

Quantum classical correspondence of Dirac equation

Pranaav Sinz

Bangalore institute of technology, Bangalore 560004, INDIA

pranav.virgo.1989@gmail.com

Abstract: it has been shown that unphysical results of quantum classical correspondence pertaining to Dirac equation have their roots in unjustified calculation of commutation relation involving 4×4 component operators acting on single component non normalized wave function. Zitterbewegung like unphysical phenomena have been completely eliminated as the treatment establishes a seamless connection between operators and observables both in relativistic and non relativistic limits. Intrinsic nature of spin angular momentum has been found questionable.

Keywords: zitterbewegung; intrinsic angular momentum; Dirac equation; quantum classical correspondence; commutation relations.

Background and motivation: A review of Dirac treatment of electron [1] has become essential due to seemingly odd difficulties cropping up regarding various physical features of electron like single valued magnetic moment and velocity Eigen values. While the equation effortlessly reduces to its non-relativistic counter parts (Schrödinger and Pauli equations) there has been a considerable amount of attempt [6, 7] to understand various unphysical features it brings regarding the reduction of expectation value of observables in non-relativistic limit. We first study two anomalous results

$$\frac{[\hat{H}, \hat{x}]}{i\hbar} = \alpha c$$

$$\frac{[\hat{H}, \hat{T}]}{i\hbar} = 0 \text{ Where } \hat{T} = \hat{L} + \hat{S} \quad \hat{S} = \sigma \frac{\hbar}{2}$$

Let us consider the commutation relations of position operator \hat{x} with relativistic Dirac Hamiltonian. Velocity Eigen function thus obtained αc is a constant (independent of energy-momentum of particle) matrix function and its only Eigen value corresponds to velocity of light; a result deemed strictly forbidden by special theory of relativity as an observable for a massive particle. Our well established non relativistic expression of velocity expectation value in low energy limit (Schrödinger limit) is expectation value of momentum operator divided by the mass of the given particle. Therefore, it's puzzling why velocity spectrum of a massive particle is contracted to a single velocity c .

It's well known that complete time dependence of position operator according to Schrödinger's treatment [2] has features of rapid oscillations ($\nu \approx 10^{21} \text{ Hz}$) of very small amplitude called zitterbewegung. It however remains unclear how a solitary particle exhibit rapid acceleration in absence of a force field.

Usually such inconsistency is speculated as a fundamental feature of Dirac equation which caters to both +ve and -ve energy Eigen states of particle [6] and somehow overlapping of these Eigen states may cause such unphysical microscopic phenomenon. Contrary to theoretical observation there have been no conclusive evidence of zitterbewegung like motion and nature seems avoiding it at best. Furthermore, various attempts to relate such motion with the structure of electron appear to be fraught with difficulties of theoretical nature and have not much experimental validation either. Therefore, it can be contended that such attributes completely defeat the spirit of quantum mechanics that stresses observables as integral and validating to the dynamics of system it describes.

Similarly, we shall admit that commutation relation of total angular momentum and Dirac Hamiltonian which shares the same pathology (a constant matrix operator as spin angular momentum operator) is but a fictitious relationship. Value of intrinsic angular momentum thus obtained should not be a single valued function but a momentum energy dependent term. Therefore even the intrinsic nature of additional angular momentum is debatable and can be discarded as a property of fermionic particle.

In the foregoing work it has been established that these discrepancies are not due to some misunderstood physical structure of electron but only a product of premature calculation. By operating with 4×4 components operators on 1 component scalar Eigen functions a fatal error is introduced. Commutation relations involving 4×4 component operators operating on 4 components spinor wave functions immediately resolve this long standing problem. Any additional attempts to modify the definitions of operators [3], [4] and secondary unitary transformations [8] seem only superfluous.

Section 1

Before swiftly proceeding to calculation of various expectation values, we perform a merely cosmetic transformation of Dirac equation by multiplying both sides with matrix α in order to get all the derivative terms on the same side of expression. Matrix α is given by

$$\alpha = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

After multiplication we get

$$\hat{H} = \sum_i \gamma^i \hat{P}c + \gamma^0 mc^2 \rightarrow \alpha \hat{H} + \sum_i^3 \beta^i \hat{P}c = Imc^2 \quad (1A)$$

