will be the transform of the decoupling of U under the unitary operator R .** Once we have obtained this U^\diamond , then we also get a unitary

ψ do (called $U^\circ(t)$), now depending on t , decoupling the Dirac equation $\partial_t u + i\tilde{H}(t)u = 0$ obtained by changing coordinates under the boost (6.0.2). It turns out that

$$(6.0.10) \quad U^\circ(t) = e^{i\eta t D_1} U^\circ(t) e^{-i\eta t D_1} .$$

So, under $U^\circ(t)$ we still have the R -transformed original decoupling of U - just combined with a time dependent translation $T_{\eta t} = e^{i\eta t D_1}$ (which leaves the spaces $\mathcal{H}'_e = R\mathcal{H}_e$, $\mathcal{H}'_p = R\mathcal{H}_p$ unchanged with time).

Also, since now we have a time-dependent Hamiltonian, the algebras \mathcal{P} and $\mathcal{P}\mathcal{X}$ now should depend on the initial point τ . Indeed, we get $\tilde{\mathcal{P}}(\tau) = e^{i\eta t D_1} \mathcal{P}'$ with $\mathcal{P}' = R\mathcal{P}R^*$ describing the proper precisely predictable algebra.

This then, finally, should describe the Lorentz covariance of precise predictability we have to offer.

Proving these facts (i.e., thm. 6.4.1) will engage us in a complicated discussion, finally focusing on the problem of solving a certain ODE with ψ do-coefficients - rather, in proving symbol properties of their solutions. This is discussed in sec's 6.5-6.7. We close the chapter with a discussion of integral kernels of some of the operators used in this section - just to let us get a feeling for them.

Interestingly, the 1-dimensional (abelian) subgroup of boosts (6.0.1), for $\theta \in \mathbb{R}$, generates a group $R = R_\theta$ of unitary operators. This R_θ may be seen to be the evolution operator of a certain hyperbolic system, and, approximately, $\text{symb}(A')$ is the transport of $\text{symb}(A)$ along the (pair of) Hamiltonian flow(s) generated. We will not work this out, however.

Note, we are keeping the 'time evolution interpretation' of the Dirac theory intact, although normally this is abandoned in the extensive literature on Dirac theory: For relativistic discussions equation (1.0.2) usually is multiplied by β and thus assumes a form symmetric in the 4 variables $(t, x) = (x_0, x_1, x_2, x_3)$. The symmetry invites forgetting about the distinction of time variable.

Perhaps we here should mention the work of A.Unterberger [Un_j] who independently has offered an abstract theory of Dirac observables, also involving pseudodifferential operators. For vanishing potentials the operator $Z = \beta(-i\partial_t + H) - 1$ is a "square root" of the wave operator: We have $Z^2 = \Delta - \partial_t^2$, due to the properties of the Dirac matrices α_j, β . Accordingly, a solution ψ of $\dot{\psi} + iH\psi = 0$ will also solve the Klein-Gordon equation $\psi_{|tt} = \Delta\psi - \psi$. Their (t, x) -Fourier transform ψ^\wedge must satisfy $(\tau^2 - \xi^2 - 1)\psi^\wedge(\tau, \xi) = 0$, hence must have support on the "mass-hyperboloid" $\mathbf{M} = \{\tau^2 = 1 + \xi^2\}$. Similarly to his earlier discussions for Klein-Gordon theory, Unterberger introduces a class of pseudodifferential operators with symbol defined on a "phase space" with momentum and location given

by the “world lines” in (t, x) -space. His operators preserve solutions of the Dirac equation, and have covariance under Poincare transforms built in. This is worked out for vanishing potentials only.

Perhaps we also should mention, at this point, the extensive literature on the subject of relativity and the Dirac equation (cf. Thaller’s book [Th1], chapters 2 and 3). For us, looking at observables of the Dirac equation, the only thing important seems to be the covariance of our algebras, looked at in terms of conjugation with the unitary operator R introduced above. In fact, while mathematically quite interesting, many of the properties discovered within the past 75 years might only distract from the real physical issues.

6.1 A New Time Frame for a Dirac State

We are looking at the Dirac equation with time-dependent⁴ potentials, and symbol of the Hamiltonian $H(t)$ given by

$$(6.1.1) \quad h(t; x, \xi) = \sum_{j=1}^3 \alpha_j (\xi_j - \mathbf{A}(t, x)) + \beta + \mathbf{V}(t, x),$$

A physical state will be a unit vector $\psi(x)$ in the Hilbert space \mathcal{H} . When thinking of this same physical state in the new space-time frame given by the boost (6.0.2) we first extend $\psi(x)$ into Minkowsky space $\{(t, x)\}$ as a solution of the Dirac equation $\dot{\psi} + iH\psi = 0$ to obtain a function $\psi(t, x)$, and then restrict $\psi(t, x)$ to the space-like hyperplane $t' = 0$ in the new space-time coordinates (t', x') .

This transformed state $\psi^\Delta = \psi^\Delta(x')$ should be a unit vector in the Hilbert space \mathcal{H}^Δ of squared integrable 4-vector functions on \mathbf{S}' . And, indeed, we will show this to be correct, but with a slight amendment: The inner product of \mathbb{C}^4 on \mathcal{S}' will no longer be $\psi^* \chi$. Rather, we must use $\psi^* \kappa^2 \chi$, with a certain constant positive definite hermitian symmetric matrix⁵ κ .

The boost (6.0.2) will be abbreviated as

$$(6.1.2) \quad t' = tc - x_1 s, \quad x'_1 = -ts + x_1 c, \quad x'_2 = x_2, \quad x'_3 = x_3,$$

with $c = \cosh \theta$ and $s = \sinh \theta$. Its inverse is given by

$$(6.1.3) \quad t = t'c + x'_1 s, \quad x_1 = t' s + x'_1 c, \quad x_2 = x'_2, \quad x_3 = x'_3.$$

⁴Lorentz-transforming the Dirac equation will work for time-dependent potentials, but eventually we will return to time-independent A and V , since we want to study covariance of our algebras \mathcal{P} and $\mathcal{P}\mathcal{X}$ partly defined only for that case.

⁵But, to compensate for this, we rather will left-multiply the restriction to $t' = 0$ with the constant matrix κ - applying a “relativistic distortion” to the state.

Given a state ψ (and its extension $\psi(t, x)$ into \mathbb{R}^4). Assume $\psi(x) \in C_0^\infty(\mathbb{R}^3)$, then also $\psi_t \in C_0^\infty(\mathbb{R}^3)$, for all times t . Indeed, the Dirac equation is a symmetric hyperbolic system, hence it displays *finite propagation speed*. A quick study of hyperbolic theory shows the upper speed limit to be $= 1$ — the speed of light — as expected. Thus, if $\text{supp } \psi$ is contained in a ball $\{|x| \leq \eta\}$ then $\text{supp } \psi_t$ will be contained in $\{|x| \leq \eta + |t|\}$.

The transformed state ψ^Δ then should be given as the restriction $\psi(t, x)|_{\{t'=0\}}$, in the proper coordinates x' on \mathbf{S}' . Note that $t' = 0$ amounts to $t = \eta x_1$, with $\eta = \tanh \theta$. In order to verify a relation between $\|\psi\|^2 = \int \psi^* \psi dx = \int |\psi(x)|^2 dx$ and some L^2 -norm on \mathcal{S}' we consider the difference

$$(6.1.4) \quad Z = \int |\psi(\eta x_1, x)|^2 dx - \int |\psi(x)|^2 dx.$$

For convenience we assume that $t > 0$, and that $\text{supp } \psi_t$ is contained in the half space $x_1 \geq 0$, for all $0 \leq \tau \leq t$. This is no restriction of generality, due to the fact that supports are compact, and that we have arbitrary space-time translations available to shift supports, before attempting our discussion.

Then we may write (using our Dirac equation $\partial\psi/\partial t = -iH\psi$):

$$\begin{aligned} Z &= \int_{x_1 \geq 0} dx \int_0^{\eta x_1} d\tau \left\{ \frac{d}{d\tau} |\psi(\tau, x)|^2 \right\} = \int_{x_1 \geq 0} dx \int_0^{\eta x_1} d\tau \{ \psi_t^* \psi + \psi^* \psi_t \}(\tau, x) \\ &= - \int_0^\infty d\tau \iint dx_2 dx_3 \int_{\tau/\eta}^\infty dx_1 \{ (iH\psi)^* \psi + \psi^* (iH\psi) \}(\tau, x_1, x_2, x_3). \end{aligned}$$

But the differential operator H is hermitian symmetric. Therefore the latter inner integral transforms into a boundary integral.

More precisely, we get $iH = \alpha_1 \partial_{x_1} + \dots$. The crucial term of above inner integral is $\int_{\tau/\eta}^\infty dx_1 \partial_{x_1} \{ \psi^* \alpha_1 \psi \}(\tau, x_1, x_2, x_3) = -\{ \psi^* \alpha_1 \psi \}(\tau, \tau/\eta, x_2, x_3)$. The partial integrations with respect to x_2 and x_3 do not give boundary terms since the integrals extend from $-\infty$ to ∞ . It follows that

$$(6.1.5) \quad Z = \int_0^\infty d\tau \iint dx_2 dx_3 \{ \psi^* \alpha_1 \psi \} \left(\tau, \frac{\tau}{\eta}, x_2, x_3 \right) = -\eta \int dx \{ \psi^* \alpha_1 \psi \}(\eta x_1, x),$$

where we have used the substitution $\frac{\tau}{\eta} = x_1$, $d\tau = \eta dx_1$, and extended the integral to all of \mathbb{R}^3 , using the support condition. Finally we introduce the coordinates x' (also in the first integral of Z): On \mathcal{S}' we have $t = x_1 \tanh \theta$, $x'_1 = x_1 \cosh \theta - t \sinh \theta = x_1 / \cosh \theta$, $x'_2 = x_2$, $x'_3 = x_3$. Introducing this in the first integral (6.1.8), and in the integral of (6.1.5), we get — with $\psi(\eta x_1, x) = \psi^\Delta(x')$ —

$$(6.1.6) \quad \int \psi^{\Delta*} (\cosh \theta - \alpha_1 \sinh \theta) \psi^\Delta(x') dx' = \int |\psi(x)|^2 dx.$$

This confirms the above discussion — we find that the positive definite matrix κ mentioned is given by $\kappa^2 = \cosh \theta - \alpha_1 \sinh \theta$. Indeed, κ^2 is hermitian, since α_1 is. Also, α_1 has eigenvalues ± 1 , since $\alpha_1^2 = 1$. Hence the eigenvalues of κ^2 are $\cosh \theta \pm \sinh \theta > 0$.

In order to round off this discussion let us next transform the Dirac equation onto the coordinates (t', x') of (6.1.2). Equation $\dot{\psi} + iH(t)\psi = 0$ assumes the form

$$(6.1.7) \quad \{(c - \alpha_1 s)\partial_t + (\alpha_1 c - s)\partial_{x_1} + \alpha_2 \partial_{x_2} + \alpha_3 \partial_{x_3} + i(\beta + \mathbf{V} - \sum_1^3 \alpha_j \mathbf{A}_j)\}\psi^\Delta = 0.$$

We find our positive matrix κ^2 as coefficient of ∂_t . It is practical to introduce $\psi' = \kappa\psi^\Delta$, with the positive square root κ of $\kappa^2 = c - \alpha_1 s$. Then the left hand side of (6.1.6) will be $\|\psi'\|^2$, and (6.1.6) shows that the map $\psi \rightarrow \psi'$ is a unitary operator of \mathcal{H} . On the other hand, (6.1.7) with ψ' , after a left multiplication by $\kappa^{-1} = \sqrt{c + \alpha_1 s}$, assumes the form

$$(6.1.8) \quad \{\partial_{t'} + \alpha'_1 \partial_{x'_1} + \alpha'_2 \partial_{x'_2} + \alpha'_3 \partial_{x'_3} + i\beta' + i\kappa^{-1}(\mathbf{V} - \sum_1^3 \alpha_j \mathbf{A}_j)\kappa^{-1}\}\psi' = 0,$$

where

$$(6.1.9) \quad \alpha'_1 = \alpha_1, \quad \alpha'_2 = \kappa^{-1}\alpha_2\kappa^{-1}, \quad \alpha'_3 = \kappa^{-1}\alpha_3\kappa^{-1}, \quad \beta' = \kappa^{-1}\beta\kappa^{-1}.$$

The last term in (6.1.8) assumes the form

$$(6.1.10) \quad \begin{aligned} & i\{(c + \alpha_1 s)(\mathbf{V} - \alpha_1 s) - \sum_2^3 \alpha'_j \mathbf{A}_j\} \\ & = i\{(c\mathbf{V} - s\mathbf{A}_1) - \alpha_1(-s\mathbf{V} + c\mathbf{A}_1) - \sum_2^3 \alpha'_j \mathbf{A}_j\}. \end{aligned}$$

Introducing the transformed vector potential

$$(6.1.11)$$

$$(\mathbf{V}', \mathbf{A}'_1, \mathbf{A}'_2, \mathbf{A}'_3)(t', x') = (\mathbf{V} \cosh \theta - \mathbf{A}_1 \sinh \theta, \mathbf{A}_1 \cosh \theta - \mathbf{V} \sinh \theta, \mathbf{A}_2, \mathbf{A}_3)(t, x)$$

(which conforms with the covariant transformation rules for vector potentials) we then obtain the Dirac equation (6.0.3) in the old form again, with the α_j, β replaced by α'_j, β' of (6.1.13). However, a calculation shows that $\beta' = \beta, \alpha'_j = \alpha_j$, for $j = 1, 2, 3$. Indeed, we get

$$(6.1.12) \quad \kappa = \delta_+ - \alpha_1 \delta_-, \quad \kappa^{-1} = \delta_+ + \alpha_1 \delta_-, \quad \delta_+ = \cosh(\theta/2), \quad \delta_- = \sinh(\theta/2),$$

using $\alpha_1^2 = 1$, and the fact that the matrices at right are positive.

We already have $\alpha'_1 = \alpha_1$. We use that $\alpha_1\alpha_2 + \alpha_2\alpha_1 = 0$, for $\alpha'_2 = \kappa^{-1}\alpha_2\kappa^{-1} = (\delta_+ + \alpha_1\delta_-)\alpha_2(\delta_+ + \alpha_1\delta_-) = \alpha_2(\delta_+ - \alpha_1\delta_-)(\delta_+ + \alpha_1\delta_-) = \alpha_2$. Similarly for α_3 and β , using $\alpha_1\alpha_3 + \alpha_3\alpha_1 = 0$ and $\alpha_1\beta + \beta\alpha_1 = 0$.

It follows that $\psi'(t', x') = \kappa\psi(t, x) = (\delta_+ - \alpha_1\delta_-)\psi(t, x)$ satisfies the Dirac equation again, in the new coordinates (t', x') , with the (covariantly) transformed potentials $\mathbf{V}', \mathbf{A}'_j$ of (6.1.11), but with exactly the same Dirac matrices α_j, β .

We summarize:

Proposition 6.1.1 *The map $R : \psi \rightarrow \psi' = \kappa\psi^\Delta$, with κ of (6.1.12), and the restriction $\psi^\Delta(x')$ to \mathcal{S}' (the plane $t' = 0$) of $\psi(t, x) = e^{-itH}\psi$, in the new coordinates (6.1.2), defines a unitary map of $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ onto itself. This map takes the physical state $\psi(x)$ on $\mathcal{S} = \{t = 0\}$ (with $\|\psi\| = \{\int \psi^*\psi dx\}^{1/2} = 1$) to a transformed physical state $\psi'(x')$, defined on the plane $\mathcal{S}' = \{t' = 0\}$, in the new coordinates (t', x') , again with $\|\psi'\| = \{\int \psi'^*\psi'(x')dx'\}^{1/2} = 1$, in such a way that the solution $\psi'(t', x')$ of the Cauchy problem*

$$(6.1.13) \quad \partial\psi'/\partial t' + i\tilde{H}\psi' = 0, \quad \psi'(0, x') = \psi'(x'),$$

(with \tilde{H} of the same form as H , in new coordinates (t', x')),

$$(6.1.14) \quad \tilde{H} = h'(t', x', D'), \quad h' = \mathbf{V}' + m\beta + \sum_1^3 \alpha_j(\xi'_j - \mathbf{A}'_j),$$

with the old α_j, β of (6.0.2), but potentials $\mathbf{V}', \mathbf{A}'_j$ of (6.1.11) and the solution $\psi(t, x) = e^{-itH}\psi$ of (1.0.1) with $\psi(0, x) = \psi(x)$ are transforms of each other in the coordinate transform (6.1.2), combined with the map $\psi \rightarrow \kappa\psi^\Delta$ as transform of dependent variable.

Remark 6.1.2 *When trying to look at our algebras \mathcal{P} and \mathcal{PX} of sec.3.3, sec.3.5, sec.5.7, sec.5.8, and their behaviour under this coordinate change, we must keep in mind that \mathcal{PX} generally was only defined for time-independent \mathbf{A} and \mathbf{V} , while, in general, \mathcal{P} will depend on the initial point τ , if potentials depend on time. However, after performing above coordinate transform, our new \mathbf{A}', \mathbf{V}' of (6.1.11) in general now will depend on t' . We will assume time-independence of \mathbf{A} and \mathbf{V} , in the following, then getting our \mathcal{P} and \mathcal{PX} , in the old coordinates, with the constructions of ch.3 and ch.5. But these constructions normally will not be available in the new coordinates. Still, of course, we may transform the algebras already obtained to the new coordinates, using our operator R , above, and we will show that they display similar properties, also in the new coordinates, regarding the possibility of decoupling by means of a unitary ψ do, etc. Also, these algebras will be independent of the initial Hilbert space of states, in spite of now time-dependence*

of A', V' . However, as the constructions of sec.3.5 are not available for \mathbf{A}', \mathbf{V}' , we cannot expect a comparison between the different methods of obtaining these algebras.

Remark 6.1.3 *No symbol properties are needed for \mathbf{A} and \mathbf{V} , above, although we will assume bounded C^∞ -potentials \mathbf{V}, \mathbf{A}_j . This implies essential self-adjointness of H in its minimal domain C_0^∞ , hence existence of a unique self-adjoint realization of H (cf.[Th1], thm. 4.2). So, also, our unitary group e^{-iHt} is well defined under such weaker assumptions. However, for convenience we always will assume *cdn.*(X) for A and V , which implies *cdn.*(X) also for A', V' together with all their time-derivatives.*

Then this group consists of operators of order 0 - bounded $\mathcal{H}_s \rightarrow \mathcal{H}_s$ for all s , with the weighted Sobolev spaces \mathcal{H}_s of sec.1.4 (cf. [Co5], VI, thm.3.1 - also look at sec.5.7, above, for further comments). In particular, this ensures that we may calculate with C_0^∞ -states, all the way.

6.2 Transformation of \mathcal{P} and $\mathcal{P}\mathcal{X}$ for Vanishing Fields

Let us look first at invariance of our algebras \mathcal{P} and $\mathcal{P}\mathcal{X}$ for vanishing potentials. This is a case where not only the operator R of (6.0.2) but also conjugation $A \rightarrow RAR^*$ taking observables to the new space-time frame can be described explicitly. It will be confirmed indeed that we have

$$(6.2.1) \quad RPR^* = \mathcal{P} \ , \ R\mathcal{P}\mathcal{X}R^* = \mathcal{P}\mathcal{X} \ .$$

Interestingly, however, we do not have $H' = RHR^* = H$, reflecting the fact, that, in the “moving frame”, the total energy of the particle (at rest in the old frame) is “augmented” by the energy of the uniform motion in the x_1 -direction at speed η .

Let us assume $\mathbf{V} = \mathbf{A}_j \equiv 0$ in all of the present section. In that case the FW-transform U of (3.1.5) is just given by

$$(6.2.2) \quad U = \frac{1}{\sqrt{2+2S_0}}(1 + S_0 - \beta\alpha S) = u(D) \ ,$$

with $u(\xi) = \frac{1}{\sqrt{2+2s_0}}(1 + s_0 - \beta\alpha s)$, where $s_0(\xi) = \frac{1}{(\xi)}$, $s(\xi) = \frac{\xi}{(\xi)}$, and, as usual, $u(D) = F^{-1}u(\xi)F$.

We have

$$(6.2.3) \quad \mathcal{H}_e = U\{(u_1, u_2, 0, 0)^T = \binom{u}{0}\} \subset \mathcal{H}, \quad \mathcal{H}_p = U\{(0, 0, v_3, v_4)^T = \binom{0}{v}\} \subset \mathcal{H},$$

and our algebras are explicitly given as

$$(6.2.4) \quad \mathcal{P} = U\left\{\begin{pmatrix} A & B \\ C & D \end{pmatrix} : A, D \in \text{Op}\psi c, B, C \in \mathcal{O}(-\infty)\right\}U^*,$$

$$(6.2.5) \quad \mathcal{PX} = U\left\{\begin{pmatrix} A & 0 \\ 0 & D \end{pmatrix} : A, D \in \text{Op}\psi c\right\}U^*.$$

Or, alternately, using the two eigenprojections

$$(6.2.6) \quad P_{\pm} = p_{\pm}(D), \quad p_{\pm}(\xi) = \frac{1}{2}(1 \mp (\alpha\xi + \beta)/\langle\xi\rangle),$$

we have

$$(6.2.7) \quad \mathcal{P} = \{A \in \text{Op}\psi c : P_+AP_-, P_-AP_+ \in \mathcal{O}(-\infty)\},$$

$$(6.2.8) \quad \mathcal{PX} = \{A \in \text{Op}\psi c : P_-AP_+ = P_+AP_- = 0\}.$$

In terms of 2×2 -block matrices the two projections P_{\pm} satisfy

$$(6.2.9) \quad U^*P_+U = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad U^*P_-U = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$

and we have

$$(6.2.10) \quad H = \langle D \rangle P_+ - \langle D \rangle P_- ,$$

since $h(\xi) = \alpha\xi + \beta$ has eigenvalues $\pm\langle\xi\rangle = \pm\sqrt{1 + \xi^2}$. The P_{\pm} satisfy

$$(6.2.11) \quad P_{\pm}^* = P_{\pm}, \quad P_{\pm}^2 = P_{\pm}, \quad P_+P_- = P_-P_+ = 0, \quad P_+ + P_- = 1.$$

We get

$$(6.2.12) \quad e^{-iHt} = e^{-i\langle D \rangle t}P_+ + e^{i\langle D \rangle t}P_- ,$$

where the $P_{\pm} = p_{\pm}(D)$ are ψ do-s with symbol $p_{\pm} \in \psi c_0$, while $e^{\pm i\langle D \rangle t}$ also are ψ do-s, but with symbol $e^{\pm i\langle \xi \rangle t}$ only in ψt_0 , not in ψc . Leibniz formulas do not apply in the asymptotic form, for such operators. Their composition obeys some more complicated rules.

We will need fla. (6.2.12) for construction of our unitary operator R : The solution of Diracs equation for a given initial value $\psi_0(x)$, at $t = 0$, is determined by

$$(6.2.13) \quad \psi(t, x) = e^{-i\langle D \rangle t} P_+ \psi_0 + e^{i\langle D \rangle t} P_- \psi_0 .$$

Recall, R was constructed by the sequence

$$(6.2.14)$$

$$\psi_0(x) \rightarrow \psi(t, x) = e^{-iHt} \psi_0 \rightarrow \psi(\eta x_1, x) = \psi^\diamond(x) \rightarrow \kappa \psi^\diamond(cx_1, \tilde{x}) = \psi'_0(x) = R\psi_0(x).$$

In (6.2.13) the terms $\psi_{0,\pm} = P_\pm \psi_0$ are independent of t . Thus, if we set $t = \eta x_1$, $\eta = \tanh \theta$, then we will obtain terms of the form $E\psi_{0,\pm}$ with an operator $E = E_\eta$ of the form

$$(6.2.15) \quad Eu(x) = (2\pi)^{-3/2} \int d\xi e^{ix\xi} e^{i\eta x_1 \langle \xi \rangle} u^\wedge(\xi), \quad |\eta| < 1 .$$

Again, E looks like a ψ do with symbol $e(x, \xi) = e^{i\eta x_1 \langle \xi \rangle}$. But this symbol does not even belong to ψ t since repeated ξ -differentiation brings out higher and higher powers of x_1 . Still, the operator E is well defined by the integral (6.2.15), at least for $u \in \mathcal{S}$, as easily seen⁶. Let us discuss some properties of the map E . Note, this is a scalar operator - it commutes with every constant 4×4 -matrix.

Proposition 6.2.1 *The scalar operator (formal ψ do) $E = e(x, D)$ with symbol $e(x, \xi) = e^{i\eta x_1 \langle \xi \rangle}$ may be written as*

$$(6.2.16) \quad E = F^{-1} Q \frac{1}{\varphi(x)} F ,$$

with the operator $Q : u(x) \rightarrow u(\mu(x), x_2, x_3)$, and the multiplication $u(x) \rightarrow u(x)/\varphi(x)$ where the real-valued functions μ and φ are given by

$$(6.2.17) \quad \mu(x) = \frac{1}{1 - \eta^2} (x_1 - \eta \sqrt{x_1^2 + (1 - \eta^2) \langle \tilde{x} \rangle^2}) , \quad \tilde{x} = (x_2, x_3) ,$$

and

$$(6.2.18) \quad \varphi(x_1) = 1 + \eta \frac{x_1}{\sqrt{1 + x_1^2 + \tilde{x}^2}} > 0 .$$

In other words, E is the Fourier transform of a product of a substitution Q of the independent variable x_1 and a multiplication operator $u(x) \rightarrow u(x)/\varphi(x)$.

⁶These operators still have Leibniz formulas with integral remainder, but that remainder is uncontrollable. Moreover, as another fact: While ψ do-s leave the location of singularities (of the functions they are applied to) fixed, Fourier integral operators - like E - may transport singularities elsewhere - according to interesting laws or prescriptions. Similar facts appear at $|x| = \infty$, for our type of (global) ψ do-s and the global Fourier integral operators, similar to E .

Proof. We may write the operator E in the form

$$\begin{aligned}
 (6.2.19) \quad Eu(x) &= (2\pi)^{-3/2} \int d\xi e^{i(x\xi + \eta x_1 \langle \xi \rangle)} u^\wedge(\xi) \\
 &= (2\pi)^{-3/2} \int d\tilde{\xi} e^{i\tilde{x}\tilde{\xi}} \int d\xi_1 e^{ix_1 \lambda(\xi_1, \tilde{\xi})} u^\wedge(\xi_1, \tilde{\xi}) ,
 \end{aligned}$$

where we have written $\xi = (\xi_1, \tilde{\xi})$ again, and where

$$(6.2.20) \quad \lambda(\xi) = \lambda(\xi_1, \tilde{\xi}) = (\xi_1 + \eta \sqrt{1 + \xi_1^2 + \tilde{\xi}^2}) .$$

Observe that φ of (6.2.18) equals the partial derivative $\varphi = \partial\lambda/\partial\xi_1$. Since $|\eta| < 1$ we get $\partial\lambda/\partial\xi_1 > 0$ for all ξ , and conclude that $\lambda(\xi_1, \tilde{\xi})$ is an increasing function of ξ_1 for fixed $\tilde{\xi}$. This function has an inverse function, explicitly given by μ of (6.2.17), as seen by a calculation.

The function μ clearly is a symbol in $\psi_{c_{e^2}}$, and it satisfies

$$(6.2.21) \quad \mu^{(\theta)}(\xi) = O(\langle \xi \rangle^{1-|\theta|}) .$$

Furthermore, the functions $\varphi(\xi)$ of (6.2.18) and

$$(6.2.22) \quad \nu(\xi) = \frac{1}{\varphi(\xi)} = \frac{\langle \xi \rangle}{\langle \xi \rangle + \eta\xi_1}$$

clearly belongs to ψ_{c_0} .

Now fla. (6.2.16) arises from the following trick: We get

$$\begin{aligned}
 (6.2.23) \quad E\varphi(D)u &= (e\varphi)(x, D)u \\
 &= (2\pi)^{-3/2} \int d\tilde{\xi} e^{i\tilde{x}\tilde{\xi}} \int d\xi_1 e^{ix_1 \lambda(\xi_1, \tilde{\xi})} \partial\lambda/\partial\xi_1(x_1, \tilde{\xi}) u^\wedge(\xi_1, \tilde{\xi}) .
 \end{aligned}$$

Here we may introduce λ as new integration variable, in the inner integral. With the inverse function μ of λ we then get

$$(6.2.24) \quad E\varphi(D)u = (2\pi)^{-3/2} \int d\xi e^{ix\xi} u^\wedge(\mu(\xi_1), \tilde{\xi}) = F^{-1}QFu , \quad u \in \mathcal{S} .$$

All above integral manipulations are easily verified, and we then indeed get (6.2.16) from (6.2.24), q.e.d.

The following consequences of prop.6.2.1 will be helpful.

Proposition 6.2.2 (i) *For any (possibly matrix-valued) function $f(\xi)$ of polynomial growth we have*

$$\begin{aligned}
 (6.2.25) \quad Ef(D)E^* &= f^\sim(D), \quad \text{where } f^\sim = S_c f^\Delta, \quad \text{with} \\
 f^\Delta(\xi) &= (c^2 - sc \frac{\xi_1}{\langle \xi \rangle}) f(c\xi_1 - s\langle \xi \rangle, \tilde{\xi}) .
 \end{aligned}$$

(ii) We have

$$(6.2.26) \quad E^*E = \nu(D) \quad \text{with} \quad \nu(\xi) = \frac{\langle \xi \rangle}{\langle \xi \rangle + \eta \xi_1} ,$$

again with $c = \cosh \theta$, $s = \sinh \theta$, $\eta = \tanh \theta$, and the ξ_1 -dilations $S_c : u(\xi) \rightarrow u(c\xi_1, \tilde{\xi})$.

(iii) The operator E_η , as a function of η , satisfies the differential equation

$$(6.2.27) \quad \frac{dE_\eta}{d\eta} = ix_1 E_\eta \langle D \rangle .$$

Proof. For fla.(6.2.27) we differentiate $E_\eta u(x) = (2\pi)^{-3/2} \int d\xi e^{i(x\xi + \eta x_1 \langle \xi \rangle)} u^\wedge(\xi)$ under the integral sign. For (6.2.26) use (6.2.16) - i.e., $E = F^*Q\nu F$ - , implying $E^* = F^*\nu Q^*F$ with $Q^* = \varphi Q^{-1}$, so that $E^* = F^*Q^{-1}F$ and $E^*E = F^*Q^{-1}FF^*Q\nu F = \nu(D)$. Similarly get $Ef(D)E^* = F^*Q(\nu f)Q^{-1}F = f^\sim(D)$, where a calculation yields that $f^\sim(x) = (\nu f)(\mu(x_1, \tilde{x}), \tilde{x})$ assumes the form stated in (6.2.25). Q.E.D.

Now we can approach the following result.

Theorem 6.2.3 For vanishing potentials the operator R of prop.6.1.1 commutes with the projections P_\pm , so that we have

$$(6.2.28) \quad P'_\pm = RP_\pm R^* = P_\pm .$$

Also, we have

$$(6.2.29) \quad H' = RHR^* = \cosh \theta \{H + \tanh \theta D_1\} , \quad D_1 = \frac{1}{i} \frac{\partial}{\partial x_1}$$

as transform of the total energy observable H .

For any ψ do $A \in \mathcal{P}_m$ the operator $A' = RAR^*$ belongs to \mathcal{P}_m again. For any $A \in \mathcal{PX}_m$ we also have $A' \in \mathcal{PX}_m$.

Proof. Looking at (6.2.14) we may write (with the x_1 -dilation $S_c : u(x) \rightarrow u(cx_1, \tilde{x})$ and its adjoint $S_c^* = \frac{1}{c}S_{1/c}$, where $c = \cosh \theta$)

$$(6.2.30) \quad R = \kappa S_c (E_{-\eta} P_+ + E_\eta P_-) , \quad R^* = \frac{1}{c} (P_+ E_{-\eta}^* + P_- E_\eta^*) S_{1/c} \kappa .$$

Let

$$(6.2.31) \quad A = A_{++} + A_{--} + A_{+-} + A_{-+} , \quad A_{\varepsilon\delta} = P_\varepsilon A P_\delta , \quad \varepsilon, \delta = \pm .$$

An operator A belongs to \mathcal{P}_m if and only if $A_{++}, A_{--} \in Op\psi c_m$, but $A_{+-}, A_{-+} \in \mathcal{O}(-\infty)$. It even belongs to $\mathcal{P}\mathcal{X}_m$ if also $A_{+-} = A_{-+} = 0$. Combining (6.2.30) and (6.2.31) we get

(6.2.32)

$$A' = RAR^* = \frac{1}{c} \kappa S_c \{ E_{-\eta} A_{++} E_{-\eta}^* + E_{\eta} A_{--} E_{\eta} + E_{-\eta} A_{+-} E_{\eta}^* + E_{\eta} A_{-+} E_{-\eta}^* \} S_{1/c} \kappa.$$

For $A \in \mathcal{P}\mathcal{X}$ the last two terms in the sum of 4 in (6.2.32) vanish, and only the first two must be considered. For $A \in \mathcal{P}$ we want to show that we get $E_{\eta} C E_{-\eta}^* \in \mathcal{O}(-\infty)$ for all $|\eta| < 1$ and $C \in \mathcal{O}(-\infty)$. This follows from the fact that the operator E belongs to $\mathcal{O}(0)$. That is, $E \in \cap L(\mathcal{H}_s)$ - for every s the operator E extends to a continuous operator⁷ $\mathcal{H}_s \rightarrow \mathcal{H}_s$. But E_{η} is the evolution operator of a first order symmetric hyperbolic pseudodifferential equation: Using (6.2.27) and (6.2.25),(6.2.26) we get

$$(6.2.33) \quad \frac{dE_{\eta}}{d\eta} = ix_1(E_{\eta}(\langle D \rangle \varphi(D))E_{\eta}^*)E_{\eta} = ik(\eta, x, D)E_{\eta}, \quad E_0 = 1,$$

where $k(\eta, x, \xi) = x_1(\langle \xi \rangle \varphi(\xi)) \sim$ in the sense of (6.2.25). Here the function $k(\eta, x, \xi)$ satisfies the assumptions of [Co5],VI,thm.3.1, so that, indeed, the evolution operator E_{η} is of order 0. Thus, indeed, it follows that the last two terms in (6.2.32) are in $\mathcal{O}(-\infty)$ whenever $A \in \mathcal{P}$.

We will show that the first two terms of (6.2.32) belong to ψc_m whenever $A \in Op\psi c_m$. But first now let us prove (6.2.28).

Apply fla. (6.2.25), setting $f(\xi) = p(\xi) = \frac{1}{2}(1 - (\alpha\xi + \beta)/\langle \xi \rangle)$. We get $p^{\Delta}(\xi) = (c^2 - cs \frac{\xi_1}{\langle \xi \rangle})p(c\xi_1 - s\langle \xi \rangle, \tilde{\xi}) = \frac{1}{2}(c^2 - cs \frac{\xi_1}{\langle \xi \rangle}) \{ 1 - \frac{\alpha_1(c\xi_1 - s\langle \xi \rangle) - \tilde{\alpha}\tilde{\xi} - \beta}{c\langle \xi \rangle - s\xi_1} \}$
 $= \frac{1}{2} \frac{c}{\langle \xi \rangle} \{ c\langle \xi \rangle - s\xi_1 - \alpha_1(c\xi_1 - s\langle \xi \rangle) - \tilde{\alpha}\tilde{\xi} - \beta \} = \frac{1}{2} \frac{c}{\langle \xi \rangle} \{ (c + \alpha_1 s)\langle \xi \rangle - (s + \alpha_1 c)\xi_1 - \tilde{\alpha}\tilde{\xi} - \beta \}.$

Recall from sec.6.1 that we have $c + \alpha_1 s = \kappa^{-2}$, $s + \alpha_1 c = \alpha_1 \kappa^{-2}$, and that we may write

$$(6.2.34) \quad \alpha_2 = \kappa^{-1} \alpha_2 \kappa^{-1}, \quad \alpha_3 = \kappa^{-1} \alpha_3 \kappa^{-1}, \quad \beta = \kappa^{-1} \beta \kappa^{-1}.$$

So, it follows that

$$(6.2.35) \quad \kappa p^{\Delta}(\xi) \kappa = cp(\xi).$$

Now we must look at the construction of $p(D)'$: Clearly we get $p(D) = p(D)_{++}$. So, in fla. (6.2.32), only the first term at right will appear. Formula (6.2.25) may

⁷As an alternate proof of this fact - perhaps more direct - one may use (6.2.16) again, where then F, F^* map $\mathcal{H}_{(s_1, s_2)} \rightarrow \mathcal{H}_{(s_2, s_1)}$, so that one just must show that the multiplication (by $\nu(x)$) and the substitution operator Q both map $\mathcal{H}_s \rightarrow \mathcal{H}_s$. The first is evident, since $\nu(x), \varphi(x) \in \psi c_0$. The second again may be verified, using that Q, Q^{-1} are L^2 -bounded while again thm.1.6.1 may be used on the operator $Q^{-1}\langle x \rangle^{m_2} \langle D \rangle^{m_1} Q$ to show that it belongs to $Op\psi c_m$, with corresponding $L(\mathcal{H}_s, \mathcal{H}_{s-m})$ -boundedness, according to sec.1.4.

be written as

$$(6.2.36) \quad Ep(D)E^* = F^*S_c p^\Delta(x)S_{1/c}F .$$

Furthermore note, we get $F^*S_c u(x) = (2\pi)^{-3/2} \int d\xi u(c\xi_1, \tilde{\xi})e^{ix\xi} = \frac{1}{c}(S_{1/c}Fu(x))$, and $S_{1/c}F = cFS_c$, and, $S_c^* = \frac{1}{c}S_{1/c}$. So, (6.2.36) may be written as

$$(6.2.37) \quad Ep(D)E^* = S_{1/c}p^\Delta(D)S_c = c\kappa^{-1}S_{1/c}p(D)S_c\kappa^{-1} .$$

Combining (6.2.37) with (6.2.32) - where only the first term, at right, counts, we indeed get $P' = p(D)' = Rp(D)R^* = p(D)$ - this is for $p = p_+$, while a similar argument implies $P'_- = RP_-R^* = P_-$.

Next we look at the transform of the Fourier multiplier

$$(6.2.38) \quad H = \langle D \rangle p_+(D) - \langle D \rangle p_-(D) ,$$

i.e., we seek for the observable H' corresponding to the Hamiltonian H in the old coordinates. We then get

$$(6.2.39) \quad H_{++} = \langle D \rangle p_+(D) , \quad H_{--} = -\langle D \rangle p_-(D) .$$

It is easy to get $f^\Delta(D)$ for $f(\xi) = \langle \xi \rangle p_+(\xi)$: There just is the additional (scalar) factor $\langle (c\xi_1 - s(\xi), \tilde{\xi}) \rangle = c\langle \xi \rangle - s\xi_1$ to be inserted into the result for $f = p_+$. So, we will get

$$(6.2.40) \quad H'_{++} = c\langle D \rangle p_+(D) - sD_1 p_+(D) ,$$

and similarly,

$$(6.2.41) \quad H'_{--} = -c\langle D \rangle p_-(D) + sD_1 p_-(D) .$$

However, before we put both formulas together, to form H' , we must recall, that (6.2.40) is to be used for $E = E_{-\eta}$, but (6.2.41) for $E = E_\eta$. This means that, in (6.2.40) and (6.2.41), we must replace $(c, s) = (\cosh \theta, \sinh \theta)$ by $(c, -s)$ and (c, s) , respectively. In other words, in (6.2.25) we still must replace $-s$ by s . Thus (6.2.40) and (6.2.41) imply (6.2.29).

Finally, to show that the first two terms of (6.2.32) belong to $Op\psi c_m$ whenever $A \in Op\psi c_m$, it suffices to look at the map

$$(6.2.42) \quad A \rightarrow EAE^* = F^*Q\nu(x)FAF^*\nu(x)Q^*F = F^*Q\nu(x)FAF^*Q^{-1}F ,$$

using (6.2.16) again. First of all, the map $A \rightarrow FAF^*$ takes $Op\psi c_{(m_1, m_2)}$ onto $Op\psi c_{(m_2, m_1)}$. Indeed, we get

$$(FAF^*u)(\xi) = \frac{1}{8\pi^3} \int dx e^{-ix\xi} \int d\zeta e^{ix\zeta} a(x, \zeta) d\zeta = \frac{1}{8\pi^3} \int dx \int d\zeta e^{ix(\zeta-\xi)} a(x, \zeta) u(\zeta).$$

Reorganizing the variables, we may write

$$(FAF^*u)(x) = \frac{1}{8\pi^3} \int d\xi \int dy e^{i\xi(x-y)} a(-\xi, y) u(y) .$$

Comparing this with (1.0.15) we find that

$$(6.2.43) \quad FAF^* = (a^*(-D, x))^* , \quad F^*AF = (a^*(D, -x))^* .$$

Here we see that the roles of x and ξ of the symbol $a(x, \xi)$ have been interchanged: For a symbol $a(x, \xi) \in \psi c_{(m_1, m_2)}$ the symbols $b(x, \xi) = a^*(-\xi, x)$ and $c(x, \xi) = a^*(\xi, -x)$ belong to $\psi c_{(m_2, m_1)}$. But this change $(m_1, m_2) \rightarrow (m_2, m_1)$ will be reversed by the later transform $B \rightarrow F^*BF$ occurring in our procedure.

We already noted that the function $\nu(x)$ of (6.2.22) (and its inverse $\varphi(x)$) belong to ψc_0 . Hence, the multiplication $b(x, D) \rightarrow \nu(x)b(x, D) = c(x, D)$ will preserve the property “ $b(x, D) \in Op\psi c_m$ ”. So, we are left with showing that $C \rightarrow Q C Q^{-1}$ takes $\psi c_m \rightarrow \psi c_m$. So, the question will be whether the coordinate transform $v : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ defined by $x = (x_1, \tilde{x}) \rightarrow (\mu(x_1, \tilde{x}), \tilde{x})$ will leave the classes $Op\psi c_m$ invariant.

Now, local coordinate invariance of Hoermander classes of ψ do-s is well known. For the global coordinate invariance needed here we will need thm.1.6.1 - or, equivalently, thm.3.3 of ch.IV in [Co5]. This will require the condition that the map

$$(6.2.44) \quad s \circ v \circ s^{-1} \text{ with } s(x) = \frac{x}{\langle x \rangle} , \quad s^{-1}(x) = \frac{x}{\sqrt{1-x^2}}$$

of the open unit ball $\{|x| < 1\}$ onto itself extends continuously to a diffeomorphism $\Upsilon : \{|x| \leq 1\} \rightarrow \{|x| \leq 1\}$.

To check on this condition, note, it will be equivalent to show that the inverse map, $s \circ v^{-1} \circ s^{-1}$ (where μ is replaced by λ) has this property. A calculation shows that⁸

$$(6.2.45) \quad \Upsilon^{-1}(x) = \frac{1}{\sqrt{1+\eta^2+2\eta x_1}}(x_1 + \eta, \tilde{x}) ,$$

a $C^\infty(|x| \leq 1)$ -function, indeed, since the denominator does not vanish (due to $|\eta| < 1$ and $|x_1| \leq |x| \leq 1$).

