

Symmetry Conditions on Dirac Observables

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Using our Dirac invariant algebra we attempt a mathematically and philosophically clean theory of Dirac observables, within the environment of the 4 books [10,9,11,4]. All classical objections to one-particle Dirac theory seem removed, while also some principal objections to von Neumann’s observable theory may be cured. Heisenberg’s uncertainty principle appears improved. There is a clean and mathematically precise pseudodifferential Foldy–Wouthuysen transform, not only for the supersymmetric case, but also for general (C^∞ -) potentials.

1 Introduction

The free Dirac Hamiltonian $H_0 = \alpha D + \beta$ is a self-adjoint square root of $1 - \Delta$, with the Laplace operator Δ . The free Schrödinger Hamiltonian $H_0^S = 1 - \frac{1}{2}\Delta$ (where “1” is the “rest energy” mc^2) seems related to H_0 like $\sqrt{1+x}$ its approximation $1 + \frac{1}{2}x$ – second partial sum of its Taylor expansion.

From that aspect the early discoverers of Quantum Mechanics were lucky that the energies of the bound states of hydrogen (a few eV) are small, compared to the mass energy of an electron (approx. 500 000 eV), because this should make “Schrödinger” a good approximation of “Dirac”. But what about the continuous spectrum of both operators – governing scattering theory. Note that today big machines scatter with energies of about 10,000 – compared to the above $1 = mc^2$. So, from that aspect the precise scattering theory of both Hamiltonians (with potentials added) should give completely different results, and one may have to put ones trust into one of them, because at most one of them can be applicable.

We decide for the Dirac Hamiltonian which can explain the fine structure of spectral lines, Schrödinger cannot. This afortiori, because we believe to have a cure for the classical deficiencies of Dirac’s theory – a different one as offered by quantum field (multi-particle) theory. Moreover, the resulting observable theory appears more consistent and offers insights, the Schrödinger Hamiltonian cannot supply.

Our main point is that the Dirac equation (with time-independent electromagnetic potentials) possesses an *invariant algebra of pseudodifferential operators* we want to exhibit as the algebra of “precisely predictable observables”¹. The Dirac Hamiltonian itself

$$H = \alpha \cdot (D - \mathbf{A}(x)) + \beta + \mathbf{V}(x) \tag{1}$$

is precisely predictable. But other dynamical observables, like location, are not. However, location possesses “precisely predictable approximations”, with an “error” of the order of magnitude of the Compton wave length – that is what Physicists assume anyway: The electron also may be observed as a wave, one should not expect a prediction of its location more accurate than its wave length.

Furthermore, no transition from “electron states” to “positron states” is ever precisely predictable – and no approximation to it exists. That should save us from the “electron see”, and make one-particle Dirac theory consistent. A restriction to anti-symmetric states for multi-particle theory may be required for the Pauli principle, but is superfluous for Dirac’s theory.

¹Similar algebras exist for the “Dirac-type” equations of Yang–Mills theory.

There exist precisely predictable approximations to observables like spin (or current), but *only* if we already know for sure that the particle is an electron (a positron).

We might assume that this algebra was not known by Dirac or his contemporaries.

Some details: First an explanation why it might be reasonable to insist on observables which are pseudodifferential operators (abbrev.: ψ do). An observable interests us only if we can hope that our theory is able to *predict* it. We must expect our observable does not change too fast if we translate – rotate – dilate our coordinates, and both so, in configuration space and momentum space, because there always are errors of such kind in our measurements.

In above statement, if we replace “*does not change too fast*” by “*changes smoothly*”, then we arrive at a mathematical concept we might start working with. Namely, translation, rotation and dilation describe 3 Lie groups under the action of which our observable should be “smooth” – both in configuration space and momentum space. Well, there are (precise mathematical) theorems stating that such a (Hilbert space) operator *must* be a ψ do (cf. [1] or, [4, Ch. 8]). Moreover, then, a “symbol calculus” – giving Leibniz-type formulas – is correct.

This is why we think it natural to assume observables as ψ do’s.