The above equation renders rest energy Eigen values +ve definite and is **completely equivalent to Dirac equation** provided that fundamental Eigen value equation is changed accordingly. For operator \hat{P} acting on Eigen function ψ the transformation appears as

$$\hat{P}\psi = p\psi \rightarrow \alpha\hat{P}\psi = \alpha p\psi \quad (1B)$$

Therefore identity operator and commutation relations need to be transformed in similar way

$$\hat{I}\psi = \psi \rightarrow \alpha\hat{I}\psi = \alpha\psi \quad (1C)$$

$$[\hat{H}, \hat{P}] = \langle \psi | \hat{H}\hat{P} - \hat{P}\hat{H} | \psi \rangle \rightarrow \langle \psi | \alpha\hat{H}\hat{P} - \alpha\hat{P}\hat{H} | \psi \rangle \quad (1D)$$

It can be verified that preserving the bilinear form of relativistic relation $\hat{H}^2 - \hat{P}^2 c^2 = m^2 c^4$, α and β matrices satisfy following well known non-commutation relations.

$$\beta^i \beta^j + \beta^j \beta^i = 2I\delta_{ij}$$

$$\alpha\beta^i + \beta^i\alpha = 0$$

These matrices when written explicitly in terms of Pauli matrices appear as

$$\alpha = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \beta^1 = \begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix} \quad \beta^2 = \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix} \quad \beta^3 = \begin{pmatrix} 0 & \sigma_z \\ -\sigma_z & 0 \end{pmatrix}$$

where, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ are Pauli matrices.

After substituting these matrices in equation (1A) and providing a gauge substitution $\frac{\partial}{\partial t} \rightarrow \frac{\partial}{\partial t} - \frac{e\phi}{i\hbar}$ for weak electric field we obtain the following expression

$$\begin{pmatrix} \hat{H} - e\phi & 0 \\ 0 & -\hat{H} + e\phi \end{pmatrix} + \begin{pmatrix} 0 & \sigma \cdot \hat{P}c \\ -\sigma \cdot \hat{P}c & 0 \end{pmatrix} = \begin{pmatrix} mc^2 & 0 \\ 0 & mc^2 \end{pmatrix} \quad (1E)$$

Conjugate of the above equation can be readily written down after substituting various operators with their hermitian conjugates.

$$\begin{pmatrix} \hat{H}^\dagger - e\phi & 0 \\ 0 & -\hat{H}^\dagger + e\phi \end{pmatrix} + \begin{pmatrix} 0 & \sigma \cdot \hat{P}^\dagger c \\ -\sigma \cdot \hat{P}^\dagger c & 0 \end{pmatrix} = \begin{pmatrix} mc^2 & 0 \\ 0 & mc^2 \end{pmatrix} \quad (1F)$$

Or equivalently as

$$\begin{pmatrix} -\hat{H} - e\phi & 0 \\ 0 & \hat{H} + e\phi \end{pmatrix} + \begin{pmatrix} 0 & -\sigma \cdot \hat{P} c \\ \sigma \cdot \hat{P} c & 0 \end{pmatrix} = \begin{pmatrix} mc^2 & 0 \\ 0 & mc^2 \end{pmatrix} \quad (1G)$$

Section 2

2.1 Solutions of wave equation and its conjugate

Let us define two 4 component column vectors $\langle U |, \langle V |$ and two row vectors $|U \rangle, |V \rangle$ as the solutions of equation and its conjugate defined as such

$$\langle V | \alpha \hat{H} |U \rangle + \sum_i^3 \langle V | \beta^i \hat{P}^i c |U \rangle = \langle V | \mathbf{I} mc^2 |U \rangle \quad (2A)$$

$$\langle U | \alpha \hat{H}^\dagger |V \rangle + \sum_i^3 \langle U | \beta^i \hat{P}^i c |V \rangle = \langle U | \mathbf{I} mc^2 |V \rangle \quad (2B)$$

To obtain complete set of solutions we need to determine these row and column vectors by solving the above equations separately for each. Proceeding

Let column vector $|U \rangle$ be of form $|U \rangle = \begin{pmatrix} u \\ u' \end{pmatrix}$

Its components can be easily determined by solving eqn. (2A) separately for $|U \rangle$

$$\alpha \hat{H} |U \rangle + \sum_i^3 \beta^i \hat{P}^i c |U \rangle = \mathbf{I} mc^2 |U \rangle$$