The function of (6.2.45) is invertible as map between the open balls $\{|x| < 1\}$, by construction. But its inverse also exists in the closed ball: Setting $y = (y_1, \tilde{y}) = \Upsilon^{-1}(x)$ we focus on the first of these 3 equations:

$$(6.2.46) \quad y_1 = \frac{x_1 + \eta}{\sqrt{1 + \eta^2 + \eta x_1}} .$$

⁸We get $v^{-1}(x) = (x_1 + \eta(x), \tilde{x})$ hence $(v^{-1} \circ s^{-1})(x) = (x_1 + \eta, \tilde{x})/\sqrt{1-x^2}$, using that $\langle x/\sqrt{1-x^2} \rangle = 1/\sqrt{1-x^2}$. Next we need $\langle (x_1 + \eta, \tilde{x})/\sqrt{1-x^2} \rangle = \sqrt{1+\eta^2+2\eta x_1}/\sqrt{1-x^2}$. Using this we will get (6.2.45).

The function at right is smooth and increases from -1 to $+1$, as $-1 \leq x_1 \leq 1$. Thus it has a smooth inverse $x_1 = \gamma(y_1, \eta)$ in $|y_1| \leq 1$. Substituting this we get

$$(6.2.47) \quad \tilde{x} = \sqrt{1 + \eta^2 + 2\eta\gamma(y_1, \eta)} \tilde{y} .$$

This supplies the desired smooth inverse map Υ .

Since application of κ and of the dilation S_c both leave $Op\psi c_m$ and $\mathcal{O}(-\infty)$ invariant, we then indeed get

$$(6.2.48) \quad A'_{\varepsilon, \delta} = P_\varepsilon A' P_\delta = (A_{\varepsilon\delta})' = \frac{1}{c} \kappa S_c E_{-\varepsilon\eta} A_{\varepsilon\delta} E_{-\delta\eta} S_{1/c} \kappa, \quad \varepsilon, \delta = \pm ,$$

and may conclude that $R\mathcal{P}R^* \subset \mathcal{P}$, as well as

$R\mathcal{P}\mathcal{X}R^* \subset \mathcal{P}\mathcal{X}$, completing the proof of thm.6.2.3.

Corollary 6.2.4 *In the case of vanishing potentials \mathbf{V}, \mathbf{A}_j the two algebras \mathcal{P} and $\mathcal{P}\mathcal{X}$ are left invariant by the transformation $A \rightarrow A' = RAR^*$ generated by introducing new space-time coordinates with an x_1 -boost (6.1.2).*

This is just a consequence of the symmetry of conditions - comparing (6.1.2) and (6.1.3) -, allowing application of thm.6.2.3 for the inverse Lorentz transform.

6.3 Relating Hilbert Spaces; Evolution of the Spaces H' and \tilde{H}

From now on - for the remainder of this chapter, we always will assume time-independent potentials A, V satisfying cdn.(X) - but no longer vanishing identically.

In constructing the operator R relating the spaces of physical states between different space-time-coordinates we were, so far, only relating the L^2 -spaces of the hyperplanes $t = 0$ and $t' = 0$ with each other, by a unitary operator we called R .

Let us now try the same, but with the modification that we will relate the space for $t = 0$ with the L^2 -space on the hyperplane $t' = \tau'$, with given fixed τ' - in the corresponding space-coordinates x' . Recall the boost (6.1.2) and its inverse (6.1.3).

Given a state $\psi_0(x)$ (at $t = 0$) we will extend it into \mathbb{R}^4 as solution of our Dirac equation :

$$(6.3.1) \quad \psi(t, x) = (e^{-iHt} \psi_0)(x) .$$

Introducing the new space-time coordinates t', x' we then get

$$(6.3.2) \quad \tilde{\psi}(t', x') = \psi(t'c + x'_1s, t's + x'_1c, \tilde{x}') .$$

Here we now set $t' = \tau'$ = a given fixed constant:

$$(6.3.3) \quad \check{\psi}(x') = \check{\psi}(x'_1, \tilde{x}') = \psi(\tau'c + x'_1s, \tau's + x'_1c, \tilde{x}') .$$

This again is a function of (x'_1, \tilde{x}') . To normalize it and create a state in $L^2(\{x' \in \mathbb{R}^3\})$ we will have to multiply it by the constant matrix $\kappa = \cosh(\theta/2) - \alpha_1 \sinh(\theta/2)$ again, creating $\psi'(x') = \kappa\check{\psi}(x')$.

Repeating the construction of $R\psi$ in sec.6.1, let us write

$$(6.3.4) \quad \psi^\diamond(x_1, \tilde{x}) = \psi(\tau'/c + \eta x_1, x) ,$$

with $\eta = \tanh\theta = s/c$, and with the function $\psi(t, x)$ of (6.3.1). Then we get

$$(6.3.5) \quad R^{\tau'}\psi_0(x') = \psi'_0(x') = \kappa\psi^\diamond(x'_1c + \tau's, \tilde{x}') ,$$

defining a unitary operator $R^{\tau'}$ relating the initial states $t = 0$ and $t' = \tau'$.

The question now is whether R and R^τ can be related, using the families e^{-iHt} and $U_{\tilde{H}}(\tau, t)$ - evolution operator of the Dirac equation with the coordinate transformed Hamiltonian \tilde{H} . Note, we have

$$(6.3.6) \quad \psi'(t', x') = (U_{\tilde{H}}(0, t')R\psi_0)(x') = \kappa\tilde{\psi}(t', x') = \kappa\psi(t'c + sx'_1, x'_1c + st', \tilde{x}') .$$

On the other hand, we get

$$(6.3.7) \quad (Re^{-iH\tau'/c}\psi_0)(x') = \kappa S_c\psi(\tau'/c + \eta x'_1, x'_1, \tilde{x}') = \kappa\psi(\tau'/c + sx'_1, cx'_1, \tilde{x}') .$$

Onto (6.3.7) we apply a translation $T_\lambda : u(x) \rightarrow u(x_1 + \lambda, \tilde{x})$ (with $\lambda = \eta\tau'$) for

$$(6.3.8) \quad \begin{aligned} (T_\lambda Re^{-iH\tau'/c}\psi_0)(x') &= \kappa\psi(\tau'/c + s(x'_1 + \lambda), c(x'_1 + \lambda), \tilde{x}') \\ &= \kappa\psi(\tau'c + sx_1, cx'_1 + s\tau' .\tilde{x}') , \end{aligned}$$

using that $c\eta = s$ and $1 + s^2 = c^2$. Comparing (6.3.8) with (6.3.6) - where we set $t' = \tau'$, we get

$$(6.3.9) \quad R^{\tau'}\psi_0(x') = (U_{\tilde{H}}(0, \tau')R\psi_0)(x') = (T_{\eta\tau'}Re^{-iH\tau'/c}\psi_0)(x') ,$$

where also (6.3.2),(6.3.3) and (6.3.5) were involved. This gives an interesting relation between evolution operators, as an immediate consequence of (6.3.9):

Proposition 6.3.1 *The evolutions $U_{\tilde{H}}$ and $e^{-iH't}$ with $H' = RHR^*$ are related by the formula*

$$(6.3.10) \quad U_{\tilde{H}}(0, t) = T_{\eta t}Re^{-iHt/c}R^* = T_{\eta t}e^{-iH't/c} .$$

Note, this gives the occasion for a check: For $\mathbf{V} = \mathbf{A}_j = 0$ we obtained the formula

$$(6.3.11) \quad H' = c(H + \eta D_{x_1})$$

(cf.(6.2.29)). The terms at right of (6.3.11) commute - they are $f(D)$ -s - hence (6.3.10) implies

$$(6.3.12) \quad U_{\tilde{H}}(0, t) = T_{\eta t} e^{-iHt} e^{-i\eta t D_{x_1}} .$$

But the operator $e^{-i\eta t D_{x_1}}$ equals the translation $T_{-\eta t} : u(x) \rightarrow u(x_1 - \eta t, \tilde{x})$, inverting $T_{\eta t}$ occurring in (6.3.12). Accordingly we have

$$(6.3.13) \quad U_{\tilde{H}}(0, t) = e^{-iHt} ,$$

as it should be for vanishing potentials. - The test checks.

In connection with prop.6.3.1 we will go back to sec.6.1, for the following observation.

Remark 6.3.2 *Our potentials - in the old coordinates - did not depend on t , by assumption. This has the effect that V', A'_j of (6.1.11) only depend on the 3 variables $x'_1 + \eta t', \tilde{x}' = (x'_2, x'_3)$. Introducing the "translation operator" $T_{\eta t} : u(x) \rightarrow u(x_1 + \eta t, \tilde{x})$, we may write*

$$(6.3.14) \quad (V', A')(t', x') = T_{\eta t'}(V^\diamond, A^\diamond) ,$$

where now the potentials

$$(6.3.15) \quad (V^\diamond, A^\diamond)(x') = (Vc - A_1s, A_1c - Vs, A_2, A_3)(cx'_1, x'_2, x'_3)$$

depend only on x' , no longer on t' . In particular, the multiplication operator $u(x) \rightarrow V^\sim(t, x)u(x)$ may be written as $V^\sim = T_{\eta t} V^\diamond T_{-\eta t}$, where now V^\diamond is independent of t . Similarly for A^\sim and A^\diamond .

However, the translation operator $T_{\eta t}$ commutes with every x -differentiation and constant matrix. Looking at (6.1.2), we thus get

$$(6.3.16) \quad \tilde{H}(t) = T_{\eta t} H^\diamond T_{-\eta t} , \quad \text{with} \quad H^\diamond = \sum_j \alpha_j (D_j - A_j^\diamond) + \beta + V .$$

Again, let us emphasize, that the operator H^\diamond - formally, a Dirac operator - is time-independent.

One finds that the relation (6.3.10) between the evolution operators of $\tilde{H}(t)$ of (6.1.14) and $H' = RAR^*$ also implies a relation between $\tilde{H}(t)$ and H' .

Proposition 6.3.3 *We have*⁹

$$(6.3.17) \quad H' = RHR^* = c(H^\diamond + \eta D_{x_1}) = c(T_{-\eta t} \tilde{H} T_{\eta t} + \eta D_{x_1}) ,$$

with the (time-independent) operator H^\diamond of (6.3.16).

Proof. We have $(T_{\eta t}u)(x) = u(x_1 + \eta t, \tilde{x})$, hence $\partial_t(T_{\eta t}u) = \eta u_{|x_1}(x_1 + \eta t, \tilde{x}) \Rightarrow \dot{T}_{\eta t} = \eta T_{\eta t} \partial_{x_1}$. Differentiating (6.3.10) for t we get $-i\dot{\tilde{H}}(t)T_{\eta t}e^{-iH't/c} = \dot{U}_{\tilde{H}}(0, t) = \partial_t(T_{\eta t}e^{-iH't/c}) = \eta T_{\eta t} \partial_{x_1} e^{-iH't/c} - \frac{i}{c} T_{\eta t} H' e^{-iH't/c}$.

Multiply left by $iT_{-\eta t}$ and right by $e^{iH't/c}$ for $T_{-\eta t} \tilde{H} T_{\eta t} = i\eta \partial_{x_1} + \frac{1}{c} H'$, implying (6.3.17), in view of (6.3.16). Q.E.D.

Finally, as a generalization of prop.6.3.1 useful for considering the algebras $\mathcal{P}'(\tau)$, $\mathcal{P}\mathcal{X}'(\tau)$:

Proposition 6.3.4 *The evolution operator $U_{\tilde{H}}(\tau, t)$, for a general initial point τ , is given by the formula*

$$(6.3.18) \quad U_{\tilde{H}}(\tau, t) = T_{\eta t} e^{-iH'(t-\tau)/c} T_{-\eta\tau} \text{ with } H' = c(H^\diamond + \eta D_{x_1}) .$$

This follows easily, using that $\tilde{H}(t + \tau) = T_{\eta\tau} \tilde{H}(t) T_{-\eta\tau}$, by (6.3.16).

6.4 The General Time-Independent Case

Suppose now, we have a Dirac Hamiltonian $H = \alpha(D - \mathbf{A}) + \mathbf{V}$ with general (time-independent) potentials \mathbf{V} , \mathbf{A} satisfying cdn.(X). We then have a decoupling unitary ψ do $U \in Op\psi c_0$, in the sense of sec.3.5 such that¹⁰

$$(6.4.1) \quad H = U \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix} U^* , \text{ where } X = \langle D \rangle + X_1 , Y = -\langle D \rangle + Y_1 , X_1, Y_1 \in Op\psi c_{-e^2} .$$

We also have the operator R of sec.6.1, and the operator $H' = RHR^*$, explicitly related to the transformed Hamiltonian \tilde{H} by fla. (6.3.17). Since H' is time-independent and also has a somewhat modified standard Dirac Hamiltonian form

⁹We should observe that one might feel tempted to apply the Baker-Campbell-Hausdorff formula onto (6.3.9), observing that $T_{\eta t} = e^{i\eta t D_{x_1}}$, in order to get a representation of the operator $U_{\tilde{H}}(t)$: Formally, we get $e^{At} . e^{Bt} = e^{C(t)}$ with a power series $C(t) = C_1 t + C_2 t^2 + \dots$, where $C_1 = A + B$ and C_j is a combination of iterated commutators of A and B - of order j . With our special operators $A = i\eta D_{x_1}$, $B = iH'$ these commutators will be of lower and lower order, and the formal infinite series $C(t)$ will converge asymptotically, resulting in a corresponding asymptotic expansion for $U_{\tilde{H}}(t)$.

¹⁰Here we refer to a split $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ with \mathcal{H}_\pm coinciding with $L^2(\mathbb{R}^3, \mathbb{C}^2)$, except that a finite dimensional space \mathcal{Z} of rapidly decreasing functions may have been shifted from “+” to “-” (or “-” to “+”) (cf.sec.3.5).

we might as well also ask whether H' may be decoupled by a unitary ψ do. Trivially we have

$$(6.4.2) \quad (RU)^* H' (RU) = H^\Delta = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix}.$$

However, this is **NOT** a decoupling of the transformed Dirac equation in the sense of ch.3, because the new unitary operator RU is not a ψ do in $Op\psi c_0$.

On the other hand, we shall see that (6.4.2) may be modified, using another (decoupled) unitary operator $Z = \begin{pmatrix} Z_- & 0 \\ 0 & Z_+ \end{pmatrix}$, again not a ψ do, such that

$$(6.4.3) \quad (RUZ)^* H' (RUZ) = \begin{pmatrix} \check{X} & 0 \\ 0 & \check{Y} \end{pmatrix}, \text{ with } \check{X} = Z_-^* X Z_- , \check{Y} = Z_+^* Y Z_+ ,$$

where now

$$(6.4.4) \quad \check{X} = c(\langle D \rangle + \eta D_{x_1}) \text{ mod } (Op\psi c_{-e^2}) , \check{Y} = c(-\langle D \rangle + \eta D_{x_1}) \text{ mod } (Op\psi c_{-e^2}) ,$$

are ψ do-s in $Op\psi c_{e_1}$, while also $U^\diamond = RUZ \in Op\psi c_0$, and

$$(6.4.5) \quad U^\diamond = U_0 \text{ mod } (Op\psi c_{-e}) ,$$

with the operator $U_0 = u_0(D)$ of¹¹ sec.3.1.

The task of getting the above operator Z will encounter considerable technical difficulties (cf. sec's 6.5 and 6.7). Even though decoupling H' by a unitary ψ do does not mean that we have decoupled the (now time dependent) Dirac equation $\dot{u} + i\tilde{H}(t)u = 0$, this still will help us to accomplish the latter task for the following reason.

In decoupling equ. $\dot{u} + iH^\sim(t)u = 0$ we look for a unitary map - call it $V(t)$ here - such that the substitution $u(t) = V(t)v(t)$ brings forth

$$(6.4.6) \quad \dot{v} + iH^\Delta(t)v = 0 \text{ with } H^\Delta(t) = V^* H V - iV^* \dot{V} ,$$

where now $H^\Delta = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix}$ is decoupled.

Writing $v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$, equation (6.4.6) then splits into the 2 completely separate equations

$$(6.4.7) \quad \dot{v}_1 + iX(t)v_1 = 0 , \dot{v}_2 + iY(t)v_2 = 0 .$$

Each of these two equations has its own evolution operator - we call them $A(t)$ and $B(t)$, resp. Then the evolution operator $U_{H^\Delta}(t)$ will be decoupled:

$$(6.4.8) \quad U_{H^\Delta}(t) = \begin{pmatrix} A(t) & 0 \\ 0 & B(t) \end{pmatrix}.$$

¹¹it really is u of (3.1.5).

Now, the initial-value problem at $t = 0$ for (6.4.6) is solved by $v(t) = U_{H^\Delta}(t)v(0)$. So, then, the initial-value problem for $H^\sim(t)$ will be solved by $u(t) = V(t)v(t) = V(t)U_{H^\Delta}(t)v(0) = V(t)U_{H^\Delta}(t)V^*(0)u(0)$, implying $U_{H^\sim}(t) = V^*(t)U_{H^\Delta}(t)V(0)$. Or, in other words, for a unitary operator decoupling H^\sim , in the above sense, we have

$$(6.4.9) \quad V^*(t)U_{H^\sim}(t)V(0) = \begin{pmatrix} A(t) & 0 \\ 0 & B(t) \end{pmatrix}.$$

Now, in our case, we have $U_{H^\sim}(t) = T_{\eta t}e^{-iH^\sim t/c}$. And, we already decoupled $e^{-iH^\sim t/c}$ by a (time-independent) operator we called U° . Notice, we may just set $V(t) = T_{\eta t}U^\circ$. Then $V^*(t) = U^{\circ*}T_{-\eta t}$, and we get (6.4.9) satisfied with $A(t) = e^{-iX^\circ t/c}$ and $B(t) = e^{-iY^\circ t/c}$.

But, clearly, this $V(t)$ is no longer a strictly classical ψ do - except for $t\eta = 0$, since it contains the translating factor $T_{\eta t}$.

On the other hand, it again turns out that we may compensate for this by using the unitary operator $U^\circ(t) = V(t)T_{-\eta t} = T_{\eta t}U^\circ T_{-\eta t}$ instead of $V(t)$. The additional conjugation of H^Δ with the translation $T_{-\eta t}$ does not “undecouple” H^Δ and will give us the desired ψ do decoupling eq. (6.1.13).

Also, we note:

Since the transformed Hamiltonian $\tilde{H}(t)$ is time-dependent, we should expect the corresponding algebra $\tilde{\mathcal{P}}$ of sec.5.2 to depend on the initial point τ . This indeed will be confirmed: While the algebra \mathcal{P}' is independent of t , we will get $\tilde{\mathcal{P}}(\tau) = T_{\eta\tau}\mathcal{P}'T_{-\eta\tau}$.

Incidentally, while the algebra $\mathcal{P}\mathcal{X}$ was defined so far only for time-independent potentials - since only then we have results like sec.3.5 - we well may define algebras $\mathcal{P}\mathcal{X}^\sim(\tau)$ for the present (time-dependent) $\tilde{H}(t)$. Then, again, we have $\mathcal{P}\mathcal{X}^\sim(\tau) = T_{\eta\tau}\mathcal{P}\mathcal{X}'T_{-\eta\tau}$ as we shall see.

Let us summarize and state the following.

Theorem 6.4.1 *After a Lorentz transform in the form of an x_1 -boost of the form (6.0.2) we may consider the Hilbert space \mathcal{H} of physical states transformed by the unitary operator R of prop.6.1.1: A state $\psi \in \mathcal{H}$ transforms into the state $\psi' = R\psi$. An observable A (acting on a subspace of \mathcal{H}) transforms into $A' = RAR^*$.*

The Dirac equation may be transformed onto the new coordinates in two different ways:

(i) *By substitution of independent variables (6.0.2) (together with left-multiplying the dependent variable with the constant matrix κ of (6.1.12)) we get*

$$(6.4.10) \quad \dot{\psi} + iH^\sim\psi = 0, \quad \psi = \psi_0 \text{ at } t' = 0, \quad \text{with}$$

(6.4.11)

$$(\mathbf{V}^\sim, \mathbf{A}_1^\sim, \mathbf{A}_2^\sim, \mathbf{A}_3^\sim)(t', x') = (\mathbf{V}c - \mathbf{A}_1s, \mathbf{A}_1c - \mathbf{V}s, \mathbf{A}_2, \mathbf{A}_3)(x'_1c + t's, x'_2, x'_3) .$$

(ii) By just introducing $\psi' = R\psi$ as new dependent variable we get

$$(6.4.12) \quad \dot{\psi} + iH'\psi = 0, \quad \psi = \psi_0 \text{ at } t = 0, \quad \text{with } H' = RAR^*,$$

where we found that (the time-independent) operator H' has the form

$$(6.4.13) \quad H' = c(H^\diamond + \eta D_{x_1}) \text{ with } H^\diamond = \alpha(D - \mathbf{A}^\diamond) + \beta + \mathbf{V},$$

with potentials

(6.4.14)

$$(\mathbf{V}^\diamond, \mathbf{A}_1^\diamond, \mathbf{A}_2^\diamond, \mathbf{A}_3^\diamond)(t, x) = (\mathbf{V}c - \mathbf{A}_1s, \mathbf{A}_1c - \mathbf{V}s, \mathbf{A}_2, \mathbf{A}_3)(cx_1, x_2, x_3) .$$

The two initial value problems of (6.4.10) and (6.4.12) are solved (respectively) by $\psi = U_{H^\sim}(t)\psi_0$, $U_{H^\sim}(t) = U_{H^\sim}(0, t)$, and by $\psi = e^{-iH't}\psi_0$, where we have

$$(6.4.15) \quad U_{H^\sim}(t) = T_{\eta t} e^{-iH't/c} .$$

For each of these initial-value problems there exists a unitary strictly classical ψ do of order 0 [called $U^\circ(t)$ and U^\diamond , respectively] decoupling the equation [(6.4.10) or (6.4.13), resp.].

Moreover then, our transformed algebras $\mathcal{P}' = R\mathcal{P}R^*$ and $\mathcal{P}\mathcal{X}' = R\mathcal{P}\mathcal{X}R^*$ may be characterized as the classes of strictly classical ψ do-s A with $P'AQ', Q'AP' \in \mathcal{O}(-\infty)$, (or = 0, resp.), where

$$(6.4.16) \quad P' = U^\diamond \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} U^{\diamond*}, \quad Q' = U^\diamond \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} U^{\diamond*} .$$

In other words, \mathcal{P}' and $\mathcal{P}\mathcal{X}'$ consist of all ψ do-s in $Op\psi c$ which are decoupled mod($\mathcal{O}(-\infty)$) or strictly decoupled by conjugation with the unitary ψ do $U^\diamond \in Op\psi c_0$, respectively.

On the other hand, the operator $U^\circ(t) \in Op\psi c_0$ decoupling the (time-dependent) transformed Dirac equation (6.4.10) is given by

$$(6.4.17) \quad U^\circ(t) = T_{\eta t} U^\diamond T_{-\eta t} .$$

The family of algebras $\tilde{\mathcal{P}}(\tau)$ defined (as in sec.5.2 but) for the transformed Dirac equation (6.4.10) is given by

$$(6.4.18) \quad \tilde{\mathcal{P}}(\tau) = T_{\eta\tau} \mathcal{P}' = \{A \in Op\psi c : T_{-\eta\tau} A T_{\eta\tau} \in \mathcal{P}'\} .$$

Then $\tilde{\mathcal{P}}(\tau)$ consists precisely of all $A \in Op\psi c$ with $P^\circ(\tau)AQ^\circ(\tau), Q^\circ(\tau)AP^\circ(\tau) \in \mathcal{O}(-\infty)$, where

$$(6.4.19) \quad P^\circ(t) = U^\circ(t) \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} U^{\circ*}(t) , \quad Q^\circ(t) = U^\circ(t) \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} U^{\circ*}(t) .$$

Moreover, since $U^\circ(t)$ represents a precise decoupling of (6.4.10) we also may define algebras $\mathcal{P}\mathcal{X}^\sim(\tau)$ by setting

$$(6.4.20) \quad \mathcal{P}\mathcal{X}^\sim(\tau) = \{A \in Op\psi c : P^\circ(\tau)AQ^\circ(\tau) = Q^\circ(\tau)AP^\circ(\tau) = 0\} .$$

These algebras then are transforms of $\mathcal{P}\mathcal{X}$ - of the (given time-independent) Dirac equation, in the sense that

$$(6.4.21) \quad \mathcal{P}\mathcal{X}^\sim(\tau) = \{A \in Op\psi c : R^*T_{-\eta\tau}AT_{\eta\tau}R \in \mathcal{P}\mathcal{X}\} .$$

Only the statements (6.4.15) through (6.4.21) remain to be verified. This will require some efforts to be accomplished in sec.6.6, after a more careful study of the operator R in sec.6.5.

6.5 The Fourier Integral Operators around R

While (so far, in earlier chapters) we always tended to avoid an explicit discussion of the operator e^{-iHt} , or the more general evolution operator $U_H(\tau, t)$ in the time-dependent case, it already was necessary to consider an explicit representation of our Fourier integral operator R in sec.6.2, in the case of vanishing fields. In the present section we will tend to achieve similar results for more general fields - still time-independent. Again R will be seen to be a Fourier integral operator. Again, however, we will not involve results about composition of general Fourier integral operators.

Note, our operator U of (6.4.1) is of the form

$$(6.5.1) \quad U = U_0 + U_1 , \quad U_0 = u_0(D) , \quad U_1 \in Op\psi c_{-e} , \quad u_0(\xi) = \frac{1}{\sqrt{2 + 2s_0}}(1 + s_0 - \beta\alpha s) ,$$

where $s_0 = 1/\langle \xi \rangle$, $s = \xi/\langle \xi \rangle$ [cf. thm.3.2.2 - combined with an additional term of $\mathcal{O}(-\infty)$, as seen in sec.3.5].

Let $P = U \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} U^*$, $Q = U \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} U^*$, and, $P_0 = U_0 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} U_0^*$, $Q_0 = U_0 \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} U_0^*$, the latter with the splitting $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^2) \oplus L^2(\mathbb{R}^3, \mathbb{C}^2)$ corresponding to the fieldless $H_0 = \alpha D + \beta$. Then P_0, Q_0 are the projections of the fieldless Hamiltonian H_0 while P, Q are the analogous splitting projections corresponding to our present H (with fields). Clearly we have

$$(6.5.2) \quad P = P_0 + P_1 , \quad Q = Q_0 + Q_1 , \quad \text{with } P_1, Q_1, \in Op\psi c_{-e} .$$

Our relation (6.2.12) of the fieldfree case may be set up again here, we get

$$(6.5.3) \quad e^{-iHt} = e^{-iH_+t}P + e^{-iH_-t}Q, \quad H_+ = U \begin{pmatrix} X & 0 \\ 0 & 0 \end{pmatrix} U^*, \quad H_- = U \begin{pmatrix} 0 & 0 \\ 0 & Y \end{pmatrix} U^*,$$

where $X = \langle D \rangle + X_1$, $Y = -\langle D \rangle + Y_1$, $X_1, Y_1 \in \text{Op}\psi c_{-e^2}$. Using the expansions (6.5.1),(6.5.2) we may write $H_+ = U_0 \langle D \rangle \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} U_0^* + H_{1+}$ with $H_{1+} \in \text{Op}\psi c_{-e^2}$. Also, $U_0 = u_0(D)$ commutes with $\langle D \rangle$, so that we get $H_+ = \langle D \rangle P_0 + H_{1+}$. Similary for H_- : We get

$$(6.5.4) \quad H_+ = \langle D \rangle P_0 + H_{1+}, \quad H_- = -\langle D \rangle Q_0 + H_{1-}, \quad H_{1\pm} \in \text{Op}\psi c_{-e^2}.$$

Construction of our operator R (now with fields) again will start along the diagram (6.2.14): Given an initial state ψ_0 get $\psi(t, x) = (e^{-iHt}\psi_0)(x)$, using (6.5.3): $\psi = \psi_+ + \psi_- = e^{-iH_+t}P\psi_0 + e^{-iH_-t}Q\psi_0$, and then look at $\psi_{\pm}(\eta x_1, x)$. Here H_{\pm}, P, Q, ψ_0 are independent of t . We focus on the term with e^{-iH_+t} and look at

$$(6.5.5) \quad S(t) = e^{i\langle D \rangle t} e^{-iH_+t} P = e^{i\langle D \rangle t} e^{-i(\langle D \rangle P_0 + H_{1+})t} P,$$

hoping to show that $S(t)$ is a ψ do.

We get $S(0) = P$. Noting that P and e^{-itH_+} commute, we differentiate for t and get

$$(6.5.6) \quad \dot{S}(t) = -iK(t)S(t) \text{ where } K(t) = e^{i\langle D \rangle t}(H_{1+} + \langle D \rangle(P_0 - P))e^{-i\langle D \rangle t}.$$

Now an important observation: The operator $K(t)$ is a ψ do in $\text{Op}\psi c_{-e^2}$ - using [Co5],VI, thm.5.1. We even know the symbol $k(t, x, \xi)$ of $K(t)$, up to lower order terms: The conjugation $a(x, D) \rightarrow e^{i\langle D \rangle t} a(x, D) e^{-i\langle D \rangle t}$ generates the Hamiltonian system

$$(6.5.7) \quad \dot{x} = \langle \xi \rangle|_{\xi} = \frac{\xi}{\langle \xi \rangle}, \quad \dot{\xi} = \langle \xi \rangle|_x = 0,$$

with flow

$$(6.5.8) \quad x = x^0 + t \frac{\xi^0}{\langle \xi^0 \rangle}, \quad \xi = \xi^0 = \text{const.}$$

Thus the symbol $k(t, x, \xi)$ will be of the form

$$(6.5.9) \quad k(t, x, \xi) = k_0(x + t\xi/\langle \xi \rangle, \xi) + k_1(t, x, \xi),$$

where

$$(6.5.10) \quad k_0(t, x, D) = H_{1+} + \langle D \rangle(P_0 - P), \quad k_1 \in \psi c_{-e-e^2}.$$

It is clear thus that $S(t)$ describes an evolution

$$(6.5.11)$$

$$\dot{S}(t) + ik(t, x, D)S(t) = 0, \quad S(0) = P = p(x, D), \quad \text{where } k(t, x, \xi) \in \psi c_{-e^2}.$$

Proposition 6.5.1 $S(t)$ is a ψ do $\in Op\psi c_0$.

This proposition is an immediate consequence¹² of thm.1.5.4.

Next we observe that (6.5.3) may be written as

$$(6.5.12) \quad e^{-iHt} = S^*(-t)e^{-i\langle D \rangle t}P + S_-^*(-t)e^{i\langle D \rangle t}Q,$$

whith another ψ do $S_-(t) = e^{-i\langle D \rangle t}e^{-iH-t}Q$ with properties¹³ similar to $S(t)$. Let $S^*(-t) = s(t, x, D)$, and $S_-^*(-t) = s_-(t, x, D)$, and $\psi_{0+} = P\psi_0$, $\psi_{0-} = Q\psi_0$. Setting $t = \eta x_1$ in the first term at right of (6.5.12) we get

$$(6.5.13) \quad \begin{aligned} & (S^*(-t)e^{-i\langle D \rangle t}P\psi_0)(x)|_{t=\eta x_1} \\ &= (2\pi)^{-3/2} \int d\xi e^{ix\xi} s(\eta x_1, x, \xi) \{(e^{-i\langle D \rangle t}\psi_{0+})^\wedge(\xi)\}|_{t=\eta x_1} \\ &= (2\pi)^{-3/2} \int d\xi s(\eta x_1, x, \xi) e^{i(x\xi - \eta x_1 \langle \xi \rangle)} \psi_{0+}^\wedge(\xi) \\ &= (2\pi)^{-3/2} \int d\xi s(\eta x_1, x, \xi) e^{i(\tilde{x}\tilde{\xi} + x_1(\xi_1 - \eta \langle \xi \rangle))} \psi_{0+}^\wedge(\xi). \end{aligned}$$

We again find the function $\lambda(\xi) = \xi_1 + \eta \langle \xi \rangle$ of (6.2.20) in the exponent of the last term [with η replaced by $-\eta$], hence again might try the substitution of integration variable $\xi_1 = \mu(\zeta_1)$, $\tilde{\xi} = \tilde{\zeta}$ to arrive at

$$(6.5.14) \quad \begin{aligned} R\psi_0 &= (2\pi)^{-3/2} \kappa S_c \int d\xi e^{ix\xi} s(\eta x_1, x, \nu_{-\eta}(\xi)) (\nu_{-\eta}\psi_{0+}^\wedge)(\nu_{-\eta}(\xi)) \\ &+ (2\pi)^{-3/2} \kappa S_c \int d\xi e^{ix\xi} s_-(\eta x_1, x, \nu_\eta(\xi)) (\nu_\eta\psi_{0-}^\wedge)(\nu_\eta(\xi)), \end{aligned}$$

where we used κ of (6.1.12) and $S_c : u(x) \rightarrow u(cx_1, \tilde{x})$ of (6.2.25), and the functions $\mu(x), \nu(x) = 1/\varphi(x)$ of (6.2.17), (6.2.18), (6.2.22) (and $\nu(x) = (\mu(x), \tilde{x})$), calling them $\mu_\eta, \nu_\eta, \nu_\eta$, since they are used for η and $-\eta$.

¹²Recall, we used “the parametrix method”: Substitute a symbol $s(t, x, D)$ into (6.5.11) and neglect all “lower order terms”. Solve the corresponding ODE, and show the solution is a symbol $s_0(x, \xi)$. Start an iteration by going into the equation with $s = s_0 + w$ with w of lower order. Again solve the resulting ODE, etc. Take the asymptotic sum $s = s_0 + w + \dots$ and show it solves (6.5.12) mod $\mathcal{O}(-\infty)$. Then, finally, use Picard’s successive approximation for an ODE with coefficient in $\mathcal{O}(-\infty)$ to obtain a “clean” solution of (6.5.11).

¹³The arguments while analyzing $S(t)$ may be exactly repeated.

Note, we may re-express fla.(6.5.14) writing

$$(6.5.14') \quad R\psi_0 = \kappa S_c k_+(\eta, x, D)E_{-\eta}P\psi_0 + \kappa S_c k_-(\eta, x, D)E_{\eta}Q\psi_0 ,$$

with the (formal) symbols

$$k_+(\eta, x, \xi) = s(\eta x_1, x, v_{-\eta}(\xi)) , \quad k_-(\eta, x, \xi) = s_-(\eta x_1, x, v_{\eta}(\xi)).$$

Formula (6.5.14') may be compared with (6.2.30) with $E_{\pm\eta}$ of (6.2.16), in the fieldless case. This, however, can be useful for us only if we are able to prove a symbol property for the terms $s(\eta x_1, x, \xi)$, $s_-(\eta x_1, x, \xi)$. We indeed will achieve this, but using a different approach.

Proposition 6.5.2 *Consider the operator $V = V_{\eta}$ defined by*

$$(6.5.15) \quad V_{\eta}\psi_0(x) = \{e^{-iH_+t}\psi_0\}(x)|_{t=\eta x_1} , \quad \psi_0 \in \mathcal{S} .$$

This operator solves the evolution initial-value problem

$$(6.5.16) \quad \frac{dV_{\eta}}{d\eta} + ix_1 V_{\eta} H_+ = 0 , \quad V_0 = 1 .$$

Proof. First consider $\psi_+(t, x) = e^{-iH_+t}\psi_0$. We get $\dot{\psi}_+(t, x) = -ie^{-iH_+t}\omega_0$ with (time-independent) $\omega_0 = H_+\psi_0$, and $V_{\eta}\psi_0(x) = \psi_+(\eta x_1, x)$, so that

$$(6.5.17) \quad \begin{aligned} \frac{\partial}{\partial \eta} V_{\eta}\psi_0 &= x_1 \dot{\psi}(\eta x_1, x) = -ix_1 \{e^{-iH_+t}\omega_0\}|_{t=\eta x_1} \\ &= -ix_1 (V_{\eta}\omega_0)(x) = -ix_1 (V_{\eta}H_+\psi_0)(x) , \end{aligned}$$

confirming the differential equation (6.5.16). The initial condition follows trivially. Q.E.D.

At this time let us recall the (scalar) operator E_{η} of (6.2.15). Recall, that we control this operator explicitly, using prop.6.2.1 and prop.6.2.2.

Let us introduce the operator $W_{\eta} = V_{\eta}PE_{-\eta}^*$. Differentiating for η (using fla.-s (6.5.16) and (6.2.27)) we get

$$(6.5.18) \quad \frac{dW_{\eta}}{d\eta} = -ix_1 V_{\eta}PH_+E_{-\eta}^* + iV_{\eta}P\langle D \rangle E_{-\eta}^* x_1 .$$

With $H_+ = \langle D \rangle P_0 + H_{1+}$, by (6.5.4), and $P^2 = P$, write $PH_+ = PP_0\langle D \rangle + PH_+ = P\langle D \rangle + P((P_0 - P)\langle D \rangle + H_{1+}) = P\langle D \rangle + PH_{2+}$, where $H_{2+} = (P_0 - P)\langle D \rangle + H_{1+} \in Op\psi c_{-\epsilon^2}$, this assumes the form

$$(6.5.19) \quad \frac{dW_{\eta}}{d\eta} + i[x_1, V_{\eta}P\langle D \rangle E_{-\eta}^*] = -ix_1 V_{\eta}PH_{2+}E_{-\eta}^* , \quad H_{2+} \in Op\psi c_{-\epsilon^2} .$$

From (6.2.26) we get

$$(6.5.20) \quad E_{-\eta}^* E_{-\eta} \varphi(D) = 1 \quad \text{with} \quad \varphi(\xi) = 1 - \eta \xi_1 / \langle \xi \rangle .$$

Substituting this into (6.5.19) we get

$$(6.5.21) \quad \frac{dW_\eta}{d\eta} + i[x_1, W_\eta(E_{-\eta} \langle D \rangle \varphi(D) E_{-\eta}^*)] = -ix_1 W_\eta(E_{-\eta} \varphi(D) H_{2+} E_{-\eta}^*) .$$

In this ODE for the operator function W_η , $|\eta| < 1$, all coefficients are ψ do-s. Specifically, we have

$$(6.5.22) \quad x_1 \in Op\psi c_{e^2}, \quad E_{-\eta} \langle D \rangle \varphi(D) E_{-\eta}^* \in Op\psi c_{e^1}, \quad E_{-\eta} \varphi(D) H_{2+} E_{-\eta}^* \in Op\psi c_{-e^2} .$$

Moreover, the first two (occurring in the commutator of (6.5.21)) are scalars; we even have $E_{-\eta} \langle D \rangle \varphi(D) E_{-\eta}^* = f^\sim(D)$ with the f^\sim for $f(x) = \langle x \rangle \varphi(x)$ of (6.2.25)¹⁴. For the last term in (6.5.22) we must apply thm.5.1 of [Co5], VI again.

Proposition 6.5.3 *The unique solution W_η of the ODE (6.5.21) with initial value $W_0 = P$ also takes values in $Op\psi c_0$.*

The proof again uses the parametrix method, but it is more complicated, since certain first order linear systems of PDE-s must be examined, regarding their preservation of symbol properties. We shall discuss it in sec.6.7.

It should be clear that there is an analogous discussion for the operator V_η^- defined by

$$(6.5.23) \quad V_\eta^- \psi(x) = \{e^{-iH-t\psi(x)}\}|_{t=\eta x_1} ,$$

leading to the construction of $W_\eta^- = V_\eta^- Q E_\eta^* \in Op\psi c_0$. Assuming this we get the following:

Theorem 6.5.4 *The operators $V_\eta P$, $V_\eta^- Q$ of (6.5.15), (6.5.23) may be written as*

$$(6.5.24) \quad V_\eta P = V_\eta P E_{-\eta}^* \varphi(D) E_{-\eta} = (W_\eta \varphi(D)) E_{-\eta} \quad \text{and} \quad V_\eta^- = V_\eta^- = (W_\eta^- (E_\eta \varphi(D)) E_\eta ,$$

where the expressions $W_\eta \varphi(D)$ and $W_\eta^- \varphi(D)$ belong to $Op\psi c_0$.

¹⁴A calculation shows that $f^\sim(\xi) = \frac{1}{1-\eta^2} \{ \sqrt{\xi_1^2 + (1-\eta^2)(\tilde{\xi})^2 + \eta \xi_1} \}$. We observe that we get $f^\sim > 0$ for all ξ and $|\eta| < 1$. Moreover, for large $|\xi_1|$, we have a convergent power series expansion

$$(6.5.25) \quad f^\sim = \frac{|\xi_1|}{1-\eta^2} \{ (1-\eta \operatorname{sgn}(\xi_1)) + \sum_{j=1}^{\infty} c_j \left(\frac{\sigma^2(1-\eta^2)}{\xi_1^2} \right)^j \} ,$$

with $\sigma = \langle \tilde{x} \rangle$ and constants c_j , showing that $f^\sim \approx \frac{|\xi_1|}{1 \pm \eta}$, (with $\pm = \operatorname{sgn}(\xi_1)$), with an error bounded by $c(1-\eta^2)\langle \tilde{\xi} \rangle^2 / \xi_1^2$.

The operator R of sec.6.1 (for general time-independent potentials satisfying *cdn.(X)*) may be written as

$$(6.5.26) \quad R = \kappa S_c \{ V_\eta^0 E_{-\eta} P + V_\eta^{0-} E_\eta Q \}$$

with ψ do-s $V_\eta^{0\pm} \in Op\psi c_0$, and the x_1 -dilation $S_c : u(x) \rightarrow u(x_1 \cosh \theta, \tilde{x})$ and (constant 4×4 -) matrix $\kappa = \cosh(\theta/2) - \alpha_1 \sinh(\theta/2)$, also, with $\eta = \tanh \theta$.

6.6 Decoupling with Respect to H' and $\tilde{H}(t)$

With the above theorem we now can approach a “repair” of the splitting [using the operator RU] of (6.4.2) - that is, in effect, the completion of the proof of thm.6.4.1.