Next, *time propagation* of an observable A . is given by the *Heisenberg transform*

$$A_t = e^{iHt} A e^{-iHt}. \quad (2)$$

The class of (*strictly classical*) ψ do-s A with the property that A_t is a *smooth* function of t forms an algebra \mathcal{P} . Here we are using a somewhat special concept of *smoothness* with derivatives $\partial_t^k A_t$ required to exist and be continuous as maps between certain polynomially weighted L^2 -Sobolev spaces.

In our earlier theory (first published in 1983) we suggested using the self-adjoint operators of \mathcal{P} as “precisely predictable observables”.

In that respect we remind of the concept formulated precisely by J. von Neumann (in his book “Principles of Quantum Mechanics” of 1932): *To predict an observable A (with discrete spectrum) in the state ψ (a unit vector of the Hilbert space \mathcal{H}) we expand ψ into a series, after the eigenfunctions φ_j of A :*

$$\psi = \sum_{j=1}^{\infty} a_j \varphi_j, \quad a_j = (\varphi_j, \psi), \quad (3)$$

with an orthonormal base $\{\varphi_j, j = 1, 2, \dots\}$ of eigenvectors of A . One predicts the value λ for A with probability $\pi = \sum |a_j|^2$, with the sum over all j with $A\varphi_j = \lambda\varphi_j$. Only an eigenvalue of A can be measured, and the expectation value of the measurement is (predicted as) $\sum_{j=1}^{\infty} \lambda_j |a_j|^2 = (\psi, A\psi)$ (Extension for A with general spectrum well known but omitted).

Now, we propose to apply above prediction rules **only** to observables (i.e., self-adjoint operators) within our above algebra \mathcal{P} which then are called “precisely predictable”. For other observables (not contained in \mathcal{P}) we devised an *approximation scheme*. Some observables – like location, momentum, may be approximated by observables in \mathcal{P} , and then there is an infinite series of (closer and closer) approximations, asymptotically convergent. For others, like spin and current, an approximation is possible only for specific physical states.

Now, before entering further physical discussions, we must explain a series of (precise mathematical) theorems. The first is related to the well known Foldy–Wouthuysen transform: That transform was introduced as an *approximate decoupling* (of electronic and positronic states) with an error of the order $\frac{1}{c^2}, \frac{1}{c^4}, \dots$, (with $c =$ speed of light). For a supersymmetric Hamiltonian this decoupling could be made precise. In 1983 we proved (without supersymmetry):

Theorem 1. *Under the general assumptions (X), below, there exists a unitary operator U of \mathcal{H} which also is a strictly classical ψ do of order $0 = (0, 0)$ such that the Dirac operator (1) is*

decoupled modulo a reminder of order $-\infty$. That is,

$$U^*HU - \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix} \in \mathcal{O}(-\infty), \quad (4)$$

with certain (2×2 -blocks of) ψ do-s X, Y having well described asymptotic expansions, and with $\mathcal{O}(-\infty)$ denoting the class of (globally defined) integral operators with kernel $k(x, y)$ in the Schwartz-space $\mathcal{S}(\mathbb{R}^6)$ of rapidly decreasing functions in all 6 variables x, y .

Theorem 2. A strictly classical ψ do A belongs to the algebra \mathcal{P} if and only if it decouples exactly as H above, under the unitary transform U of Theorem 1. That is, we have

$$U^*AU - \begin{pmatrix} M & 0 \\ 0 & N \end{pmatrix} \in \mathcal{O}(-\infty), \quad (5)$$

with U of Theorem 1 and ψ do-s M, N of the same order than A .

Theorem 2 also requires the general assumptions (X), as follows:

The potentials \mathbf{A}, \mathbf{V} are C^∞ and their partial derivatives of order k decay like $(1 + |x|)^{-k-1}$ at infinity.

Note that the Coulomb potential will need a ‘‘cap’’ near 0 to make it C^∞ , but then will satisfy assumptions (X).