Or explicitly $\begin{pmatrix} \hat{H} - e\phi & 0 \\ 0 & -\hat{H} + e\phi \end{pmatrix} \begin{pmatrix} u \\ u' \end{pmatrix} + \begin{pmatrix} 0 & \sigma \cdot \hat{P} c \\ -\sigma \cdot \hat{P} c & 0 \end{pmatrix} \begin{pmatrix} u \\ u' \end{pmatrix} = \begin{pmatrix} mc^2 & 0 \\ 0 & mc^2 \end{pmatrix} \begin{pmatrix} u \\ u' \end{pmatrix}$

u and u' as solutions of above equation can be expressed in terms of each other as

$$u = \frac{c\sigma \cdot \hat{p}}{-\hat{H} + e\phi + mc^2} u' \quad \text{and} \quad u' = \frac{-c\sigma \cdot \hat{p}}{\hat{H} - e\phi + mc^2} u$$

2.2 Choice of small and large component

It can be promptly shown that upper component characterizes a particle moving in the direction of +ve gradient of applied potential (electron like behavior) while lower component characterizes a particle moving in -ve direction (positron like behavior). Since in low energy limit an electron behaves predominantly in electronic fashion, we assume upper component to be larger component and lower component to be smaller one. An

opposite choice renders a world where electrons move in the direction of –ve gradient of applied potential and therefore is not a valid option.

For an electron polarized along +ve z axis we can assume

$$u = \begin{pmatrix} 1 \\ 0 \end{pmatrix} u \quad \text{Accordingly} \quad u' = \frac{-c\sigma \cdot \hat{p}}{\hat{H} - \phi e + mc^2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} u$$

Therefore, complete column solution can be written as

$$|U\rangle = \begin{pmatrix} u \\ u' \end{pmatrix} = \frac{1}{N} \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} u \\ \frac{-c\sigma \cdot \hat{p}}{\hat{H} - \phi e + mc^2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} u \end{pmatrix} \quad \frac{1}{N} \text{ is a normalization operator.}$$

In a similar fashion, solving the conjugate equation we obtain

$$\langle U| = (u \quad u') = \left((1 \quad 0)u \quad \frac{-(1 \quad 0)uc\sigma \cdot \hat{p}}{-\hat{H} - \phi e + mc^2} \right) \frac{1}{N}$$

Similarly for $|V\rangle$ and $\langle V|$

$$|V\rangle = \begin{pmatrix} v \\ v' \end{pmatrix} = \frac{1}{N} \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} v \\ \frac{c\sigma \cdot \hat{p}}{-\hat{H} - \phi e + mc^2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} v \end{pmatrix}$$

$$\langle V| = (v \quad v') = \left((1 \quad 0)v \quad \frac{(1 \quad 0)vc\sigma \cdot \hat{p}}{\hat{H} - \phi e + mc^2} \right) \frac{1}{N}$$

Section 3

3.1 State density and normalization of wave function

Expectation value integral of probability density according to postulates of quantum mechanics is

$$\int \rho \, dx dy dz = \int \psi^* \psi \, dx dy dz = \int \langle V | \hat{I} | U \rangle \, dx dy dz = \int \langle U | \hat{I} | V \rangle \, dx dy dz \quad (3A)$$

But in the view of transformation discussed in eqn. (1c) we have transformed probability density as;

$$\int \rho \, dx dy dz = \int \langle V | \alpha \hat{I} | U \rangle \, dx dy dz = \int \langle U | \alpha \hat{I} | V \rangle \, dx dy dz \quad (3B)$$

After substituting solution vectors;

$$\int \rho \, dx dy dz = \int \left[\begin{pmatrix} 1 & 0 \end{pmatrix} v \frac{(1 \ 0) v c \sigma \cdot \hat{p}}{\hat{H} - \phi e + mc^2} \right] \frac{1}{N} \alpha \hat{I} \frac{1}{N} \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} u \\ \frac{-c \sigma \cdot \hat{p}}{\hat{H} - \phi e + mc^2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} u \end{pmatrix} dx dy dz$$

We shall analyze two important cases here.

Case 1: $E \approx mc^2$ and $mc^2 > 0$ (**Low energy limit of a massive particle**)

In this case momentum energy dependent terms of the above matrix equation can be ignored due to their smallness and normalization operator $\frac{1}{N}$ can be set to unity; we obtain

$$\int \rho \, dx dy dz = \int v u \, dx dy dz \Rightarrow \rho = v u$$

Case 2: First order relativistic approximation in weak electrostatic field ($\hat{H} - \phi e + mc^2 \approx 2mc^2$)

Here, the expression for probability density obtained from eqn. (3B) yields

$$\int \rho \, dx dy dz = \int v \frac{1}{N^2} u + v \frac{1}{N} \frac{\hat{P}^2}{4m^2 c^2} \frac{1}{N} u \, dx dy dz$$

Stipulating $\frac{1}{N} = \frac{1}{\sqrt{1 + \frac{\hat{P}^2}{4m^2 c^2}}}$ normalized wave functions can be obtained.