We noted that RU is a unitary operator decoupling $H' = c(H^\circ + \eta D_{x_1})$, but it is **not** a strictly classical ψ do. To repair this we introduce the (decoupled) unitary operator¹⁵

$$(6.6.1) \quad Z = \begin{pmatrix} Z_- & 0 \\ 0 & Z_+ \end{pmatrix} \quad \text{with} \quad Z_\pm = \frac{1}{\sqrt{c}} \sqrt{\varphi_{\pm\eta}(D)} E_{\pm\eta}^* S_{1/c}$$

[it is unitary, by (6.5.20)], and then the unitary operator

$$(6.6.2) \quad U^\circ = RUZ \quad .$$

Since Z already is decoupled, this will not change the decoupling property, - i.e. we still have (6.4.2), with RU replaced by U° , but with the same spaces $\mathcal{H}_e, \mathcal{H}_p$. Relation (6.4.4) will change, insofar as X, Y must be replaced by other ψ do-s \check{X}, \check{Y} ,

¹⁵The matrix listed in (6.7.1) refers to the splitting $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ where \mathcal{H}_\pm are built from the functions in $L^2(\mathbb{R}^3, \mathbb{C}^4)$ with vanishing last two (first two) entries, respectively. We should recall that the splitting used for the two projections P, Q differs from that by having a finite dimensional space \mathcal{Z} shifted. Calling these two splittings the *standard* and the *effective* splitting, we should be aware that the projections $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = U^* P U$ and $\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = U^* Q U$ of the effective splitting assume the form $\begin{pmatrix} 1 & 0 \\ 0 & F \end{pmatrix}$ and $\begin{pmatrix} 0 & 0 \\ 0 & 1-F \end{pmatrix}$ in the standard splitting where $F \in \mathcal{O}(-\infty)$ is a finite dimensional orthogonal projection [onto the space \mathcal{Z} we assume shifted from \mathcal{H}_- to \mathcal{H}_+ , for example]. The operator $U^\circ = RUZ$ will give $U^{\circ*} P' U^\circ = Z^* \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} Z$ and $U^{\circ*} Q' U^\circ = Z^* \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} Z$ in the effective splitting. This assumes the form $Z^* \begin{pmatrix} 1 & 0 \\ 0 & F^\circ \end{pmatrix} Z = \begin{pmatrix} 1 & 0 \\ 0 & F^\circ \end{pmatrix}$, $F^\circ = Z_-^* F Z_-$ and $Z^* \begin{pmatrix} 0 & 0 \\ 0 & 1-F \end{pmatrix} Z = \begin{pmatrix} 0 & 0 \\ 0 & 1-F^\circ \end{pmatrix}$, in the standard splitting. Here F° still is an orthogonal projection with finite rank $\mathcal{Z}^\circ \subset \mathcal{H}_-$. Moreover, since Z_- is of order 0 we still get $F^\circ \in \mathcal{O}(-\infty)$, and $\mathcal{Z}^\circ = \text{im } F^\circ$ consists of rapidly decreasing functions. This means that the unitary operator U° still decouples H' , but now with respect to a new splitting - we must shift the space $\mathcal{Z}^\circ \subset \mathcal{H}_-$ from \mathcal{H}_- to \mathcal{H}_+ . Similar for shifts $\mathcal{H}_+ \rightarrow \mathcal{H}_-$.

but still ψ do-s in $Op\psi c_{e^1}$, and still, formulas like (3.2.1) or (6.4.1) are valid for \check{X}, \check{Y} , and still, this is a decoupling¹⁶.

On the other hand, using (6.5.25), it is easy to show¹⁷, that U^\diamond also is a ψ do in $Op\psi c_0$.

Also, it is clear that the transformed algebras $\mathcal{P}', \mathcal{P}\mathcal{X}'$ are characterized by the condition that $P'AQ', Q'AP' \in \mathcal{O}(-\infty)$ (or, = 0, resp.) with P', Q' defined by (6.4.16).

This will complete the proof of thm.6.4.1, as far as decoupling with respect to H' is concerned.

Now, regarding the decoupling of the transformed Dirac equation (6.1.13), i.e., $\dot{\psi} + \tilde{H}(t)\psi = 0$, we already noted that $\psi(t) = V(t)\omega(t)$ with $V(t) = T_{\eta t}U^\diamond$, U^\diamond of (6.6.2) will take (6.1.13) into

$$(6.6.3) \quad \dot{\omega} + i(U^{\diamond*}(T_{-\eta t}\tilde{H}(t)T_{\eta t} + \eta D_{x_1})U^\diamond)\omega = 0,$$

where $T_{-\eta t}\tilde{H}T_{\eta t} + \eta D_{x_1} = H'$, (by (6.3.17)), is independent of t , and where, moreover, $U^{\diamond*}H'U^\diamond = \check{H} = \begin{pmatrix} \check{X} & 0 \\ 0 & \check{Y} \end{pmatrix}$ is decoupled - with asymptotic expansions (6.4.4).

Again, this is not a decoupling of (6.1.13) by a unitary ψ do, since $V(t)$ contains the factor $T_{\eta t}$. However, we now may define

$$(6.6.4) \quad U^\circ(t) = V(t)T_{-\eta t} = T_{\eta t}U^\diamond T_{-\eta t}.$$

This clearly is a ψ do, since the translation $T_{\eta t}$ leaves all classes ψc_m invariant. On the other hand, the substitution $\omega(t) = T_{-\eta t}\chi(t)$ will take (6.6.3), or $\dot{\omega} + i\check{H}\omega = 0$ into

$$(6.6.5) \quad \dot{\chi} + i(T_{-\eta t}\check{H}T_{\eta t} - \eta D_{x_1})\chi = 0,$$

¹⁶It is not hard to see that the new \check{X}, \check{Y} have the proper asymptotic expansion, required for an analogous of (6.4.1).

¹⁷Assume first that $Z = 0$ - i.e., that standard and effective splitting coincide. Then, using (6.5.26) and the fla.'s $P = U\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}U^*$, $Q = U\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}U^*$ we get $RU = \kappa S_c V_{-\eta}^0 E_{-\eta} U\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \kappa S_c V_{\eta}^{0-} E_{\eta} U\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$.

After a right multiplication by Z the first term ends up with a factor $E_{-\eta}U\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}E_{-\eta}^*$. This is a ψ do in $Op\psi c_0$, since $\Omega = U\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \in Op\psi c_0$, using prop.6.2.1. [We get $E_{-\eta}\Omega E_{-\eta}^* = F^*Q\nu(\xi)F\Omega F^*\nu(\xi)Q^*F \in Op\psi c_0$ since the funtion $\nu(\xi) = \frac{1}{\varphi(\xi)}$ belongs to ψc_0 while the substitution of variables executed by Q leaves $Op\psi c_0$ invariant.] It follows that the first term is of the form $S_c \Xi S_{1/c}$, where $\Xi \in Op\psi c_0$. But the coordinate transform $S_c : x \rightarrow (cx_1, \bar{x})$ leaves $Op\psi c_m$ invariant. Thus the first term gives a ψ do in $Op\psi c_0$, if right multiplied by Z . Similarly for the second term.

If standard and effective splitting do not agree, then our matrix $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ above must be replaced by $\begin{pmatrix} 1 & 0 \\ 0 & F \end{pmatrix}$, bringing forth extra terms such as $E_{-\eta}U\begin{pmatrix} 0 & 0 \\ 0 & F \end{pmatrix}E_{\eta}$. But such terms are of order $-\infty$ since $F \in \mathcal{O}(-\infty)$ and $E_{\pm\eta} \in \mathcal{O}(0)$. Hence they belong to $Op\psi c_{-\infty} \subset Op\psi c_0$. So, still, U^\diamond remains as a ψ do in $Op\psi c_0$.

and this equation clearly is decoupled; we may write it as

$$(6.6.6) \quad \dot{\chi} + iH^\circ(t)\chi = 0 \text{ with } H^\circ = T_{-\eta t} \check{H} T_{\eta t} - \eta D_{x_1} = \begin{pmatrix} X^\circ & 0 \\ 0 & Y^\circ \end{pmatrix},$$

where we have

$$(6.6.7.) \quad X^\circ = T_{-\eta t} \check{X} T_{\eta t} - \eta D_{x_1}, \quad Y^\circ = T_{-\eta t} \check{Y} T_{\eta t} - \eta D_{x_1}.$$

In other words, we have

Proposition 6.6.1 *The Dirac equation $\dot{\psi} + i\check{H}(t)\psi = 0$ with the x_1 -boost transformed Hamiltonian $\check{H}(t)$ of (6.1.14) is decoupled by the unitary ψ do $U^\circ(t)$ of (6.6.4).*

Let us then look for the decoupling of the evolution operator $U_{\check{H}}(\tau, t)$, already evaluated in fla. (6.3.18). Clearly the evolution operator of the (decoupled) equation $\dot{\chi} + iH^\circ(t)\chi = 0$ is given by

$$(6.6.8) \quad U_{H^\circ}(\tau, t) = U^{\circ*}(t)U_{\check{H}}(\tau, t)U(\tau),$$

as may be derived by an argument as used for (6.4.9).

Proposition 6.6.2 *The graded algebra $\tilde{\mathcal{P}}(\tau)$ for the (time-dependent) transformed Hamiltonian $\check{H}(t)$, in the sense of sec.5.2, is given by*

$$(6.6.9) \quad \tilde{\mathcal{P}}(\tau) = T_{\eta\tau} \mathcal{P}' = \{A \in Op\psi c : T_{-\eta\tau} \in \mathcal{P}'\}.$$

Indeed, we may solve (6.6.8) for

$$(6.6.10) \quad U_{\check{H}}(0, t) = T_{\eta t} \{U^\circ(T_{\eta t} U_{H^\circ}(0, t)) U^{\circ*}\},$$

where the term $(.)$ is decoupled so that the unitary ψ do $\{U^\circ(.)U^{\circ*}\}$ takes $\mathcal{P}' = \tilde{\mathcal{P}}(0)$ onto itself. Since $\tilde{\mathcal{P}} = U_{\check{H}}(0, t)\tilde{\mathcal{P}}(0)U_{\check{H}}^*(0, t)$, by (5.2.2), we indeed conclude (6.6.9).

It then is clear that the remaining statements of thm.6.4.1. are falling into place. In particular, conjugation by the (decoupled) unitary ψ do-s Z and $T_{\pm\eta t}$ leaves all the classes $Op\psi c_m$ (and also the class $\mathcal{O}(-\infty)$) invariant, so that indeed the characterizations of \mathcal{P} and \mathcal{P}' proposed in thm.6.4.1 are equivalent, as well as those of $\mathcal{P}\mathcal{X}$, $\mathcal{P}\mathcal{X}'$.

Thus thm.6.4.1 is established - except that we still need the proof of prop.6.5.3, to be discussed in the section, below.

We might finish this section with some remarks:

First we might point to fla. (6.6.4) which emphasizes the special kind of time-dependence we have for our Hamiltonian $\tilde{H}(t)$, obtained by using an x_1 -boost on a time-independent Dirac Hamiltonian: The unitary ψ do decoupling it will depend on time, but only through a time-dependent x_1 -translation.

Second, let us recall that our decoupling of H was not with respect to the split $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ but with respect to (what we called) an “effective splitting” - having a certain space \mathcal{Z} shifted. If we now examine the splittings achieved by our unitary ψ do-s $U^\circ(t)$ then it must be noted that now the splitting will depend on t , insofar as the space \mathcal{Z}° to be shifted will depend on t .

6.7 A Complicated ODE with ψ do-Coefficients

In this section we want to generalize thm.1.5.2 so as to make it fit the ODE (6.5.21) needed for the proof of thm.6.5.3.

Theorem 6.7.1 *Given an initial-value problem of the form*

$$(6.7.1) \quad \frac{dZ}{d\eta} + i[x_1, Zf(\eta, D)] + ix_1 Zc(\eta, x, D) = 0, \quad -1 < \eta < 1, \quad Z(0) = b(x, D),$$

for an unknown operator-valued function $Z(\eta)$ taking values in $\mathcal{O}(m)$, for a given fixed $m \in \mathbb{R}^2$, with real-valued (scalar) $f(\eta, \xi) = \frac{1}{1-\eta^2} \{ \sqrt{\xi_1^2 + (1-\eta^2)\langle \tilde{\xi} \rangle^2} + \eta \xi_1 \}$, and a coefficient symbol $c(\eta, x, \xi) \in C^\infty(|\eta| < 1, \psi c_{-e^2})$ taking values in the class of self-adjoint 4×4 -matrices, modulo ψc_{-e^2} . Also we assume that $b(x, \xi) \in \psi c_m$.

This problem admits a unique solution $Z(\eta)$ belonging to $C^\infty(|\eta| < 1, Op\psi c_m)$.

We will attempt a proof along the lines of thm.1.5.2. Thus the first step will be to assume existence of a solution of the form $Z(\eta) = z(\eta, x, D) \in Op\psi c_0$, and then write down (6.7.1) in terms of symbols:

$$(6.7.2) \quad z_{|\eta} + i \sum_{j=1}^{\infty} \frac{(-i)^j}{j!} \{x_1, (zf)\}_j + ix_1 \sum_{j=0}^{\infty} \frac{(-i)^{|l|}}{l!} z^{(l)} c_{(l)} = 0.$$

In the first sum all terms vanish except for $j = 1$, where we get $+i(zf)_{|\xi_1}$. In the second sum we neglect all terms but the one for $j = 0$. We get

$$(6.7.3) \quad z_{|\eta} - (zf)_{|\xi_1} - ix_1 zc = 0 \pmod{\psi c_{m-e}},$$

and will attempt to solve (6.7.3) as a sharp equation, not only mod ψc_{-e} , with initial value $z(0, x, \xi) = b(x, \xi)$, just as suggested by (6.7.1). We must show then that this solution $z(\eta, x, \xi)$ exists in the “slab” $|\eta| < 1, x, \xi \in \mathbb{R}^3$, and, moreover, that it represents a symbol in $C^\infty(|\eta| < 1, \psi c_m)$.

Before we construct such z , let us discuss the iteration to follow: We will try to improve on z by going with the Ansatz $z + w$ (instead of z) into equ. (6.7.2), with a correction symbol $w \in \psi c_{m-e}$. Assuming that z satisfies a sharp (6.7.3) with initial value b , and neglecting terms of order $m - 2e$, we then get a new equation for w , of the form

$$(6.7.4) \quad w|_s - (wf)|_{\xi_1} - ix_1wc = -z|\xi c|_x, w = 0 \text{ as } s = 0 .$$

Comparing (6.7.3) and (6.7.4) one may observe that both equations are identical, except that we have inhomogeneous initial condition but a homogeneous equation in (6.7.3) but an inhomogeneous equation with homogeneous boundary condition in (6.7.4) - but the corresponding homogeneous equation is the same, in each case.

It also becomes clear that the equation of this type arising in any of the further improvements again will be of the form (6.7.4) with zero-initial condition and more and more complicated right hand side, determined by the earlier iterations.

This simplifies matters, insofar as there is only one first order PDE-initial value problem to be considered.

In (6.7.3) we consider $x = (x_1, x_2, x_3)$ and ξ_2, ξ_3 as constant parameters and regard only η and ξ_1 as variables. We then have a first order PDE in two variables η, ξ_1 of the form

$$(6.7.5) \quad z|_\eta - fz|_{\xi_1} = z\check{c}, \text{ with } \check{c} = f|_{\xi_1} + ix_1c ,$$

where f assumes real (scalar) values, although the coefficient \check{c} assumes matrix values. Still, we may apply the standard technique used before: For any curve $\xi_1 = \xi_1(\eta)$ with $\xi_1(\eta)$ solving the ODE

$$(6.7.6) \quad \dot{\xi}_1 = \xi_1|_\eta = -f(\eta, \xi_1) ,$$

the (matrix-valued) function $\tilde{z}(\eta) = z(\eta, \xi_1)$ satisfies the ODE

$$(6.7.7) \quad \frac{d\tilde{z}}{d\eta} = \tilde{z}\tilde{c} \text{ with } \tilde{c}(\eta) = \check{c}(\eta, \xi_1(\eta)) .$$

Under our assumptions the solution curves of the ODE (6.7.4) cover the entire $\{(\eta, \xi_1) : |\eta| < 1, \xi_1 \in \mathbb{R}\}$: One curve through each point, and for all x, ξ_2, ξ_3 . Thus we get a unique solution $z(\eta, x, \xi)$ of (6.7.3), with initial values $b(x, \xi)$ at $s = 0$, defined in $|s| < 1$. The point again is that we must show $z(\eta, x, \xi)$ to be a symbol.

Actually, the solution $\xi_1(\eta, \xi_1^0)$ of the ODE (6.7.6) through the point $(0, \xi_1^0)$ may be explicitly calculated. We get¹⁸

$$(6.7.8) \quad \xi_1(\eta, \xi_1^0) = \sqrt{1 - \eta^2} \{ ((\xi_1^0, \tilde{\xi}) \sinh(\log \sqrt{\frac{1 - \eta}{1 + \eta}}) + \xi_1^0 \cosh(\log \sqrt{\frac{1 - \eta}{1 + \eta}}) \} .$$

Moreover, it also is easy to calculate explicitly the inverse function $\xi_1^0 = \xi_1^0(\eta, \xi_1)$ - keeping η fixed. We get

$$(6.7.9) \quad \xi_1^0 = \frac{1}{\sqrt{1-\eta^2}} \left\{ \xi_1 \cosh\left(\log \sqrt{\frac{1-\eta}{1+\eta}}\right) - \sqrt{\xi_1^2 + (1-\eta^2)\langle \tilde{\xi} \rangle^2} \sinh\left(\log \sqrt{\frac{1-\eta}{1+\eta}}\right) \right\}.$$

We now can get control of the task regarding solving (6.7.3) or (6.7.4) by verifying

Proposition 6.7.2 *Let the functions of (6.7.8) and (6.7.9) be denoted by $\xi_1 = v(\eta, \xi_1^0, \sigma)$ and $\xi_1^0 = \theta(\eta, \xi, \sigma)$, respectively, with $\sigma = \langle \tilde{\xi} \rangle$. Then, for each fixed $|\eta| < 1$ the two transformations of variables*

$$(6.7.10) \quad \Upsilon_\eta : a(x, \xi) \rightarrow a(x, v(\eta, \xi_1, \langle \tilde{\xi} \rangle), \tilde{\xi})$$

and

$$(6.7.11) \quad \Theta_\eta : a(x, \xi) \rightarrow a(x, \theta(\eta, \xi_1, \langle \tilde{\xi} \rangle), \tilde{\xi})$$

take the symbol classes ψ_{c_m} onto themselves. Moreover, the maps $a_\eta = a(\eta, x, \xi) \rightarrow \Upsilon_\eta a_\eta$ and $a_\eta \rightarrow \Theta_\eta a_\eta$ even take $C^\infty(|\eta| < 1, \psi_{c_m}) \rightarrow C^\infty(|\eta| < 1, \psi_{c_m})$.

The proof is a matter of differential calculus and proper use of estimates (1.2.2). [See also [Co5], sec.9.2, and [Co2].]

Now the map Υ_η takes (6.7.3) into (6.7.7) as we have seen, where now prop.6.7.2 implies that $\tilde{c} = \Upsilon_\eta \check{c} \in \psi_{c_0}$ while $\tilde{z} = \Upsilon_\eta z$. We must show that $\tilde{z} \in \psi_{c_m}$. Then $z = \Theta_\eta \tilde{z} \in \psi_{c_m}$ as well, again by prop.6.7.2, and we have obtained the desired symbol property for the first approximation z . Very similarly one will handle all further approximations, looking at (6.7.4), leading into an inhomogeneous linear first order ODE with vanishing initial conditions.

¹⁸We may verify (6.7.8) directly: Clearly we get $\xi_1 = \xi_1^0$ as $\eta = 0$. Notice that (6.7.8) may be rewritten as

$$\xi_1 = \sqrt{1-\eta^2} \langle \tilde{\xi} \rangle \sinh\left\{\log \frac{1-\eta}{1+\eta} + \gamma\right\} \quad \text{where} \quad \sinh \gamma = \frac{\xi_1^0}{\langle \tilde{\xi} \rangle}.$$

Rewrite this as

$$\sinh^{-1}\left\{\frac{\xi_1}{\langle \tilde{\xi} \rangle \sqrt{1-\eta^2}}\right\} = \log \sqrt{\frac{1-\eta}{1+\eta}} + \gamma$$

and differentiate for η . We get

$$\frac{\sqrt{1-\eta^2}}{\sqrt{\xi_1^2 + (1-\eta^2)\langle \tilde{\xi} \rangle^2}} \left\{ \frac{\xi_1}{\sqrt{1-\eta^2}} \right\}|_\eta = -\frac{1}{1-\eta^2}.$$

This coincides with our ODE (6.7.6).

However, solving equ. (6.7.7) with a symbol \tilde{z} is just a matter of prop.1.5.3. Thus, indeed, solving equ. (6.7.1) mod($\mathcal{O}(-\infty)$) is accomplished.

Finally we must find an operator $V \in C^\infty(|\eta| < 1, \mathcal{O}(-\infty))$ solving the ODE-initial-value problem

$$(6.7.12) \quad \frac{dV}{d\eta} + i[x_1, Vf(\eta, D)] + ix_1Vc(\eta, x, D) = G(\eta) , \quad |\eta| < 1 , \quad V(0) = 0 ,$$

with a given $G(\eta) \in C^\infty(|\eta| < 1, \mathcal{O}(-\infty))$.

Let us transform this equation a bit: First note that the function $f(\xi)$ does never vanish, and that

$$(6.7.13) \quad g(\xi) = 1/f(\xi) = \frac{1}{\langle \xi \rangle^2} (\sqrt{\xi_1^2 + (1 - \eta^2)\langle \tilde{\xi} \rangle^2} - \eta\xi_1)$$

belongs to ψc_{-e^1} . Furthermore, we also have

$$(6.7.14) \quad g|_\eta = -\frac{1}{\langle \tilde{\xi} \rangle^2} \left(\xi_1 + \frac{\eta \langle \tilde{\xi} \rangle^2}{\sqrt{\xi_1^2 + (1 - \eta^2)\langle \tilde{\xi} \rangle^2}} \right) \in \psi c_{-e^1} .$$

In (6.7.12) introduce the operator $K = Vf(D)$ - i.e., set $V = Kg(D)$, $V|_\eta = K|_\eta g(D) + Kg|_\eta(D)$. Right-multiply by $f(D)$, and get

$$(6.7.15) \quad \frac{\partial K}{\partial \eta} + K \frac{g|_\eta}{g}(D) + i[x_1, K]f(D) + ix_1Kg(D)c(x, D)f(D) = Gf(D) = L \in \mathcal{O}(-\infty) .$$

Write $x_1Kg(D)c(x, D)f(D) = K(x_1g(D)c(x, D)f(D)) + [x_1, K](g(D)c(x, D)f(D))$, then (6.7.15) assumes the form

$$(6.7.16) \quad \frac{\partial K}{\partial \eta} + i[x_1, K](f(D) + g(D)c(x, D)f(D)) \\ + K \left(\frac{g|_\eta}{g}(D) + ix_1g(D)c(x, D)f(D) \right) = Gf(D) .$$

Clearly, equ. (6.7.16) is of the form

$$(6.7.17) \quad \frac{\partial K}{\partial \eta} + i[x_1, K]A + KB = L ,$$

with ψ do-s $A \in Op\psi c_{e^1}$, $B \in Op\psi c_0$, and given $L \in \mathcal{O}(-\infty)$.

Now - since we expect a solution $K \in \mathcal{O}(-\infty)$, which is an integral operator with kernel $k(x, y)$ in $\mathcal{S}(\mathbb{R}^6)$, by prop.1.4.6 - let us interpret equ.(6.7.17) as an equation for the kernel $k(x, y)$ of K . If C is any ψ do , then CK and KC have the kernels $(C^x k)(x, y)$ and $(C^{y*} k)(x, y)$, respectively, where the superscripts x, y

indicate that the operator is to be applied to the x - or y -variable, respectively. With this convention equ.(6.7.17) assumes the form

$$(6.7.18) \quad \frac{\partial k}{\partial \eta} + i(x_1 \bar{A}^{y*} - \bar{A}^{y*} y_1)k + \bar{B}^{y*}k = l .$$

Now, one finds at once that equ. (6.7.18) is a symmetric hyperbolic system of pseudodifferential equations of type e in the 6 variables (x,y) , in the sense of [C5],ch.6. In particular we must use that the symbol of A is hermitian symmetric modulo lower order, and also that the commutator $[x_1, A]$ is of order 0. Thus, using the fact that the evolution operator of such an equation is an operator of order 0, it follows at once that the solution of (6.7.18) (with initial-value 0) exists, and belongs to $\mathcal{S}(\mathbb{R}^6)$. In other words existence of the solution of the initial-value problem (6.7.1) and the symbol property of the solution is established.

Moreover, we then also get uniqueness of that solution: A transformation of (6.7.1) to equ. (6.7.18) (with $l = 0$) works in general – not only for solutions in $\mathcal{O}(-\infty)$, except that then the kernel k is a distribution kernel belonging to $\mathcal{S}'(\mathbb{R}^6) = \cup \mathcal{H}_s(\mathbb{R}^6)$. Any solution of (6.7.1) with initial-value $Z(0) = 0$, and $Z(t) \in C^\infty(|\eta| < 1, \mathcal{O}(m))$ thus must vanish identically, implying uniqueness of the solution of (6.7.1). Q.E.D.

6.8 Integral Kernels of $e^{i|D|t}$, $e^{i\sqrt{1-\Delta}t}$ and e^{iH_0t}

We were involved in the action of conjugation by e^{iHt} (or the evolution operator $U(\tau, t)$ of (1.0.1)) throughout this book, but avoided discussing these operators explicitly, so far - except that we now were forced into a closer study, within the present chapter. Let us thus take this final occasion to discuss these operators as (highly singular) integral operators, although this will not be used anywhere here.

Note, the integral kernels of $e^{i|D|t}$ and $e^{i\sqrt{1+D^2}t}$ are distribution kernels - i.e., Schwartz kernels. They are given as inverse Fourier transforms $(2\pi)^{-3/2}k^\vee(|x-y|)$ where $k(\xi) = e^{i|\xi|t}$ or else $= e^{it\sqrt{1+\xi^2}}$, respectively. Since k is radially symmetric, in each case, the inverse Fourier transforms are Hankel transforms: For a function $f(x) = \omega(|x|)$ we have $f^\wedge(\xi) = f^\vee(\xi) = \chi(|\xi|)$ with

$$(6.8.1) \quad \chi(r) = \frac{1}{r} \int_0^\infty \sqrt{r\rho} J_{\frac{1}{2}}(r\rho) \rho \omega(\rho) d\rho ,$$

with the Bessel function $J_{\frac{1}{2}}(z) = \sqrt{\frac{2}{\pi z}} \sin z$ - [for half-numbers $\nu = j + \frac{1}{2}$ Bessel functions are expressible by trigonometric functions; cf. [MO],p.27 or [MOS], p.73]. For formula (6.8.1) cf. [Co5], p.22, for example, where the dimension n equals 3.

Thus we get,

$$(6.8.2) \quad \chi(r) = \sqrt{\frac{2}{\pi}} \frac{1}{r} \int_0^\infty \rho \sin(r\rho) \omega(\rho) d\rho .$$

Here we may substitute $\omega(\rho)$, as supplied - noting that these integrals will diverge, but should be ok as distribution integrals.

Incidentally, note that we may write $\square = \partial_t^2 - \Delta = (\partial_t + i|D|)(\partial_t - i|D|)$ and $\square + 1 = (\partial_t + i\langle D \rangle)(\partial_t - i\langle D \rangle)$, which explains why the operators $e^{i|D|t}, e^{i\langle D \rangle t}$ are related to the initial-value problems of the wave operator \square and the Klein-Gordon operator $\square + 1$, as discussed in ch. 0 of [Co5].

In our case we have $\omega(r) = e^{itr}$, or else, $\omega(r) = e^{it\sqrt{1+r^2}}$, but we might as well then also look at $\omega_\gamma(r) = e^{it\sqrt{\gamma^2+r^2}}$, $0 \leq \gamma \leq 1$, connecting the two above ω .

Of course, the integral (6.8.2) diverges, as improper Riemann integral, and formula (6.8.1) is valid only for $L^1(\mathbb{R}^3)$ -functions, strictly speaking.

The simplest case happens for $\gamma = 0$ where we must make sense of the integral

$$(6.8.3) \quad \int_0^\infty \rho d\rho \sin(r\rho) e^{it\rho} .$$

We do this by writing

$$(6.8.4) \quad \chi(r) = -\sqrt{\frac{2}{\pi}} \frac{1}{r} \partial_t^2 \left\{ \int_0^\infty \frac{d\rho}{\rho} e^{it\rho} \sin r\rho \right\} ,$$

where now the integral exists as improper Riemann integral, while we interpret the derivative ∂_t^2 as a *distribution derivative*.

Focus on the integral in (6.8.4), called I , for a moment: $I = \frac{1}{2i} \int_0^\infty \frac{d\rho}{\rho} (e^{i\rho(t+r)} - e^{i\rho(t-r)}) = \frac{1}{2i} \{I_1 + iI_2\}$, with

$$(6.8.5) \quad I_1 = \int_0^\infty (\cos(t+r)\rho - \cos|t-r|\rho) \frac{d\rho}{\rho} , \quad I_2 = \int_0^\infty (\sin(t+r)\rho - \text{sgn}(t-r) \sin|t-r|\rho) \frac{d\rho}{\rho} .$$

We may split the integral I_2 and make a substitution of variable, for

$$(6.8.6) \quad I_2 = \frac{\pi}{2} (1 - \text{sgn}(t-r)) = -\pi H(r-t) ,$$

with the Heaviside function $H(\tau) = 1$ as $\tau > 0$, $= 0$, as $\tau < 0$. On the other hand, write $I_1 = \lim_{\epsilon \rightarrow 0} \int_\epsilon^\infty = \lim(I_{3,\epsilon} - I_{4,\epsilon})$, and then make similar integral substitutions in $I_{j,\epsilon}$, $j = 3, 4$. Get $I_1 = -\lim_{\epsilon \rightarrow 0} \int_{|r-t|}^{r+t} \cos(\tau\epsilon) \frac{d\tau}{\tau}$. Or,

$$(6.8.7) \quad I_1 = -\log \frac{t+r}{|t-r|} .$$

Alltogether, we get

$$(6.8.8) \quad (2\pi)^{-3/2} \chi(r) = \frac{1}{4\pi r} \partial_t^2 \left\{ H(r-t) + \frac{i}{\pi} \log \left| \frac{t-r}{t+r} \right| \right\} = -\frac{1}{4\pi r} \partial_t \left\{ \delta(t-r) + \frac{2ir}{\pi} \text{p.v.} \frac{1}{r^2 - t^2} \right\} .$$

Let us remind of the fact that ∂_t in (6.8.8) is a distribution derivative. So, (6.8.8) will contain a derivative of a delta-function, and of a “principal value”, both holding singularities at $r = t$.

Now let us try to do the same or similar things for the operator $e^{i\langle D \rangle_\gamma t}$, with $\langle D \rangle_\gamma = \sqrt{\gamma^2 + D^2}$.

Formula (6.8.2) now may be written in the form

$$(6.8.9) \quad \chi(r) = -i\sqrt{\frac{2}{\pi}} \frac{1}{r} \partial_t \int_0^\infty \sin(r\rho) e^{it\langle \rho \rangle_\gamma} \frac{\rho}{\langle \rho \rangle_\gamma} d\rho,$$

with $\langle \rho \rangle_\gamma = \sqrt{\gamma^2 + \rho^2}$. We choose this form (with only a first derivative ∂_t) in spite of the fact that the integral \int_0^∞ still is a distribution integral, because a formula due to Sonine and Gegenbauer may be used to evaluate it [cf. [MO], p.53, first formula, or else, [MOS], p.104, 4-th fla., where we set $\mu = \nu = \frac{1}{2}$, $a = t$, $b = r$, $x = \gamma$, and the integration variable now will be called ρ .] We also use the formulas $J_{\frac{1}{2}}(z) = \sqrt{\frac{2}{\pi z}} \sin z$, $H_{\frac{1}{2}}^{(1)}(z) = -i\sqrt{\frac{2}{\pi z}} e^{iz}$, and that $K_{-1} = K_1$, $H_{-1}^{(1)} = -H_1^{(1)}$. Furthermore, we took the complex conjugate of the formula in [MO] and [MOS], and use that K_1 is real and that the complex conjugate of $H_1^{(1)}$ is $H_1^{(2)}$, for real argument. From (6.8.9) we get

$$(6.8.10) \quad \begin{aligned} \chi(r) &= \frac{-i}{\sqrt{r}} \partial_t \left\{ \int_0^\infty d\rho \left(\sqrt{\frac{2}{\pi r \rho}} \sin(r\rho) \right) \left(\frac{e^{it\langle \rho \rangle_\gamma}}{\sqrt{t\langle \rho \rangle_\gamma}} \right) \rho^{3/2} \langle \rho \rangle_\gamma^{-1/2} \sqrt{t} \right\} \\ &= -\sqrt{\frac{\pi}{2r}} \partial_t \left\{ t^{1/2} \int_0^\infty d\rho J_{\frac{1}{2}}(r\rho) H_{\frac{1}{2}}^{(1)}(t\langle \rho \rangle_\gamma) \rho^{3/2} \langle \rho \rangle_\gamma^{-1/2} \right\}. \end{aligned}$$

Applying Sonine-Gegenbauer the integral assumes the form

$$(6.8.11a) \quad \int_0^\infty = -\left(\frac{r}{t}\right)^{\frac{1}{2}} \frac{\gamma}{\sqrt{t^2 - r^2}} H_1^{(1)}(\gamma\sqrt{t^2 - r^2}), \quad \text{as } r < t,$$

and

$$(6.8.11b) \quad = \frac{2i}{\pi} \left(\frac{r}{t}\right)^{\frac{1}{2}} \frac{\gamma}{\sqrt{r^2 - t^2}} K_1(\gamma\sqrt{r^2 - t^2}), \quad \text{as } r > t.$$

Therefore

$$(6.8.12a) \quad (2\pi)^{-3/2} \chi(r) = -\frac{\gamma}{4\pi} \partial_t \left\{ \frac{H_1^{(1)}(\gamma\sqrt{t^2 - r^2})}{\sqrt{t^2 - r^2}} \right\} \quad \text{as } r < t,$$

and

$$(6.8.12b) \quad (2\pi)^{-3/2} \chi(r) = \frac{i\gamma}{2\pi^2} \partial_t \left\{ \frac{K_1(\gamma\sqrt{r^2 - t^2})}{\sqrt{r^2 - t^2}} \right\} \quad \text{as } r > t.$$

We need not to mention that J_ν , $H_\nu^{(j)}$, K_ν denote the well known (modified) Bessel functions, and that ∂_t in (6.8.9) denotes the distribution derivative. The

integral in (6.8.9) defines a distribution we evaluated only for $r \neq t$, as a C^∞ -function there, while no statement was made for the singularity $r = t$.

Note that we have

$$(6.8.13) \quad \lim_{z \rightarrow 0} z H_1^{(1)}(z) = -\frac{2i}{\pi}, \quad \lim_{z \rightarrow 0} z K_1(z) = 1,$$

with limit taken over $z > 0$. So, in the limit, as $\gamma \rightarrow 0$, we get

$$(6.8.14) \quad (2\pi)^{-3/2} \chi(r) \rightarrow -\frac{i}{2\pi^2} \partial_t \left\{ \frac{1}{r^2 - t^2} \right\} \quad \text{as } t \neq r,$$

as γ tends to 0, in agreement with (6.8.8). Note, that only the imaginary part appears, since the real part has its support at $t = r$. One finds that this (singular) real part does not change with γ . Accordingly, for $\gamma = 1$, with the function

$$(6.8.15a) \quad \lambda(r, t) = r \frac{H_1^{(1)}(\sqrt{t^2 - r^2})}{\sqrt{t^2 - r^2}}, \quad r < t,$$

and

$$(6.8.15b) \quad \lambda(r, t) = \frac{2ir}{\pi} \frac{K_1(\sqrt{r^2 - t^2})}{\sqrt{r^2 - t^2}}, \quad t < r.$$

we arrive at the formula (for the integral kernel of $e^{i(D)t}$)

$$(6.8.16) \quad k(x, y) = (2\pi)^{-3/2} \chi(|x - y|) = \frac{1}{4\pi|x - y|} \partial_t \{ \delta(t - |x - y|) + \text{p.v.} \lambda(t, |x - y|) \},$$

where it may be readily checked (along (6.8.13)) that the principal value of the function $\lambda(t, |x - y|)$ (along the ‘singular sphere’ $|x - y| = t$) exists.

Let us only then write down the final formula for the operators: In each of the two cases we will have

$$(6.8.17) \quad e^{i|D|t} u(x) = \int dy k_0(x, y) u(y) dy, \quad e^{i(D)t} u(x) = \int dy k_1(x, y) u(y) dy, \quad u \in \mathcal{S},$$

with distribution integrals, where k_0 and k_1 are formed as in (6.8.16), using the functions χ of (6.8.8) and (6.8.16), respectively.

Since we now control the operator $e^{i(D)t}$, and, of course, then also the operator $e^{-i(D)t}$ (by taking proper complex conjugates), we then may construct the operator $e^{iH_0 t}$ as well, with the field free Dirac operator $H_0 = \alpha \cdot D + \beta$, using the unitary diagonalization discussed in sec.3.1 - note that the unitary operator U there is a ψ do of order 0. Its symbol is given explicitly by fla. (3.1.5), and it may be recalled that the operators S_0 , S all can be explicitly expressed with integral kernels built from modified Hankel functions. The factor $\frac{1}{\sqrt{2+2S_0}}$ is inessential, by the way. If

we omit it, the operator U no longer will be unitary, but it will be bounded and invertible, and it still will decouple H_0 : We will get $U^{-1}H_0U = \begin{pmatrix} \Lambda_+ & 0 \\ 0 & \Lambda_- \end{pmatrix} = \Lambda$.)

For the evolution operator e^{-iH_0t} we then get

$$(6.8.18) \quad e^{-iH_0t} = e^{-i\langle D \rangle t} P_+ + e^{i\langle D \rangle t} P_- ,$$

with $P_+ = U \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} U^*$, $P_- = U \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} U^*$. [That is, in essence, P_+ and P_- may be constructed, using the first two (last two) columns of the 4×4 -matrix U , and, again, the factor $\sqrt{1+S_0}$ may be dealt with similarly as in sec.4.4.]

Chapter 7

Spectral Theory of Precisely Predictable Approximations

7.0 Introduction

In this chapter we will analyze the spectral theory of a few of our “precisely predictable approximations” of dynamical observables, which are not precisely predictable. Let us emphasize again: *We are not attempting to redefine these observables.* The approximations only are good for calculating an “approximate expectation value” for predicting outcome of a measurement of the observable in question.

Note, the operators we consider are not really precisely predictable - they are only results of the first (or second, or third) iteration of a process leading to a precisely predictable approximation. Besides, they are not uniquely fixed.

Still, when we analyze their spectrum, we might be able to get an idea of meaningfulness of the procedure offered in this book.

The reader familiar with work on spectral theory of the (precisely predictable) Hamiltonian will understand that we are approaching a huge task, requiring much detailed work for a more complete covering. Here, at this level, we essentially will focus on only two observables: *location and electrostatic potential*, perhaps with relativistic mass in the background.

It turns out that we will run into a type of singular Sturm-Liouville problem - after a suitable separation of variables - which seems not well studied, so far, insofar as there is a “third singularity” of the ODE in question - inside the interval of definition, where the equation is “non-elliptic” hence has distribution solutions which are not C^∞ there.

We shall start this investigation with discussing a simple model problem, in sec.7.1, involving a second order ODE. The principles developed there will be applied in sec.7.2 to discuss the correction of the location observable we derived in sec.4.3 [fla. (4.3.10)].

In sec.7.3 we then start with a discussion of the split $H = \mathbf{M} + \mathbf{V}$ of the (precisely predictable) total energy observable $H = \alpha D + \beta + \mathbf{V}$ into “relativistic mass” $\mathbf{M} = H_0 = \alpha D + \beta$ and electrostatic potential \mathbf{V} . Here we assume $\mathbf{A} \equiv 0$ and a radially symmetric $\mathbf{V} = \mathbf{V}(|x|)$.

Note, the two summands \mathbf{M} and \mathbf{V} are not precisely predictable, while their sum H belongs to \mathcal{PX} . However, the symbols of $\mathbf{V}(r)$ and H_0 commute with the symbol of H . Therefore our approximation procedure of ch.’s 4 and 5 works. This produces an (asymptotically convergent) infinite sequence A_j^\sim , $j = 1, 2, \dots$, of corrections, for $A = \mathbf{V}(r)$ or $A = H_0$ with the limit A_∞^\sim still needing a correction O_A of order $-\infty$ such that $A^\sim = A_\infty^\sim + O_A$ belongs to \mathcal{PX} . We can supply only the initial (first two, or first 3) approximations A_1^\sim, A_2^\sim , below, and hope that they may be used as a substitute for A^\sim . [By the way, for any “capped” Coulomb potential the difference $A^\sim - A_2^\sim$ is of trace class, so that, by the Kato-Rosenblum theorem [Ka1], ch.10 at least a statement about the absolutely continuous spectrum of A^\sim can be made.]

We will study the precisely predictable correction \mathbf{V}_{corr} (of the first order) for the electrostatic potential \mathbf{V} derived in (4.3.13) - here called $(\mathbf{V})^\sim$. There will be a corresponding corrected relativistic mass $(M)^\sim = (H_0)^\sim$ defined by the (analogous) split $H = (H_0)^\sim + (\mathbf{V}(r))^\sim$, we leave to a future investigation.

A more detailed investigation of the spectral theory of $(\mathbf{V}(r))^\sim$ will fill the remainder of this chapter. It turns out that the eigenvalue problem $(\mathbf{V}(r))^\sim \psi = \lambda \psi$ may be reduced to an eigenvalue problem of a (4-th order system of) PDE-s, of the form $Au = \lambda Bu$ with (formally self-adjoint) partial differential operators A, B , where, in addition, B is positive definite. One might recall the fact that, for self-adjoint finite matrices A, B , such problems possess a basis of eigenvectors, orthonormal with respect to the inner product $\langle u, v \rangle^\circ = u^* B v$. Correspondingly, the eigenvalue problem of the operator $(\mathbf{V}(r))^\sim$ will lead into a rather complete Sturm-Liouville-type investigation of a self-adjoint 4-th order $\times 2$ -system of ODE-s, again of the form $Au = \lambda Bu$, with differential operators A, B , $B > 0$, defined over the half-line $r > 0$. This will use the radial symmetry of the problem, enabling us to use exactly the kind of separation of variables also splitting the eigenvalue problem of the Dirac operator H .

And again, there will be a point of non-ellipticity inside the interval of definition

$0 < r < \infty$ (depending on the parameter λ), so that the model of sec.7.1 might give some directives.

Interestingly again, and similar to the result of sec.7.2 for the location coordinates, the first correction for the operator $\mathbf{V}(r)$ is unitarily equivalent to $\mathbf{V}(r)$ itself - at least as far as the continuous spectrum is concerned, and by a unitary transform which is a Wiener-Hopf-Cauchy type singular integral operator. Very similar facts seem to emerge for $(H_0)^\sim$, but we will postpone details to a later occasion.

Clearly, such unitary transforms can become “effective” only if the electron is close to the nucleus, since otherwise the operators $\mathbf{V}(r)$ and H_0 undergo only very small changes. When close to the nucleus one perhaps might offer $(\mathbf{V}(r))^\sim$ and $(H_0)^\sim$ as **renormalized** potential and kinetic energies, bearing on thoughts leading to similar properties of the electron developed in quantum field theory.

It also might be interesting that the unitary transform we obtained again is a pseudodifferential operator, at least in its separated form. Indeed, the Cauchy-type singular integral operator U of (7.3.9) is a local (1-dimensional) ψ do, while the operators of our algebras \mathcal{P} and $Op\psi c$ mentioned in (iii) above are 3-dimensional

Our theorem - in its separated form - is stated in sec.7.3. In order to be self-contained we are discussing the required separation of variables in sec.7.4 [This is the well known separation of variables of the Dirac operator for radially symmetric potentials, discussed also in [So2] or [Th1], for example].