A physical reflection will cause us now to look for a removal of the reminder in $\mathcal{O}(-\infty)$.

Question. Does there exist another unitary map $V = 1 + \mathcal{O}(-\infty)$ such that, with notations of Theorem 1, we have

$$V^*U^*HUV = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix}, \quad (6)$$

with slightly changed X, Y – just with some term of $\mathcal{O}(-\infty)$ to be added?

The answer to this question is a ‘‘YES’’, but **only** after correcting the underlying direct decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$, with \mathcal{H}_\pm denoting the subspaces with vanishing last to (first two) components by subtracting a *finite dimensional* subspace \mathcal{Z} (with components in $\mathcal{S}(\mathbb{R}^3)$) from one of the spaces and adding it to the other one (cf. [7]).

This ‘‘obstruction’’ may mean that the potentials are so strong that some electron eigenvalues have entered into the ‘‘positron’s continuous spectrum’’ (or, vice versa). Note, however, that our techniques of proof do not allow to decide if, for example, the (capped) Coulomb potential (with fine structure constant coefficient) needs this correction.

Why do we find this result interesting?

Note that this really will amount to a clean split of $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ into a direct sum of spaces of electron and positron physical states. We will correct our older notion of precisely predictable observables by introducing the smaller algebra \mathcal{Q} of strictly classical ψ do-s which decouple strictly under the unitary transform $W = UV$. This means that a precisely predictable observable leaves the two subspaces of electronic and positronic physical states invariant.

Then, in view of prediction of measurements, those two spaces are strictly separated by a ‘‘fire-wall’’ Nothing can move across.

Note, by the way, even an observable of finite rank (and of order $-\infty$) which sends \mathcal{H}_+ into \mathcal{H}_- would oscillate in time with more than twice the frequency of the Compton wave length. So, how could anybody hope to predict its value?

We will offer more (mathematical) details in the section below, but here will close with the following final remarks:

Remark 1. In our opinion, our modification of von Neumann’s observable concept will remove *all* the old objections to Dirac’s theory – there will be no need for the Pauli principle and an electron sea, and no “Zitterbewegung”, nor a Klein Paradox.

Remark 2. On the other hand, we have become very curious about explicit spectral theory of some precisely predictable observables. For example – assuming $\mathbf{A} = 0$ – the energy observable H of (1) splits into kinetic and potential energy, the potential energy represented by \mathbf{V} . Now, while H is precisely predictable, \mathbf{V} and $H - \mathbf{V}$ are not. But both have precisely predictable approximations. However these approximations seem to get very bad near $x = 0$. We have been curious about their spectral theory, reflecting on the possibility of getting some hints about special forces acting on an electron very close to the nucleus.

2 Some mathematical details

In this section we shall review some details, augmenting the statements of Section 1.

A (zero order) strictly classical ψ do A is of the form

$$Au(x) = (2\pi)^{-3/2} \int a^{\vee 2}(x, x-y)u(y)dy, \quad u \in \mathcal{S}, \quad (7)$$

where “ $(\cdot)^{\vee 2}$ ” denotes the inverse Fourier transform with respect to the second (set of) variable(s), and where the integral is a distribution integral – value of the distribution at $u \in \mathcal{S}$. The “symbol” $a(x, \xi)$ is a C^∞ -function with this property: x -differentiation of order k followed by ξ -differentiation of order l gives a function bounded by $c(1 + |x|)^{-k}(1 + |\xi|)^{-l}$ with constant c . This class of symbols is called ψc_0 ; the class of all such operators $Op\psi c_0$. Note, $Op\psi c_0$ forms an adjoint invariant subalgebra of $L(\mathcal{H})$ with symbol of product and adjoint given by Leibniz-type rules as asymptotically convergent infinite series.