3.2 Quantum classical correspondence

3.2.1 Velocity expectation value

In the view of transformation discussed in eqn. (1D) Heisenberg equation of motion for operator \hat{x} is modified as

$$\left\langle \frac{dx}{dt} \right\rangle = \langle V | \alpha \hat{H} \hat{x} - \alpha \hat{x} \hat{H} | U \rangle + \langle V | \alpha \frac{\partial x}{\partial t} | U \rangle \quad (3C)$$

Assuming \hat{x} has no explicit time dependence or $\alpha \frac{\partial x}{\partial t} = 0$; velocity expectation value in absence of external electromagnetic field has following expression

$$\left\langle \frac{dx}{dt} \right\rangle = \langle V | \alpha \hat{H} \hat{x} - \alpha \hat{x} \hat{H} | U \rangle$$

Substituting various values from eqn. (1A) and solution vectors, we get

$$\left\langle \frac{dx}{dt} \right\rangle = \left((1 \ 0) v \frac{(1 \ 0) v c \sigma \cdot \hat{p}}{\hat{H} + mc^2} \right) \frac{1}{N} \begin{pmatrix} mc^2 \hat{x} - \hat{x} mc^2 & -\sigma \cdot \hat{p} c \hat{x} + \hat{x} \sigma \cdot \hat{p} c \\ \sigma \cdot \hat{p} c \hat{x} - \hat{x} \sigma \cdot \hat{p} c & mc^2 \hat{x} - \hat{x} mc^2 \end{pmatrix} \frac{1}{N} \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} u \\ \frac{-c \sigma \cdot \hat{p}}{\hat{H} + mc^2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} u \end{pmatrix}$$

In low energy limit the expression $\hat{H} + mc^2$ can be approximated as $\hat{H} + mc^2 \approx 2mc^2$. we can also set normalization operator $\frac{1}{N}$ to unity if we are not interested in higher order terms. Subsequently,

$$\begin{aligned} \left\langle \frac{dx}{dt} \right\rangle &= \left((1 \ 0) v \frac{(1 \ 0) v c \sigma \cdot \hat{p}}{2mc^2} \right) \begin{pmatrix} mc^2 \hat{x} - \hat{x} mc^2 & -\sigma \cdot \hat{p} c \hat{x} + \hat{x} \sigma \cdot \hat{p} c \\ \sigma \cdot \hat{p} c \hat{x} - \hat{x} \sigma \cdot \hat{p} c & mc^2 \hat{x} - \hat{x} mc^2 \end{pmatrix} \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} u \\ \frac{-c \sigma \cdot \hat{p}}{2mc^2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} u \end{pmatrix} \\ &= v mc^2 \hat{x} u - v \hat{x} mc^2 u + v \frac{\sigma \cdot \hat{P} \hat{x} \sigma \cdot \hat{P}}{2m} u - v \frac{\hat{x} \hat{P}^2}{2m} u - v \frac{\sigma \cdot \hat{P} \hat{x} \sigma \cdot \hat{P}}{2m} u + v \frac{\hat{P}^2 \hat{x}}{2m} u + \text{higher order terms} \\ &= v \frac{\hat{P}^2 \hat{x}}{2m} u - v \frac{\hat{x} \hat{P}^2}{2m} u \\ &= v \frac{\hat{P}}{m} u \end{aligned}$$

We observe that after omitting higher order corrections velocity expectation value is in full agreement with that obtained in the context of non relativistic Schrödinger equation.

3.2.2 Total angular momentum

For solving Dirac equation in spherically symmetric field's angular momentum Eigen basis is the obvious choice. It's usually believed that total angular momentum $\hat{T} = \hat{L} + \hat{S}$ is a constant of motion in all energy limits and somehow spin angular momentum \hat{S} is integral to a fermionic particle. We shall gauge that such is not the case

if $\hat{T} = \hat{L} + \hat{S}$ is a constant of motion; according to Heisenberg equation of motion

$$\left\langle \frac{d\hat{T}}{dt} \right\rangle = \langle V | \alpha \hat{H} \hat{T} - \alpha \hat{T} \hat{H} | U \rangle = 0$$