In sec.7.5 we give a summary of the various steps needed. In sec.7.6 and sec.7.7 we discuss the 3 singularities of our generalized singular Sturm-Liouville problem, at the 3 points $r = 0$, $r = \frac{1}{\lambda}$, $r = \infty$. The first two are regular singularities, while the last one, at ∞ requires a “Thomé-normal-series-treatment” of a special kind, where we borrow some ideas from J.Horn [Ho1]. In sec.7.8 we finish our proof, discussing a variety of technical facts. In sec’s 7.6-7.8 we are still omitting straight-forward calculations, quoting only the results.

7.1 A Second Order Model Problem

We find it useful to explain our technique for handling a special class of singular Sturm-Liouville problems with applications to Dirac Theory on hand of a model problem, working in the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$, $\mathbb{R} = \{-\infty < x < \infty\}$ on a perturbation of the “location operator” $u(x) \rightarrow xu(x)$, namely,

$$(7.1.1) \quad L_\varepsilon = x + \varepsilon \frac{1}{1 - \partial^2} , \quad \partial = \partial/\partial x , \quad \frac{1}{1 - \partial^2} u(x) = \frac{1}{2} \int_{-\infty}^{\infty} e^{-|x-y|} u(y) dy , \quad 0 \leq \varepsilon \leq 1 .$$

Specifically we focus on $\varepsilon = 0$, where the unperturbed operator $L_0 = x$ has the well known spectral decomposition induced by the “wave distributions” $\delta(x - \lambda)$, and on $\varepsilon = 1$.

The eigenvalue problem $L_\varepsilon u = \lambda u$ is related to the singular Sturm- Liouville problem

$$(7.1.2) \quad (1 - \partial)x(1 + \partial)v + \varepsilon v = \lambda(1 - \partial^2)v, \quad v = (1 + \partial)^{-1}u \in \mathcal{H}_1 = (1 + \partial)^{-1}\mathcal{H},$$

or,

$$(7.1.3) \quad (1 - \partial)(x - \lambda)(1 + \partial)v + \varepsilon v = 0.$$

For $\varepsilon = 1$ this will be the Bessel equation (with variable $s = x - \lambda$): $s^2v'' + sv' - s^2v = 0$.

Note, the differential equation (7.1.3) has 3 singularities, now at $0, \pm\infty$. Surprisingly there are 3 linearly independent global distribution solutions (instead of 2). Using the modified Hankel functions I_0, K_0 (cf.[MOS],p.66) we may explicitly write them down as

$$(7.1.4) \quad v_1(s) = I_0(s), \quad v_2(s) = K_0(|s|), \quad v_3(s) = I_0(s), \quad s > 0, = 0, \quad s \leq 0.$$

It is clear that only $v_2(s) = K_0(|s|)$ will be L^2 (with all derivatives) at $\pm\infty$ (both). Taking $(1 + \partial)$ (with ∂ =distribution derivative) we then get the “wave distribution”¹

$$(7.1.5) \quad u_\lambda(x) = (1 + \partial)K_0(|x - \lambda|) = p.v.k(x - \cdot), \quad k(s) = K_0(|s|) + \text{sgn}(s)K_1(|s|),$$

(that is, a distribution solution u_λ of $L_1 u = \lambda u$ which is L^2 at $\pm\infty$, and such that the “eigenpackets”

$$(7.1.6) \quad f(x) = p.v. \int_{-\infty}^{\infty} k(x - \lambda)\kappa(\lambda)d\lambda, \quad \kappa \in C_0^\infty(\mathbb{R})$$

belong to \mathcal{H}).

Clearly there are no eigenfunctions - i.e., no nontrivial linear combination of (7.1.4) can be in \mathcal{H}_1 . One will expect an “orthogonality” of the form

$$(7.1.7) \quad p.v. \int_{-\infty}^{\infty} k(x - \lambda)k(x - \mu)dx = 0, \quad \lambda \neq \mu$$

with that principal value well defined as $\lambda \neq \mu$.

¹ $p.v.k(x - \cdot)$ denotes the “principal value” distribution $\langle p.v.k(x - \cdot), \varphi \rangle = p.v. \int k(x - \lambda)\varphi(\lambda)d\lambda$, $\varphi \in \mathcal{S}$, with $p.v. \int = \lim_{\varepsilon \rightarrow 0} \int_{|x - \lambda| > \varepsilon}$.

Completeness of the absolutely continuous spectrum generated by (7.1.7) is a matter of proving solvability of (7.1.6) for every f of a set dense in \mathcal{H} . Again, (7.1.6) is a singular convolution equation, equivalent to $f^\wedge(\xi) = \sqrt{2\pi}k^\wedge(\xi)\kappa^\wedge(\xi)$ with Fourier transform “ \wedge ”. Using that application of $(1 + \partial)$ amounts to multiplying the Fourier transform by $(1 + i\xi)$ one finds that $\kappa^\wedge = \sqrt{\frac{\pi}{2}} \frac{1+i\xi}{\sqrt{1+\xi^2}}$. So, we get the equation $f^\wedge(\xi) = \pi v(\xi)\kappa^\wedge(\xi)$ with $v(\xi) = \frac{1+i\xi}{\sqrt{1+\xi^2}}$ having $|v(\xi)| = 1$, so that the multiplication operator is unitary. Then, with $g(x) = \pi\kappa(x)$ we get $f^\wedge = v g^\wedge$, with $v = \sqrt{\frac{2}{\pi}}k^\wedge$. Going back we get

$$(7.1.8) \quad f = Ug, \quad Ug(x) = \frac{1}{\pi}p.v. \int_{-\infty}^{\infty} k(x-y)g(y)dy, \quad U^*L_1U = L_0,$$

with $k(s)$ of (7.1.5), where U is a unitary singular convolution operator, as a new generalized Fourier integral transform. Completeness of the absolutely continuous spectrum thus generated then is evident.

For $\varepsilon = 0$ we already have control of the spectral resolution, but we might repeat the same chain of arguments - formally - to then get $sv'' + v' + (1-s)v = 0$ solved by e^{-s} . Since one solution is known, two other distribution solutions may be explicitly obtained. Only $w(s) = e^{-s}$, $s > 0$, $= 0$, $s < 0$ will be L^2 at $\pm\infty$ (both). This will give the (already known) wave distribution $u_\lambda(x) = \delta(x - \lambda)$, and the corresponding eigenpackets and(trivial) generalized Fourier expansion - with the identity as Fourier transform.

For general $0 < \varepsilon < 1$ we get the differential equation $sv'' + v' + (1-\varepsilon-s)v = 0$, equivalent to the Whittaker equation (W): $4t^2w'' = (t^2 - 4\kappa t + 4\mu^2 - 1)w$. [We use [MO],Ch.VI,2 as a reference]. Let $w(\kappa, \mu, t)$ be any solution of (W). Then

$$(7.1.9) \quad v(s) = s^{-\frac{1}{2}}w\left(\frac{1}{2}(1-\varepsilon), 0, 2s\right)$$

solves our equation. In this case we again will get a 3-dimensional space of global distribution solutions in $(-\infty, \infty)$. From the solutions of (W) we pick the “Whittaker function” $W_{\kappa,0}(z)$, $\kappa = \frac{1}{2}(1-\varepsilon)$ as $z > 0$, but $W_{-\kappa,0}(-z)$, as $z < 0$. In other words, we select

$$(7.1.10) \quad v(s) = p_{wc0}(s)|s|^{-\frac{1}{2}}W_{\kappa(s),0}(2|s|), \quad s \in \mathbb{R},$$

with a piecewise constant function $p_{wc0}(s) = a_\pm$ jumping only at 0, where $\kappa(s) = \text{sgn}(s)\frac{1}{2}(1-\varepsilon)$. This solves for $s \neq 0$ since $w(-\kappa, \mu, -z)$ also solves (W).

The behaviour near $\pm\infty$ of the function (7.1.10) is determined by the asymptotic formulas on p.116 of [MO] (second last formula) [Note that derivatives again may be expressed by $W_{\lambda,0}$ with good coefficients (cf.[MO],p.117)]. This makes

sure that $(1 + \partial)v \in L^2$ near $\pm\infty$. The behaviour near $s = 0$ is determined by the second formula on p.116 of [MO], giving

$$(7.1.11) \quad v(s) = -\frac{a_+}{\Gamma(\frac{\varepsilon}{2})} \{2C + \psi(\frac{\varepsilon}{2}) + \log |2s|\} + h.p. , \quad s > 0 ,$$

and

$$(7.1.12) \quad v(s) = -\frac{a_-}{\Gamma(1 - \frac{\varepsilon}{2})} \{2C + \psi(1 - \frac{\varepsilon}{2}) + \log |2s|\} + h.p. , \quad s < 0 .$$

Here $C \approx 0.577\dots$ denotes the Euler constant, and, $\psi(z) = \Gamma'(z)/\Gamma(z)$. “h.p.” stands for a term of the form $p(s) + q(s) \log |s|$ with power series p, q vanishing at 0.

Proposition 7.1.1 *$v(s)$ of (7.1.10) is a distribution solution of (7.1.3) if (and only if) we choose the constants a_{\pm} such that the logarithmic terms in (7.1.11) and (7.1.12) bear the same constant factor.*

Indeed, we then get $v(s) = c_1 \log |s| + c_2 H(s) + v_1(s)$ with the Heaviside function $H(s)$, and $v_1(s) = p(s) + q(s) \log |s|$, again with power series p, q , where still $q(0) = 0$, coefficients jumping at 0, except $p(0)$. We may write (7.1.3) in the form $(sv')' + (2\kappa - s)v = 0$. Note that $H'(s) = \delta(s)$, hence $sH'(s) \equiv 0$. Also, $(\log |s|)' = p.v. \frac{1}{s}$, hence $s(\log |s|)' = 1 = const.$, and $(s(\log |s|)')' = 0$. It follows that $(sv')' = (sv_1')' \in L^1_{loc}$, as readily checked from the special form of v_1 . Accordingly we also have (the distribution) $z = (sv')' + (2\kappa - s)v \in L^1_{loc}$. But v solves the equation for $s \neq 0$. Accordingly $z = 0$ for $s \neq 0$. Since $z \in L^1_{loc}$ it must be the zero distribution, and hence v must be a global distribution solution. The converse is evident, following the argument backward. Q.E.D.

From the proposition we derive the condition

$$(7.1.13) \quad a_- = -\frac{\varepsilon}{2} \frac{\Gamma(-\frac{\varepsilon}{2})}{\Gamma(\frac{\varepsilon}{2})} a_+ .$$

This then will again give a solution $v(s)$ independent of λ . Defining $k_{\varepsilon}(s) = (1 + \partial)v(s)$ we again get an orthogonal integral expansion of the above kind. This time the integral expansion theorem if of the form

$$(7.1.14) \quad f(x) = \int_{-\infty}^{\infty} k_{\varepsilon}(x - \lambda) \kappa(\lambda) d\lambda , \quad k_{\varepsilon} = c_1^{\varepsilon} \delta(s) + c_2^{\varepsilon} p.v. \frac{1}{s} + L^1_{loc} ,$$

with certain constants c_j^{ε} (where $k_{\varepsilon} \in L^2$ near $\pm\infty$). Explicitly we get (with $\psi = \Gamma'/\Gamma$)

$$(7.1.15) \quad c_1^{\varepsilon} = -\frac{a_+}{\Gamma(\frac{\varepsilon}{2})} \left\{ \psi(\frac{\varepsilon}{2}) - \psi(-\frac{\varepsilon}{2}) - \frac{2}{\varepsilon} \right\} , \quad c_2^{\varepsilon} = -\frac{a_+}{\Gamma(\frac{\varepsilon}{2})} .$$

First we confirm that c_j^ε are well defined in $0 \leq \varepsilon \leq 1$, and that $c_2^0 = c_1^1 = 0$, in agreement with earlier calculations. The orthogonality $\int_{-\infty}^{\infty} k_\varepsilon(x-\lambda)k_\varepsilon(x-\mu)dx = 0$ (with distribution integral) is readily confirmed, using symmetry of the operator L_ε . This implies that the convolution operator $(k_\varepsilon^*)^*(k_\varepsilon^*) = (l_\varepsilon^*)$ must be of the form $l_\varepsilon = c^2\delta(x)$ with a constant $c > 0$. Then define $U_\varepsilon = \frac{1}{c}k_\varepsilon^*$ and get a unitary operator again, diagonalizing L_ε - i.e., $U_\varepsilon^*L_\varepsilon U_\varepsilon = L_0$.

7.2 The Corrected Location Observable

We were confronted with problems of the above kind while trying to do a *clean* quantum mechanics of the Dirac equation. One may remember that Dirac's equation - while doing an incredible job explaining the hydrogen spectral lines - was attacked because of unexplainable contradictions and paradoxa with the theory of its *observables*, not to speak of the infinite negative energy band.

At that time it seemed to be unknown (or was left without consideration) that the Dirac equation - similar to other (semi-strictly hyperbolic) symmetric hyperbolic first order systems - possesses an invariant *algebra of observables* [also relativistically covariant], and that it perhaps should be *imperative* to admit only the self-adjoint operators of that algebra - of course, this is our algebra \mathcal{P} (or else the algebra \mathcal{PX}) of ch.5 - as **precisely predictable observables**. Total energy and total angular momentum are precisely predictable, but most other dynamical observables are **not** precisely predictable - although most of them possess *precisely predictable approximations*.

Transitions from "electron states" to "positron states" seem to be "*unpredictable*" - so that the negative energy band should not be a disturbance at all.

To come back to our above problem: We have set out to study the spectral theory of precisely predictable approximations of special observables, such as *location*, *orbital angular momentum*, *electrostatic potential*, *relativistic mass* and, at that occasion, found that they may be treated with above method, to get a unitary equivalence between the precisely predictable approximation and the original observable, by a unitary map which is a pseudodifferential operator, similar to above singular convolutions.

Let us discuss the perhaps simplest of such problems. We now are in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$, and consider the *location operator* $x = (x_1, x_2, x_3)$, i.e. the 3 multiplication operators $u(x) \rightarrow x_j u(x)$, $j = 1, 2, 3$. These 3 operators are not precisely predictable. But their precisely predictable approximations² are given

²Actually, fla. (7.2.1) gives only first improvement of a list of infinitely many, where only the

as³

$$(7.2.1) \quad x_{corr} = x - \frac{1}{2} \frac{1}{1 - \Delta} (\mu + \rho \times D),$$

where “ \times ” denotes the vector product, and with the 4×4 -matrices $\rho = \begin{pmatrix} \sigma^0 \\ 0 \sigma \end{pmatrix}$ and⁴ $\mu = \begin{pmatrix} 0 \sigma \\ \sigma 0 \end{pmatrix}$ - also $D = \frac{1}{i} \partial_x$ and $\Delta = \sum_1^3 \partial_{x_j}^2 = \text{Laplacian}$. [Also, we set the electromagnetic potentials equal to 0 but allow an arbitrary electrostatic potential.]

Let us focus on the operator A_1 representing the first coordinate

$$(7.2.2) \quad A_1 = x_1^{corr} = x_1 - \frac{1}{2} \frac{1}{1 - \Delta} (\mu_1 + \rho_2 D_3 - \rho_3 D_2),$$

In order to convert the equation $A_1 u = \lambda u$ into an ODE we apply the Fourier transform with respect to the second and third variable, for

$$(7.2.3) \quad B_1 = F_2^{-1} F_3^{-1} A_1 F_2 F_3 = x_1 - \frac{1}{2} \frac{1}{1 + \xi_2^2 + \xi_3^2 - \partial_{x_1}^2} (\mu_1 + \rho_2 \xi_3 - \rho_3 \xi_2).$$

Here we realize that the operator B_1 almost looks like L_ε of section 7.1, except that we have a self-adjoint matrix involved. Introduce a new independent variable $y = \kappa x_1$, with $\kappa = \sqrt{1 + \xi_2^2 + \xi_3^2}$. With that we get

$$(7.2.4) \quad B_1 = \frac{1}{\kappa} \left\{ y - \frac{1}{2} a(\xi_2, \xi_3) \frac{1}{1 - \partial_y^2} \right\},$$

with the self-adjoint 4×4 -matrix

$$(7.2.5) \quad a(\xi_2, \xi_3) = \frac{1}{\kappa} \mu_1 - \frac{\xi_2}{\kappa} \rho_3 + \frac{\xi_3}{\kappa} \rho_2.$$

Then it will be a matter of a principal axes transform of the matrix (7.2.5) to generate exactly the operator (7.1.1) with $-2\varepsilon = \lambda(\xi_2, \xi_3) = \text{eigenvalue of } a(\xi_2, \xi_3)$. The unitary operator diagonalizing A_1 then will be the inverse Fourier transform (with respect to the two parameters ξ_2, ξ_3) of the unitary operator we obtained in section 7.1. The detailed form of that operator will emerge if we get more details about above diagonalization of the matrix a .

final result will really be precisely predictable. But this last operator is not explicitly accessible, so, we hope, that a study of (7.2.1) will provide a hint in the right direction.

³Recall our physical dimensions: The unit of length is the *Compton wave length* of the electron $\hbar/mc \approx 3.861 \times 10^{-13} m$. The unit of time is $\hbar/mc^2 \approx 1.287 \times 10^{-21} sec$. The unit of energy is $mc^2 \approx 0.5 MeV$ (cf. footnote 1 of ch.1).

⁴Recall our “Pauli matrices” $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ of (3.1.6), where

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

Regarding the matrix $a(\xi_2, \xi_3)$, note that

$$(7.2.6) \quad \mu_1^2 = \rho_2^2 = \rho_3^2 = 1, \quad \rho_1\rho_2 + \rho_2\rho_1 = 0, \quad \mu_1\rho_j + \rho_j\mu_1 = 0, \quad j = 2, 3.$$

This implies

$$(7.2.7) \quad a^2(\xi_2, \xi_3) = 1,$$

so that $a(\xi_2, \xi_2)$ can only have the eigenvalues $\lambda = \pm 1$. Note that ρ_2 has both eigenvalues ± 1 with multiplicity 2, each. For reason of continuity this must prevail for all ξ_2, ξ_3 .

In order to obtain a diagonalization of $A_1 = x_1^{corr}$ we then will need an explicit unitary 4×4 -matrix $\Phi = \Phi(\xi^\circ)$ (with $\xi^\circ = (\xi_2, \xi_3)$) such that

$$(7.2.8) \quad \Phi^*(\xi^\circ)a(\xi^\circ)\Phi(\xi^\circ) = \text{diag}(1, 1, -1, -1).$$

To solve that eigenvalue problem we may write the 3 matrices occurring as tensor products:

$$(7.2.9) \quad \mu_1 = \sigma_2 \otimes \sigma_1, \quad \rho_2 = 1 \otimes \sigma_2, \quad \rho_3 = 1 \otimes \sigma_3.$$

Then, looking for u solving

$$(7.2.10) \quad a(\xi^\circ)u = \lambda u,$$

let $u = v_\pm \otimes w$ with $v_\pm = \frac{1}{\sqrt{2}}(\pm 1)$ being one of the normalized eigenvectors of σ_2 . Then (7.2.10) amounts to

$$(7.2.11) \quad b(\xi^\circ)w = \left(\pm \frac{1}{\kappa} \sigma_1 + \frac{\xi_3}{\kappa} \sigma_2 - \frac{\xi_2}{\kappa} \sigma_3 \right) w = \lambda w,$$

involving the matrix

$$(7.2.12) \quad b(\xi^\circ) = \frac{1}{\kappa} \begin{pmatrix} -\xi_2 & \xi_3 \pm i \\ \xi_3 \mp i & \xi_2 \end{pmatrix}.$$

A calculation gives the following eigenvectors of b :

$$(7.2.13) \quad \text{For } \lambda = 1: \quad w = w_+ = (2\kappa(\kappa + \xi_2))^{-\frac{1}{2}} \begin{pmatrix} \xi_3 \pm i \\ \kappa + \xi_2 \end{pmatrix} = (2(1 + \zeta_2))^{-\frac{1}{2}} \begin{pmatrix} \zeta_3 \pm i \zeta_0 \\ 1 + \zeta_2 \end{pmatrix},$$

and

$$(7.2.14) \quad \text{For } \lambda = -1: \quad w = w_- = (2\kappa(\kappa - \xi_2))^{-\frac{1}{2}} \begin{pmatrix} \xi_3 \pm i \\ \kappa - \xi_2 \end{pmatrix} = (2(1 - \zeta_2))^{-\frac{1}{2}} \begin{pmatrix} \zeta_3 \pm i \zeta_0 \\ 1 - \zeta_2 \end{pmatrix},$$

where we have written $\zeta_j = \frac{\xi_j}{\kappa}$, $j = 2, 3$, and $\zeta_0 = \frac{1}{\kappa} = \sqrt{1 - \zeta_2^2 - \zeta_3^2}$.

In this way we end up with the orthonormal system

$$(7.2.15) \quad \begin{aligned} (u_1, u_2) &= (v_+ \otimes w_+, v_- \otimes w_+) \text{ for } \lambda = 1, \\ (u_3, u_4) &= (v_+ \otimes w_-, v_- \otimes w_-) \text{ for } \lambda = -1, \end{aligned}$$

and a desired unitary matrix is given as

$$(7.2.16) \quad \Phi(\xi^\diamond) = (u_1, u_2, u_3, u_4).$$

Let us observe that the unitary matrix $\Phi(\xi^\diamond)$ of (7.2.16) has one shortcoming: Considered as a function of $\zeta^\diamond = (\zeta_1, \zeta_2)$ in the disk $|\zeta^\diamond| \leq 1$ with $\zeta_0 = \sqrt{1 - |z^\diamond|^2}$ the components of Φ are bounded but some of them are discontinuous at $\zeta^\diamond = (\pm 1, 0)$. Actually the absolute values are continuous in the entire circle, but the argument of some components of w_\pm fails to be continuous there. However, using that the eigenvectors w_\pm are unique only up to a multiple of norm 1, this may be cured locally by multiplying the discontinuous argument away. And, since the unit disk is contractible, there also is a global cure, effected by multiplying w_\pm by a suitable function of norm 1.

Continuity of $\Phi(\zeta^\diamond)$ becomes important when we return to the spectral theory of the operator A_1 by taking the inverse Fourier transform. Combining (7.2.3),(7.2.4) and (7.2.8) we get

$$(7.2.17) \quad (F^\diamond T_\kappa \Phi^\diamond)^* A_1 (F^\diamond T_\kappa \Phi^\diamond) = \frac{1}{\kappa} \text{diag}(L_{-\frac{1}{2}}, L_{-\frac{1}{2}}, L_{\frac{1}{2}}, L_{\frac{1}{2}}),$$

with $F^\diamond = F_2 F_3$, and the (unitary) dilation operator

$$(7.2.18) \quad (T_\kappa u)(x_1, \xi^\diamond) = \sqrt{\kappa} u(\kappa x_1, \xi^\diamond),$$

and with $L_{\pm\frac{1}{2}} = L_\varepsilon$, $\varepsilon = \pm\frac{1}{2}$ of fla.(7.1.1). This operator will be diagonalized with (the singular convolution operator) $V = \text{diag}(U_{-\frac{1}{2}}, U_{-\frac{1}{2}}, U_{\frac{1}{2}}, U_{\frac{1}{2}})$, using the operator U_ε introduced at the end of sec.7.1. Then we still must reverse the dilation and the Fourier transform F^\diamond . So, we end up with

$$(7.2.19) \quad W^* x_1^{corr} W = x_1, \text{ where } W = F^\diamond T_\kappa \Phi^\diamond T_{1/\kappa} F^{\diamond*}, \quad W^* W = W W^* = 1.$$

It should be interesting to look at the detailed properties of the unitary operator W , but we will not look at this here.

7.3 Electrostatic Potential and Relativistic Mass

Let us next analyze a precisely predictable approximation of the electrostatic potential $\mathbf{V}(x)$.

Again our Hilbert space is $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$. Consider the multiplication operator $u(x) \rightarrow \mathbf{V}(|x|)u(x)$ with⁵ $V(r) = \frac{1}{r}$, and the (first order constant coefficient) (4×4 -matrix-) differential operator $H_0 = \sum_1^3 \alpha_j D_j + \beta$. In the absence of electromagnetic fields our Dirac Hamiltonian - the (precisely predictable) *total energy observable* then is of the form

$$(7.3.1) \quad H = H_0 + \mathbf{V}(|x|) .$$

Note that $H_0, \mathbf{V}(r)$ also represent *dynamical observables* of Dirac theory. They represent *relativistic mass*, and *potential* (energy) of the particle. However, H_0 and $\mathbf{V}(r)$ are not precisely predictable - but they have precisely predictable approximations we call $(H_0)^\sim$ and $(\mathbf{V}(r))^\sim$, respectively. Explicitly, we write⁶

$$(7.3.2) \quad (H_0)^\sim = H_0 - \Lambda - \Lambda^* , \quad (\mathbf{V}(r))^\sim = \mathbf{V}(r) + \Lambda + \Lambda^* , \quad \Lambda = -\frac{1}{4} \mathcal{E} \cdot (\mu + \rho \times D) \frac{1}{1 - \Delta} ,$$

with $\mathcal{E} = -grad \mathbf{V}(|x|)$ and constant 4×4 -matrices $\mu = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}$, $\rho = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}$, where $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ are the 2×2 -Pauli matrices.

Note, we still have the split $H = (H_0)^\sim + (\mathbf{V}(r))^\sim$, since the perturbations cancel each other. Our point, making this new split, is that we claim that the new energies $(H_0)^\sim$ and $(\mathbf{V}(r))^\sim$ can be predicted (in the sense of quantum mechanical rules) while H_0 and $\mathbf{V}(|x|)$ cannot. Yet, on superficial examination, the perturbation Λ seems to be small, as $|x|$ is large, due to $\mathcal{E} = O(\frac{1}{|x|^2})$ and $\frac{1}{1-\Delta}$ and $\frac{D}{1-\Delta}$ being bounded operators of \mathcal{H}^4 . In that sense one may safely talk about potential and kinetic energy, assuming the electron moves in its normal (hydrogen-) orbits, but **NOT SO** if the electron is directly on the nucleus.

When we talk about spectral theory of the (unbounded self-adjoint) operators $A = (H_0)^\sim$ or $A = (\mathbf{V}(r))^\sim$, we mean to study the eigenvalue problem $Au = \lambda u$. Formally, these eigenvalue problems may be reduced to the problem

$$(7.3.3) \quad (1 - \Delta)H_0(1 - \Delta)v - \frac{1}{4} \{ (1 - \Delta)\mathcal{E}(\mu + \rho \times D) + (\mu + \rho \times D)\mathcal{E}(1 - \Delta) \} v = \lambda(1 - \Delta)^2 v$$

⁵Actually, we should use $\mathbf{V}(r) = -\frac{c_f}{r}$ with the fine structure constant $c_f \approx \frac{1}{137}$. But $-c_f$ is a factor of \mathbf{V} and of its perturbation (in (7.3.4)). It may be taken into the eigenvalue λ , saving complications.

⁶Actually, Λ of (7.3.2) represents only the first of infinitely many corrections to be applied to make these observables “precisely predictable”. We still control the next one, generated by replacing Λ with $\Lambda + \Upsilon$, where $\Upsilon = \frac{3}{8} i(\mathcal{E} \cdot D)(\mathcal{E} \cdot (\mu + \rho \times D)) \frac{H_0}{(1 - \Delta)^3}$. These (higher order) perturbations seem to generate very similar spectral theory, but lead to differential equations of order 12 (or 13) - using only the Υ - perhaps too complicated for a detailed discussion.

(for H_0), and,

(7.3.4)

$$(1 - \Delta) \frac{1}{r} (1 - \Delta)v + \frac{1}{4} \{ (1 - \Delta)\mathcal{E}(\mu + \rho \times D) + (\mu + \rho \times D)\mathcal{E}(1 - \Delta) \} v = \lambda(1 - \Delta)^2 v$$

(for $\mathbf{V}(r)$). In each case we were setting $u = (1 - \Delta)v$ and multiplying the equation by $(1 - \Delta)$.

In the form (7.3.3) or (7.3.4) we have an eigenvalue problem of the form $Au = \lambda Bu$ with self-adjoint differential operators A, B , and $B = (1 - \Delta)^2$ positive definite. For finite matrices A, B this would be a self-adjoint problem with respect to the inner product $\langle u, v \rangle^\circ = u^* Bv$, and we then get a base of eigenvectors, orthonormal with respect to that inner product.

The problems (7.3.3) and (7.3.4) involve (4×4 -systems of) PDE-s of order 5 and 4, respectively. Fortunately the standard separation of variables applicable to a Dirac operator H with rotationally invariant potentials may be applied for (7.3.3) and (7.3.4) as well. We are going to discuss details of this separation in sec.7.4, below. Looking at thm.7.4.1, we are summarizing this conversion:

Proposition 7.3.1 *Our Hilbert space splits: $\mathcal{H} = \oplus \mathcal{H}_{l,p,\varepsilon}$ with l, p, ε as defined in sec.7.4, where each Hilbert space $\mathcal{H}_{l,p,\varepsilon}$ coincides with the space $\mathcal{H}^2 = L^2(\mathbb{R}^+, \mathbb{C}^2)$, so consists of 2-vector functions defined and squared integrable⁷ over the half-line $0 < r < \infty$. Then problems (7.3.3) and (7.3.4) reduce to the (1-dimensional) eigenvalue problems (7.3.5) and (7.3.6), below:*

$$(7.3.5) \quad \{ZH_0Z - GZ - ZG\}v = \lambda Z^2 v, \quad v = Z^{-1}u,$$

and

$$(7.3.6) \quad \{ZV(r)Z + GZ + ZG\}v = \lambda Z^2 v, \quad v = Z^{-1}u,$$

where (with the 2×2 -Pauli matrices of (3.1.6), cf. (7.4.50))

$$(7.3.7) \quad H_0 = -i\sigma_1 \partial_r + \frac{\kappa}{r} \sigma_2 + \sigma_3.$$

(We use the same notation for the separated H_0 .) In (7.3.5) and (7.3.6) we used the second order (2×2 -matrix-) differential operator $Z = \begin{pmatrix} Z_- & 0 \\ 0 & Z_+ \end{pmatrix}$ where⁸ $Z_\pm = 1 + \frac{\kappa(\kappa \pm 1)}{r^2} - \partial_r^2$, and the 2×2 -matrix multiplication $G(r) = -\frac{cf}{4r^3} \{1 - \sigma_3 \kappa + r\sigma_2\}$. Also, κ denotes a nonvanishing integer - separation parameter, determined by the space $\mathcal{H}_{l,p,\varepsilon}$ -, and the Hilbert space is $\mathcal{H}^2 = L^2(\mathbb{R}^+, \mathbb{C}^2)$, mentioned above. The perturbed operators now are

$$(7.3.8) \quad (H_0)^\sim = H_0 - GZ^{-1} - Z^{-1}G, \quad (\mathbf{V}(r))^\sim = V(|x|) + GZ^{-1} + Z^{-1}G.$$

⁷Note, also a change $rv = w$ of dependent variable is involved, where we then return to the notation v for w again.

⁸Actually, Z is the separated operator $1 - \Delta$.

This proposition follows at once from thm.7.4.1, below.

It is clear then, that the spectral theory of our corrected operators will be a “superposition” of the spectral theories of all the operators (7.3.8), so that we must look at the “singular Sturm-Liouville problems” (7.3.5) and (7.3.6), involving only ODE-s (instead of the PDE-s (7.3.3) and (7.3.4)).

In the remainder of this chapter we will focus on $(\mathbf{V}(r))^\sim$, leaving $(H_0)^\sim$ for a later occasion. Notice that (7.3.6) is a 4-th order ordinary differential equation - rather, a system of 2 ODE-s in 2 unknown functions. Such a system will lead into a self-adjoint theory if we introduce the (Sobolev-type) Hilbert space $\mathcal{K} = Z^{-1}\mathcal{H}^2$ with norm $\|u\|_2 = \|Zu\|$ and inner product $\langle u, v \rangle_2 = \langle Zu, Zv \rangle$.

We then will attempt a diagonalization of the corrected potential $(\mathbf{V}(r))^\sim$. We focus on $(\mathbf{V}(r))^\sim$ - that is, on the eigenvalue problem (7.3.6) - but expect the same facts for the second correction discussed in sec.5.6, although the calculations there were not fully carried through. Also, we work with the *uncapped* Coulomb potential⁹ $\mathbf{V}(r) = -\frac{cf}{r}$ (saving some complications) although we pointed out that our observable theory is rigorous only with a cap on the singularity at 0.

Theorem 7.3.2 *For the eigenvalue problem (7.3.6), that is, for the radial part of the corrected potential $(\mathbf{V}(r))^\sim$, - after adding a suitable “self-adjoint boundary condition” at 0 for certain (finitely many) values of the separation parameter κ - the entire continuous spectrum is absolutely continuous. The continuous spectrum extends (with multiplicity 2) over all of the positive real axis \mathbb{R}_+ . It corresponds to the subspace \mathcal{H}_{ac}^2 of $\mathcal{H}^2 = L^2(\mathbb{R}_+, \mathbb{C}^2)$ defined as the image of a unitary map $U : L^2(\mathbb{R}_+, \mathbb{C}^2) \rightarrow \mathcal{H}_{ac}^2 \subset \mathcal{H}^2$, where U is explicitly given as singular integral operator of the form*

$$(7.3.9) \quad Uu(r) = A(r)u(r) + p.v. \int_0^\infty B(\rho)u(\rho) \frac{d\rho}{r-\rho} + \int_0^\infty C(r, \rho)u(\rho)d\rho, \quad u \in C_0^\infty(\mathbb{R}_+, \mathbb{C}^2),$$

with smooth 2×2 -matrix functions $A(\rho), B(\rho) \in C^\infty(\mathbb{R}_+)$ satisfying

$$(7.3.10) \quad A(r)^*A(r) + \pi^2 B(r)^*B(r) = 1, \quad A(r)^*B(r) - B(r)^*A(r) = 0 \text{ for all } r > 0,$$

and such that the 2×4 -matrix $(A, B)(\rho)$ is of maximal rank 2, for all $\rho > 0$; also, with $C(\cdot, \rho) \in \mathcal{H}^2$ for all $\rho > 0$, and smooth in ρ as well. The integral kernel of (7.3.9), i.e.,

$$(7.3.11) \quad A(r)\delta(r-\rho) + B(\rho) p.v. \frac{1}{r-\rho} + C(r, \rho),$$

⁹Our theory of precisely predictable observables so far is valid only for smooth potentials; so we must modify $\mathbf{V}(r)$ in some small neighbourhood of 0, to make it smooth. We call that a *capped* Coulomb potential.

is of the form Zv , with a distribution solution v (in the variable r) of the differential eqn. (7.3.6) with $\lambda = \frac{1}{\rho}$, and the distribution kernel (7.3.11) is L^2 , both near 0 and near ∞ .

The operator U , as a map $\mathcal{H}^2 \rightarrow \mathcal{H}^2$, is an isometry with range \mathcal{H}_{ac}^2 , and we have¹⁰.

$$(7.3.12) \quad U^*U = 1, \quad U^*(V(r)) \sim U = \frac{1}{r} = V(r).$$

In other words, the unitary U transforms the corrected potential $(\mathbf{V}(r)) \sim$ into the unperturbed $\mathbf{V}(r)$.

In the negative real axis we at most have discrete spectrum.

A discussion of the proof of the above theorem, and its link to the PDE-eigenvalue problem (7.3.4), will fill the remainder of this chapter. Especially we thought it necessary to give a detailed discussion of the separation of variables involved, although this is the standard separation of variables used for Dirac Hamiltonians with rotationally symmetric potentials.

This again is an eigenvalue problem with the “third singularity” of sec.7.1, but with many more complications appearing underway. Actually the standard methods of treating singular eigenvalue problems involving ODE-s come into play, but with very large technical difficulties, due to the fact, that this is a 4-th order problem, involving 2×2 -systems.

7.4 Separation of Variables in Spherical Coordinates

We will discuss the well known separation of variables for a Dirac equation with potentials depending on $r = |x|$ only. Here we are leaning on [So2] or [Th1].

We introduce spherical coordinates in \mathbb{R}^3 :

$$(7.4.1) \quad x_1 = r \sin \theta \cos \varphi, \quad x_2 = r \sin \theta \sin \varphi, \quad x_3 = r \cos \theta,$$

where $0 \leq r < \infty$, $0 \leq \theta \leq \pi$, $0 \leq \varphi \leq 2\pi$. Inverted get

$$(7.4.2) \quad r = |x|, \quad \theta = \arctan \frac{x_3}{\sqrt{x_1^2 + x_2^2}}, \quad \varphi = \arctan \frac{x_2}{x_1}.$$

¹⁰Note, this theorem does not make statements about completeness of the continuous spectrum addressed, nor does it discuss a possible point spectrum - or even a possibly dense domain of the operators $(\mathbf{V}(r))_j \sim$. In the proof we just will gather information about wave distributions, using well known techniques about singularities of ODE-s, and construct the unitary singular integral operator (7.3.9).

We get $\partial_x = (\partial_{x_1}, \partial_{x_2}, \partial_{x_3})^T$ in the form

$$(7.4.3) \quad \partial_x = \underbrace{\begin{pmatrix} \sin \theta \cos \varphi \\ \sin \theta \sin \varphi \\ \cos \theta \end{pmatrix}}_{e_r} \partial_r + \frac{1}{r} \underbrace{\begin{pmatrix} \cos \theta \cos \varphi \\ \cos \theta \sin \varphi \\ -\sin \theta \end{pmatrix}}_{e_\theta} \partial_\theta + \frac{1}{r \sin \theta} \underbrace{\begin{pmatrix} -\sin \varphi \\ \cos \varphi \\ 0 \end{pmatrix}}_{e_\varphi} \partial_\varphi,$$

Note, the 3 unit vectors e_r, e_θ, e_φ , at right, satisfy $e_r = \frac{x}{|x|}$, $e_\theta = \partial_\theta e_r$, $e_\varphi = \frac{1}{\sin \theta} \partial_\varphi e_r$, as well as

$$(7.4.4) \quad e_r \times e_\theta = e_\varphi, \quad e_\theta \times e_\varphi = e_r, \quad e_\varphi \times e_r = e_\theta.$$

Formula (7.4.3) may be rewritten as

$$(7.4.3') \quad \partial_x = e_r \partial_r + \frac{1}{r} e_\theta \partial_\theta + \frac{1}{r \sin \theta} e_\varphi \partial_\varphi.$$

In Diracs theory the orbital angular momenta L , the spin S , and the total angular momentum J are defined as

$$(7.4.5) \quad L = -ix \times \partial_x, \quad S = \frac{1}{2} \rho, \quad J = L + S,$$

with $\rho = \begin{pmatrix} \sigma_0 \\ 0 \end{pmatrix}$. Using $e_r \times e_r = 0$, $e_r \times e_\theta = e_\varphi$, $e_r \times e_\varphi = -e_\theta$, $x = r e_r$, and use of (7.4.3') gives

$$(7.4.6) \quad L = -ie_\varphi \partial_\theta + \frac{i}{\sin \theta} e_\theta \partial_\varphi,$$

and a calculation yields

$$(7.4.7) \quad L^2 = -\frac{1}{\sin \theta} \partial_\theta (\sin \theta \partial_\theta) - \frac{1}{\sin^2 \theta} \partial_\varphi^2.$$

Note that $-L^2$ coincides with the Beltrami-Laplace operator on the unit sphere. In particular, the Laplace operator $\Delta = \sum_1^3 \partial_{x_j}^2$ of \mathbb{R}^3 admits the form

$$(7.4.8) \quad \Delta = \partial_r^2 + \frac{2}{r} \partial_r - \frac{1}{r^2} L^2 = \frac{1}{r^2} \{ \partial_r r^2 \partial_r - L^2 \}.$$

From (7.4.3'), (7.4.4) and (7.4.6) we get

$$(7.4.9) \quad -i \partial_x = -ie_r \partial_r - \frac{1}{r} (e_r \times L).$$

The important point for this separation is that the total angular momentum

$$(7.4.10) \quad J = \frac{1}{2} \rho + \frac{i}{\sin \theta} e_\theta \partial_\varphi - ie_\varphi \partial_\theta$$

commutes with the free Dirac operator¹¹ H_0 - and also, of course, with *any* scalar potential $\mathbf{V}(r) = \mathbf{V}(|x|)$, depending on $r = |x|$ only.

Constructing H_0 in spherical coordinates we first focus on $-i\alpha\partial_x$. Here use the identity

$$(7.4.11) \quad (a\sigma)(b\sigma) = a \cdot b + ia \times b \cdot \sigma_3 ,$$

valid for the Pauli matrices $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ and any pair a, b , of 3-vectors. Similarly, if $a \cdot b = 0$, we conclude that (for $\alpha = \begin{pmatrix} 0 & i\sigma \\ -i\sigma & 0 \end{pmatrix}$ of (3.1.7)), we get

$$(7.4.12) \quad \alpha(a \times b) = -i(\alpha a)(\rho b) .$$

Using (7.4.9) and (7.4.12) get $-i\alpha\partial_x = -i(\alpha e_r)\partial_r + \frac{i}{r}(\alpha e_r)(\rho L)$, hence

$$(7.4.13) \quad H_0 = -i\alpha\partial_x + \beta = -i(\alpha e_r)\{\partial_r - \frac{1}{r}(\rho L)\} + \beta .$$

With a potential $\mathbf{V}(r)$ then H assumes the form

$$(7.4.14) \quad H = -i(\alpha e_r)\{\partial_r - \frac{1}{r}(\rho L)\} + \beta + \mathbf{V}(r) .$$

In (7.4.14) we still replace the term (ρL) by

$$(7.4.15) \quad K = \beta(\rho L + 1) ,$$

called the *spin-orbit operator*. Clearly $\rho L = \beta K - 1$, hence

$$(7.4.16) \quad H = -i(\alpha e_r)\{\partial_r + \frac{1}{r} - \frac{1}{r}\beta K\} + \beta + \mathbf{V}(r) .$$

Notice, K has the matrix form

$$(7.4.17) \quad K = \begin{pmatrix} K_0 & 0 \\ 0 & -K_0 \end{pmatrix} , \quad K_0 = \sigma L + 1 ,$$

where the 2×2 -matrix K_0 depends on angular variables θ , φ only. We have $J^2 = (L + \frac{1}{2}\rho)^2 = L^2 + \rho L + \frac{3}{4} = L^2 + \beta K - \frac{1}{4}$. So,

$$(7.4.18) \quad K = \beta(J^2 - L^2 + \frac{1}{4}) .$$

Note, the matrix (7.4.17) K commutes with β .

Regarding our separation of variables in spherical coordinates: Note, the 3 operators J^2 , J_3 , K all commute with each other; they act only on angular

¹¹For the first component L_1 of L (of 7.4.5)) one finds $[L_1, H_0] = \alpha_2\partial_{x_3} - \alpha_3\partial_{x_2}$. Also, $[\rho_1, H_0] = -i[\rho_1, \alpha_2]\partial_{x_2} - i[\rho_1, \alpha_3]\partial_{x_3}$, where $[\rho_1, \alpha_2] = -2i\alpha_3$, $[\rho_1, \alpha_3] = 2i\alpha_2$, using that $\sigma_1\sigma_2 = i\sigma_3$... So, we get $[J_1, H_0] = 0$. Similarly for the other components.

coordinates, and hence may be regarded as operators on the sphere $\mathbb{S}^3 = \{|x| = 1\}$. Actually, they are self-adjoint operators there, in proper domains, and they have a joint orthonormal base of eigenvectors¹² in the Hilbert space $L^2(\mathbb{S}^3, \mathbb{C}^4)$.