For strictly classical ψ do-s of arbitrary order the symbol $a(x, \xi)$ is a polynomial in x, ξ with coefficients in ψc_0 . The classes are called ψc and $Op\psi c$. Operators may still be written as (7), or also,

$$a(x, D) = \sum x^\alpha a_{\alpha\beta}(x, D)D^\beta, \quad a_{\alpha\beta} \in \psi c_0. \quad (8)$$

Again, $Op\psi c$ is an algebra (with Leibniz formulas), $\mathcal{O}(-\infty)$ a 2-sided ideal of $Op\psi c_0$ and $Op\psi c$.

Note, the distribution $a^{\vee 2}(x, x - \cdot)$ is singular only at the point x , and behaves like a function in \mathcal{S} otherwise. At $x = y$ the integral (7) may be a Cauchy-type singular integral, or, generally, an “Hadamard finite part”. Away from 0 (8) is a Lebesgue integral.

In (8), if all functions $a_{\alpha\beta}$ are independent of ξ , then $a(x, D)$ is a differential operator. Especially, **all of the common dynamical observables of Dirac theory** belong to our algebra $Op\psi c$ of strictly classical ψ do-s. Here we may remind of the fact that Dirac observables are 4×4 -matrices, so we are really working here with $Op\psi c$ consisting of 4×4 -matrices of operators of the form (8).

While $Op\psi c_0$ is a subalgebra of $L(\mathcal{H})$, $\mathcal{H} = L^2(\mathbb{R}^3)$, a general ψ do $\in Op\psi c$ is continuous $\mathcal{H}_s \rightarrow \mathcal{H}_{s-m}$ (for all s) with the “polynomially weighted” L^2 -Sobolev spaces $\mathcal{H}_s = \langle D \rangle^{-s_1} \langle x \rangle^{-s_2} \mathcal{H}$ with $\langle x \rangle = \sqrt{1 + x^2}$, $\langle D \rangle = \sqrt{1 + D^2} = \sqrt{1 - \Delta}$, and with $m = (m_1, m_2) = (D, x)$ -degree of the polynomial (8). Such m is called an *order* of the ψ do A . There are other (perhaps better) orders, and m may be a pair of reals (of arbitrary sign). “Order = $-\infty$ ” means that $A : \mathcal{H}_s \rightarrow \mathcal{H}_t$ is continuous for all s, t . Such operators form the ideal $\mathcal{O}(-\infty)$.

With this preparation we can give a better description of above facts:

Essentially, the algebra \mathcal{P} may be built from (4×4 -matrices of) ψ do-s $A = a(x, D)$ with the property that $a(x, \xi)$ commutes with the symbol $h(x, \xi) = \alpha(\xi - \mathbf{A}) + \mathbf{V}$ of the Hamiltonian H .

If $[a, h] = 0$ for some a of order m then a z of order $m - e = (m_1 - 1, m_2 - 1)$ may be found such that $A + Z = a(x, D) + z(x, D)$ belongs to \mathcal{P} . Moreover, every $P \in \mathcal{P}$ of order m splits: $P = A + Z$, where $[a, h] = 0$, z of order $m - e$. Given a ψ do A – such as the location operator x , for example – with the property that its symbol commutes with h one may explicitly construct an infinite series of “corrections” Z_j such that $A + \sum Z_j$ is asymptotically convergent and represents an operator of \mathcal{P} . For the location coordinate x_j one gets the symbol²

$$x_j^{\text{corr}} = x_j + \frac{1}{2i\sqrt{1 + (\xi - \mathbf{A})^2}}(\alpha_j h_0 - \xi_j) + \dots, \quad h_0 = \alpha\xi + \beta, \quad (9)$$

and we will propose this operator (still a bit more corrected, adding an $\mathcal{O}(-\infty)$ to get into \mathcal{Q}) as the precisely predictable approximation of the location.

For other observables – spin or current, for example – the symbol does not commute with h . But then we may find a “ \mathcal{Q} -approximation” for the operator with symbol pap – with the (4×4) projection matrix $p(x, \xi)$ onto one of the two eigenspaces of $h(x, \xi)$. One finds that pap is a symbol in ψ c commuting with h . Physically this means that *spin or current can be approximately predicted, but only if it is known with certainty that the particle is an electron (a positron)*.