Or,

$$\left((1 \ 0) v \frac{(1 \ 0) v c \sigma \cdot \hat{p}}{\hat{H} + mc^2 - e\phi} \right) \frac{1}{N} \begin{pmatrix} mc^2 \hat{T} - \hat{T} mc^2 & -\sigma \cdot \hat{p} c \hat{T} + \hat{T} \sigma \cdot \hat{p} c \\ \sigma \cdot \hat{p} c \hat{T} - \hat{T} \sigma \cdot \hat{p} c & mc^2 \hat{T} - \hat{T} mc^2 \end{pmatrix} \frac{1}{N} \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} u \\ \frac{-c \sigma \cdot \hat{p}}{\hat{H} + mc^2 - e\phi} \begin{pmatrix} 1 \\ 0 \end{pmatrix} u \end{pmatrix} = 0 \quad (3C)$$

Just by observation it becomes abundantly clear that the constant of motion must be a function of dynamical variables like energy and momentum appearing in various orders. As discussed earlier, additional angular momentum \hat{S} must be a dynamical quantity rather than a constant valued matrix operator. We should calculate it to the order of accuracy required depending on the sensitivity of experimental setup. Thereby, in absence of a closed form Eigen basis, even the simplest system like hydrogen atom can be studied only perturbatively and an exact expression for energy Eigen value shall elude us.

3.3.3 A curious case of null rest energy

With appropriate apparatus for calculating expectation values in our hands, we investigate an interesting behavior of ultra relativistic electron. We wish to calculate the non normalized contribution of rest energy to the total energy of electron in high energy limit.

From equation (2A);

$$\langle \hat{H} \rangle = \langle V | \alpha \hat{H} | U \rangle = \langle V | mc^2 | U \rangle - \langle V | \beta^i \hat{P}_i c | U \rangle$$

As we are interested only in contribution from rest energy, momentum term can be neglected for a while

$$\langle \hat{H} \rangle = \langle V | mc^2 | U \rangle$$

$$= \left((1 \ 0) v \frac{(1 \ 0) v c \sigma \cdot \hat{p}}{\hat{H} + mc^2} \right) \begin{pmatrix} mc^2 & 0 \\ 0 & mc^2 \end{pmatrix} \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} u \\ \frac{-c \sigma \cdot \hat{p}}{\hat{H} + mc^2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} u \end{pmatrix}$$

On simplifying, the equation reduces to

$$= v mc^2 u - v \frac{c^2 \hat{P}^2}{(\hat{H} + mc^2)^2} u$$

In the ultra relativistic limit ($\hat{P} \rightarrow \infty$)

$$= \lim_{\hat{P} \rightarrow \infty} v m c^2 u - v \frac{c^2 \hat{P}^2}{(\hat{H} + m c^2)^2} u = 0$$

From above exercise it's evident that rest energy contribution to total energy of electron in ultra relativistic limit is null. This apparent mass less behavior implies that electron shows characteristics similar to light quantum in high energy limit.

Comment and conclusion

The work attempts to thoroughly establish a smooth reduction of some aspects of Dirac equation to non relativistic domain and its quantum classical correspondence becomes clear and free of contradictions of both theoretical and experimental nature. A valid total angular momentum can be calculated satisfying eqn. (3C) and be used as an Eigen basis for finding energy levels of hydrogen atom. The author speculates some contribution from new angular momentum in lifting the degeneracy prevalent in earlier treatments of hydrogen atom. Since additional angular momentum is now a dynamical operator characterization of elementary fermions as particles carrying intrinsic angular momentum is not well suited. Projection Eigen values in context of Stern Gerlach type experiments must be delinked from and should not be interpreted as a consequence fictitious spin angular momentum of particle.

Bibliography

- [1] P.A.M Dirac "The Quantum Theory of Electron", Proc. R. Soc. A (1928) VOL. 117. No. 778, 610-624
- [2] E. Schrodinger "On the free movement in relativistic quantum mechanics" Berliner. Ber., pp. 418-428 (1930)
- [3] T D Newton and E P Wigner , *Rev. Mod. Phys.* 21, 400 (1949)
- [4] M.H.L Pryce, *Proc. Roy. Soc* 195(A), 62 (1948)
- [5] A Messiah , *Quantum Mechanics* volume 2, Chapter xx, Section 37 pp 950-952 (1962)
- [6] Hastenes D. "The Zitterbewegung interpretation of Quantum mechanics" *Found. Physics.* Vol. 20 No. 10 (1990) 1213-1232
- [7] Gyula David, "General theory of Zitterbewegung" *Phys. Rev.* B81, 121417[®] (2010)
- [8] L. L Foldy , S A Wouthuysen, *Phys. Rev* 78, 29 (1950)