Moreover, the (matrix-)multiplication operator αe_r also depends on θ , φ only, and it also commutes with J^2 , J_3 , K , and so does the constant matrix β . But, of course, αe_r and β do not commute - they anti-commute.¹³

Let us then focus on some joint eigenvector ψ of the 3 operators J^2 , J_3 , K , on the sphere. The simplest of the 3 operators will be $J_3 = -i\partial_\varphi + \frac{1}{2}\rho_3$, by (7.4.3), (7.4.6), (7.4.10). So, we get $J_3\psi = m\psi$, with some real m . But $\rho_3 = \begin{pmatrix} \sigma_3 & 0 \\ 0 & \sigma_3 \end{pmatrix}$ where (our) $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. So $\frac{1}{2}\rho_3 - m$ is a diagonal matrix with diagonal elements equal to $-m \pm \frac{1}{2}$. The solution $\exp i(m - \frac{1}{2}\rho_3)\varphi$ of the eigenvalue equation can be continuous on \mathbb{S}^3 only if $m \pm \frac{1}{2}$ is an integer. That is, m must be a *half-number*: $m = \pm \frac{1}{2}, \pm \frac{3}{2}, \pm \frac{5}{2}, \dots$ Then, however, we get the four components ψ_j all in the form

$$(7.4.19) \quad \psi_j = c_j(\theta)e^{i(m \mp \frac{1}{2})\varphi},$$

with “-” for $j = 1, 3$, and “+” for $j = 2, 4$.

For our joint eigenvector ψ we then have

$$(7.4.20) \quad J^2\psi = \nu\psi, \quad J_3\psi = m\psi, \quad K\psi = \kappa\psi,$$

¹²The operator J^2 is self-adjoint and elliptic, on the compact manifold \mathbb{S}^3 , because its (scalar-valued) principal part equals the negative Laplace operator L^2 on \mathbb{S}^3 . Accordingly, J^2 has discrete spectrum. All its eigenspaces are finite dimensional subspaces of $C^\infty(\mathbb{S}^3, \mathbb{C}^4)$, left invariant by the operators J_3 , K . By theory of commuting self-adjoint operators in a finite dimensional space every eigenspace of J^2 is spanned by an orthonormal base of joint eigenvectors of the 3 operators. These bases may be united for an orthonormal base of $L^2(\mathbb{S}^3, \mathbb{C}^4)$, consisting of joint eigenfunctions of the 3 operators.

¹³We trivially get $[J_3, J^2] = [J_3, \beta K]$, looking at (7.4.18). In the UL-corner of this commutator matrix we get $[J_3, \sigma_1 L_1 + \sigma_2 L_2]$, evaluating to 0, using the standard commutator relations for $[\sigma_j, \sigma_i]$ and $[L_j, L_l]$. Similarly for the LR-corner. So, $[J_3, J^2] = 0$. This also implies $[J_3, K] = 0$, using (7.4.18), since J_3, K both commute with β . Furthermore, $[J^2, K] = [L^2, K]$, by (7.4.18) again. Again look at the UL-(and LR-)corner(s) only to verify that the commutator vanishes. A similar calculation, finally, shows that also $[\alpha e_r, K] = 0$. The latter implies that $[\alpha e_r, J^2] = 0$, again using the commutator relations (7.4.28) for $[L_j, L_l]$.

Let us prove $[\alpha e_r, J_3] = 0$: First look at $J_3 = -i\partial_\varphi + \frac{1}{2}\rho_3 = \begin{pmatrix} \tau & 0 \\ 0 & \tau \end{pmatrix}$, $\tau = -i\partial_\varphi + \frac{1}{2}\sigma_3$. and, $\alpha e_r = \begin{pmatrix} 0 & i\sigma e_r \\ -i\sigma e_r & 0 \end{pmatrix} = \begin{pmatrix} 0 & i\nu \\ -i\nu & 0 \end{pmatrix}$ $\nu = \sigma e_r$. So, J_3 is ψ -diagonal, and, the commutator equals $[\alpha e_r, J_3] = \begin{pmatrix} 0 & i[\tau, \nu] \\ -i[\tau, \nu] & 0 \end{pmatrix}$. So, let's get $[\tau, \nu]$: Recall, $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\sigma_1 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$, $\sigma_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, so that, with e_r of (7.4.3),

$$\nu = \sigma e_r = \begin{pmatrix} \cos \theta & ie^{-i\varphi} \sin \theta \\ -ie^{i\varphi} \sin \theta & -\cos \theta \end{pmatrix}.$$

Get $[\partial_\varphi, \nu] = [\partial_\varphi, \sigma e_r] = \begin{pmatrix} 0 & e^{-i\varphi} \sin \theta \\ e^{i\varphi} \sin \theta & 0 \end{pmatrix} = \begin{pmatrix} 0 & \zeta \\ \zeta & 0 \end{pmatrix}$, $\zeta = e^{i\varphi} \sin \theta$. Also, $[\sigma_3, \begin{pmatrix} a & b \\ c & d \end{pmatrix}] = 2\begin{pmatrix} 0 & b \\ -c & 0 \end{pmatrix}$, hence, $\frac{1}{2}[\sigma_3, \nu] = i\begin{pmatrix} 0 & \zeta \\ \zeta & 0 \end{pmatrix}$. It follows that $[\tau, \nu] = -i[\partial_\varphi, \nu] + \frac{1}{2}[\sigma_3, \nu] = 0$. So, indeed, (αe_r) commutes with J_3 .

with reals ν , κ , and a half-number m . Using formula (7.4.18) we then get $\kappa\psi = \beta(\nu\psi - L^2\psi + \frac{1}{4}\psi)$. That is,

$$(7.4.21) \quad L^2\psi = \left\{ \left(\nu + \frac{1}{4} \right) - \beta\kappa \right\} \psi$$

for the scalar differential operator $L^2 = -\Delta_S$. Writing $\psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}$ we find that (7.4.21) amounts to

$$(7.4.22) \quad L^2\psi_+ = \left(\nu - \kappa + \frac{1}{4} \right) \psi_+, \quad L^2\psi_- = \left(\nu + \kappa + \frac{1}{4} \right) \psi_- .$$

But we know all the eigenfunctions of $L^2 = -\Delta_S$: They are the spherical harmonics $Y_p^l(\theta, \varphi)$, where $l = 0, 1, \dots$, $p = 0, \pm 1, \dots, \pm l$. The corresponding eigenvalue is $\lambda_l = l(l+1)$. Organized as a suitable orthonormal base of $L^2(\mathbb{S}^3)$ we may use the functions (cf. [Mu], p.50)

$$(7.4.23) \quad Y_p^l(\theta, \varphi) = c_{lp} e^{ip\varphi} P_l^{|p|}(\cos \theta) ,$$

with certain normalization constants c_{lp} , and with the associated *Legendre* functions

$$(7.4.24) \quad P_l^k(x) = (-1)^k \frac{1}{2^l l!} (1-x^2)^{k/2} \partial_x^{k+l} (x^2-1)^l, \quad k = 0, \dots, l .$$

We choose the c_{lp} as

$$(7.4.25) \quad c_{lp} = \sqrt{\frac{2l+1}{4\pi} \frac{(l-|p|)!}{(l+|p|)!}} ,$$

then we have a complete orthonormal system of $L^2(\mathbb{S}^3)$.

Since J^2, J_3, K commute with β they also commute with $(1 \pm \beta)$. Conclusion: With $\psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}$ also the two vectors $\begin{pmatrix} \psi_+ \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ \psi_- \end{pmatrix}$ are simultaneous eigenvectors of the 3 operators. Thus we may assume that either $\psi = \begin{pmatrix} \psi_+ \\ 0 \end{pmatrix}$ or $\psi = \begin{pmatrix} 0 \\ \psi_- \end{pmatrix}$, and even our joint orthonormal base may be assumed to consist of vectors $\begin{pmatrix} \psi_+ \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ \psi_- \end{pmatrix}$ as well.

Moreover, looking at the multiplication operator $\alpha e_r(\theta, \varphi)$ we get

$$(7.4.26) \quad (\alpha e_r) \begin{pmatrix} \psi_+ \\ 0 \end{pmatrix} = -i(\sigma e_r) \begin{pmatrix} 0 \\ \psi_+ \end{pmatrix}, \quad (\alpha e_r) \begin{pmatrix} 0 \\ \psi_- \end{pmatrix} = i(\sigma e_r) \begin{pmatrix} \psi_- \\ 0 \end{pmatrix} .$$

Notice, the 4×4 -matrix αe_r is unitary and self-adjoint (i.e., a symmetry), as well as the 2×2 -matrix σe_r , for every θ, φ . Accordingly, the right hand sides in (7.4.26) again are unit vectors, and they also form an orthonormal system. Therefore, we may arrange our joint orthonormal base into a sequence of pairs $\begin{pmatrix} \psi_+ \\ 0 \end{pmatrix}$, $\begin{pmatrix} 0 \\ \psi_- \end{pmatrix}$, in such a way that for each pair the action of β is given by the 2×2 -matrix $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$,

and the action of αe_r by the 2×2 -matrix $\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$. Also, each pair spans a space of joint eigenvectors of the 3 operators, to a triple v, m, κ of eigenvalues, and we have

$$(7.4.27) \quad \psi_- = i(\sigma e_r)\psi_+, \quad \psi_+ = -i(\sigma e_r)\psi_- .$$

So, let us assume first that $\psi = \begin{pmatrix} \psi_+ \\ 0 \end{pmatrix}$. Then, looking at (7.4.22), we must have $v - \kappa + \frac{1}{4} = l(l+1)$, for some integer $l \geq 0$, and the two components ψ_+^j , $j = 1, 2$ of ψ_+ must be linear combinations of the Y_p^l , $|p| \leq l$. However, looking at (7.4.19), we conclude that $\psi_+^1 = c_1 Y_{m-\frac{1}{2}}^l$, $\psi_+^2 = c_2 Y_{m+\frac{1}{2}}^l$, this being the only way to establish proper dependence on φ .

We can establish other relations between v and κ : Observe that $(\sigma L)^2 = L^2 + \sigma_1 \sigma_2 [L_1, L_2] + \sigma_2 \sigma_3 [L_2, L_3] + \sigma_3 \sigma_1 [L_3, L_1]$, using the (anti-)commutator rules for the σ_j . Then use that $\sigma_1 \sigma_2 = i\sigma_3$, $\sigma_2 \sigma_3 = i\sigma_1$, $\sigma_3 \sigma_1 = i\sigma_2$, and also, that

$$(7.4.28) \quad [L_1, L_2] = iL_3, \quad [L_2, L_3] = iL_1, \quad [L_3, L_1] = iL_2 .$$

as verified by a calculation. So, we get $(\sigma L)^2 = L^2 - (\sigma L)$. Or, $L^2 = (\sigma L)((\sigma L) + 1)$. Looking at (7.4.17) we get

$$(7.4.29) \quad L^2 = K_0(K_0 - 1) .$$

Also, since $\rho = \begin{pmatrix} \sigma^0 \\ 0 \sigma \end{pmatrix}$, we may write $L^2 = (\rho L)^2 + (\rho L)$. So, $J^2 = L^2 + \rho L + \frac{3}{4} = (\rho L)^2 + 2(\rho L) + \frac{3}{4} = (\rho L + 1)^2 - \frac{1}{4}$. This implies

$$(7.4.30) \quad J^2 = K^2 - \frac{1}{4} ,$$

and, the corresponding for the eigenvalues v and κ :

$$(7.4.31) \quad v = \kappa^2 - \frac{1}{4} = \left(\kappa + \frac{1}{2}\right)\left(\kappa - \frac{1}{2}\right) .$$

Inserting this into (7.4.22) get

$$(7.4.22') \quad L^2 \psi_+ = \kappa(\kappa - 1)\psi_+, \quad L^2 \psi_- = \kappa(\kappa + 1)\psi_- .$$

Now, coming back to our construction of ψ_+ , we must have

$$(7.4.32) \quad \psi_+^1 = c_1 Y_{m-\frac{1}{2}}^l, \quad \psi_+^2 = c_2 Y_{m+\frac{1}{2}}^l ,$$

where the integer $l \geq 0$ satisfies

$$7.4.33) \quad l(l+1) = \kappa(\kappa - 1) ,$$

while the half-number m must be chosen such that $|m \pm \frac{1}{2}| \leq l$, either for “-” or for “+”, or for both “ \pm ”. In the latter case we can allow both $c_j \neq 0$, $j = 1, 2$. For “-” and “+” we may allow $c_1 \neq 0$ and $c_2 \neq 0$, respectively.

Note, (7.4.33) implies $\kappa = \frac{1}{2} \pm (l + \frac{1}{2})$, so, either $\kappa = l + 1$, or, $\kappa = -l$. It follows that (the eigenvalue) κ must be a (positive or negative) integer. (Note, $\kappa = 0$ is impossible, since this would give the negative eigenvalue $-\frac{1}{4}$ to the positive self-adjoint operator J^2 , by (7.4.30).)

In this way we will get a scheme of vectors ψ_+ for $\kappa = 1, 2, 3, \dots$, $j = m - \frac{1}{2} = -\kappa, \dots, \kappa - 1$, and for $\kappa = -1, -2, \dots$, with $j = m - \frac{1}{2} = \kappa - 1, \dots - \kappa$.

Specifically, for $\kappa = 1$ we get the two vectors

$$(7.4.34) \quad \psi_+^{1, -\frac{1}{2}} = \begin{pmatrix} 0 \\ Y_0^0 \end{pmatrix}, \quad \psi_+^{1, \frac{1}{2}} = \begin{pmatrix} Y_0^0 \\ 0 \end{pmatrix},$$

belonging to $(\kappa, m) = (1, -\frac{1}{2})$, and, $(1, \frac{1}{2})$, resp., where $Y_0^0 = \frac{1}{\sqrt{4\pi}}$ is the constant, of course. These two states will be related to the ground state of the atom.

Next, for $\kappa = 2$, and, $\kappa = -1$, each, we will get 4 sorts of vectors, each times:

$$(7.4.35) \quad \begin{pmatrix} 0 \\ Y_{-1}^1 \end{pmatrix}, \dots, \begin{pmatrix} Y_1^1 \\ 0 \end{pmatrix},$$

for $(\kappa, m) = (2, -\frac{3}{2})$, $(2, -\frac{1}{2})$, $(2, \frac{1}{2})$, $(2, \frac{3}{2})$, and, the one for $\kappa = -1$ is identical to (7.4.35), so far. Similarly for $\kappa = 3, -2$, $\kappa = 4, -3$, etc.

But, so far, we have not fully exploited the condition $K\psi = \kappa\psi$, or, $(\sigma L)\psi_+ = (\kappa - 1)\psi_+$, for our special ψ . This condition holds trivially for $\psi = \begin{pmatrix} \psi_+ \\ 0 \end{pmatrix}$ with the functions ψ_+ of (7.4.34), since these ψ_+ are constant, so that $\Lambda\psi_+ = 0$, $K_0\psi_+ = \psi_+$. However, for the other cases we now must fully evaluate this condition. Clearly

$$(7.4.36) \quad K_0 = \begin{pmatrix} 1 + L_3 & L_2 + iL_1 \\ L_2 - iL_1 & 1 - L_3 \end{pmatrix}.$$

We need to know how this operator applies to a spherical harmonic Y_p^l . Clearly $L_3 = -i\partial_\varphi$, so, $L_3 Y_p^l = p Y_p^l$.

So, let us focus on $L_2 \pm iL_1 = X$. From (7.4.3) and (7.4.6) we get $L_2 \pm iL_1 = (-i \cos \varphi \partial_\theta + i \cot \theta \sin \varphi \partial_\varphi) \pm i(i \sin \varphi \partial_\theta + i \cot \theta \cos \varphi) = -i(\cos \varphi \mp i \sin \varphi) \partial_\theta + \cot \theta (i \sin \varphi \mp \cos \varphi) \partial_\varphi$. This gives

$$(7.4.37) \quad X = L_2 \pm iL_1 = e^{\mp i\varphi} (-i \partial_\theta \mp \cot \theta \partial_\varphi).$$

Apply to (7.4.23): $XY_p^l / c_{lp} = e^{i(p\mp 1)\varphi} (i(P_l^{|p|})'(\cos \theta) \sin \theta \mp ip \cot \theta P_l^{|p|}(\cos \theta)) = i e^{i(p\mp 1)\varphi} \{ (P_l^{|p|})'(x) \sqrt{1-x^2} \mp p \frac{x}{\sqrt{1-x^2}} P_l^{|p|}(x) \} |_{x=\cos \theta}$.

Let us recall the meaning of P_l^k (of (7.4.24)): $P_l^k(x) = b_l^k \sqrt{1-x^2}^k \partial_x^{k+l} (x^2-1)^l$, with some constant b_l^k . Thus we get $(P_l^k)' = -\frac{kx}{1-x^2} P_l^k + \frac{1}{\sqrt{1-x^2}} \frac{b_l^k}{b_l^{k+1}} P_l^{k+1}$, and hence

$$(7.4.38) \quad \sqrt{1-x^2} (P_l^k)' + \frac{kx}{\sqrt{1-x^2}} P_l^k = \frac{b_l^k}{b_l^{k+1}} P_l^{k+1}, \quad k = 0, \dots, l.$$

Actually, to have (7.4.38) valid also for $k = l$, we must define $P_l^{l+1}(x) = 0$ as is quite natural, looking at (7.4.24), since the $(2l + 1)$ -th derivative of $(x^2 - 1)^l$ vanishes identically. Generally, for formal reason, we then also define $Y_k^l = 0$ for $|k| > l$. Looking at (7.4.24) we find that $\frac{b_l^k}{b_l^{k+1}} = -1$. Let us write $p = k\varepsilon$, $k = |p|$, $\varepsilon = \text{sgn}(p)$. So, if “ \pm ” in (7.4.37) equals $-\varepsilon$, and we write $X = X_{\pm} = X_{-\varepsilon}$, then (7.4.38) will give

$$(7.4.39) \quad X_{-\varepsilon} Y_{k\varepsilon}^l = -i \frac{c_{l,k}}{c_{l,k+1}} Y_{(k+1)\varepsilon}^l .$$

In the other case - “ \pm ” = ε the crucial term below (7.4.37) will have the wrong sign; it will read

$$(7.4.40) \quad \sqrt{1-x^2} (P_l^k)' - \frac{kx}{\sqrt{1-x^2}} P_l^k = -P_l^{k+1} - \frac{2kx}{\sqrt{1-x^2}} P_l^k .$$

Here we use a formula listed in [MO] (p.74, first formula):

$$(7.4.41) \quad P_l^{k+1} + \frac{2kx}{\sqrt{1-x^2}} P_l^k = -(l-k+1)(l+k) P_l^{k-1}, \quad 1 \leq k \leq l-1 .$$

Actually, (7.4.41) is valid also for $k = l$, if we assume $P_l^{l+1} = 0$, as introduced above. Combining then (7.4.37),..., (7.4.41) we get $X_{\varepsilon} Y_{k\varepsilon}^l = i(l-k+1)(l+k)c_{l,k} e^{i(k-1)\varepsilon\varphi} P_l^{k-1}$. Or,

$$(7.4.42) \quad X_{\varepsilon} Y_{k\varepsilon}^l = i(l-k+1)(l+k) \frac{c_{l,k}}{c_{l,k-1}} Y_{(k-1)\varepsilon}^l, \quad k = 1, \dots, l .$$

Summarizing formulas (7.4.39) and (7.4.42), we get

$$\begin{aligned} X_{\pm} Y_k^l &= q_{l,k,\pm} Y_{k\mp 1}^l, \quad k = 0, \dots, l, \\ X_{\pm} Y_{-k}^l &= q_{l,-k,\pm} Y_{k\mp 1}^l, \quad k = 0, \dots, l, \end{aligned}$$

with certain constants $q_{l,j,\pm}$. A calculation gives the following result:

- (a) $(L_2 - iL_1) Y_k^l = -i\sqrt{(l+k+1)(l-k)} Y_{k+1}^l, \quad k = 0, 1, 2, \dots, l,$
- (b) $(L_2 - iL_1) Y_{-k}^l = i\sqrt{(l-k+1)(l+k)} Y_{-k+1}^l, \quad k = 1, 2, \dots, l,$
- (c) $(L_2 + iL_1) Y_k^l = i\sqrt{(l-k+1)(l+k)} Y_{k-1}^l, \quad k = 1, 2, \dots, l,$
- (d) $(L_2 + iL_1) Y_{-k}^l = -i\sqrt{(l+k+1)(l-k)} Y_{-k-1}^l, \quad k = 0, 1, 2, \dots, l.$

Actually, since $Y_{\pm(l+1)}^l$ was defined to be 0, equation (a) and (d) are valid with any constant $q_{l,l,+}$ or $q_{l,-l,-}$, so, need to be derived only for $k < l$.

The above formulas can be brought onto a simpler (more compact) form by changing the definition of Y_p^l for $p < 0$: As Thaller does, for example, let us replace Y_p^l by $(-1)^p Y_p^l$, for $p < 0$, (while leaving Y_p^l unchanged for $p \geq 0$). The modified Y_p^l will form an orthonormal base of $L^2(\mathbb{S}^3)$ just as well, and will substitute those of (7.4.23) in every respect. Thus, from now on, (7.4.23) will define Y_p^l only for $p \geq 0$, while we have

$$(7.4.23') \quad Y_p^l(\theta, \varphi) = (-1)^p c_{lp} e^{ip\varphi} P_l^{|p|}(\cos \theta), \quad p < 0.$$

With the modified Y_p^l we now may write (c),(d), above, as

$$(7.4.43a) \quad (L_2 + iL_1)Y_p^l = i\sqrt{(l-p+1)(l+p)} Y_{p-1}^l, \quad p = 0, \pm 1, \dots, \pm l,$$

while (a),(b) assume the form

$$(7.4.43b) \quad (L_2 - iL_1)Y_p^l = -i\sqrt{(l+p+1)(l-p)} Y_{p+1}^l, \quad p = 0, \pm 1, \dots, \pm l.$$

Formulas (7.4.43) give complete control of an application of K_0 of (7.4.36) to a vector of the form $z = \begin{pmatrix} c_1 Y_p^l \\ c_2 Y_{p+1}^l \end{pmatrix}$, $p = -l - 1, -l, \dots, l$. We have

$$(7.4.44) \quad K_0 z = \begin{pmatrix} 1+p & i\sqrt{(l-p)(l+p+1)} \\ -i\sqrt{(l+p+1)(l-p)} & -p \end{pmatrix} z.$$

So, the eigenvalue problem $K_0 \psi_+ = \lambda \psi_+$ is reduced to that of the 2×2 -matrix in (7.4.44), called A , for a moment. Let $A - \frac{1}{2} = B$, then $\det(B - \mu) = 0$ amounts to $\mu = \pm(l + \frac{1}{2})$, so, A has the eigenvalues $\lambda = \frac{1}{2} \pm (l + \frac{1}{2})$, i.e., $\lambda = l + 1, -l$, as expected.

The matrix B assumes a more transparent form if we introduce the half-numbers $m = p + \frac{1}{2}$, $j = l + \frac{1}{2}$:

$$(7.4.45) \quad B = \begin{pmatrix} m & i\sqrt{j^2 - m^2} \\ -i\sqrt{j^2 - m^2} & -m \end{pmatrix}.$$

Subtracting and adding $m = p + \frac{1}{2}$ from B of (7.4.45) it becomes evident that the corresponding eigenvectors are

$$(7.4.46) \quad \psi_+ = \begin{pmatrix} i\sqrt{(l+p+1)} Y_p^l \\ \sqrt{(l-p)} Y_{p+1}^l \end{pmatrix},$$

for the eigenvalue $j = l + \frac{1}{2}$ of B - i.e., for $\kappa = l + 1$ of K_0 , and ,

$$(7.4.47) \quad \psi_+ = \begin{pmatrix} i\sqrt{(l-p)} Y_p^l \\ -\sqrt{(l+p+1)} Y_{p+1}^l \end{pmatrix},$$

for the eigenvalue $-j$ of B - i.e., for $\kappa = -l$ of K_0 .

There are some exceptions here: Above we appointed to have $p = -l - 1, -l, -l + 1, \dots, l - 1, l$, where it seems that for each such p there appear two eigenvectors ψ_+ of K_0 - one for $\kappa = l + 1$, the other for $\kappa = -l$. However, we observe that for $p = -l - 1$ (and also for $p = l$) the vector (7.4.47) is not an eigenvector. We then get $\psi_+ = \binom{i\sqrt{2l+1}Y_{-l-1}^l}{0} = \binom{0}{0}$ (and $\psi_+ = \binom{0}{\sqrt{2l+1}Y_{l+1}^l} = \binom{0}{0}$) using that we appointed $Y_{\pm(l+1)}^l = 0$. So, both components of ψ_+ vanish in these cases, and only the vector (7.4.46) - belonging to $\kappa = l + 1$ is left. The latter vector is a multiple of $\binom{0}{Y_{-l}^l}$, for $p = -l - 1$ (and of $\binom{Y_l^l}{0}$, for $p = l$). This, of course, nicely agrees with (7.4.34).

All other vectors (7.4.46),(7.4.47) have both components $\neq 0$. They are not yet normalized, but (7.4.46),(7.4.47), for a given l , form an orthogonal system spanning the space of all 2-component vectors the components of which are spherical harmonics to the eigenvector $l(l + 1)$. Evidently then, the collection of these vectors, for $l=0,1,\dots$, will form a base of the space $L^2(\mathbb{S}^3, \mathbb{C}^2)$.

It is easy to normalize our vectors ψ_+ : Since the Y_p^l are normalized, we will get the sum of the square integrals of the components equal to $2l + 1$ for each vector (7.4.46) and (7.4.47). It follows that we must divide the right hand sides of (7.4.47) and (7.4.48) by $\sqrt{2l + 1}$.

Summarizing then, introduce the (2-vector) functions $Z_{p,+}^l, l = 0, 1, 2, \dots, p = -l - 1, -l, \dots, l$, and $Z_{p,-}^l, l = 0, 1, 2, \dots, p = -l, -l + 1, \dots, l - 1$, by setting

$$(7.4.46') \quad Z_{p,+}^l = \frac{1}{\sqrt{2l + 1}} \binom{i\sqrt{(l+p+1)}Y_p^l}{\sqrt{(l-p)}Y_{p+1}^l},$$

$$(7.4.47') \quad Z_{p,-}^l = \frac{1}{\sqrt{2l + 1}} \binom{i\sqrt{(l-p)}Y_p^l}{-\sqrt{(l+p+1)}Y_{p+1}^l}.$$

These (2-vector) functions $Z_{p,\pm}^l$ we call *spin spherical harmonics* (SSH(-functions)). For each such SSH-function $z = Z_{p,+}^l$ (or $z = Z_{p,-}^l$) we then introduce the pair of (4-vectors) $\psi = \binom{z}{0}, \omega = \binom{0}{\sigma_{e_r,z}}$. Then we have the following

Theorem 7.4.1 (a) *The 4-vectors ψ and ω , taken over all SSH-functions $Z_{p,\pm}^l$, form an orthonormal base of the Hilbertspace $L^2(\mathbb{S}^3, \mathbb{C}^4)$.*

(b) *For any $z = Z_{p,\varepsilon}^l, \varepsilon = +, -,$ introduce the 2-dimensional space $\mathbf{h} = \text{span}\{\psi, \omega\}$, and then the tensor product $\mathbf{h} \otimes L^2(0 \leq r < \infty, r^2 dr)$, called $\mathcal{H}_{l,p,\varepsilon}$. Then the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ equals the orthogonal direct sum of all $\mathcal{H}_{l,p,\varepsilon}$.*

Moreover, the Dirac operator H of (7.4.14) with radially symmetric potential $\mathbf{V}(r)$ is reduced by the above orthogonal decomposition: It transforms each $\mathcal{K} = \mathcal{H}_{l,p,\varepsilon}$ into itself, and so do the 5 operators $J^2, J_3, K, \beta, \alpha e_r$.

(c) A vector u of such subspace \mathcal{K} may be uniquely written as $u = u_1(r)\psi(\theta, \varphi) + u_2(r)\omega(\theta, \varphi)$, and then may be represented by the column $\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$. Then, if $u \sim \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$, the (multiplication) operators β , (αe_r) are represented by the matrices

$$(7.4.48) \quad \beta \sim \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (\alpha e_r) \sim \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix},$$

while J^2 and J_3 and K are represented as multiplications by the real scalars κ and $\kappa^2 - \frac{1}{4}$ and $m = p + \frac{1}{2}$ (while $\kappa = l + 1$ for $\varepsilon = +$, $\kappa = -l$ for $\varepsilon = -$). The operator H then is represented by

$$(7.4.49) \quad H \sim -i \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \left\{ \partial_r + \frac{1 - \beta\kappa}{r} \right\} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \mathbf{V}(r), \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Furthermore, the operators $(1 - \Delta)$ and $\mathcal{E}](\mu + \rho \times D)$ occurring in fla's (7.4.3) and (7.4.4) are represented as

$$(7.4.50) \quad 1 - \Delta \sim \frac{1}{r} \begin{pmatrix} Z_- & 0 \\ 0 & Z_+ \end{pmatrix} r \quad \text{with } Z_{\pm} = 1 + \frac{\kappa(\kappa \pm 1)}{r^2} - \partial_r^2,$$

and

$$(7.4.51) \quad \mathcal{E} \cdot (\mu + \rho \times D) \sim G(r) = -\frac{c_f}{4r^3} \{1 - \sigma_3 \kappa + r\sigma_2\}.$$

Only the last two formulas still need a discussion: From (7.4.8) get $r(1 - \Delta)\frac{1}{r} = 1 - \partial_r^2 - \frac{1}{r^2}L^2$. But on the spaces $\mathcal{H}_{l,p,\varepsilon}$ we have $L^2 = \{\kappa^2 - \beta\kappa\}$, where β must be represented according to (7.4.49) above. This indeed confirms (7.4.50).

Regarding (7.4.51), we recall the formula

$$(7.4.52) \quad \mu + \rho \times D = -i(\alpha H_0 - D),$$

easily verified, using fla's (1.0.3). Also, with $\mathcal{E} = -\text{grad } \mathbf{V}$ and $\mathbf{V} = -c_f/r$ we get $\mathcal{E} = -\frac{c_f}{r^2}e_r$. Thus, $\mathcal{E} \cdot (\mu + \rho \times D) = i\mathcal{E}(\alpha H_0 - D) = -\frac{c_f}{r^2} \{i(\alpha e_r)H_0 - i\partial_r\}$. Using (7.4.48) and (7.4.49) we then get (7.4.51).

7.5 Highlights of the Proof of Theorem 7.3.2

In this section we will *sketch* a proof for our theorem. The various steps will be discussed in more detail in sec.'s 7.6 and 7.7, below. To simplify the discussion we will just set $c_f = -1$ here, i.e., work with $\mathbf{V}(r) = \frac{1}{r}$, noting that $-c_f$ in (7.3.6) is a factor contained in \mathbf{V} and G , hence may be taken into the eigenvalue parameter λ . One major point is that, for $\lambda > 0$, eq. (7.3.6) fails to be elliptic at the point

$r = \frac{1}{\lambda}$, inside the interval $(0, \infty)$ of definition, because the coefficient of its highest derivative vanishes there. As a consequence, not all global distribution solutions of (7.3.6) are also smooth solutions.

Curiously, eq. (7.3.6) has 10 linearly independent distribution solutions defined in the entire \mathbb{R}_+ , while normally a 4-th order 2×2 -system should have only 8. The two “extra-solutions” mean the existence of a (2-dimensional) absolutely continuous spectrum of the observable, in all of $0 \leq \lambda < \infty$.

The construction of this absolutely continuous spectrum follows the old and well known method of integrating a family $\varphi_\lambda(r)$ of “wave functions” after its parameter λ , to obtain “eigenpackets” but with the important difference that the $\varphi_\lambda(r)$ will be not functions, but distributions with singular support at $r = \frac{1}{\lambda}$. In fact, near $r = \frac{1}{\lambda}$ the singular part will be a linear combination of a delta-function and a principal value.

Checking for completeness of this absolutely continuous spectrum could be a matter of solving a Wiener-Hopf type singular integral equation over the half-line. This seems to invite application of well known Fredholm criteria for such equations (cf.[GK] or [Co12], for example) but ,so far, we do not control the behaviour of kernels near $\lambda = 0$ and $\lambda = \infty$ well enough for this.

One may have to be on guard for “spectrum at ∞ ”: For some κ the operator Z is self-adjoint and positive definite only after imposing boundary conditions at $r = 0$; We circumvent the difficulty of finding a proper domain of definition for $(\mathbf{V}(r))_j^\sim$ for uncapped Coulomb $\mathbf{V}(r)$ by defining $\text{dom}(\mathbf{V}(r))_j^\sim$ as the span of all eigenvalues and eigenpackets we will construct below.

Let us focus on (7.3.6): For $\lambda > 0$ this ODE has regular singularities at $r = 0$ and $r = \frac{1}{\lambda}$, and a Thomé-Poincaré-type singularity at $r = \infty$. At 0 and ∞ we may fix (real-valued) local bases $\varphi_j(r, \lambda)$, $\omega_j(r, \lambda)$, $j = 1, \dots, 8$, defined in $(0, \frac{1}{\lambda})$ and $(\frac{1}{\lambda}, \infty)$ according to standard rules¹⁴, and such that, at fixed r , they are power series in $\lambda - \lambda_0$ for $\lambda_0 > (or <) \frac{1}{r}$, respectively. At ∞ eq. (7.3.6) looks like $(1 - \partial_r^2)^2 v = 0$, solved by $e^{\pm r}$, $re^{\pm r}$ since all other terms carry a factor $\frac{1}{r^j}$, $j = 1, 2, 3, \dots$. Unfortunately, the two roots ± 1 of the indicial equation, for getting the Thomé normal series’ have multiplicity 2, so the standard approach does not work. However, we found that, near ∞ , the 4-th order 2×2 -system (7.3.6) may be reduced to a second order 4×4 -system of the form

$$(7.5.1) \quad w'' + a\left(\frac{1}{r}\right)w' + b\left(\frac{1}{r}\right)w = 0,$$

with convergent (4×4 -matrix-valued) power series $a(s), b(s)$, in such a way that the discussion we found in [Ho1], §62 through §65, carries over with few changes

¹⁴cf. for example [JvN], or, [Km1], or, [Ho1], or, [Na1].

and indeed supplies a set of 8 linearly independent solutions with asymptotic behaviour of the form $e^{\pm r}(c_0 + c_1 \frac{1}{r} + \dots)$, and depending analytically on λ , for fixed r and $\lambda > \frac{1}{r}$. Clearly then, at ∞ , exactly 4 of the ω_j - say, for $j = 5, \dots, 8$ - are exponentially decaying (with all derivatives). They span a space $\mathcal{T}_\infty(\lambda)$ (of dimension 4). At $r = 0$ the 8 indicial exponents are symmetric with respect to 2, insofar as $\varepsilon = (\gamma - 2)^2$ solves a product of 2 quadratic equations. Again there will be a 4-dimensional subspace $\mathcal{T}_0(\lambda)$ of local solutions - spanned by $\varphi_5, \dots, \varphi_8$ - such that $Zu \in L^2$ near 0 for $u \in \mathcal{T}_0$. [For special κ we may have to add self-adjoint boundary conditions¹⁵ to make that dimension 4.]

At the regular singularity $r = \frac{1}{\lambda}$ the indicial exponents are 2, 1, 0 with 1 of multiplicity 4 and 0, 2 each of multiplicity 2. One might expect then a local system of 8 “Frobenius-type” solutions, involving higher powers of $\log|r - \frac{1}{\lambda}|$, in view of the fact that there are multiple roots, and that any two roots differ by an integer. A careful analysis shows, however, that only the first power of $\log|r - \frac{1}{\lambda}|$ ever occurs, and then only in the form $s^j \log|s|$, $j = 1, 2, \dots$, $s = r - \frac{1}{\lambda}$. One may isolate a basis of 10 global distribution solutions, with singular support at $r = \frac{1}{\lambda}$ only - call them χ_1, \dots, χ_{10} - such that $Z\chi_j \in L^2_{loc}$ for $j = 5, \dots, 10$, while, for $j = 1, 2$,

$$(7.5.2) \quad Z\chi_j = e^j \delta(r - \frac{1}{\lambda}) + L^2_{loc}, \quad e^1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad e^2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

and, for $j = 3, 4$,

$$(7.5.3) \quad Z\chi_j = e^{j-2} p.v. \frac{1}{r - \frac{1}{\lambda}} + L^2_{loc},$$

with “ $p.v. \frac{1}{s}$ ” denoting the “principal-value distribution”

$$(7.5.4) \quad \langle p.v. \frac{1}{s}, \varphi \rangle = \lim_{\varepsilon \rightarrow 0} \int_{|s| \geq \varepsilon} \varphi(s) \frac{ds}{s}, \quad \varphi \in \mathcal{D}.$$

All $\chi_j(r, \lambda)$ are power series in $\lambda - \lambda_0$ for every $r \neq \frac{1}{\lambda_0}$, including their derivatives, so, including $Z\chi_j$.

Now we want to look for eigenfunctions and wave distributions: For $0 < \lambda < \infty$ we get

$$(7.5.5) \quad \chi_j(r, \lambda) = \sum_{l=1}^8 c_{jl}(\lambda) \omega_l(r, \lambda), \quad r > \frac{1}{\lambda}, \quad \chi_j(r, \lambda) = \sum_{l=1}^8 d_{jl}(\lambda) \varphi_l(r, \lambda), \quad r < \frac{1}{\lambda},$$

¹⁵The discussion of self-adjoint boundary conditions at singular end points follows the standard principles laid out by many authors (cf. the book [CL], for example). Note, in particular, that the indicial exponents are independent of the eigenvalue parameter λ , so they are also valid for $\lambda = \pm i$, as necessary for the study of defect spaces.

with constants c_{jl}, d_{jl} depending on λ . These relations may be differentiated arbitrarily for r , and we may introduce the “Wronskian matrices” $W_\omega(r, \lambda) = (\omega, \omega', \omega'', \omega''')$, etc. Note then that W_ω and W_φ are invertible 8×8 -matrices, while $W_\chi(r, \lambda)$ is a 10×8 -matrix, defined for $r \neq \frac{1}{\lambda}$, and of maximal rank 8. With $c = ((c_{jl}(\lambda)))$, $d = ((d_{jl}(\lambda)))$, (7.5.5) implies that $W_\chi(r, \lambda) = c(\lambda)W_\omega(r, \lambda)$, $r > \frac{1}{\lambda}$, and, $W_\chi(r, \lambda) = d(\lambda)W_\varphi(r, \lambda)$, $r < \frac{1}{\lambda}$. Therefore,

(7.5.6)

$$c(\lambda) = W_\chi(r, \lambda)W_\omega(r, \lambda)^{-1}, \quad r > \frac{1}{\lambda}, \quad d(\lambda) = W_\chi(r, \lambda)W_\varphi(r, \lambda)^{-1}, \quad r < \frac{1}{\lambda}.$$

(7.5.6) implies that $c(\lambda)$ and $d(\lambda)$ have maximal rank 8 and have convergent expansions in powers of $(\lambda - \lambda_0)$ for every $\lambda_0 > 0$.

A family $v(r, \lambda)$ of global distribution solutions will be of the form

$$(7.5.7) \quad v(r, \lambda) = \sum_{j=1}^{10} p_j(\lambda)\chi_j(r, \lambda) = \sum_{l=1}^8 \omega_l(r, \lambda) \sum_{j=1}^{10} p_j(\lambda)c_{jl}(\lambda), \quad r > \frac{1}{\lambda},$$

and,

$$(7.5.8) \quad v(r, \lambda) = \sum_{l=1}^8 \varphi_l(r, \lambda) \sum_{j=1}^{10} p_j(\lambda)d_{jl}(\lambda), \quad r < \frac{1}{\lambda}.$$

The condition $v(r, \lambda) \in \mathcal{T}_0(\lambda) \cap \mathcal{T}_\infty(\lambda)$ means that the coefficients of $\omega_1, \dots, \omega_4$, and of $\varphi_1, \dots, \varphi_4$ must vanish. that is,

$$(7.5.9) \quad \sum_{j=1}^{10} c_{jl}(\lambda)p_j(\lambda) = 0, \quad \sum_{j=1}^{10} d_{jl}(\lambda)p_j(\lambda) = 0, \quad l = 1, \dots, 4,$$

giving 8 linear conditions for the 10 unknown functions $p_j(\lambda)$. There are at least two linearly independent solutions of (7.5.9). For a point-eigenvalue λ_0 , on the other hand, we also must set $p_j(\lambda_0) = 0$, $j = 1, \dots, 4$, so that only the 6 unknowns p_5, \dots, p_{10} are left, and (7.5.8) gives an overdetermined system of 8 equations in 6 unknowns. This should be nontrivially solvable only for special λ . To prove this we need orthogonality of eigenfunctions and wave functions:

Proposition 7.5.1 (i) *Eigenfunctions to different eigenvalues are orthogonal [always with respect to the inner product of \mathcal{H}^2]. (ii) Wave distributions to different λ -values are orthogonal - in particular the [distribution-] integral $\langle u_1, u_2 \rangle$ is well defined as long as the λ -values of u_1 and u_2 are distinct. (iii) Any eigenfunction (to λ) is orthogonal to any wave function (to $\lambda' \neq \lambda$).*

This proposition follows with the standard argument, using partial integration and vanishing of boundary terms. For example, for two eigenfunctions $u_j = Zv_j$

we get

$$(7.5.10) \quad \langle u_1, u_2 \rangle = \langle Z^2 v_1, v_2 \rangle = \langle v_1, Z^2 v_2 \rangle ,$$

with partial integration and vanishing of boundary terms at 0 and ∞ [and also at $r = \frac{1}{\lambda_j}$]. Then $Z^2 v_j = \frac{1}{\lambda_j} X v_j$ with the left hand side operator in (7.3.6) called X , for a moment. Then also, we must confirm that

$$(7.5.11) \quad \langle X v_1, v_2 \rangle = \langle v_1, X v_2 \rangle .$$

Again this is a standard partial integration, and vanishing of boundary terms, using what we know about the spaces $\mathcal{T}_\zeta(\lambda)$, $\zeta = 0, \infty$.

The orthogonalities (ii) and (iii) follow similarly - one must keep in mind that the singularities of the distributions on either side never can get together, so that inner product integrals can be defined.

Any orthonormal system in our separable Hilbert space \mathcal{H}^2 is finite or countable. Hence there are at most countably many eigenvalues, i.e., the system (7.5.9) with $p_1 = \dots = p_4 = 0$ cannot be identically of rank < 6 . Notice, a 6×6 -minor $\mu(\lambda)$ will be a real power series in $\lambda - \lambda_0$, for all $\lambda_0 > 0$, and so will be its square, and even the finite sum $\Sigma(\lambda)$ of such squares. It follows that $\Sigma(\lambda)$ does not vanish identically, and, hence, that it has (at most) countably many isolated zeros, clustering only at 0 and ∞ , at most.