Regarding Theorem 1. The construction of the symbol u of the unitary operator U starts with choosing a (unitary 4×4 -) matrix $u_0(x, \xi)$ diagonalizing the symbol $h(x, \xi) = \alpha(\xi - \mathbf{A}) + \mathbf{V}$ as zero-th approximation (of order 0). Then an infinite series of correction symbols u_j of order $-je$ (resembling those of the Foldy–Wouthuysen transform) is constructed by an iteration, such that the asymptotic sum $u = \sum u_j$ satisfies $u(x, D)^*u(x, D) = 1 + \mathcal{O}(-\infty)$, $u(x, D)^*Hu(x, D) = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix} + \mathcal{O}(-\infty)$. Then the removal of $\mathcal{O}(-\infty)$ only requires work within the algebra $\mathbb{C} + \mathcal{O}(-\infty)$ of Fredholm type integral operators with very regular kernel – no singular integrals anymore. For more details cf. [3].

For the discussion of Theorem 2 we refer to [6, Theorem 1.3].

It is clear that the relations

$$U^*U = 1, \quad U^*HU = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix} \quad (10)$$

indicate a spectral split of H which we are tempted to identify with a split of the form

$$1 = (1 - E_\lambda) + E_\lambda, \quad (11)$$

with the spectral family E_λ of H . We then will expect that $|\lambda| < 1$, so that one may hope for a split within the gap between continuous spectra of electron and positron. Interestingly, there seems to exist an obstruction: One may attempt to *build* the decoupling (10) (by a ψ do U) to correspond to (11) for some specific $\lambda = \lambda_0$, but then it will be necessary to first modify the two spaces $\mathcal{H}_- = E_\lambda\mathcal{H}$, $\mathcal{H}_+ = (1 - E_\lambda)\mathcal{H}$ by shifting a finite dimensional subspace \mathcal{Z} from one of the spaces to the other one, according to a “deficiency index” $\iota_\lambda = \dim \mathcal{Z}$. This index changes monotonely as λ increases from -1 to $+1$. If it goes through zero, then we have found a split (10). If not then we first must make a finite dimensional “residual” correction of the spaces \mathcal{H}_\pm with first two (last two) components zero, before we can reach (10). For more details cf. [7].

3 Final comments

It should be noted, that our above clean separation between electron and positron states still needs some “physical input”, insofar as it is *not* unique: It will insist on the total dimension of

²Note our unit of length here is the Compton wave length.

either space, in the sense that we may not arbitrarily cast a finite dimensional subspace from \mathcal{H}_\pm to \mathcal{H}_\mp . However, for example, we might exchange a (finite number of) positronic eigenvector(s) for an (equal number of) electronic one(s), while getting an equivalent mathematical theory.

It is, of course, evident that an abstract decoupling (by just a unitary U , not necessarily in $Op\psi c_0$) exists for just any spectral split (11), arbitrary λ . Our unitary $U \in Op\psi c_0$ must also be continuous $\mathcal{H}_s \rightarrow \mathcal{H}_s$, for every $s = (s_1, s_2)$, not only for $s = 0$, while that property does not alone make $U \in Op\psi c_0$. Note also, our construction of U (in [3] or [4]) leaves lots of ambiguity.

It may be important to observe that our “induced Hamiltonians” X, Y for the electronic (positronic) states (while not differential operators anymore) are strictly classical ψ do-s, of order (1,0), with known asymptotic expansions. They are semi-bounded from below (above), as proper Hamiltonians should be. The “residual” (finite dimensional) space \mathcal{Z} , if it occurs, might indicate yet that *not all electronic (positronic) states obey their corresponding Hamiltonian*. In principle, for example, there could be some very negative energy states still be possible for electrons under a Coulomb type potential, assuming that there indeed would exist a residual \mathcal{Z} of electronic states governed by the operator Y .

In conclusion we note that we are aware of a large number of older attempts to deal with deficiencies of the Dirac theory. For a survey of literature we refer to the book [11], especially its notes.

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