After this we now turn to the wave distributions. So far we only know that the system (7.5.9) is not identically (in λ) of rank < 6 . But another use of orthogonality of wave distributions shows that this system really is of rank 8 (with exceptions clustering only at $0, \infty$). [For every component of the 2-vector we can have only one (nontrivial) linear combination of δ and $p.v.$ being L^2 near $0, \infty$, or else we run into a contradiction with orthogonality.] So, then an argument described more closely in sec.7.8.1 allows construction of a pair of two global families $v^1(r, \lambda)$, $v^2(r, \lambda)$, defined for all $\lambda > 0$, writing p_j in (7.5.9) as $p_j^1(\lambda)$ or $p_j^2(\lambda)$, where the $p_j^k(\lambda)$ are smooth in λ . Then we get

$$(7.5.12) \quad Z v^k(r, \lambda) = u_1^k(\lambda) \delta(r - \frac{1}{\lambda}) + u_2^k(\lambda) p.v. \frac{1}{r - \frac{1}{\lambda}} + z^k(r, \lambda) ,$$

with $u_1^k(\lambda) = \begin{pmatrix} p_1^k \\ p_2^k \end{pmatrix}(\lambda)$, and, $u_2^k(\lambda) = \begin{pmatrix} p_3^k \\ p_4^k \end{pmatrix}(\lambda)$ [where¹⁶ the real 2×4 -matrix $U(\lambda) = (U_1, U_2)(\lambda)$, $U_j = (u_j^1, u_j^2)$ is of maximal rank 2 for all λ], and with the 2×2 -matrix $U_c = (z^1(r, \lambda), z^2(r, \lambda))$ smooth in λ and with values in L^2 , in the variable r , even if differentiated for λ . With that notation we may write the two eqs. (7.5.12) as one matrix equation:

¹⁶At first there may be a discrete exception set of λ , but it may be eliminated (cf.sec.7.8.1).

$$(7.5.12') \quad Z(v^1, v^2)(r, \lambda) = U_1(\lambda)\delta(r - \frac{1}{\lambda}) + U_2(\lambda) p.v. \frac{1}{r - \frac{1}{\lambda}} + U_c(r, \lambda) .$$

Or, if we now come back to the corresponding eigenpackets $\int d\lambda \kappa(\lambda) Z v_j(\lambda) = \int d\rho v(\rho) Z v_j(\frac{1}{\rho})$, - with $v(\rho) = \frac{1}{\rho^2} \kappa(\frac{1}{\rho}) \in C_0^\infty(\mathbb{R}_+)$, by a change of integration variable - the right hand side of (7.5.12) will supply the term

$$(7.5.13) \quad U_1(\frac{1}{\rho})v(r) + p.v. \int_0^\infty U_2(\frac{1}{\rho})v(\rho) \frac{d\rho}{r - \rho} + \int_0^\infty U_c(r, \frac{1}{\rho})v(\rho)d\rho = F(r) \in \mathcal{H}^2 ,$$

where now $v(\rho)$ must be assumed as a 2-vector-valued C_0^∞ -function. [Note, that $F(r)$ no longer is a distribution, but a function in \mathcal{H}^2 .]

In (7.5.13) there appears the distribution kernel

$$(7.5.14) \quad U^0(r, \rho) = U_1(\frac{1}{\rho})\delta(r - \rho) + p.v. \frac{U_2(\frac{1}{\rho})}{r - \rho} + U_c(r, \frac{1}{\rho}) .$$

This kernel has the following properties: (i) For fixed ρ , as a function of r only, $U^0(., \rho)$ is L^2 near 0 and ∞ (both), and has singular support at $r = \rho$ only. (ii) By orthogonality we have

$$(7.5.15) \quad W(\rho, \rho') = \int_0^\infty U^0(s, \rho)U^0(s, \rho')ds = 0 , \quad \rho \neq \rho' .$$

(iii) The distribution $W(\rho, \rho')$ defined by the above integral has singular support at $\rho = \rho'$ only and must be a $(2 \times 2$ -matrix-) multiple of $\delta(\rho - \rho')$.

All in all this indicates that we have $U^{0*}U^0$ equal to a multiplication operator (by a matrix $a^2(\rho)$, with $a(\rho)$ nonsingular). The desired unitary operator U of our theorem - unitary only as a map from \mathcal{H}^2 to the (closed) span of the functions $F(r)$ of (7.5.13) - then is defined as the operator $U = U^0 a^{-1}(r)$. This completes the discussion of our theorem.

We will get completeness of above eigenpackets if we can show that the functions F of the form (7.5.13) are dense in \mathcal{H}^2 . Or else, if the space spanned by them is not \mathcal{H}^2 then one perhaps expects that its orthocomplement is spanned by the eigenvalues obtained above.

At any rate, the issue of completeness clearly is related to the solvability of the [Wiener-Hopf-type] singular integral eq. (7.5.13), when a function $F \in \mathcal{H}^2$ is given and a function v is to be found. However, in addition we also have the orthogonality (7.5.15), perhaps leading to a better approach.

7.6 The Regular Singularities

7.6.1 The Regular Singularity at 0

The series Ansatz $v = r^\gamma(v_0 + v_1r + \dots)$ will lead to a product of 2 quadratic equations in $\varepsilon = (\gamma - 2)^2$ solved by

$$(7.6.1) \quad \varepsilon = \frac{5}{2} + (\kappa + \frac{1}{4})(\kappa - \beta) \pm \frac{1}{4}\sqrt{144(\kappa - 2\beta)(\kappa + \beta) + (\kappa - \beta + 18)^2},$$

where we must set $\beta = \pm 1$, while κ may be any nonvanishing integer.

Some special κ, β : For $\kappa = \beta$ we get $\gamma = 0, 1, 3, 4$. For $\kappa = 2\beta$ we get $\gamma = \pm\sqrt{9 + \beta/2} + 2, 2, 2$. For $\kappa = -\beta$ we get $\gamma = \pm\sqrt{9 - \beta} + 2, 2, 2$.

The radicand in (7.6.1) may become negative, but not for our choices of β, κ , so ε will always be real. Moreover, a detailed check shows that, for our choices of β, κ , ε will never be negative, so that all exponents γ remain real. We will get $\gamma = 2 \pm \sqrt{\varepsilon}$. Looking at (7.6.1) it is clear that the two terms go like $|\kappa|^2$ and $\pm|\kappa|$, so that $\varepsilon \approx |\kappa|^2$ for large $|\kappa|$, and $\sqrt{\varepsilon} \approx |\kappa|$. One verifies that the cases $\kappa = 2\beta$ and $\kappa = -\beta$ are the only cases where $\varepsilon = 0$ occurs, so that there are some roots $\gamma = 2$.

Note that we must check for squared integrability of Zu for the Frobenius type solutions $u_0r^\gamma + \dots$ (or, possibly, a term like $(u_0r^\gamma + \dots)\log r$ also might occur). But we have

$$(7.6.2) \quad Zu = Z_0u_0r^{\gamma-2} + \dots, \quad Z_0 = \kappa(\kappa - \sigma_3) - \gamma(\gamma - 1).$$

The diagonal matrix Z_0 has the elements $\kappa(\kappa - \beta) - (2 \pm \sqrt{\varepsilon})(1 \pm \sqrt{\varepsilon}) = d_\beta$, $\beta = \pm 1$, and we get $r^{\gamma-2} = r^{\pm\sqrt{\varepsilon}}$. Clearly then the $\gamma = 2 + \sqrt{\varepsilon}$ will give Frobenius solutions in L^2 , near 0, since the smallest r -exponent of Zu is nonnegative. This remains true, even if there still is a logarithmic factor. For $\gamma = 2 - \sqrt{\varepsilon}$ that exponent will be negative (except for $\kappa = -\beta$ and $\kappa = 2\beta$, and assuming that the corresponding d_β does not vanish). We need $d_\beta \neq 0$ and $\sqrt{\varepsilon} \geq \frac{1}{2}$, in order to secure a solution $u \notin L^2$ near 0. We get

$$(7.6.3) \quad d_\beta = (\kappa - \frac{\beta}{2})^2 - (\frac{3}{2} - \sqrt{\varepsilon})^2 = (|\kappa| + \sqrt{\varepsilon} - c_\beta)(|\kappa| - \sqrt{\varepsilon} + c_\beta)$$

with $c_\beta = \frac{1}{2}(3 - \beta\text{sgn}(\kappa))$. Note we get either $c_\beta = 1$ or $c_\beta = 2$. The first factor, at right of (7.6.3) will be $\neq 0$ for $|\kappa| > 2$. The second factor depends on a more careful evaluation of ε (of (7.6.1)): Set $v = |\kappa|$, $\sigma = \text{sgn}(\kappa)$, $\tau = \beta\text{sgn}(\kappa)$, for

$$(7.6.4) \quad 4\varepsilon = \{4v^2 + (\sigma - 4\tau)v + (10 - \sigma\tau)\} \pm \sqrt{145v^2 - (146 - 36\sigma)v + (37 - 36\sigma\tau)}.$$

There are 8 possibilities for the signs σ, τ and \pm in (7.6.4). In each of the 8 cases one may expand $\sqrt{\varepsilon} = |\kappa| + b_{\sigma\tau\pm} + \frac{1}{|\kappa|}p(\frac{1}{|\kappa|})$ with a constant $b_{\sigma\tau\pm}$. This gives an

expansion for the second factor at right of (7.6.3) at ∞ , of the form

$$(7.6.5) \quad |\kappa| - \sqrt{\varepsilon} + c_\beta = a_{\sigma\tau\pm} + \frac{1}{|\kappa|} p\left(\frac{1}{|\kappa|}\right),$$

where, in the 8 cases, $16a_{\sigma\tau\pm} = 19 \pm \sqrt{145}$, $29 \pm \sqrt{145}$, $27 \pm \sqrt{145}$, $21 \pm \sqrt{145}$, respectively. The smallest constant $a_{\sigma\tau\pm}$ will be ≈ 0.43 . It follows that we will have “limit point case” for all but finitely many κ - i.e., precisely 4 linearly independent solutions (of the 8) which are L^2 near 0.

Furthermore, one finds that the coefficients of the 8 Frobenius solutions are polynomials in λ , hence, for fixed r , the solutions $v(r, \lambda)$ have convergent power series expansions at λ_0 , for each $\lambda_0 < \frac{1}{r}$.

7.6.2 The Regular Singularity at $r = \frac{1}{\lambda}$

As mentioned, the indicial exponents are 2, 1, 0 with 1 a double root. Setting $s - r - \frac{1}{\lambda}$ we get 8 Frobenius solutions, of the form

$$(7.6.6) \quad \psi_1(s) = \binom{1}{0}s^2 + \dots, \psi_2(s) = \binom{0}{1}s^2 + \dots, \psi_3(s) = \binom{1}{0}s + \dots, \psi_4(s) = \binom{0}{1}s + \dots,$$

and

$$(7.6.7) \quad \psi_5(s) = \psi_3 \log |s| + \psi_{52}s^2 + \dots, \psi_6(s) = \psi_4 \log |s| + \psi_{62}s^2 + \dots,$$

and

$$(7.6.8) \quad \psi_7(s) = \binom{1}{0} + \dots + (\psi_{71}s + \dots) \log |s|, \psi_8(s) = \binom{0}{1} + \dots + (\psi_{81}s + \dots) \log |s|.$$

Eqs. (7.6.6)-(7.6.8) define just functions, in the r -intervals $(0, \frac{1}{\lambda})$ and $(\frac{1}{\lambda}, \infty)$. To obtain distributions in $\mathcal{D}'(\mathbb{R}_+)$ we must fit them together at $r_\lambda = \frac{1}{\lambda}$, and, in addition, we must check for solutions with support at the point r_λ only. It turns out that (i) there are no solutions of the latter kind (except 0). Also, (ii) one finds that *only* ψ_3 and ψ_4 may be broken at r_λ , giving raise to yet another pair $H(s)\psi_j(s)$, $j = 3, 4$, with the Heaviside function $H(s) = \frac{1}{2}(1 + \text{sgn}(s))$, we call ψ_9, ψ_{10} . For $j \neq 3, 4$, $j < 9$, the $\psi_j(r - r_\lambda) \in L^1_{loc}(\mathbb{R}_+)$ define solutions of (7.3.6) with derivatives taken in the distribution sense. But this is not true, if they are broken at r_λ (i.e., continued on the other side of r_λ with a different linear combination of the ψ_l).

We finally set $\chi_1 = \psi_9, \chi_2 = \psi_{10}, \chi_3 = \psi_5, \chi_4 = \psi_6$, and then list the remaining ψ_j as χ_5, \dots, χ_{10} - except that suitable linear combinations of ψ_5, ψ_6 must be subtracted from ψ_7, ψ_8 to eliminate the terms $\psi_{l1}s \log |s|, l = 7, 8$. It is clear then that $Z\chi_j \in L^2_{loc}$ for $j = 5, \dots, 10$, so that conditions for the system of 10 global distributions are fulfilled.

7.7 The Singularity at ∞

7.7.1 Asymptotic Behaviour of Solutions at Infinity

Observe that (7.3.6) -i.e., $\{Z R Z + G Z + Z G\}v = 0$, with $Z = 1 - \partial_r^2 + \kappa(\kappa - \sigma_3)\frac{1}{r^2}$ and the multiplications $R = \frac{1}{r} - \lambda$ and $G = \frac{1}{4r^3}(1 - \sigma_3\kappa + r\sigma_2)$ may be written in the form

$$(7.7.1) \quad (L R L + L M + M L + N)v = 0, \quad L = 1 - \partial_r^2,$$

where $M = \frac{1}{r^2}p(\frac{1}{r})$, $N = \frac{1}{r^4}q(\frac{1}{r})$ with power series $p(s), q(s)$. [In this subsection we use “ $X = p(\frac{1}{r})$ ” (or “ $Y = q(\frac{1}{r})$ ”) just to indicate that X (or Y) equals *some* power series in $\frac{1}{r}$, with positive radius of convergence]. Clearly $\frac{1}{R} = p(\frac{1}{r})$. We may write (7.7.1) in the form

$$(7.7.2) \quad \{(L+S)R(L+S)+T\}v = 0, \quad S = \frac{M}{R} = \frac{1}{r^2}p(\frac{1}{r}), \quad T = N - RS^2 = \frac{1}{r^4}q(\frac{1}{r}).$$

Introduce $u = (L + S)v$ as additional dependent variable, so that (7.7.2) is equivalent to

$$(7.7.3) \quad (L + S)v - u = 0, \quad (L + S)Ru + Tv = 0.$$

The second eq. (7.7.3) may be converted into $(L + S)u - \frac{1}{R}[\partial_r^2, R]u + \frac{T}{R}v = 0$, where (with $R = \frac{1}{r} - \lambda$) we get $-[\partial_r^2, R] = -[\partial_r^2, \frac{1}{r}] = \frac{2}{r^2}\partial_r - \frac{2}{r^3}$, so that, (7.7.3) assumes the form

$$(7.7.4) \quad (L + S)v - u = 0, \quad \frac{T}{R}v + (L + S - \frac{1}{r^2}\frac{2}{R})u + \frac{1}{r^2}\frac{2}{R}\partial_r u = 0.$$

Writing (7.7.4) matrixwise - for the 4-vector $w = \begin{pmatrix} v \\ u \end{pmatrix}$ - we get this:

$$(7.7.5) \quad \left\{ \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix} - \partial_r^2 \right\} w + \frac{1}{r^2} \frac{2}{R} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \partial_r w + \frac{1}{r^2} p(\frac{1}{r}) w = 0,$$

where $0, \pm 1$ in the matrices stand for 2×2 -blocks, so that we have 4×4 -matrices.

So, indeed, we now have converted (7.7.1) (or (7.3.6)) into a second order equation of the form (7.5.1) with (the 4×4 -matrices) $a(\frac{1}{r}) = -\frac{1}{r^2} \frac{2}{R} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$, $b(\frac{1}{r}) = -\begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix} - \frac{1}{r^2} p(\frac{1}{r})$.

It is important to notice that the first two coefficients a_0, a_1 of the power series p vanish while also $b_1 = 0$ and $b_0 = -\begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}$. The singularity of this equation at ∞ is “non-regular”, so that the standard (Frobenius) method for regular singularities fails. A *scalar* equation of this form has been discussed in all details in [Ho1], §.10, with a well readable proof - regarding asymptotic behaviour of its solutions near ∞ . An essential condition there is that the algebraic equation $\gamma^2 + a_0\gamma + b_0 = 0$

(called *indicial equation*) has distinct roots $\gamma_1 \neq \gamma_2$ [this is for scalar a, b where the γ_j are complex numbers]. Our main reason for transforming (7.7.1) into (7.7.5) is the fact, that, in the form (7.7.5), the indicial equation reads

$$(7.7.6) \quad \gamma^2 - \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix} = 0 .$$

This equation may be solved by two distinct 4×4 -matrices $\gamma = \pm\theta$, $\theta = 1 - \frac{1}{2}\nu$ where $\nu = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$. [Note, ν is nilpotent, we have $\nu^2 = 0$, hence $\theta^2 = 1 - \nu = \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}$.]

This suggests to try a generalization of Horn's technique to our case of 4×4 -matrices. It turns out that, indeed, [Ho1], ch.10 may be carried out, although with some special guidance. This is important, because the general method of Thomé normal series discussed in [CL], ch.5, for example seems to fail. Aiming at (asymptotically convergent) Thomé normal series solutions of the form

$$(7.7.7) \quad w(r) = e^{\pm\theta r} r^\gamma p\left(\frac{1}{r}\right) ,$$

(with a scalar γ), we make the matrix-substitution $w = e^{\pm\theta r} z$ in (7.7.5). Using “+” (with “-” behaving quite similarly) we get $\partial_r w = e^{\theta r}(\partial_r + \theta)z$. Accordingly, (7.7.5) assumes the form [with $\iota = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$, and switching back from z to the old notation w]

$$(7.7.8) \quad L^\sim w + \frac{1}{r^2} \frac{2}{R} \iota w' + \frac{1}{r^2} p\left(\frac{1}{r}\right) w = 0 , \quad L^\sim = -\partial_r^2 - 2\theta\partial_r .$$

Here we may make an ansatz $w = w_0 r^\gamma + w_1 r^{\gamma-1} + \dots$ with a scalar γ : The term with the highest power will be $-2\gamma\theta r^{\gamma-1}$. Since θ is nonsingular, we conclude that $\gamma = 0$, so that w appears as an ordinary power series in $\frac{1}{r}$ (taking values in \mathbb{C}^4). Starting with an arbitrary constant 4-vector w_0 one will get the usual recursion to calculate w_1, \dots , and there will be no vanishing denominators, but the formal power series obtained tend to be divergent. (Clearly one will get 4 linearly independent formal series.) For details cf. [Ho1], §62.

The formal power series obtained are asymptotically convergent to solutions of the system (7.7.8) obtained as exponential integrals, as follows: First another substitution $w \rightarrow rw$ converts (7.7.8) into

$$(7.7.9) \quad Xw = 0 , \quad X = -\partial_r^2 - 2\theta\partial_r + \frac{1}{r} p\left(\frac{1}{r}\right) \partial_r + \frac{1}{r} q\left(\frac{1}{r}\right) ,$$

with convergent power series $p(s), q(s)$ - the constant terms now are $p_0 = -2$, $q_0 = -2\theta$. In (7.7.9) we substitute a Laplace integral

$$(7.7.10) \quad w(r) = \int_0^\infty e^{rt} z(t) dt ,$$

with integration path a halfline $\arg t = \text{const.}$, in the complex t -plane. Assuming a suitable exponential behaviour of $z(t)$ this will lead us to a pair of (Volterra-type) integral equations¹⁷, to be satisfied by $z(t)$:

$$(7.7.14) \quad (2\theta + t)tz(t) + \int_0^t \{\tau P(\tau - t) + Q(\tau - t)\}z(\tau)d\tau = 0 ,$$

with the power series

$$(7.7.15) \quad P(t) = \sum_0^\infty p_j \frac{t^j}{j!} , \quad Q(t) = \sum_0^\infty q_j \frac{t^j}{j!} ,$$

using the coefficients p_j, q_j of the series for p and q .

Or also, equivalent to (7.7.14), a Volterra-type integral equation of the second kind

$$(7.7.16) \quad z(t) = (t + 2\theta)c + Yz(t) , \quad Yz(t) = -(t + 2\theta) \int_0^t \frac{d\tau}{\tau(\tau + 2\theta)} \int_0^\tau \Phi(\tau, t')z(\tau')d\tau' ,$$

with a constant 4-vector c , and

$$(7.7.17) \quad \Phi(t, \tau) = \{(2\theta + t)^{-1}(\tau P(\tau - t) + Q(\tau - t))\}_{|t} .$$

¹⁷Formally, assuming all integrals to exist, and all boundary terms of partial integrations performed to vanish we will get the correspondences

$$(7.7.11) \quad w \sim z(t) , \quad w' \sim tz(t) , \quad w'' \sim t^2z(t) , \quad \frac{1}{r^{j+1}}w \sim - \int_0^t \frac{(\tau - t)^j}{j!} z(\tau)d\tau , \quad j = 1, \dots .$$

[To see the last correspondence, let, for a moment, $\varphi_j = - \int_0^t \frac{(\tau - t)^j}{j!} z(\tau)d\tau$. Then $\varphi'_0 = -z$, and $\varphi'_j = -\varphi_{j-1}$, so that a repeated partial integration gives $\int_0^\infty e^{rt}\varphi_j(t)dt = \frac{1}{r} \int_0^\infty e^{rt}\varphi_{j-1}(t)dt = \dots = \frac{1}{r^j} \int_0^\infty e^{rt}z(t)dt$, assuming all boundary terms to vanish.] This will lead us to eq. (7.7.14) with P, Q of (7.7.15). [Note, since the power series p and q converge near 0, the series P, Q converge for all t , due to the additional denominators $j!$. Hence P, Q are entire functions of t .]

Eq. (7.7.14) is converted into (7.7.16) as follows: Multiply by $(t + 2\theta)^{-1}$ and differentiate for t , to get

$$(7.7.12) \quad (tz(t))' + (2\theta + t)^{-1}(q_0 + tp_0)z(t) + \int_0^t \Phi(t, \tau)z(\tau)d\tau = 0 ,$$

with $\Phi(t, \tau) = \{(2\theta + t)^{-1}(\tau P(\tau - t) + Q(\tau - t))\}_{|t}$. Link (7.7.12) with the homogeneous first order ODE

$$(7.7.13) \quad (tz(t))' + \frac{1}{t + 2\theta}(p_0 + \frac{1}{t}q_0)(tz(t)) = 0 .$$

Here we cast in our knowledge about $p_0 = -2$, $q_0 = -2\theta$ to get (7.7.12) into the form $(tz(t))' - \omega(t)(tz(t)) = 0$, $\omega(t) = 2 \frac{t + \theta}{t(t + 2\theta)} = \frac{1}{t} + \frac{1}{t + 2\theta}$, integrated by $z(t) = (t + 2\theta)c$, with a constant 4-vector c . [In Horn's case, this is trivial, while here we must use that p_0 and q_0 commute to get an exponential function as solution.] In (7.7.12) write the last term as $\Psi(t)$, for a moment. Then get $(tz(t))' - \omega(t)(tz(t)) + \Psi(t) = 0$. With "variation of constants" we then get (7.7.12) into the form $tz(t) = t(t + 2\theta)c - t(t + 2\theta) \int_0^t \frac{1}{\tau(\tau + 2\theta)} \Psi(\tau)d\tau$, i.e., (7.7.16), remembering the special form of Ψ .

Eq. (7.7.16) may be solved¹⁸ by a Neumann series $z(t) = z_0 + Yz_0 + Y^2z_0 + Y^3z_0 + \dots$, $z_0(t) = (t + 2\theta)c$, uniformly convergent in compact sets of the t -plane slitted along the negative real axis below -2 . Such (unique) solution $z = z_c$ is obtained for every constant 4-vector c . It is holomorphic in t in $\mathbb{C} \setminus \{t \leq -2\}$ and satisfies both (7.7.14) and (7.7.16).

To make the integral (7.7.10) exist and the equivalences (7.7.11) work, one then will need exponential estimates on such $z(t)$ along suitable rays $\arg t = \text{const}$. Reexamining coefficients of (7.7.9), they are meromorphic functions in the entire complex r -plane with poles only at $r = 0$ and $r = \frac{1}{\lambda}$. We need existence of the integral (7.7.10) for r on the half-line $r > \frac{1}{\lambda}$. For this, as it turns out, we must choose a ray $\arg t = \omega$ with $\frac{\pi}{2} \leq |\omega| \leq \pi$. Our $z(t)$ satisfies both integral eqs. (7.7.14) and (7.7.16), for any ray $\arg t = \omega$, any ω , except $\omega = \pi$. The factor e^{rt} in (7.7.10), as $r > \frac{1}{\lambda}$, will decay exponentially for $\pi \geq |\omega| > \frac{\pi}{2}$. So, we will need an exponential estimate for z along such a ray. That will follow from (7.7.14) if we obtain proper exponential estimates for the entire functions P, Q of (7.7.15). To obtain such estimates we fix a path $\mathcal{P}_{\varepsilon, \eta}$ in the complex r -plane encircling the two singularities 0 and $\frac{1}{\lambda}$ of the coefficients of (7.7.10), by following a straight segment parallel to (and above) the line $\mathcal{L}_\eta = \{y = -\eta + \lambda\eta x\}$ (with $\eta > 0$), at distance $\varepsilon > 0$ from 0 (and above 0), passing the two singularities $0, \frac{1}{\lambda}$ on \mathcal{L}_η , and then to return in the half-plane below \mathcal{L}_η (Fig.7.7.1), encircling $0, \frac{1}{\lambda}$. The line \mathcal{L}_η has unit normal $\frac{1}{\sqrt{1+\lambda^2\eta^2}}(-\lambda\eta) = \begin{pmatrix} \cos \omega \\ \sin \omega \end{pmatrix}$ with some $\omega = \omega_\eta$ between $\frac{\pi}{2}$ and π (Fig.7.7.1). Then \mathcal{L}_η is given by $\Re(re^{-i\omega}) = -\frac{\eta}{\sqrt{1+\lambda^2\eta^2}} = -\sigma(\omega)$. We have “ $>$ ” and “ $<$ ” in this relation above and below \mathcal{L}_η , respectively. Thus we have

$$(7.7.18) \quad \Re(re^{-i\omega}) \leq \varepsilon$$

along the entire path $\mathcal{P} = \mathcal{P}_{\varepsilon, \eta}$, With \mathcal{P} positively oriented we get

$$(7.7.19) \quad \int_{\mathcal{P}} p\left(\frac{1}{r}\right)r^{m-1}dr = 2\pi ip_m, \quad m = 0, 1, \dots$$

¹⁸This is a matter of estimating the operator Y to get convergence. Specify a region \mathcal{R} by taking the disk $|t| \leq \eta$ in the complex t -plane - with η large, cutting out the sector $|\arg t - \pi| \leq \varepsilon$, $|t| \geq 2 - \varepsilon$, for small $\varepsilon > 0$. Then confirm: $\frac{1}{t+2\theta} = \frac{1}{t+2} + \frac{1}{(t+2)^2}\nu$ is meromorphic with only pole at $t = -2$. Hence,

$$\begin{aligned} |t + 2\theta| &\leq c_1, \quad \left|\frac{1}{t+2\theta}\right| \leq c_2, \quad |\Phi(t, \tau)| \leq c_3, \\ \text{as } t, \tau &\in \mathcal{R}. \text{ Also, } |z_0| \leq c_1|c|. \text{ Let } z_n = Y^n z_0. \text{ Then,} \\ |z_1(t)| &\leq |c|c_1c_1c_2c_3|t| = |c|c_1^2c_2c_3|t|, \quad |z_2(t)| \leq |c|c_1^3c_2^2c_3^2\frac{|t|^2}{2!}, \dots, \\ |z_n(t)| &\leq |c|c_1^{n+1}c_2^n c_3^n \frac{|t|^n}{n!}, \dots, \text{ for all } t \in \mathcal{R}. \end{aligned}$$

This indeed insures convergence of the series $\sum Y^j z_0$ for all $t \in \mathcal{R}$. So, it defines a unique solution $z = z_c$ of (7.7.16), as specified. But we have differentiated to obtain (7.7.16) from (7.7.14). So, apriori, (7.7.16) implies only that the left hand side of (7.7.14) is constant. However, for $z(t)$ continuous near 0 that constant vanishes at $t = 0$, hence it is 0 , and we indeed have equivalence of (7.7.14) and (7.7.16). [Uniqueness of the solution is evident, of course.]

Rewrite this as

$$(7.7.20) \quad p_m = \frac{1}{2\pi i} \int_{\mathcal{P}} \left(\frac{1}{r} p\left(\frac{1}{r}\right)\right) r^m dr .$$

Then get

$$(7.7.21) \quad P(t) = \sum p_m \frac{t^m}{m!} = \frac{1}{2\pi i} \int_{\mathcal{P}} \sum \frac{t^m}{m!} r^m \left(\frac{1}{r} p\left(\frac{1}{r}\right)\right) dr = \frac{1}{2\pi i} \int_{\mathcal{P}} \left(\frac{1}{r} p\left(\frac{1}{r}\right)\right) e^{rt} dr ,$$

and, similarly,

$$(7.7.22) \quad Q(t) = \frac{1}{2\pi i} \int_{\mathcal{P}} \left(\frac{1}{r} q\left(\frac{1}{r}\right)\right) e^{rt} dr .$$

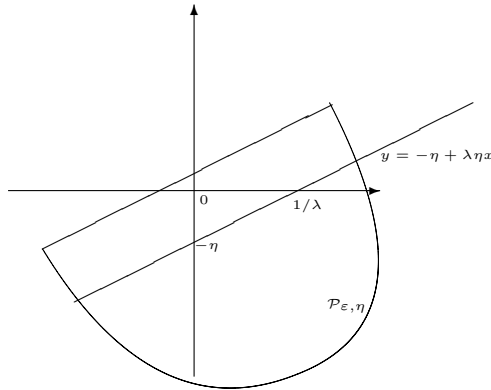


Fig. 7.7.1. A path $\mathcal{P}_{\epsilon, \eta}$ with $\Re(re^{-i\omega\eta}) \leq \epsilon$ around 0 and $\frac{1}{\lambda}$.

From (7.7.21),(7.7.22) get $|P(t)|, |Q(t)| \leq c \text{Max}\{e^{\Re(rt)} : r \in \mathcal{P}\}$ with a constant c incorporating length of \mathcal{P} and maximum of coefficients p, q along \mathcal{P} . For t with $\arg t = -\omega$ we have $t = e^{-i\omega}|t|$, $\Re(rt) = |t|\Re(re^{-i\omega}) \leq \epsilon|t|$ on all of $\mathcal{P} = \mathcal{P}_{\epsilon, \eta}$, by (7.7.18). Thus we get

$$(7.7.23) \quad |P(t)|, |Q(t)| \leq c_{\epsilon} e^{\epsilon|t|} , \text{ as } t = e^{-i\omega}|t| ,$$

with some constant c_{ϵ} for every $\epsilon > 0$. Now we estimate $z(t)$:

Proposition 7.7.1 *The solution $z(t)$ of our integral eqs. (7.7.14) and (7.7.16) satisfies*

$$(7.7.24) \quad z(e^{-i\omega}t) = O(e^{\epsilon t}) , t > 0 ,$$

for any fixed $\omega = \omega_{\eta}$ satisfying $\frac{\pi}{2} < \omega < \pi$, with $\sigma(\omega)$ of (60) - choosing $0 < \eta < \infty$.

Proof. With (7.7.14) and (7.7.23) we get

$|z(e^{-i\omega t})| \leq \frac{c}{t} \frac{1+t}{1+t} \int_0^t d\tau e^{\varepsilon(t-\tau)} |z(e^{-i\omega\tau})|$. For $\zeta(t) = \int_0^t e^{-\varepsilon\tau} |z(e^{-i\omega\tau})| d\tau$ we thus get $\zeta'/\zeta = (\log\zeta)' \leq \frac{c}{t} = (\log t^c)'$. Integrating we get

$\log(\zeta(t)/\zeta(1)) \leq \log(t^c)$. Or, $\zeta(t) \leq \zeta(1)t^c$, as $t \geq 1$. Or,

$e^{-\varepsilon t} |z(e^{-i\omega t})| \leq \frac{c}{t} \zeta(t) \leq \zeta(1)ct^{c-1}$. Finally,

$|z(e^{-i\omega t})| \leq ct^{c-1}e^{\varepsilon t} \leq ce^{2\varepsilon t}$ for all $t > 0$, q.e.d.

Now we look at $w(r)$ defined by (7.7.10), and fix the integration path as $\arg t = -\omega$ with above $\omega = \omega_\eta$, while assuming r in the half-plane below line \mathcal{L}_η . For the e -function of (7.7.10) we get $|e^{rt}| = e^{|t|\Re(re^{-i\omega})} \leq e^{-\sigma(\eta)|t|}$. Therefore, integrating along that ray $t = e^{-i\omega}\tau$, and using (7.7.24) we get

$$(7.7.25) \quad w(r) = \int_0^\infty z(t)e^{rt} dt = O\left(\int_0^\infty d\tau e^{\tau(\varepsilon - \sigma(\omega))}\right).$$

Notice the coefficient of τ in the exponent is negative (for small $\varepsilon > 0$, and the r chosen). Therefore this integral exists for all r in the half-plane below the line \mathcal{L}_η , in particular, on the real axis, for $r > \frac{1}{\lambda}$. To make the correspondences (7.7.11) work we must insure that $e^{tr} \int_0^t d\tau \int_0^\tau (\tau - \kappa)^m z(\kappa) d\kappa \rightarrow 0$ as $t \rightarrow \infty$, for r in that halfplane and t going along the integration path, and for $m = 0, 1, \dots$. But we have $z(t) = O(e^{\varepsilon|t|})$ there, hence the inner integral is $O(|t|^m e^{\varepsilon|t|}) = O(e^{(2\varepsilon|t|)})$ while the factor e^{tr} decays like $e^{-\sigma|t|}$ as $|t| \rightarrow \infty$. Thus, indeed, the above condition holds, and the $w(r)$ constructed will solve our eq. (7.7.9). All in all, thus, we constructed the desired solution of (7.7.8), for every constant 4-vector c , giving a 4-dimensional space of solutions of (7.7.5) of the form $w_c(r)e^{\theta r}$, $\theta = 1 - \frac{1}{2}\nu$, $\nu = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$. Repeating the procedure for the minus sign we get another such family of the form $w_c(r)e^{-\theta r}$ - so, all together, an 8-dimensional space of solutions of (7.7.5), and thus of (7.3.6).

7.7.2 The Asymptotic Expansion at ∞ ; Dependence on λ

Finally, let us discuss the asymptotic expansion of the solution $w(r)$ we found: Recall $z(t)$ is holomorphic in the plane slitted along $t \leq -2$, so it has a power series expansion

$$(7.7.26) \quad z(t) = \sum_{m=0}^\infty z_m t^m$$

convergent in $|t| < 2$. Observe that

$$(7.7.27) \quad \int_0^\infty t^m e^{rt} = \frac{(-1)^{m+1}}{r^{m+1}} \Gamma(m+1) = (-1)^{m+1} \frac{m!}{r^{m+1}},$$

where we must recall that the integral was taken over a ray $t = \tau e^{-i\omega}$ with $\frac{\pi}{2} < \omega < \pi$. With a complex curve integral technique we may convert such integral into an integral along the negative real axis, giving us the Gamma function. We write (7.7.26) as

$$(7.7.28) \quad z(t) = \sum_{m=0}^k z_m t^m + R_k(t) ,$$

with a “remainder” R_k bounded by $c|t|^{k+1}$ near $t = 0$. Recall, we have $|z(t)| = O(e^{\varepsilon|t|})$ on the integration path, and the same also for $R_k(t)$. Thus,

$$(7.7.29) \quad w(r) = \frac{1}{r} \sum_{m=0}^k \frac{w_m}{r^m} + S_k(r) , \quad S_k = \int_0^\infty e^{rt} R_k(t) dt , \quad w_m = (-1)^{m+1} m! z_m ,$$

where (with $\Re(re^{-i\omega}) = -\frac{\lambda r \eta}{\sqrt{1+\lambda^2 \eta^2}}$, for real r)

$$(7.7.30) \quad S_k = O\left(\int_0^\infty |t|^{k+1} e^{(\varepsilon - \lambda r \eta / \sqrt{1+\lambda^2 \eta^2})|t|} dt\right) .$$

A substitution $\tau = (\frac{\lambda r \eta}{\sqrt{1+\lambda^2 \eta^2}} - \varepsilon)|t|$ in (7.7.30) gives $S_k = O(|r|^{-k-2})$, for real $r > \frac{1}{\lambda}$, q.e.d.

Finally, dependence¹⁹ on λ : The coefficients of the DE’s (7.3.6), (7.7.5), ..., (7.7.9) all are local power series in λ as long as $r > \frac{1}{\lambda}$. Hence also the operator Y of (7.7.16) and all the terms of the Neumann series defining $z(t)$ have that property. Since the Neumann series converges uniformly (also under local change of λ) we can state the same thing for $z(t)$, in that slitted t -plane. Then even our exponential estimates are uniform under local changes of λ . It follows that also the 8 linearly independent solutions of (7.3.6) we obtained have the property that $v(r)$ (and $u(r)$) are local power series in λ whenever $\lambda > \frac{1}{r}$. Exactly 4 of them grow exponentially, the other 4 decay exponentially, as we stated in sec.7.5.

7.8 Final Arguments

7.8.1 Fitting Together our Wave Distributions

First we verify that the system (7.5.9) must be of rank 8 for all $\lambda > 0$ (with discrete exceptions). Introduce the 4×10 -matrices $C^\sim = ((c_{lj}))_{l=1,\dots,10,j=1,\dots,4}$, $D^\sim = ((d_{lj}))_{l=1,\dots,10,j=1,\dots,4}$, and then the 8×10 matrix $X = (\frac{C^\sim}{D^\sim})$. Let $X'(\lambda)$ be the 8×6 -right-most corner of X . So, we know that X' has rank 6, except at the

¹⁹For a study of similar dependence on a parameter we refer to [Ki1].

eigenvalues. Let $M_j(\lambda)$ denote the sum of the squares of all $j \times j$ -minors of X . Clearly $M_j(\lambda)$ expands into a (real-valued) power series near every real $\lambda_0 > 0$ - i.e., it is a holomorphic function of λ in some neighbourhood of \mathbb{R}_+ . We know that $M_6(\lambda)$ is not $\equiv 0$, since its right hand corner X' is not identically of rank < 6 . But we claim that also $M_7(\lambda)$ and $M_8(\lambda)$ do not vanish identically.

For, assume that $M_7(\lambda) \equiv 0$ - i.e., X is of rank 6, with countable exceptions. Pick some 6×6 -minor $\mu(\lambda)$, holomorphic and not $\equiv 0$, and let $\mu(\lambda_0) \neq 0$ for some λ_0 . Assume μ is obtained by crossing out the columns ν_1, \dots, ν_4 - but we know that we may choose $\nu_j = j$, since X' is of rank 6. This means that we may choose the 4-vector (p_1, \dots, p_4) arbitrarily - say, equal to e^j (having j -th component = 1, all others zero) - and then solve for $p_5(\lambda), \dots, p_{10}(\lambda)$, not only at $\lambda = \lambda_0$ but for all λ with countable exceptions not clustering anywhere in \mathbb{R}_+ . The functions $p_j(\lambda)$, $j \geq 5$, have denominator $\mu(\lambda)$ hence are meromorphic in a neighbourhood of \mathbb{R}_+ with poles possible on \mathbb{R}_+ . As a consequence we arrive at 4 families of wave-distributions, of the form (7.5.2)(7.5.3), but with L_{loc}^2 replaced by $L^2(\mathbb{R}_+)$: For $j=1,2$, get

$$(7.8.1) \quad Zv_j(r, \lambda) = e^j \delta(r - \frac{1}{\lambda}) + v_j^0(r, \lambda), \quad v_j^0 \in L^2, \quad e^1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad e^2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

and, for $j = 3, 4$,

$$(7.8.2) \quad Zv_j = e^{j-2} p.v. \frac{1}{r - \frac{1}{\lambda}} + v_j^0(r, \lambda), \quad v_j^0 \in L^2.$$

All $Zv_j^0(r, \lambda)$ are meromorphic in λ near \mathbb{R}_+ , for each fixed $r > 0$. However, we then find that $Zv_{1\lambda}$ and $Zv_{3\mu}$ must be orthogonal, as $\lambda \neq \mu$, while we get - setting $\eta = \frac{1}{\lambda}$, $\zeta = \frac{1}{\mu}$, for a moment - $\langle \delta(r - \eta), p.v. \frac{1}{r - \zeta} \rangle = \frac{1}{\eta - \zeta}$. We get $0 = \langle Zv_1(\cdot, \lambda), Zv_3(\cdot, \mu) \rangle = \langle \delta(\cdot - \eta), p.v. \frac{1}{\cdot - \zeta} \rangle + v_3^0(\zeta, \lambda) + p.v. \int v_1^0(r, \lambda) v_3^0(r, \mu) \frac{dr}{r - \zeta} + \int v_1^0(r, \lambda) v_3^0(r, \mu) dr$ where the last term stays bounded, as $\lambda - \mu \rightarrow 0$, and the second and third term are $O(|\log |\eta - \zeta||)$ and $O((\log |\eta - \zeta|)^2)$, as may be checked by a calculation, using the fact that the singularities of v_j^0 are generated by terms of the form $s^j \log |s|$ with $j \geq 0$. Since the first term goes like $\frac{1}{\eta - \zeta}$, we get a contradiction, and must conclude that $M_7(\lambda)$ does not vanish identically. A similar argument yields that also $M_8(\lambda)$ is not $\equiv 0$.

Then, now, we may pick an 8×8 -minor $\mu(\lambda)$, not $\equiv 0$. Assume $\mu(\lambda)$ is obtained by crossing out the columns ν_1, ν_2 from X . Then specify $(p_{\nu_1}(\lambda), p_{\nu_2}(\lambda)) \equiv (1, 0)$ (or $\equiv (0, 1)$) for two families of wave distributions of the form (7.5.12).

But there may be discrete points λ where the minor $\mu(\lambda)$ vanishes. Before we discuss these points, let us note:

For a λ with $\mu(\lambda) \neq 0$ the linear span of the two vector functions $Zv^k(r, \lambda)$, $k = 1, 2$, is characterized as the 2-dimensional null space of the system (7.5.9) - via

relation (7.5.7). This space depends smoothly on λ , both, in L^2 , and as subspace $\mathcal{Q}(\lambda) \subset \mathbb{C}^{10}$, using the base $(p_1^l(\lambda), \dots, p_{10}^l(\lambda))^T, l = 1, 2$, the latter dependence even being real analytic. If, at a λ_0 with $\mu(\lambda_0) = 0$ we still have $\text{rank}(X) = 8$ then there will be another minor $\mu^1(\lambda_0) \neq 0$. This will generate another base $(p_j^{1l}(\lambda))$, not only at λ_0 , but in some neighbourhood, where also $\mu(\lambda) \neq 0$. In other words, at such a point, only the base we constructed gets singular, but the space stays smooth (and even real analytic) in λ . Similarly, at a point λ_0 where $\text{rank}(X) < 8$ we only must show that the above two-dimensional space $\mathcal{Q}(\lambda) \subset \mathbb{C}^{10}$ continues smoothly through that point, as a local subspace of the null space of $X(\lambda_0)$, but coinciding with the null space of $X(\lambda)$, near λ_0 . Given that, we have a smooth base near each point λ of \mathbb{R}_+ and may construct a smooth global base, since \mathbb{R}_+ is contractible.

Now let $\text{rank}(X(\lambda_0)) = d < 8$. Pick d rows $x_{\nu_1}, \dots, x_{\nu_d}$ of X forming a basis at λ_0 . They still are linearly independent near λ_0 , but the rank of X must be 8 there.

WLOG assume that $X = \begin{pmatrix} I & 0 \\ S & T \end{pmatrix}$. [First multiply left by a constant 8×8 -permutation such that (ν_1, \dots, ν_d) goes into $(1, \dots, d)$. Then right by a 10×10 -permutation such that the columns of a non-vanishing minor Z are taken into the first d columns. So, we then have $X = \begin{pmatrix} Z & Y \\ R & L \end{pmatrix}$ with Z invertible. Now multiply right by (the 10×10 -matrix) $\begin{pmatrix} J & K \\ 0 & I \end{pmatrix}$ where $J = Z^{-1}$, $K = -Z^{-1}Y$. All these matrix multiplications are valid for some neighbourhood of λ_0 and they are invertible. As a result indeed we have converted X to the above form.] In fact, we even may assume $S(\lambda) = 0$, using another invertible 8×8 -left multiplication of the form $\begin{pmatrix} 1 & 0 \\ -S & 1 \end{pmatrix}$.

In this normal form we look at the equation $Xp = 0$ with $X = \begin{pmatrix} I & 0 \\ 0 & T \end{pmatrix}$ and, correspondingly, $p = \begin{pmatrix} q \\ p \end{pmatrix}$. Clearly $q(\lambda) = 0$, and also, $T(\lambda)p(\lambda) = 0$, near λ_0 , where now $T(\lambda)$ is an $(8 - d) \times (10 - d)$ -matrix, and a power series $T(\lambda) = \sum_{j=k}^{\infty} T_k(\lambda - \lambda_0)^j$, with $k \geq 1$, and $T_k \neq 0$. (We have $T(\lambda_0) = 0$, since for $\lambda = \lambda_0$ the rank is d , so all other rows must be combinations of the first d .) We may divide with $(\lambda - \lambda_0)^k$ and get the same equation with $k = 0$ - changed $T(\lambda)$. With the new $(8 - d) \times (10 - d)$ -matrix $T(\lambda)$ we may have maximal rank -i.e., $\text{rank}(T(\lambda_0)) = 8 - d$. Then we are done - just fix a minor $\mu(\lambda_0) \neq 0$ and construct a linearly independent pair $p^1(\lambda), p^2(\lambda)$ of $(10 - d)$ -vectors solving $T(\lambda)p^l(\lambda) = 0$, real analytic near λ_0 , transform back to get corresponding 10-vectors real analytic near λ_0 , and spanning $\mathcal{Q}(\lambda)$ for $\lambda \neq \lambda_0$.

Or else, we still have $\text{rank } T(\lambda_0) < 8 - d$. Then we iterate the procedure. The iteration must break off since we loose at least one dimension, at each step - from the 8 dimensions we have.

In this way, we indeed have constructed the space $\mathcal{Q}(\lambda)$ for all $\lambda > 0$, and $\mathcal{Q}(\lambda)$ has a real analytic base near each point $\lambda > 0$. As mentioned, we then may piece together a global base defined for all $\lambda > 0$ [using a countable cover of open intervals Δ_j , $j = 0, \pm 1, \pm 2, \dots$ such that Δ_j intersects with $\Delta_{j\pm 1}$ but with no other Δ_l]. That global base should be used for definition of the 2 functions (7.5.12).

7.8.2 Final Construction of the Distribution Kernel

$U(r, \rho)$ of (7.3.11)

We may write the operator U^0 with distribution kernel (7.5.14) in the form

$$(7.8.3) \quad U^0 = A(r) + K_- B(r) + C,$$

with the ‘‘Mellin convolutions’’ $K_{\pm}u(r) = p.v. \int_0^{\infty} u(\rho) \frac{d\rho}{r \pm \rho} = \int_0^{\infty} u(\rho) \frac{d\rho/\rho}{r/\rho \pm 1}$, and the matrix multiplications $A(r) = U_1(\frac{1}{r})$, $B(r) = U_2(\frac{1}{r})$, and integral operator C with kernel $C(r, \rho) = U_c(r, \frac{1}{\rho})$. Note, if $\text{rank}(A(r), B(r)) < 2$ then $\lambda = \frac{1}{r}$ must be an eigenvalue, which we know happens only at discrete points r . Focus on $\langle U^0u, U^0u \rangle$, for a $u \in C_0^{\infty}(\mathbb{R}_+)$. The operators K_{\pm} are bounded over $L^2(\mathbb{R}_+)$, and they are diagonalized by the Mellin transform; one finds that

$$(7.8.4) \quad K_{\pm}^* = \pm K_{\pm}, \quad K_-^2 = -\pi^2 + K_+^2.$$

We get

$$\begin{aligned} \langle U^0u, U^0v \rangle &= \langle u, (A^*(r) - B^*(r)K_- + C^*)(A(r) + K_-B(r) + C)v \rangle = \langle u, (A^*(r)A(r) + \pi^2 B^*(r)B(r))v \rangle - \langle u, B^*(r)K_+^2 B(r)v \rangle + \langle u, (A^*K_-B - B^*K_-A)v \rangle + \langle u, (C^*K_-)Bv \rangle - \langle u, B^*(K_-C)v \rangle + \langle u, C^*Au + A^*Cv \rangle + \langle u, C^*Cv \rangle, \quad u, v \in C_0^{\infty}(\mathbb{R}_+, \mathbb{C}^2). \end{aligned}$$

We may write $\langle U^0u, U^0v \rangle = \langle W, u^*(r) \otimes v(r') \rangle$ with the distribution kernel

$$(7.8.5) \quad W(r, r') = \int_0^{\infty} U^0(\rho, r)U^0(\rho, r')d\rho = 0, \quad r \neq r'.$$

In other words, $W(r, r')$ has support at $r = r'$. However, the above calculation shows that, with $Q = A^*A + \pi^2 B^*B$, we get

$$W(r, \rho) - Q(\rho)\delta(r - \rho) = p.v. \frac{1}{r - \rho} (A^*B - B^*A)(\rho) + C^5(r, \rho)$$

where C^5 is a function. This sum must vanish identically for $r \neq \rho$, which may happen only if $(A^*B - B^*A)(r) \equiv 0$, and $C^5 \equiv 0$.

Conclusion: The operator $W = U^{0*}U^0$ defined for C_0^{∞} -functions u, v by setting $\langle u, Wv \rangle = \langle U^0u, U^0v \rangle$ is a multiplication operator; We have

$$(7.8.6) \quad U^{0*}U^0 = (A^*A + \pi^2 B^*B)(r) = Q(r).$$

We have seen that $Q(r)$ is singular at discrete points r only, since $Q(r)\varphi = 0$, $\varphi \neq 0$ implies $A(r)\varphi = B(r)\varphi = 0$, or, $\text{rank}(A(r), B(r)) < 2$. Moreover, in proper local coordinates, we have $A(r), B(r)$ analytic near such a point r_0 . One then confirms that the matrices $A^\diamond(r) = A(r)Q(r)^{-\frac{1}{2}}$ and $B^\diamond(r) = B(r)Q(r)^{-\frac{1}{2}}$ still are power series²⁰ while $A^{\diamond*}A^\diamond + B^{\diamond*}B^\diamond = 1$. Thus, defining $U = U^0Q^{-\frac{1}{2}}(r)$, we then finally have achieved our unitary map of the theorem, since we will have $U^*U = 1$. In particular, after this correction, the matrix (U_1, U_2) is smooth and has maximal rank, as stated.

7.8.3 About the Negative Spectrum

To show that there is only discrete spectrum for $\lambda < 0$ note that $r_\lambda = \frac{1}{\lambda} < 0$ no longer belongs to \mathbb{R}_+ so eq. (7.3.6) now is elliptic; distribution solutions are C^∞ . At $r = 0$ and $r = \infty$ there is no change, regarding asymptotic behaviour of solutions: We still have the bases $\varphi_j(r, \lambda)$ and $\omega_j(r, \lambda)$ of 8 solutions each, with the spaces \mathcal{T}_0 and \mathcal{T}_∞ of sec.7.5. Defining $\chi_j(r, \lambda)$ now as the system of solutions satisfying specified initial conditions at $r = 1$ - say, $\chi_1 = e^1, \chi_2 = e^2, \dots, \chi_7''' = e^1, \chi_8''' = e^2$, all other derivatives (of order < 4) = 0, all at $r = 1$, and with $e^1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, e^2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ - we now get (7.5.5), (7.5.6) for all $r > 0$. Looking for eigenvalues or wave functions we try for $p_j(\lambda)$ with $v(r, \lambda) = \sum_1^8 p_j(\lambda)\chi_j(r, \lambda) \in \mathcal{T}_\eta$, for $\eta = 0$ and $\eta = \infty$ both. This gives the 8 eqs. (7.5.9), but with sum from 1 to 8, not from 1 to 10. The matrix of this system must be singular to obtain nontrivial solutions. The coefficients are local power series in λ again we only get discrete points unless $\det((p_{jl}(\lambda))) \equiv 0$. But a nontrivial solution now defines an eigenfunction, and there may be only countably many such, due to orthogonality. Thus, indeed, the spectrum below 0 is discrete.

7.8.4 Final Comments

We expect our unitary operator U linking V^\sim to V to map **onto** \mathcal{H}^2 - equivalent to the fact that there is **no** point spectrum of V^\sim . Note, for example, that our theorem extends trivially to the operator V_η generated from (7.3.2) by replacing Λ with $\eta\Lambda$, defining a family connecting $V = V_0$ with V^\sim . This will give a family U_η , $0 \leq \eta \leq 1$ of operators, with $U_\eta^*U_\eta = 1$. Clearly, the U_η are *semi-Fredholm* -

²⁰Using analytic perturbation theory for real symmetric 2×2 -matrices one may diagonalize $Q(r)$ near r_0 , by a unitary 2×2 -matrix depending analytically on r . With that one finds the inverse square root still a Laurent series in $r - r_0$, near r_0 , and with finitely many negative powers. Then A^\diamond, B^\diamond have the same property, but are also bounded, due to $A^{\diamond*}A^\diamond + \pi^2 B^{\diamond*}B^\diamond = 1$. So, they cannot have negative powers and must be power series, i.e., analytic near r_0 .

we have $\ker U_\eta = \{0\}$ and $\text{im } U_\eta$ is closed in \mathcal{H}^2 . A simple argument shows that $U_0 = 1$, so, the Fredholm index of U_0 is 0. If it can be proven that the family U_η is continuous in operator norm of \mathcal{H}^2 , then the Fredholm index of U_η must be zero for all η , and $\text{im } U = \text{im } U_1 = \mathcal{H}^2$ would follow. Investigation of this norm continuity seems linked to a study of asymptotic behaviour²¹ of wave distributions (7.5.12) as $\lambda \rightarrow 0$ and as $\lambda \rightarrow \infty$, as would be other approaches (through [GK] or [Co9], for example).

Note also, the 4×4 -matrix-function $\begin{pmatrix} A(r) & \pi B(r) \\ -\pi B(r) & A(r) \end{pmatrix}$, with $A(r), B(r)$ of (7.3.9), is a family of unitary 4×4 -matrices, defining an “algebra-symbol” of U .

It is not hard to derive an “A-boundedness” in the sense of [Ka1] for the perturbation $\Lambda + \Lambda^*$ of V occurring in (7.3.2), using well known estimates of the form discussed in [HLP].

²¹The behaviour of solutions of the DE (7.3.6) at all 3 singularities seems uncontrollable, as $\lambda \rightarrow 0$ or $\lambda \rightarrow \infty$, except that precisely the solutions needed for our wave distributions seem to behave well, as we found out, using models. Incidentally, we believe that norm continuity of U_η can be proven if we work with (7.3.6) in a finite interval $[r', r''] \subset \mathbb{R}_+$ imposing self-adjoint boundary conditions at r', r'' . Letting $[r', r''] \rightarrow \mathbb{R}_+$ then might give the most promising approach for solving the problem of completeness of the eigenpackets we constructed, because that Ansatz should exclude the badly behaving “other solutions”.

Chapter 8

Dirac and Schrödinger Equations; a Comparison

8.0 Introduction

In this chapter we shall venture beyond the Dirac equation - so far our only object of study - and try reflecting on other wave equations in Quantum Mechanics. Perhaps we have fortified our opinion that - for the hydrogen atom - and, more generally, any “one-particle problem” considering a single charged particle in an electromagnetic field - the Dirac equation would be preferable - i.e., more accurate, and more to the point - to the Schrödinger equation, already introduced in (3.0.2).

Physics acknowledges this point of view by introducing a “Spin number” for all elementary particles, setting this number = $\frac{1}{2}$ for electrons and protons, and then specifying the Dirac equation as responsible - by axiom - for all particles of spin $\frac{1}{2}$.

On the other hand, the Schrödinger equation still may serve as an *approximate* wave equation for the hydrogen atom. However we are *forced* to accept it as *the nonrelativistic* wave equation for multiparticle systems - such as the Helium atom, having a nucleus and two electrons or other multi-electron atoms. Perhaps we may use the “approximation element” as a reason for **not** trying to discuss precisely predictable observables, in that context: *Precision of any prediction cannot be guaranteed anyway.*

We already mentioned in the preface that *it should be possible to design an analogous theory of precisely predictable observables for the “Dirac-type equations” arising from gauge theories* of Yang-Mills and Higgs. We just have not looked at

these equations, since they are an order of magnitude more technical - although quite the same approach could be used.

Returning to Schrödinger's equation, we might note yet the harmonic oscillator - with Hamiltonian $H_{sh} = \frac{1}{2}(x^2 - \Delta)$. Its wave equation $(\partial_t + iH_{sh})\psi = 0$ seems firmly entrenched in Quantum Field Theory as the wave equation of a "light quantum". A light quantum is categorized as a particle "of spin 0", and it seems that, indeed, the Schrödinger equation of the harmonic oscillator should be the proper (and precise) wave equation for it. [We even may design a relativistic "covariance" for it - cf. [BLT], for example] So, with this example, it seems that it is not proper to completely eliminate the Schrödinger equation from our discussions. We might thus ask whether any of our above principles of precisely predictable observables can be redeveloped for the Schrödinger wave equation of the harmonic oscillator.

In one dimension this would be the equation¹

$$(8.0.1) \quad \partial\psi/\partial t + iH_{sh}\psi = 0 \text{ with } H = H_{sh} = \frac{1}{2}(D^2 + x^2) = \frac{1}{2}\left(x^2 - \frac{d^2}{dx^2}\right),$$

in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3)$.

We have the algebra $Op\psi c$ of strictly classical ψ do-s (in one dimension, and scalar, complex-valued) and note that $H_{sh} \in Op\psi c_{2e}$. Its symbol is given by $h_{sh}(x, \xi) = \frac{1}{2}(x^2 + \xi^2)$, so, clearly, H_{sh} is md-elliptic of order $2e$.

There is no analogous question to that asked in ch.3, since the symbol h_{sh} is scalar. This really should be a wave equation of only one (kind of) particle. Accordingly, we should turn to the problems raised in ch.4 and ch.5, and look at the Heisenberg representation $A \rightarrow A_t = e^{iH_{sh}t} A e^{-iH_{sh}t}$ for a self-adjoint ψ do A . We shall do this - for special ψ do-s A - in sec.8.5, below, and will find a surprising difference to the findings for Dirac Hamiltonians with time-independent potentials:

In general A_t will leave the algebra $Op\psi c$ at once, as soon as $t \neq 0$. However, A_t will return - not only to the algebra, but even to the old operator $A = A_0$ periodically, as t is a multiple of π . So, if we propose $\mathcal{P}_{sh} = Op\psi c$ as algebra of precisely predictable observables, then - it seems that operators there are precisely predictable only at certain discrete times - it is as if we have a quantization of the time as well, at least in matters of predicting observables.

In case of the Dirac equation we might find- a somewhat similar behaviour for time-dependent potentials. We observed earlier - sec.5.2, 5.1 - that the total

¹This corresponds to an oscillation frequency of $\omega = 2\pi$. A general frequency results from a scaling of independent variable, not structurally affecting the algebra we will introduce.

energy always is precisely predictable, if \mathbf{V}, \mathbf{A} are time-independent, but that this fails to be true if potentials depend on time.

We are tempted, in this connection, to point to the following (hypothetical) “experiment”:

Let the potentials \mathbf{A}, \mathbf{V} be superpositions of a (time-independent) Coulomb potential $\mathbf{V}^C = \frac{cf}{|x|}$ (and $\mathbf{A}^C \equiv 0$) and an (in space compactly supported and infinitely differentiable) electromagnetic wave $\mathbf{A}^w, \mathbf{V}^w$. The wave potentials $\mathbf{A}^w, \mathbf{V}^w$ and their first time-derivatives are arbitrarily given at $t=0$ - except that we require the “Lorentz-gauge” condition

$$(8.0.2) \quad \operatorname{div} \mathbf{A}^w + \mathbf{V}^w_{|t} = 0$$

and also that $\mathbf{A}^w, \mathbf{V}^w, \mathbf{A}^w_{|t}, \mathbf{V}^w_{|t}$ are C_0^∞ -functions of x . It then follows that the field strengths \mathcal{E}, \mathcal{B} must satisfy the Maxwell equations. Together with the gauge cdn. (8.0.2) it then follows that $\mathbf{A}^w, \mathbf{V}^w$ will satisfy the wave equation $\square \mathbf{A}^w = 0, \square \mathbf{V}^w = 0$ - together with (8.0.2) for all x, t and thus are uniquely determined by their values (and values of their first time-derivatives) at $t = 0$ for all x, t . The hyperbolic wave equation has finite propagation speed ($= 1$). Hence the x -support will stay compact for all t , but the wave will spread into 3-space and die out, of course, as $t \rightarrow \pm\infty$. At any rate, the combined potentials $\mathbf{V} = \mathbf{V}^C + \mathbf{V}^w, \mathbf{A} = \mathbf{A}^w$ are uniquely determined for all $t \in \mathbb{R}$, and they will satisfy our cdn.’s (X),(XT) of ch.3. So, our theory applies.

Here are the consequences: At each time τ the total energy $H(\tau)$ qualifies for the construction of thm. 5.1.1,(ii) insofar as its symbol $h(t, x, \xi) = \alpha(\xi - \mathbf{A}) + \beta + \mathbf{V}$ commutes with itself - although $H(\tau)$ normally will not belong to the algebra $\mathcal{P}(\tau)$. However, $H(\tau)$ is approximately predictable, insofar as a correction $Z(\tau)$ of order $-e^2$ can be found - small for large $|x|$ - such that $H(\tau) + Z(\tau)$ is precisely predictable².

In other words, while at $t = \pm\infty$ we have only the Coulomb potential - with the “radiation component $\mathbf{A}^w, \mathbf{V}^w$ ” being undetectable, so that H is precisely predictable, this will not be so for a finite τ . It should be a matter of a more precise study of the correction $Z(\tau)$, in different physical states to get information on the error of expectation value.

²But $H(t)$, for a $t \neq \tau$, needs not even to have its symbol commuting with the symbol of $H(\tau)$, except if we have a periodicity of the potentials - perhaps hinted at by our assumption on the “wave” $\mathbf{A}^w, \mathbf{V}^w$. So, such $H(t)$ does not even qualify for our approximation procedure of thm. 5.1.1.

Returning to the harmonic oscillator H_{sh} , in the sections, below, we will elaborate on the scheme outlined above: To study the time-propagation under $A \rightarrow A_t = e^{iH_{sh}t} A e^{-iH_{sh}t}$ of an algebra of ψ do-s - or it could be a similar such algebra of unbounded operators on the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$ - where the self-adjoint operators of that algebra will be considered as precisely predictable observables.

At the same time we will return to the ideas of sec.1.0, paraphrasing them in a slightly different environment³: That of a C^* -algebra obtained by “mixing” multiplication and convolution operators. Such approach [to elliptic and hyperbolic theory of partial differential equations, in the light of C^* -algebras with symbol] has fascinated us for some time. It also will cast a slightly different light onto our intents, and it will give occasion to review the earlier approach, providing help for a reader who has not looked very closely at earlier chapters.

In sec.8.1 we discuss a C^* -algebra \mathcal{A} generated by a multiplication and a convolution over $L^2(\mathbb{R}) = \mathcal{H}$. This algebra is a subalgebra of the normclosure of $Op\psi c_0$ (in 1 dimension) in $L(\mathcal{H})$ (cf.thm.1.4.1); it is generated by two operators in $Op\psi c_0$. An operator A in \mathcal{A} also has a “symbol” we call the “algebra symbol” σ_A , defined as a continuous function over a certain compact space we call the “symbol space” of \mathcal{A} . σ_A is abstractly defined, and it coincides with the values at $|x| + |\xi| = \infty$ of the “ ψ do-symbol” of A , if A belongs to $Op\psi c_0$.

In sec.8.2 we discuss the action of conjugation by e^{iLt} on the “symbol space” of the algebra \mathcal{A} - the “algebra symbol” of an operator A is defined over a “boundary” $|x| + |\xi| = \infty$ of \mathbb{R}^2 we call the symbol space of \mathcal{A} . [A ψ do A has a symbol defined over \mathbb{R}^2 , possibly with a continuous extension to our symbol space. A general operator in \mathcal{A} has its “algebra symbol” defined only over that “boundary” - it needs not to have an extension into \mathbb{R}^2 .]

Here L is a self-adjoint first order differential operator. Under reasonable conditions on the coefficients of L the algebra \mathcal{A} stays invariant under such conjugation, and it is interesting to observe the action of that conjugation on the symbol space - a flow [i.e. a 1-parameter family of automorphisms] will be generated. That flow is related to a Hamiltonian flow similar to those studied in ch’s 4 and 5.

In sec.8.3 and sec.8.4 we review our concept of strictly classical ψ do-s - in this 1-dimensional case, and bring things into correspondence with earlier chapters. Especially also we will fit the case of the Dirac Hamiltonian $L = H$ with H of (1.0.2) - going into $L^2(\mathbb{R}^3, \mathbb{C}^4)$ again, where similar C^* -algebras may be studied.

³This chapter is composed, using notes of a lecture presented at Berkeley in April 2004.

One then might consider to define the self-adjoint operators of the algebra \mathcal{A} - and other self-adjoint operators “within reach of \mathcal{A} ” as *precisely predictable observables*, for the “photon Hamiltonian” H_{sh} . In sec.8.5 then we discuss the corresponding Heisenberg representation - i.e., conjugation with $e^{-iH_{sh}t}$, using our second order Hamiltonian H_{sh} . While the Hamiltonian flow generated by the first order PDE $\dot{\psi} + iL\psi = 0$ of sec.8.2 could be interpreted as “introducing a motion of the algebra symbol space”, in the first order case, this is no longer so for the second order operator $L = H_{sh}$, an explanation for the basically different behaviour we experience here.

Instead the entire algebra \mathcal{A} will suffer a “motion into a different C^* -subalgebra of $L(\mathcal{H})$ ”. But this will be a “periodic motion”, insofar as $\mathcal{A}_t = e^{itH_{sh}}\mathcal{A}e^{-itH_{sh}} = \mathcal{A}$ for all $t = j\frac{\pi}{2}$, $j = 0, \pm 1, \pm 2, \dots$

Proofs are omitted (or only sketched), in this last chapter, as this merely is to serve as a general orientation.

8.1 What is a C^* -Algebra with Symbol?

To discuss the simplest nontrivial case, let $\mathcal{H} = L^2(\mathbb{R})$, and define the two bounded linear operators

$$(8.1.1) \quad s(x) = \frac{x}{\sqrt{1+x^2}}, \quad S = s(D) = F^{-1}s(x)F,$$

where $s(x)$ acts as a multiplication operator, while F denotes the Fourier transform $Fu(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ix\xi}u(x)dx$, $u \in \mathcal{S}$. Recall S is a singular convolution operator,

$Su(x) = \frac{1}{\sqrt{2\pi}} \int dy s^\vee(x-y)u(y)dy$ with $s^\vee(z) = \frac{1}{\sqrt{\pi}}\text{sgn}(z)K_1(|z|)$ with the modified Hankel function K_1 . This function has a singularity like $\frac{1}{z}$ at $z = 0$ and the integral is a Cauchy principal value.

We have operator norms $\|s(x)\| = \|S\| = 1$ (since F is unitary). Each of the operators generates a commutative C^* -subalgebra of $L(\mathcal{H})$, called \mathcal{A}_x and \mathcal{A}_D , respectively. Clearly, $\mathcal{A}_x = C([-\infty, +\infty])$, and, $\mathcal{A}_D = F^{-1}C([-\infty, +\infty])F$, with the “closed real line” $[-\infty, +\infty]$.

We observe that **the commutator $[s(x), S]$ is a compact operator**. Moreover, if we mix both algebras - i.e., use both $s(x)$ and $S = s(D)$ to generate a C^* -subalgebra \mathcal{A} of $L(\mathcal{H})$, then

- (i) \mathcal{A} contains the entire ideal $K(\mathcal{H}) \subset L(\mathcal{H})$ of compact operators, and
- (ii) **The quotient algebra \mathcal{A}/\mathcal{K} is a commutative (abstract) C^* -algebra.**

As a commutative C^* -algebra with unit it has a compact maximal ideal space \mathcal{M} , and it must be isometrically isomorphic to the space $C(\mathcal{M})$ of continuous

(complex-valued) functions over \mathcal{M} (cf. [Lo1],[Dx1]).

To each operator $A \in \mathcal{A}$ one may associate the continuous function $\sigma_A(m) : m \in \mathcal{M}$ representing its coset modulo \mathcal{K} . σ_A is called the (*algebra*) *symbol* of A , and this defines a homomorphism $\mathcal{A} \rightarrow C(\mathcal{M})$.

Theorem 8.1.1 (elliptic theory) *An operator $A \in \mathcal{A}$ is Fredholm if and only if its symbol $\sigma_A(m)$ does not vanish anywhere on \mathcal{M} .*

One then will ask about the nature of the space \mathcal{M} , and about explicit formulas for operators - like the generators, for example: The “symbol space” \mathcal{M} is a subspace of the product $[-\infty, +\infty] \times [-\infty, +\infty]$ (with the “closed real line” $[-\infty, +\infty] = \{-\infty \leq x \leq +\infty\}$) thought of as a rectangle \mathcal{R} with coordinates (x, ξ) (see Fig.8.1.1). It coincides with the boundary of \mathcal{R} . Moreover, then, we have $\sigma_{a(x)} = a(x)$, $\sigma_{b(D)} = b(\xi)$ for $(x, \xi) \in \mathcal{M}$, and every $a(x) \in \mathcal{A}_x$, $b(D) \in \mathcal{A}_D$. Specifically, $\sigma_{s(x)} = s(x)$, $\sigma_S = s(\xi) = \frac{\xi}{\sqrt{1+\xi^2}}$.

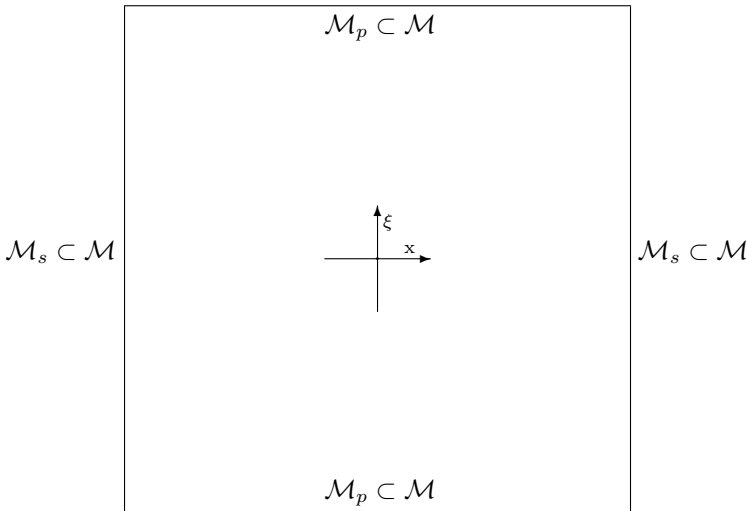


Fig. 8.1.1. The symbol space \mathcal{M} of the algebra \mathcal{A} is a square at $|x| + |\xi| = \infty$, consisting of the principal symbol space \mathcal{M}_p (at $|\xi| = \infty$) and the secondary symbol space (at $|x| = \infty$). The space \mathcal{M} is defined as the maximal ideal space of the (commutative) quotient algebra $\mathcal{A}/\mathcal{K}(\mathcal{H})$. An operator $A \in \mathcal{A}$ is Fredholm if and only if its symbol does not vanish on \mathcal{M} .

The roots of this result go back to F.Noether (cf. [No1] (in 1921)), or, in its n-dimensional (C^* -algebra-) version to I. Gohberg (cf. [Go1](in (1960))). The above theorem is a special case of the algebra \mathcal{S} discussed in [CH] (or cf. [Co11], ch.IV). We are used to call \mathcal{A} the *comparison algebra* of the differential operator $1 - \partial_x^2$ - as compared to similar algebras generated by more general second order elliptic PDO-s (cf.[Co14]).

This really holds the **key of elliptic theory** of linear PDE - there are multiple extensions to (i) differential operators; (ii) systems; (iii) domains with boundary; (iv) manifolds; (v) noncompact manifolds with edges (or conical points) on its boundary; (vi) L^p -spaces and other Banach spaces (and even Fréchet spaces).

8.2 Exponential Actions on \mathcal{A}

After “elliptic theory” we now come to “hyperbolic theory”: For this, consider a first order self-adjoint linear differential operator:

$$(8.2.1) \quad H = ia(x)\frac{d}{dx} + \frac{i}{2}a'(x) + b(x) ,$$

with real-valued functions a, b defined over \mathbb{R} . We want a, b to be $C^\infty(\mathbb{R})$ and to satisfy some growth conditions:

$$(8.2.2) \quad a^{(j)}(x), b^{(j)}(x) = O((1 + |x|)^{1-j}) , \quad j = 0, 1, 2, \dots .$$

Let us assume that the differential operator H has a unique self-adjoint realization⁴ - a (possibly unbounded) self-adjoint operator, defined in some dense subspace of \mathcal{H} . Then there is a well defined (strongly continuous) group $U(t) = e^{-itH}$ of unitary operators, with “infinitesimal generator” H , and such that (i) $U(t)\text{dom}(H) \subset \text{dom}(H)$, and (ii) $u(t) = U(t)u_0$ satisfies the differential equation $\frac{du}{dt} + iHu = 0$ and initial condition $u(0) = u_0$, for each $u_0 \in \text{dom}(H)$.

Now we ask for the “action” (by conjugation) of such $U(t)$ on our algebra \mathcal{A} with symbol. More precisely, we ask for details on the (operator-valued) function

$$(8.2.3) \quad A_t = U(t)^*AU(t) , \quad t \in \mathbb{R} ,$$

where $A \in \mathcal{A}$ is any operator. First question: For $a \in \mathcal{A}$, do we have $A_t \in \mathcal{A}$ for all (or some) t ? If yes, then this defines a family of automorphisms $\mathcal{A} \rightarrow \mathcal{A}$ (because clearly the map is invertible, since U is invertible). Such automorphism evidently would induce a homeomorphism $\mathcal{M} \rightarrow \mathcal{M}$ onto itself. So then, if the answer to (i) is affirmative, one would ask: (ii) Describe in detail this (group of) homeomorphisms.

3 special examples: For $H = D = -i\partial_x = -i\frac{d}{dx}$ we will get the translation operator $(U(t)u)(x) = u(x - t)$; For $H = x$ =multiplication by x (also fitting the assumptions) we get the “Fourier translation” (multiplication operator) $U(t) =$

⁴Actually this condition may be dropped: in [Co5],ch.6 we discuss existence of the group $U(t)$ even for $\nu \times \nu$ -matrix-valued systems H under much more general assumptions, and without looking at self-adjoint realizations

e^{-itx} (amounting to translation of the Fourier transform. It is not hard to verify that, in these cases, the action on the symbol space \mathcal{M} corresponds to these translations: For e^{-iDt} the points on the vertical lines of the square stay fixed, while those on the horizontal lines are translated. Vice versa for e^{-ixt} - horizontal and vertical interchanged. As a third example consider the case $H = ix\partial_x + \frac{i}{2}$. This operator is non-elliptic at $x = 0$, but still one easily finds that there is a unique self-adjoint realization, using the fact that $(H \pm i)u = 0$ does not have any global distribution solutions in $L^2(\mathbb{R})$. The function $u(t) = U(t)u_0 = e^{-iHt}u_0$ then will solve the (hyperbolic) PDE $u|_t = iHu = -xu|_x - \frac{1}{2}u$, or, $u|_t + xu|_x + \frac{1}{2}u = 0$. This operator H generates the group of *dilations*. Set $u(t, x) = u_0(xe^{-t})e^{-t/2}$, for some $u \in \mathcal{S}$. Clearly $u(0, x) = u_0(x)$ while $u|_t = -\frac{1}{2}u - xu|_x$. So, $u(t, x)$ solves our initial-value problem. Notice then that $U(t)$ is the unitary dilation operator, dilating x into γx , with $\gamma = e^{-t}$. The Fourier transform of that dilation operator proves to be dilation by $\frac{1}{\gamma} = e^t$. Applying this knowledge to our generators (8.1.1) one finds that (i) the algebra \mathcal{A} again is left invariant under conjugation by $U(t)$ (ii) the corresponding transformation of the symbol space \mathcal{M} is generated by dilating the sides $\xi = \pm\infty$ with $\gamma = e^{-t}$, and the sides $x = \pm\infty$ with $\frac{1}{\gamma} = e^t$.

It turns out that, in general, the 3 above cases can serve as models, insofar as our result considers 3 types of operators, along these prototypes⁵.

In the general case, it is clear that $u(t) = U(t)u_0$, for $u_0 \in \text{dom}(H)$, must solve the first order linear PDE $\partial_t u + iHu = 0$, i.e.,

$$(8.2.4) \quad \partial_t u - a\partial_x u + (-\frac{1}{2}a' + ib)u = 0, \quad u(x, 0) = u_0(x).$$

An initial value problem of this kind may be solved “explicitly”, in the following sense: Focus on curves in the (x, t) -plane given by $x=x(t)$ with

$$(8.2.5) \quad \frac{dx}{dt} = -a(x(t)), \quad x(0) = x_0.$$

Then, along such a curve, set $\varphi(t) = u(x(t), t)$, $\gamma(t) = \frac{1}{2}a'(x(t)) - ib(x(t))$. Equation (8.2.4) then amounts to

$$(8.2.6) \quad \frac{d\varphi}{dt} = u|_t + u|_x \frac{dx}{dt} = u|_t - au|_x = (\frac{1}{2}a' - ib)\varphi = \gamma\varphi, \quad \varphi(0) = u_0(x_0).$$

Note, (8.2.5) is an ODE with general solution $-\int \frac{dx}{a(x)} = t + c$. Its solutions fill the entire (x, t) -plane, as a family of non-intersecting curves. Also, (8.2.6) is a first order linear homogeneous ODE (for $\varphi(t)$), solved by

$$(8.2.7) \quad u(x(t), t) = \varphi(t) = \varphi(0)e^{\int_0^t \gamma(\tau)d\tau} = u_0(x_0)e^{\int_0^t (\frac{1}{2}a'(x(\tau)) - ib(x(\tau)))d\tau}.$$

⁵We are describing here the one-dimensional case of our result in [Co2] (also found in [Co5], ch.9).

In other words, at (x, t) one must follow the solution curve through that point backward to the line $t = 0$ to obtain some $(x_0, 0)$. Then the value $u(x, t)$ is given as $u(x(t), t)$ of (8.2.7) with that x_0 .

Now, regarding the action of $U(t)$ on our algebra, for any bounded operator $A \in L(\mathcal{H})$ let $A_t = U(t)^*AU(t)$. Then

$$(8.2.8) \quad \frac{d}{dt}A_t = i[H, A_t] , \quad A_0 = A .$$

Formally, we might regard (8.2.8) as an evolution equation determining A_t ; we might write $A_t = e^{-iad_H t}A$ with $ad_H A = [A, H]$. However, to really solve (8.2.8) it will be practical to introduce the concept of “pseudodifferential operator” (abbrev. ψ do):

Note, the special form of our second generator $S = s(D)$ using convolution with a modified Hankel function, quoted initially: This also may be written in the form (8.2.9), below, with $a(x, \xi) = s(\xi)$ (independent of x). Similarly, the first generator $s(x)$ can be given this form, with $a(x, \xi) = s(x)$. A differential operator $A = \sum_{j=1}^N a_j(x)D^j$ with coefficients $a_j(x) \in C^\infty(\mathbb{R})$ again may be written in that way, choosing $a(x, \xi) = \sum a_j(x)\xi^j$. Again, all operators of the algebra \mathcal{A}^0 finitely generated from $s(x)$ and $S = s(D)$ of (8.1.1) are ψ do’s; they may be written in that form

$$(8.2.9) \quad Au(x) = \frac{1}{2\pi} \int d\xi dy e^{i\xi(x-y)} a(x, \xi)u(y) , \quad u \in \mathcal{S} ,$$

with a function $a(x, \xi)$ also called the (ψ do-)symbol of A .

In fact, for every $A \in \mathcal{A}^0$ the “algebra symbol” σ_A equals the restriction to $\mathcal{M} = \partial\mathcal{R}$ of the continuous extension to \mathcal{R} of the corresponding ψ do-symbol $a(x, \xi)$ defining A through (8.2.9).

On the other hand, the general operator $A \in \mathcal{A}$ has a symbol *only* defined on $\mathcal{M} = \partial\mathcal{R}$, and there is not necessarily an extension a to \mathcal{R} such that $A = a(x, D)$ can be represented in the form (8.2.9).

We will be forced now to work in a (slightly) larger algebra generated by more general ψ do’s, mainly, because we need this “interpolation”, i.e., this extension of the algebra symbol from the “boundary” \mathcal{M} to the entire rectangle \mathcal{R} .

8.3 Strictly Classical Pseudodifferential Operators

Notice that (8.2.9) also may be expressed in the form (corresponding to (1.0.14) or (1.2.1))

$$(8.3.1) \quad a(x, D)u(x) = (2\pi)^{-1/2} \int d\xi e^{ix\xi} a(x, \xi)u^\wedge(\xi) , \quad u \in \mathcal{S} .$$

Or else,

$$(8.3.2) \quad a(x, D)u(x) = (2\pi)^{-1/2} \int dy a^{\vee^2}(x, x - y)u(y)dy, \quad u \in \mathcal{S},$$

with “ \vee^2 ” denoting inverse Fourier transform with respect to the second argument ξ of $a(x, \xi)$. The integral in (8.3.2) generally will be a “distribution integral” - value of the temperate distribution $a^{\vee^2}(x, x - \cdot)$ at the testing function $u \in \mathcal{S}$. We impose the following

Condition (1.2.2)₀ on our symbols $a(x, \xi)$:

$$a(x, \xi) \text{ is } C^\infty(\mathbb{R}^2). \text{ We have } \partial_x^k \partial_\xi^l a(x, \xi) = O((1 + |x|)^{-k}(1 + |\xi|)^{-l}) \quad \forall k, l \geq 0.$$

Symbols of operators $A \in \mathcal{A}_0$ [defined as the algebra finitely generated by $s(x)$ and $s(D)$] satisfy $\text{cdn.}(1.2.2)_0$. Vice versa, general symbols satisfying $(1.2.2)_0$ need not define operators in \mathcal{A} , although all such operators belong to $L(\mathcal{H})$ (cf.thm.1.4.1). We denote the class of symbols satisfying $(1.2.2)_0$ by ψc_0 , and the corresponding class of operators by $Op\psi c_0$ and denote its closure (in operator norm of \mathcal{H}) by \mathcal{A}_b . It turns out that $\mathcal{A}_b \supset \mathcal{A}$ also is a C^* -algebra with compact commutator. Its symbol is defined on a compact space \mathcal{M}_b “over” \mathcal{M} - that is, the points of \mathcal{M} split into an infinity of points of \mathcal{M}_b , in the manner of a Stone-Cech compactification (cf.[Co5],ch.V, sec.10).

We need the (slightly larger) algebra \mathcal{A}_b because we now claim that, assuming (8.2.2), with slight additional precautions, \mathcal{A}_b indeed is invariant under the action $A \rightarrow A_t$ [while we have not checked this in detail for \mathcal{A}]. Also, as will be seen shortly, use of ψ do-s seems to be unavoidable here, because the generators $s(x), S$ propagate only as ψ do’s.

Returning to equations (8.2.8), we now make the Ansatz $A_t = a(x, D; t)$ with a symbol $a_t(x, \xi) = a(x, \xi; t) \in \psi c_0$, for all t (and differentiability conditions, stated later on). Here it must be mentioned that there is a “calculus of ψ do’s” within $Op\psi c_0$ which makes it an (adjoint invariant) algebra. This is given by a couple of Leibniz-formulas (corresponding to (1.0.8) and (1.0.9))

$$(8.3.3) \quad a(x, D)b(x, D) = c(x, D), \quad a(x, D)^* = a^*(x, D),$$

where c, a^* are given as asymptotically convergent infinite series

$$(8.3.4) \quad c(x, \xi) = \sum_{j=0}^{\infty} \frac{(-i)^j}{j!} a^{(j)}(x, \xi) b_{(j)}(x, \xi), \quad a^*(x, \xi) = \sum_{j=0}^{\infty} \frac{(-i)^j}{j!} a_{(j)}^{(j)}(x, \xi),$$

Here we have $c, a^* \in \psi c_0$ whenever $a, b \in \psi c_0$. We denoted differentiation with respect to x and ξ by $\cdot^{(j)}$ and $\cdot_{(j)}$ resp. Using this we may express the commutator

$[H, a_t(x, D)]$ as a ψ do with symbol expressed as an asymptotic series

$$(8.3.5) \quad [H, a_t(x, D)] = p_t(x, D) , \quad p_t = -i(h_{1|\xi}a_{t|x} - a_{t|\xi}h_{1|x}) + \dots .$$

For this note that H of (8.2.1) is a ψ do in $\text{Op}\psi c_e$ (of order $e=(1,1)$) an extended class⁶ of (strictly classical) ψ do's for which (8.3.3) (8.3.4) holds as well, with slightly changed meanings. The symbol of H is $h(x, \xi) = -a(x)\xi + \frac{i}{2}a'(x) + b(x)$. The remainder "... " in (8.3.5) may not be small, but it will be "of lower order". That is (essentially) it will be small, as (x, ξ) approaches $\mathcal{M} = \partial\mathcal{R}$. One might thus decide to neglect this remainder, for a first approximation of A_t . Note that also the (imaginary) term $\frac{i}{2}a'(x)$ in $h(x, \xi)$ is of "lower order", compared to the first and last term, hence might be neglected too. Writing $h_1(x, \xi) = -a(x)\xi + b(x)$ this will lead us to a first order PDE (with real coefficients) of the form

$$(8.3.6) \quad a_{|t} - h_{1|\xi}a_{|x} + h_{1|x}a_{|\xi} = 0 .$$

(or, $a_{|t} - \langle h_1, a \rangle = 0$ with the "Poisson bracket" $\langle \cdot, \cdot \rangle$).

Equation (8.3.6) may be solved just as equation (8.2.4) in sec.8.2: We introduce the *Hamiltonian system*

$$(8.3.7) \quad \dot{x} = h_{1|\xi}(x, \xi) , \quad \dot{\xi} = -h_{1|x}(x, \xi) .$$

Then the solutions of (8.3.6) are the functions constant along the (reverse) "flow" in (x, ξ) -space induced⁷ by (8.3.7). [Note (8.3.6) and (8.3.7) imply $\frac{d}{dt}a(-t, x(t), \xi(t)) = -a_{|t} + \dot{x}a_{|x} - \dot{\xi}a_{|\xi} = 0$.] This, and the initial condition $a(x, \xi; 0) = a(x, \xi)$ defines a unique $a(x, \xi; t)$. One can show then, that this $a(x, \xi; t)$ is a symbol of ψc_0 again. This only gives an approximate solution of (8.2.8). However, this is enough to start an iteration, yielding an asymptotic sum giving a (unique) solution of (8.2.8) belonging to $\text{Op}\psi c_0$. Moreover, this solution then will coincide with $A(t)$, showing

⁶Actually, the algebra $\text{Op}\psi c_0 \subset L(\mathcal{H})$ only holds the (strictly classical) ψ do's of order $0 = (0, 0)$. A general (strictly classical) ψ do is a polynomial in x and $D = -i\partial_x$ with coefficients being ψ do's in $\text{Op}\psi c_0$, best written in the form $A = a(x, D) = \sum_{j,l} x^j a_{jl}(x, D) D^l$, because then formulas (8.3.1), (8.3.2), (8.3.3) all are valid with the symbol $a(x, \xi) = \sum_{j,l} a_{jl}(x, \xi) x^j \xi^l \in \psi c$. Such a symbol will satisfy a modified (1.2.2)₀, called (1.2.2)_m (or just (1.2.2)), called an *order* of $a(x, \xi)$ (or $A = a(x, D)$), the modification being that $O((1 + |x|)^{-k}(1 + |\xi|)^{-l})$ is replaced by $O((1 + |x|)^{m_2-k}(1 + |\xi|)^{m_1-l})$. The Leibniz formulas then also hold within the algebra $\text{Op}\psi c$ with the addition that *order of a product equals sum of orders of the factors*. Clearly, under assumption (8.2.2), H belongs to $\text{Op}\psi c_e \subset \text{Op}\psi c$, with $e = (1, 1)$, where $\text{Op}\psi c_m$ denotes the class of operators of order m . For details cf. sec.1.2.

⁷Clearly the flows of (8.2.5) and (8.3.7) are related: Project (8.3.7) onto (x, t) -space and get (8.2.5), since $h_{1|x} = -a(x)$ the first equation (8.3.7) does not involve ξ and may be solved on its own. Note also, for solving the initial-value problem of (8.2.5) we really needed the inverse flow which accounts for a change of sign in (8.3.7).

that $A(t)$ remains a ψ do in $Op\psi c_0$ whenever its initial value A at $t = 0$ belongs to $Op\psi c_0$.

Similarly as in sec.4.2 we then may introduce a “Hamiltonian flow”, defined as the map $\nu_{\tau t} : (x, \xi) \rightarrow (x_{\tau t}(x, \xi), \xi_{\tau t}(x, \xi))$, where $x(t) = x_{\tau t}(x, \xi)$, $\xi(t) = \xi_{\tau t}(x, \xi)$ is the solution of (8.3.7) at time t , starting at $t = \tau$ with initial values (x, ξ) . Moreover, this flow of (8.3.7) extends continuously to \mathcal{R}_b , the Stone-Cech type compactification of $\mathbb{R}^2 = \mathbb{R} \times \mathbb{R}$ generated as maximal ideal space of the closure of the function algebra ψc_0 within the bounded continuous functions over \mathbb{R}^2 . The boundary $\partial\mathcal{R}_b = \mathcal{R}_b \setminus \mathbb{R}^2$ happens to be the symbol space \mathcal{M}_b of \mathcal{A}_b . The restriction to \mathcal{M}_b of the extension to \mathcal{R}_b of our Hamiltonian flow (8.3.7) then defines the action of $U(t)$ on our algebra \mathcal{A}_b - generating a group of homeomorphisms $\mathcal{M}_b \rightarrow \mathcal{M}_b$.

The crucial result, in this respect is the following

Theorem 8.3.1 *Assuming cdn. (8.2.2) on a, b , the Hamiltonian system (8.3.7) has a unique solution $x(t; x_0, \xi_0) = x_{\tau t}(x_0, \xi_0), \xi(t; x_0, \xi_0) = \xi_{\tau t}(x_0, \xi_0)$ assuming (x_0, ξ_0) at $t = \tau$, for any given $(x_0, \xi_0) \in \mathbb{R}^2$, and all τ , defined for t close to τ . These local solutions extend for all (positive and negative) t , defining a family $\nu_{\tau t}$ of diffeomorphisms $\mathbb{R}^2 \rightarrow \mathbb{R}^2$ such that $\nu_{\tau\kappa} \circ \nu_{\kappa t} = \nu_{\tau t}$ for all $\tau, \kappa, t \in \mathbb{R}$. Moreover, the composition $a \rightarrow a \circ \nu_{\tau t} = a_{\tau t}$ leaves the function algebra ψc_0 invariant - [and it even preserves orders, i.e., $\psi c_m \circ \nu_{\tau t} \subset \psi c_m$, if we introduce general order ψ do-s in a manner analogous to that in sec.1.2].*

Theorem 8.3.1 is a special case of Thm.3.1 in [Co2] (cf. also [Co5],ch.6.6). Its proof is a matter of verifying suitable apriori estimates [see also sec.’s 5.4 and 5.5 above].

Notice that theorem 8.3.1 induces a family of automorphisms $\psi c_0 \rightarrow \psi c_0 \circ \nu_{\tau t} = \psi c_0$ of the function algebra ψc_0 extending continuously to (isometric *-) automorphisms of $C(\mathcal{R}_b)$ - since (evidently) the composition $a \rightarrow a \circ \nu_{\tau t}$ does not change the sup-norm of $a(x, \xi)$. Accordingly it follows that the homeomorphisms ν_t indeed extend continuously to the boundary \mathcal{M}_b of \mathcal{R}_b - and, of course, take \mathcal{M}_b to itself.

Finally, notice that $Op\psi c_{-e} \subset K(\mathcal{H})$, as is well known (cf. rem.1.4.3). Thus, for the study of cosets of the action $A \rightarrow A_t$, for $A \in Op\psi c_0$ it suffices to study the map $a(x, D) \rightarrow (a \circ \nu_{\tau t})(x, D)$, since $a_{\tau t} - a \circ \nu_{\tau t} \in \psi c_{-e}$. So, in this sense, \mathcal{A}_b and $U(t)^* \mathcal{A}_b U(t)$ have the same generators, so, the algebras coincide. Similarly, it follows at once, that the above mentioned homeomorphism defines the corresponding homeomorphism of the symbol space onto itself. We have proven:

Theorem 8.3.2 (hyperbolic theory) *Assuming (8.2.2) for the coefficients a, b , the map $A \rightarrow A_t = e^{iHt} A e^{-iHt}$ defines a group of automorphisms of the algebra*

\mathcal{A}_b , and the corresponding action on the symbol space \mathcal{M}_b is given by restricting the continuous extension to \mathcal{R}_b of the group of diffeomorphisms $\mathbb{R}^2 \rightarrow \mathbb{R}^2$ defined by the Hamiltonian flow of equations (8.3.7).

We call this “hyperbolic theory”, because the very same flow will govern *propagation of singularities* under the hyperbolic equation (8.2.4): If A is “non-elliptic” at $m_0 \in \mathcal{M}$ i.e., σ_A vanishes there, then the flow rules how that “singularity” will propagate in time.

Again, this only ketches the root of the problem, there are generalizations of all kinds, just as for elliptic equations. The result described does not only hold for differential operators of the form H but also for general selfadjoint ψ do’s H of order $e = (1, 1)$. A local version is known as *Egorov’s theorem*, (cf.[Eg1] published in 1969). Again this has been generalized in many ways, similar as for elliptic theory.

8.4 Characteristic Flow and Particle Flow

Returning to our “comparison algebra” \mathcal{A} of sec.8.1 we note that there is a reason to decompose the symbol space \mathcal{M} into a disjoint union

$$(8.4.1) \quad \mathcal{M} = \mathcal{M}_p \cup \mathcal{M}_s$$

of *principal* and *secondary* symbol space, respectively - where $\mathcal{M}_p = \{|\xi| = \infty\}$, and, $\mathcal{M}_s = \{|\xi| < \infty\}$ - : The Fredholm property of an N -th order differential operator L is that of the operator $A = L(1 - \partial_x^2)^{-N/2}$ possibly belonging to our algebra \mathcal{A} (if the coefficients are “good”). A (uniformly) elliptic operator L generates a symbol of A bounded away from 0 on \mathcal{M}_p . It then depends on the “secondary symbol” of \mathcal{A} - i.e., the symbol of A over \mathcal{M}_s whether or not the elliptic operator L is Fredholm. For details cf.[Co14].

Let us make the point (without detailed proof) that, for a differential operator H of the form (8.2.1) not only the symbol space of the larger algebra \mathcal{A}_b is left invariant (but is acted on) by the conjugation $A \rightarrow A_t$ but also the principal symbol space $\mathcal{M}_p \subset \mathcal{M}$ of \mathcal{A} is left invariant, and is acted upon. It turns out that this action is completely independent of the choice of the function $b(x)$ in (8.2.1), and best discussed by setting $b(x) \equiv 0$, i.e., considering the “principal symbol” only. [Then, with a local treatment, thm.8.3.2 above in effect becomes trivial.].

Of course, we still must approach this from the Hamiltonian flow defined over the space of finite x, ξ . The independence from $b(x)$ must be checked by noting that, at $|\xi| = \infty$ the flow ceases to depend on $b(x)$.

The flow of e^{-iHt} over \mathcal{M}_p is generally referred to as the *characteristic flow* (of the hyperbolic equation (8.2.4)).

In contrast to this characteristic flow we will refer to the flow of equations (8.3.7) (for finite x, ξ) as of the *particle flow* of equation (8.2.4), for a reason me might want to explain now: The name “particle flow” for this global flow will become suggestive, if we describe generalization of above results to the Dirac equation or the Schroedinger equation of the harmonic oscillator. Note, the Dirac Hamiltonian $H = H_d$ is a first order 4×4 -system (in 3 independent variables) while the Schroedinger Hamiltonian H_{sh} for the harmonic oscillator is of second order. We mainly want to comment on action of $e^{-iH_{sh}t}$ but shortly must describe things for e^{-iH_d} .

With the Dirac Hamiltonian we work in $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$. Our comparison algebra \mathcal{A} is generated by the six operators

$$(8.4.2) \quad s_j(x) = \frac{x_j}{\sqrt{1+|x|^2}} , S_j = s_j(D) = F^{-1}s_j(x)F , j = 1, 2, 3 .$$

Again the C^* -algebra \mathcal{A} contains the compact ideal \mathcal{K} of \mathcal{H} , and $\mathcal{A}/\mathcal{K} = C(\mathcal{M})$ is a commutative C^* -algebra. The subalgebras \mathcal{A}_x and \mathcal{A}_D of multipliers and Fourier multipliers, spanned by the $s_j(x)$ and by the S_j , respectively, both are (isometrically isomorphic to) $C(\mathbb{B}^3)$ with the closed ball $\mathbb{B}^3 = \{|x| \leq 1\} \cong$ directional compactification of \mathbb{R}^3 - adding one point in each direction $x_\infty^0 = \lim_{t \rightarrow \infty} tx^0$ for $|x^0| = 1$. The symbol space \mathcal{M} equals the boundary of the product $\mathcal{R} = \mathbb{B}^3 \times \mathbb{B}^3$. That is,

$$(8.4.3) \quad \mathcal{M} = \mathbb{B}^3 \times \partial\mathbb{B}^3 \cup \partial\mathbb{B}^3 \times \mathbb{B}^3 = \{(x, \xi) \in \mathcal{R} : |x| + |\xi| = \infty\} .$$

Note, \mathcal{A} is a subalgebra of $L(L^2(\mathbb{R}^3))$, not of $L(\mathcal{H})$, but the algebra \mathcal{A}^4 of all 4×4 -matrices of operators in \mathcal{A} works on \mathcal{H} . The symbol of $A \in \mathcal{A}^4$ is a 4×4 -matrix-valued function on \mathcal{M} . A is Fredholm if and only if $\sigma_A(m)$ is invertible for all $m \in \mathcal{M}$.

The Dirac operator $H_d = H$ (of (1.0.2)) is of the form

$$(8.4.4) \quad H = H_d = \sum_1^3 \alpha_j D_{x_j} + \beta + V(x) = H_0 + V(x) , D_{x_j} = -i\partial_{x_j} ,$$

with constant 4×4 -matrices α_j, β such that $H_0^2 = 1 - \Delta$, with the Laplace operator Δ . The symbol $h(x, \xi)$ of H (as a ψ do) is given by $h(x, \xi) = \sum_1^3 \alpha_j \xi_j + \beta + V(x)$. The self-adjoint matrix $h(x, \xi)$ has the two eigenvalues

$$(8.4.5) \quad \lambda_{\pm} = \pm \sqrt{1 + \xi^2} + V(x) ,$$

both of multiplicity 2 for each (x, ξ) . Both functions $\lambda_{\pm}(x, \xi)$ are symbols (in our class ψc_{e^1} , $e^1 = (1, 0)$). If it comes to $U(t) = e^{-iH_d t}$ and $A_t = U(t)^* A U(t)$, then it must be observed first that A_t remains a ψ do only for a sub-algebra $\mathcal{P}_0 \subset \mathcal{A}^4$. In ch's 4 and 5 above we describe a class $\mathcal{P}_0 \subset Op\psi c_0$ (in fact, a subalgebra algebra) characterized by a smoothness of the function A_t with respect to the parameter t , which has this property. This algebra \mathcal{P}_0 may be characterized by the fact that its operators are of the form

$$(8.4.6) \quad A = p(x, D) + s(x, D) : [p(x, \xi), h(x, \xi)] = 0 \quad \forall x, \xi ; \quad s(x, \xi) \in \psi c_{-e} .$$

For the analysis of the propagation $A \rightarrow A_t$ the decomposition (8.4.6) is crucial: Since $p(x, \xi)$ and $h(x, \xi)$ commute, there results a split of the matrix $p(x, \xi)$ into a pair $p_{\pm}(x, \xi)$ of self-adjoint 2×2 -matrices taking the (2-dimensional) eigenspaces of $h(x, \xi)$ to the (distinct) $\lambda_{\pm}(x, \xi)$ into themselves. [All of this must be thought of with respect to a suitable orthonormal base $\psi^j(x, \xi)$ of \mathbb{C}^4 , where the functions ψ_j are symbols in ψc_0 .]

Now, the symbols $p_{\pm}(x, \xi)$ propagate along different Hamiltonian flows. Namely, we have two such flows, given by the two Hamiltonian systems

$$(8.4.7) \quad \dot{x} = \lambda_{\pm|\xi}(x, \xi) , \quad \dot{\xi} = -\lambda_{\pm|x}(x, \xi) .$$

The propagation $A \rightarrow A_t$ is governed by letting p_{\pm} propagate along the flow of λ_{\pm} , and then making an infinite number of (lower and lower order) corrections. In such a way we indeed may construct a family $A_t = a_t(x, D)$ of ψ do's solving (8.2.8) for $H = H_d$, and a corresponding "propagation of symbols" for the subalgebra \mathcal{P}_0 of \mathcal{A}^4 (cf.[Co3] or [Co5]Ch.10, and, of course, ch.5, above).

Now, what fascinates us most, in this context: The self-adjoint 2×2 -matrices p_{\pm} have a unique decomposition

$$(8.4.8) \quad p_{\pm}(x, \xi) = c_{0\pm}(x, \xi) + \sum_1^3 c_{j\pm}(x, \xi) \sigma_j ,$$

with our Pauli matrices

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

[This often is called the Garding-Wightman representation.] From (8.4.8) we form the real-valued functions $c_{0\pm}(x, \xi)$ and the real 3-vectors $\vec{c}_{\pm}(x, \xi)$ with components $c_{j\pm}(x, \xi) : j = 1, 2, 3$. The point then is this [and that may justify the name "particle flow" for the finite Hamiltonian flows (within $\mathbb{R}^3 \times \mathbb{R}^3$) defined by (8.4.7) - analogous to (8.3.7)]:

Theorem 8.4.1 *The scalars $c_{0\pm}(x, \xi)$ propagate along the flow of classical orbits of electron and positron, respectively, while the vectors $\vec{c}_{\pm}(x, \xi)$ describe propagation of a magnetic moment vector along these flows - to be interpreted as the spin.*

Details were discussed in sec.4.6, where also nonvanishing electromagnetic potentials are admitted. Curiously, the strength of the magnetic moment vector is exactly one Bohr Magneton - so, even this seems built into that strange “square root” of $1 - \Delta$, called the Dirac Hamiltonian⁸.

8.5 The Harmonic Oscillator

With the harmonic oscillator we return to our Hilbert space $\mathcal{H} = L^2(\mathbb{R})$ and comparison algebra \mathcal{A} , etc., of section 8.1, but now focus on the Hamiltonian

$$(8.5.1) \quad H = H_{sh} = \frac{1}{2}(D^2 + x^2) = \frac{1}{2}(x^2 - \frac{d^2}{dx^2}) ,$$

a *second order* differential operator with symbol $h(x, \xi) = \frac{1}{2}(x^2 + \xi^2)$. This harmonic oscillator plays a crucial role in quantum theory of fields. The corresponding classical equation of motion will be $\frac{d^2x}{dt^2} + x = 0$, solved by $x(t) = a \sin(t - \varphi)$, with amplitude a and phase φ . Following our above pattern we may examine the “particle flow” of the Hamiltonian symbol $h(x, \xi)$:

$$(8.5.2) \quad \dot{x} = h_{|\xi} = \xi , \quad \dot{\xi} = -h_{|x} = -x ,$$

which indeed leads to $\ddot{x} + x = 0$, if we eliminate ξ . Solving the system (8.5.2) gives (as orbits in the interior of the rectangle \mathcal{R}) the concentric circles $x^2 + \xi^2 = c > 0$ with flow running clockwise around 0 at angular velocity 1. Indeed, this is the correct field of particle orbits in phase space. Note, this flow does not⁹

⁸These classical orbits do not exhibit a dependence on the spin. They must be regarded like light rays in geometrical optics: Phenomena like the Stern-Gerlach effect do not enter - they are like diffraction of light - appearing only with the wave nature. The Stern-Gerlach effect is quantum mechanical, already one obtains only two possible orbits - spin-up and spin-down, not a continuum of orbits. [Incidentally, the Stern-Gerlach effect may be linked to the fact that also the “commuting part” of the lower order symbol z_t (of (4.2.15)) is forced into a motion along the classical orbits, described in sec.5.1. This will suggest a split of the particle flow into two flows, using the principal axes transformation of the 2×2 -matrices c_t^{\pm} (cf. also footnote 7 of ch.5).]

⁹To see this, use the transformation $s = s(x) = \frac{x}{\sqrt{1+x^2}}, \sigma = s(\xi)$ to map \mathcal{R} homeomorphically onto the rectangle $\{|s|, |\sigma| \leq 1\}$ in (s, σ) -space. The boundary sides $|x| = \infty$ and $|\xi| = \infty$ are mapped onto $|s| = 1$ and $|\sigma| = 1$, respectively. The transformation $x_t = x \cos t - \xi \sin t, \xi_t = x \sin t + \xi \cos t$ then goes into $s_t = \frac{s[\sigma] \cos t - \sigma[s] \sin t}{\sqrt{[s]^2[\sigma]^2 + (\sigma[s] \cos t - s[\sigma] \sin t)^2}}$ (and a similar formula for σ_t), where we set $[a] = \sqrt{1-a^2}$, for a moment. Note $[s] = 0$ amounts to $s = \pm 1$. For such s

extend continuously to a homeomorphism (onto itself) of our compact rectangle $\mathcal{R} = [-\infty, +\infty] \times [-\infty, +\infty]$, except if t is a multiple of $\frac{\pi}{2}$.

Asking the question about $U(t) = e^{-iHt}$ and $A_t = U(t)^*AU(t)$ we first note that we have an explicit representation of $U(t)$ as integral operator, namely,

$$(8.5.3) \quad (U(t)\varphi)(x) = \int dy u(x, y; t)\varphi(y) \ , \ \varphi \in \mathcal{S} \ ,$$

with

$$(8.5.4) \quad u(x, y; t) = \frac{e^{\frac{i}{2}(1+t)}}{\sqrt{2\pi i \sin t}} e^{\frac{i}{2\sin t} \{(x^2+y^2) \cos t - 2xy\}} \ .$$

This may be verified either by using a ‘‘Feynman path integral¹⁰’’

$$(8.5.5) \quad u(x, y; t) = \int \exp\{i \int_0^t (x\dot{\xi} - h(x, \xi))d\tau\} \prod \frac{dx d\xi}{2\pi} \ ,$$

or also directly, using the well known spectral decomposition of H_{sh} , and the well known formula for the kernel of $U(t)$ for a self-adjoint operator H with discrete spectrum¹¹ - i.e.,

$$(8.5.6) \quad u(x, y; t) = \sum_j e^{-i\lambda_j t} \bar{\psi}_j(x)\psi_j(y) \ ,$$

with an orthonormal basis $\{\psi_j\}$ of eigenfunctions to eigenvalues λ_j . The path integral representation (8.5.5) is complicated but often preferred, since it displays the relation between the quantum mechanical Hamiltonian H and the classical ‘‘action integral’’ $\int_0^t (q\dot{p} - h(q, p))d\tau$ of Hamiltonian classical mechanics. Also, it provides a formalism useful for continuous ‘‘fields of harmonic oscillators’’.

we get $s_t = \frac{s|\sigma| \cos t}{|s|\sigma| \cos t|} = \text{sgn}(s \cos t)$ and $\sigma_t = \text{sgn}(s \sin t)$, regardless of σ as long as $|\sigma| < 1$ - i.e., $|\xi| < \infty$, and $t \neq j\frac{\pi}{2}, j = 0, \pm 1, \dots$. This means that the entire secondary symbol space $\mathcal{M}_s = \{|x| = \infty, |\xi| < \infty\}$ is mapped onto some of the 4 corners $|x| = |\xi| = \infty$ of our rectangle \mathcal{R} . Similarly with the interior of \mathcal{M}_p . It is thus clear that the map $(x, \xi) \rightarrow (x_t, \xi_t)$ is not 1 - 1 and cannot define a homeomorphism $\mathcal{R} \rightarrow \mathcal{R}$.

¹⁰Heuristically we have $U(t) \approx 1 - iHt$, hence $U(t)u(x) \approx \int \frac{dy d\xi}{2\pi} u(y)e^{i\xi(x-y)}(1 - ith(y, \xi)) \approx \int \frac{dy d\xi}{2\pi} u(y)e^{i(\xi(x-y) - th(y, \xi))} = V(t)u(x)$, for small t . To get back to a precise formula for $U(t)$, try $U(t) = \lim_{m \rightarrow \infty} (V(\frac{t}{m}))^m$, leading to a kernel u_m - a $2m - 2$ -fold integral - and its limit u for $m \rightarrow \infty$, called the Feynman path integral. [The kernel $u_m(x, y)$ of $V(t/m)^m$ appears as an integral over all polygons (in (x, ξ) -space with $m - 1$ corners) of a partial sum of the integral $\int_0^t (x\dot{\xi} - h(x, \xi))d\tau$ (with $\dot{\xi}$ replaced by a difference quotient $\Delta\xi/\Delta t$) (cf.[FS],Ch.2, for more detail).] The Feynman integral is liked in Physics because it cleanly displays the relation to the ‘‘action integral’’ $S = \int_0^t (x\dot{\xi} - h(x, \xi))d\tau$ of Hamiltonian mechanics. By some ‘‘magic’’ only those polygons contribute, in the limit $m \rightarrow \infty$, which converge to a smooth curve where the action integral makes sense - hence the name ‘‘curve integral’’.

¹¹ H has eigenvalues $n + \frac{1}{2}$, $n = 0, 1, \dots$, and eigenfunctions $e^{-x^2/2}H_n(x)$ with Hermite polynomials H_n as well known (cf.[Bu]).

Now, let A be a ψ do (of the finitely generated algebra \mathcal{A}^0 or, more generally, of $Op\psi c_0$). Then, again, we have (8.2.8), i.e., $\dot{A}_t = i[H, A]$. $H = x^2 + D^2$ also is a ψ do, hence we have the Leibniz formulas (8.3.4) for both HA and AH . But they will break off and give explicit formulas for the symbols, since $h(x, \xi) = x^2 + \xi^2$ is a polynomial in x, ξ . With $h_{|xx} = h_{|\xi\xi} = 2$, $h_{|x} = 2x$, $h_{|\xi} = 2\xi$ we get the symbol of $[H, A]$ equal to $-2i(\xi a_{|x} - x a_{|\xi}) - (a_{|xx} - a_{|\xi\xi})$.

With this we may look at (8.2.8) “symbol-wise”:

$$(8.5.7) \quad A_t = a(x, D; t), \quad a_{|t} = 2(\xi a_{|x} - x a_{|\xi}) - i(a_{|xx} - a_{|\xi\xi}).$$

In other words, the function $a(x, \xi; t)$ must satisfy the *second order*¹² partial differential equation (8.5.7).

This equation may be transformed by introducing $b(x, \xi; t) = e^{ix\xi}a(x, \xi)$ as a new dependent variable: The function $b(x, \xi; t)$ satisfies the PDE

$$(8.5.8) \quad \dot{b} + i(H_\xi - H_x)b = 0,$$

where H_x and H_ξ denote the operator H applied to the variable x and ξ , respectively. Of course, b must satisfy the initial condition $b(x, \xi; 0) = e^{ix\xi}a(x, \xi)$. Thus we may calculate $b(x, \xi; t)$ explicitly as

$b(x, \xi; t) = e^{-iH_\xi t + iH_x t}b = U_\xi(t)U_x(-t)b$, using that $U_x(-t) = e^{iH_x t}$ and $U_\xi(t) = e^{-iH_\xi t}$ commute.

All in all we come out with the formula¹³

$$(8.5.9) \quad a(x, \xi; t) = e^{-ix\xi}U_\xi(t)U_x^*(t)e^{ix\xi}a.$$

We now might want to look at the propagation of our generators $p(x)$ and $q(D)$ of the algebra \mathcal{A} . For this we write the kernel (8.5.4) of $U(t)$:

$$(8.5.10) \quad u(x, y; t) = \sqrt{\frac{e^i}{\pi}} \frac{1}{\sqrt{1 - e^{-2it}}} e^{\frac{i}{2\sin t}(x-y)^2} e^{-\frac{i}{2} \tan \frac{t}{2}(x^2+y^2)}$$

This means that we get

$$(8.5.11) \quad U(t) = a(t)e^{-ib(t)x^2} (e^{ic(t)x^2} *)^{-1} e^{-ib(t)x^2},$$

¹²One might try to repeat the construction leading to the proof of thm.8.3.2, by omitting the last term in (8.5.7), and then starting an iteration. However, it is clear that the statement of thm.8.3.1 does not hold here: The rotation of (8.5.2) - solving (8.5.7) without the last (second order) terms will not leave ψc invariant. It even will mix up the two orders m_1, m_2 of a symbol. Besides, (8.5.7) will give a clean initial-value problem for the symbol $a(x, \xi; t)$ since there is no asymptotic sum involved.

¹³Actually, formula (8.5.9) may be derived in a simpler way: The Harmonic oscillator commutes with the Fourier transform F , i.e., also $FU_x = U_\xi F$. Hence $\sqrt{2\pi}A_t u(x) = \int U_x^*(e^{ix\xi}a(x, \xi))(U_x u)^\wedge(\xi)d\xi = \int (U_\xi U_x^*(e^{ix\xi}a(x, \xi))u)^\wedge(\xi)d\xi = a(x, D; t)u(x)$ with $a(x, \xi; t)$ of (8.5.9).

with convolution $f * u = \int f(x - y)u(y)dy$ and real $a(t) = \sqrt{\frac{2e^i}{\pi}} \frac{1}{\sqrt{1 - e^{-2it}}}$, $b(t) = \frac{1}{2} \tan \frac{t}{2}$, $c(t) = \frac{1}{2 \sin t}$, independent of x . In other words, this is a product of a convolution and multiplications, each times with a quadratic exponential. Note also, that convolution with e^{icx^2} amounts to multiplication of the Fourier transform by $(e^{icx^2})^\wedge = \sqrt{\frac{i}{2c}} e^{i\xi^2/4c}$.

So, starting with $a(x, \xi) = p(x)$ (independent of ξ), we get

$$p(x) \rightarrow a^2(e^{-i(x\xi - bx^2 + b\xi^2)})(e^{-icx^2} *) \{e^{ibx^2} p(x)(e^{ic\xi^2} *) (e^{i(x\xi - b\xi^2)})\} .$$

Resolving this from inside out,

$$\int e^{ic(\xi - \eta)^2} e^{i(x\eta - b\eta^2)} d\eta = e^{ic\xi^2} \int e^{-i((b-c)\eta^2 + (2c\xi - x)\eta)} d\eta .$$

Here $d = b - c = \frac{1}{2} \cot t > 0$ for small t , but it changes sign at $t = \frac{\pi}{2}$. We thus may continue above calculation:

$$= \sqrt{-\frac{i\pi}{d}} e^{i(c\xi^2 + (2c\xi - x)^2/4d)} .$$

This also holds for $\pi/2 < t < \pi$ with the appropriate change of sign of d .

The next step will be the calculation of

$$\begin{aligned} &\int p(y) dy e^{-ic(x-y)^2} e^{iby^2} e^{i(c\xi^2 + (2c\xi - y)^2/4d)} \\ &= e^{-i(cx^2 - \xi^2(c + \frac{c^2}{d}))} \int p(y) dy e^{i(b-c + \frac{1}{4d})y^2 + i(2cx - \frac{c}{d}\xi)y} . \end{aligned}$$

$$\text{Set } b - c + \frac{1}{4d} = d + \frac{1}{4d} = \frac{1}{2}(\cot t + \tan t) = \frac{1}{\sin 2t} = f, \quad \frac{c}{2d} = \frac{\sin^2 t/2}{1 - 2\sin^2 t/2} = g .$$

$$\text{Then, } \int p(y) dy e^{i(fy^2 + 2(cx - g\xi)y)} = e^{-i(cx - g\xi)^2/f} \int p(y) e^{if(y + \frac{cx - g\xi}{f})^2} dy .$$

Let us denote the last integral by $k(x, \xi)$. Clearly

$$(8.5.12) \quad k(x, \xi) = \int p(z - \frac{c}{f}x + \frac{g}{f}\xi) e^{ifz^2} dz .$$

Then our symbol $a(x, \xi; t)$ equals the product of $k(x, \xi)$ with a bunch of quadratic exponentials, namely,

$$(8.5.13) \quad p(x, \xi; t) = \frac{|a|^2}{2\pi} \sqrt{\frac{-i\pi}{d}} k(x, \xi) e^{-i(cx - g\xi)^2/f} e^{-i(cx^2 - \xi^2(c + \frac{c^2}{d}))} e^{-i(x\xi - bx^2 + b\xi^2)} .$$

So, the exponent will be

$$(8.5.14) \quad -i\{x^2(\frac{c^2}{f} - d) + \xi^2(\frac{g^2}{f} + d - \frac{c^2}{d}) + x\xi(1 - 2\frac{cg}{f})\} .$$

Next we repeat this for $a(x, \xi) = q(\xi)$ (independent of x)

$$q(x) \rightarrow a^2(e^{-i(x\xi - bx^2 + b\xi^2)})(e^{ic\xi^2} *) \{e^{-ib\xi^2} q(\xi)(e^{-icx^2} *) (e^{i(x\xi + bx^2)})\} .$$

Resolving this from inside out,

$$\int e^{-ic(x-y)^2} e^{i(y\xi + by^2)} dy = e^{-icx^2} \int e^{i(dy^2 + (2cx + \xi)y)} dy ,$$

where again $d = b - c = \frac{1}{2} \cot t$, and, continuing,

$$= \sqrt{\frac{i\pi}{d}} e^{-i(cx^2 + (2cx + \xi)^2/4d)} .$$

The next step will be the calculation of

$$\int q(\eta) d\eta e^{ic(\xi-\eta)^2} e^{-ib\eta^2} e^{-i(cx^2+(2cx+\eta)^2/4d)}$$

$$= e^{i(c\xi^2-x^2(c+\frac{c^2}{d}))} \int q(\eta) d\eta e^{-i(d+\frac{1}{4d})\eta^2-i(2c\xi+\frac{c}{d}x)\eta} .$$

Set $b - c + \frac{1}{4d} = d + \frac{1}{4d} = \frac{1}{\sin 2t} = f$, $\frac{c}{2d} = g$.

Then, $\int q(\eta) d\eta e^{-i(f\eta^2+2(c\xi+gx)\eta)} = e^{i(c\xi+gx)^2/f} \int q(\eta) d\eta e^{-if(\eta+\frac{c\xi+gx}{f})^2}$.

Let us denote the last integral by $l(x, \xi)$. Clearly

$$(8.5.15) \quad l(x, \xi) = \int q(z - \frac{g}{f}x - \frac{c}{f}\xi) e^{-ifz^2} dz .$$

Then our symbol $a(x, \xi; t)$ equals the product of $l(x, \xi)$ with a bunch of quadratic exponentials, namely,

$$(8.5.16) \quad q(x, \xi; t) = \frac{|a|^2}{2\pi} \sqrt{\frac{i\pi}{d}} l(x, \xi) e^{i(c\xi+gx)^2/f} e^{i(c\xi^2-x^2(c+\frac{c^2}{d}))} e^{-i(x\xi-bx^2+b\xi^2)} .$$

Here the exponent works out as

$$(8.5.17) \quad i\{x^2(\frac{g^2}{f} + d - \frac{c^2}{d}) + \xi^2(\frac{c^2}{f} - d) + x\xi(2\frac{cg}{f} - 1)\} .$$

Now, a calculation shows that these exponents both vanish identically, so the exponentials both are $\equiv 1$. Moreover, we find that $\frac{c}{f} = \cos t$, $\frac{g}{f} = \sin t$. Hence (8.5.13) and (8.5.16) assume the form of (8.5.19) and (8.5.20) below, and we may summarize this as follows:

Theorem 8.5.1 *For the operator $H = H_{sh}$ of (8.5.1) and a pair of operators $p(x) \in \mathcal{A}_x$, $q(D) \in \mathcal{A}_D$ such that $p(x), q(\xi) \in \psi c_0$, conjugation with $U(t) = e^{-iHt}$ transforms $p(x)$ and $q(D)$ into formal ψ do's of the form*

$$(8.5.18)$$

$$U(t)^* p(x) U(t) = p(x \cos t - D \sin t; t) , \quad U(t)^* q(D) U(t) = q(x \sin t + D \cos t; t) ,$$

where

$$(8.5.19) \quad p(x^0; t) = (2\pi)^{-3/2} \sqrt{\frac{-2i}{\sin 2t}} \int_{-\infty}^{+\infty} p(z - x^0) e^{\frac{i}{\sin 2t} z^2} dz ,$$

and

$$(8.5.20) \quad q(\xi^0; t) = (2\pi)^{-3/2} \sqrt{\frac{2i}{\sin 2t}} \int_{-\infty}^{+\infty} q(z - \xi^0) e^{-\frac{i}{\sin 2t} z^2} dz .$$

So, for given fixed t the symbols in (8.5.18) depend only on the variable $x^0 = x \cos t - \xi \sin t$ and $\xi^0 = x \sin t + \xi \cos t$, respectively.

One may not expect the estimates of condition (1.2.2)₀ for the symbols in (8.5.18), considered as functions of x and ξ . But it is easily shown (using complex curve

integral techniques) that the functions $p(x; t), q(\xi; t)$ of (8.5.19), (8.5.20) do satisfy $\text{cdn.}(1.2.2)_0$, for the case of the (holomorphic) generators $p(x) = s(x), q(\xi) = s(\xi)$ of \mathcal{A} .

In fact, there is a periodicity:

Corollary 8.5.2 *For $t = \frac{\pi}{2}, \pi, \frac{3\pi}{2}, \dots$, the integrals in (8.5.18), (8.5.19) degenerate to delta-function integrals. For these values of t we indeed get our algebra \mathcal{A} back. Moreover, for the half-numbered multiples of π the two generating algebras \mathcal{A}_x and \mathcal{A}_D are interchanged, while for $t = j\pi$ they are reproduced.*

Interesting also, for any t , the symbols $p(x^0; t)$ (depending on x^0 only) generate a commutative algebra (with symbol depending only on the linear combination x^0 of x and ξ): We have $(pq)(x^0; t)$ given by substituting $p(x).q(x)$ instead of $p(x)$ in (8.5.19). Similarly with (8.5.20).

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General Notations

A: Generals

(1) We are using various notations for derivatives:

$\partial u / \partial x = \partial_x u = u_{|x}$ - whichever is convenient.

time derivative: $\dot{u} = \partial u / \partial t = \partial_t u$

multi-index notation - for symbols: $a_{(\iota)}^{(\theta)} = \partial_x^\iota \partial_\xi^\theta a(x, \xi)$, where $\theta = (\theta_1, \dots, \theta_n)$, $\iota = (\iota_1, \dots, \iota_n)$, $\partial_x^\iota = \partial_{x_1}^{\iota_1} \dots \partial_{x_n}^{\iota_n}$, etc., - usually $n = 3$. For a multi-index ι set $|\iota| = \iota_1 + \dots + \iota_n$.

(2) \mathbb{R}^n and \mathbb{C}^n denotes real and complex n -dimensional space; $\mathbb{R}_+ = \text{half-line } \{x > 0\}$.

(3) $f(x) = O(g(x))$ means that $|f(x)| \leq c|g(x)|$ with some positive constant independent of x - possibly only for specific x , as indicated. The constant c then is referred to as "the $O(\cdot)$ -constant".

(4) $\langle u, v \rangle$ denotes the inner product of u and v in Hilbert space, but (f, φ) denotes the value of the distribution f at the testing function φ . The first is sesqui-linear in u, v ; the second is bi-linear in f, φ .

B: Function Spaces and Distribution Spaces

(1) $L^2(\mathbb{R}^n, \mathbb{C}^m) = \text{Lebesgue-squared integrable maps } \mathbb{R}^n \rightarrow \mathbb{C}^m$ [if $m = 1$ the last argument is omitted].

(2) $C^k(\Omega) = \text{functions over } \Omega$ (an open set) with continuous partial derivatives up to order k [including $k = \infty$], values usually in \mathbb{C} , but possibly also in some \mathbb{C}^k - including matrix-valued.

(3) $\mathcal{D}(\Omega) = C_0^\infty(\Omega) = \text{compactly supported } C^\infty\text{-functions over the open set } \Omega$.

(4) $\mathcal{S} = \mathcal{S}(\mathbb{R}^k) = \text{class of "rapidly decreasing" functions over } \mathbb{R}^k$: All derivatives are $O((1 + |x|)^{-l})$ for every $l = 1, 2, \dots$

(5) $\mathcal{D}'(\Omega) = \text{set of distributions over the open set } \Omega$ - i.e., continuous linear functionals over the set $\mathcal{D}(\Omega)$ of "testing functions".

(6) $\mathcal{S}' = \mathcal{S}'(\mathbb{R}^n)$ = set of temperate distributions: continuous linear functionals over the space \mathcal{S} .

(7) $L(\mathcal{X}, \mathcal{Y})$ = class of continuous linear maps $:\mathcal{X} \rightarrow \mathcal{Y}$ [if $\mathcal{X} = \mathcal{Y}$ the last argument is omitted].

(8) $K(\mathcal{X}, \mathcal{Y})$ = class of compact linear maps $:\mathcal{X} \rightarrow \mathcal{Y}$ [the last argument is omitted if $\mathcal{X} = \mathcal{Y}$].

C: Symbol classes

(1) ψc = class of all “strictly classical” symbols: That is, of all functions $a(x, \xi) \in C^\infty(\mathbb{R}^6)$ such that derivatives of x -order k and ξ -order l are $O((1 + |x|)^{m_2-k}(1 + |\xi|)^{m_1-l})$ with some reals m_1, m_2 for all $k, l = 0, 1, \dots$ [The $O(\cdot)$ -constants may depend on k, l]. The pair $m = (m_1, m_2)$ of reals is called an order of the symbol $a(x, \xi)$. The collection of all symbols of a given order $m = (m_1, m_2)$ is denoted by ψc_m . Especially $\psi c_{-\infty} = \cap_m \psi c_m$ - the symbols of order $-\infty$.

Such a symbol $a(x, \xi)$ may be vector-valued, or matrix-valued: We will not distinguish in notation between symbols taking values in \mathbb{C} or in \mathbb{C}^n . Many of our symbols are 4×4 -matrix-valued.

(2) ψt = class of all $C^\infty(\mathbb{R}^6)$ -functions $a(x, \xi)$ such that all derivatives (of all orders) are $O((1 + |x|)^{m_2}(1 + |\xi|)^{m_1})$ with given fixed real m_1, m_2 . Then again $m = (m_1, m_2)$ is called an order of the symbol a , and ψt_m (including $\psi t_{-\infty}$) denotes the class of all symbols in ψt of order m .

(3) $\psi s = \cup_m \psi s_m$ where $\psi s_m =$ collection of all symbols in ψt_m such that any finite application of the (first order differential operators) $\eta_{jl} = \varepsilon_{jl} - \varepsilon_{lj}$, $j, l = 1, 2, 3$, $j \neq l$, and $\eta_{00} = \sum_1^3 \varepsilon_{jj}$ - where $\varepsilon_{jl} = \xi_j \partial_{\xi_l} - x_l \partial_{x_j}$ - belongs to ψt_m again.

D. Special Lie groups:

(1) $SO_3(\mathbb{R})$ = group of all real 3×3 -matrices with determinant 1 - that is, the group of all 3-dimensional rotations (about some axis in 3-space).

(2) $SU_2(\mathbb{C})$ = group of all unitary (complex) 2×2 -matrices with determinant equal to 1.

E: Abbreviations used:

DE = Differential equation

ODE = ordinary differential equation

PDE = partial differential equation

ψdo = pseudodifferential operator

FIO = Fourier integral operator

$\Re z$, $\Im z$ denote real and imaginary part of the complex number z .

WLOG = “without loss of generality”.

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