Relativistic Quantum mechanics

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1 Limitations of Schrödinger Equation

Consider the 3-dimensional Schrödinger Equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,y,z) = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi(x,y,z) + V(x,y,z)\psi(x,y,z) \tag{1}$$

The equation consists of a first derivative in time and a second derivative in space and is inherently non-relativistic because it does not treat space and time on equal footing. One can also show that the Schrödinger Equation is not invariant under Lorentz Transformations. We require either the Schrödinger Equation entirely use first derivatives or second derivatives to be relativistic.

2 The Klein Gordon Equation

In Special Relativity, a particle with 4-momentum p^μ must satisfy the relativistic dispersion relation

$$p^\mu p_\mu = E^2 - \mathbf{p}^2 = m^2, \tag{2}$$

Lets convert all derivatives in the Schrödinger Equation to second derivatives. To do this, we make the transformation to operator form with the use of natural units $\hbar = c = 1$

$$E \to i\partial_t \tag{3}$$

$$p \to i\boldsymbol{\nabla} \tag{4}$$

We postulate the wave equation for the spin-0 particle:

$$m^2\phi = \left[(i\partial_t)^2 - (i\boldsymbol{\nabla})^2\right]\phi \tag{5}$$

$$= (\boldsymbol{\nabla}^2 - \partial_t^2)\phi \tag{6}$$

$$(\partial^\mu\partial_\mu - m^2)\phi = 0 \tag{7}$$

Equation 7 is the Klein Gordon Equation and it is Lorentz Invariant by its construction. It can be shown that the solution is

$$\phi = Ne^{i\mathbf{k}\cdot\mathbf{x} - i\omega_k t} \quad \text{with} \quad \omega_k = \pm(\mathbf{k}^2 + m^2)^{3/2} \tag{8}$$

It may come as a shock that Equation 8 permits solutions with negative energy! This is a problem because the Hilbert space is formed by all possible solutions. If this has shocked you, what comes next might induce trauma. The probability density can be interpreted as:

$$\phi^*\frac{\partial^2\phi}{\partial t^2} - \phi\frac{\partial^2\phi^*}{\partial t^2} = \phi^*(\boldsymbol{\nabla}^2\phi - m^2\phi) - \phi(\boldsymbol{\nabla}^2\phi^* - m^2\phi) \tag{9}$$

$$= \phi^*\boldsymbol{\nabla}^2\phi - \phi\boldsymbol{\nabla}^2\phi^* \tag{10}$$

Using this, we form the continuity equation $\partial_t\rho + \boldsymbol{\nabla}\cdot\mathbf{j} = 0$ with

$$\rho = i\left(\phi^*\frac{\partial\phi}{\partial t} - \phi\frac{\partial\phi^*}{\partial t}\right) \quad \text{and} \quad \mathbf{j} = -i(\phi^*\boldsymbol{\nabla}\phi - \phi\boldsymbol{\nabla}\phi^*) \tag{11}$$

where we have added i to make the quantities real. For a plane wave, we have

$$\omega_k\phi^*\phi - \phi(-\omega_k)\phi^* = 2\omega_k|N|^2 \tag{12}$$

and since ω_k can be negative, density can be negative and cannot be interpreted as the usual probability density. Has the world come to an end? Thankfully, Dirac provides a solution to this issue.

3 The Dirac Equation

We saw in the last section that relativistic quantum mechanics with second derivatives has problems, but lets instead try with first derivatives. Dirac's strategy was to factor the relativistic dispersion relation into two factors which are linear in 4-momentum

$$0 = p^\mu p_\mu - m^2 \tag{13}$$
$$= (\beta^\alpha p_\alpha + m)(\gamma^\lambda p_\lambda - m). \tag{14}$$

This equation is solved if either terms go to zero

$$\beta^\alpha p_\alpha + m = 0 \quad \text{or} \quad \gamma^\lambda p_\lambda - m = 0. \tag{15}$$

We can use either equation to define a relativistic equation. Lets choose the second equationa and perform the canonical substitution $p_\mu \to i\partial_\mu$

$$i\gamma^\mu \partial_\mu \psi = m\psi \tag{16}$$
$$i\gamma^0 \partial_t \psi = \left(-i\gamma^i \frac{\partial}{\partial x^i} + m\right)\psi \tag{17}$$
$$i\partial_t \psi = \left(-i(\gamma^0)^{-1}\gamma^i \frac{\partial}{\partial x^i} + m(\gamma^0)^{-1}\right)\psi \tag{18}$$
$$\equiv \hat{H} \tag{19}$$

which is the expression for the relativistic Hamiltonian. To find the coefficients γ^λ, we expand the right side of Equation 14 out

$$(\beta^\alpha p_\alpha + m)(\gamma^\lambda p_\lambda - m) = \beta^\alpha p_\alpha \gamma^\lambda p_\lambda - m(\beta^\lambda - \gamma^\lambda)p_\lambda - m^2. \tag{20}$$

Comparing this to Equation 13 shows that $\beta^\lambda = \gamma^\lambda$ and so

$$p^\mu p_\mu = \gamma^\alpha p_\alpha \gamma^\lambda p_\lambda = (\gamma^\alpha p_\alpha)^2. \tag{21}$$

Writing Equation 21 out in components gives

$$(p^0)^2 - (p^1)^2 - (p^2)^2 - (p^3)^2 = (\gamma^0 p_0 + \gamma^1 p_1 + \gamma^2 p_2 + \gamma^3 p_3)^2. \tag{22}$$

By expanding and comparing coefficients,

$$(\gamma^0)^2 = 1 \qquad (\gamma^i)^2 = -1 \qquad (\gamma^\mu\gamma^\nu - \gamma^\nu\gamma^\mu) = 0 \tag{23}$$

These conditions can not be satisfied by ordinary commuting numbers so we require these coefficients to be matrices that satisfy the relation

$$\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}. \tag{24}$$

We require γ^0 and $\gamma^0\gamma^i$ be Hermitian matrices in order to have a Hermitian Hamiltonian. This condition is satisfied when

$$(\gamma^\mu)^\dagger = \gamma^0\gamma^\mu\gamma^0 \tag{25}$$

This is obvious for the case where $\mu = 0$ using the fact $(\gamma^0)^{-1} = \gamma^0$. For the other indicies, we use the hermiticity property

$$\gamma^0\gamma^i = (\gamma^0\gamma^i)^\dagger = \gamma^{i\dagger}\gamma^{0\dagger} \implies (\gamma^i)^\dagger = \gamma^0\gamma^i\gamma^0 \tag{26}$$

The smallest matrices which satisfy the above relations are 4×4 matrices. The set of matrices are not unique, we will use the Dirac-Pauli representation:

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix} \tag{27}$$

Where 0 is a 2×2 zero matrix and 1 is a 2×2 identity matrix and σ^i is the i-th Pauli matrix.

Using Equation 14, we use the second factor by convention to find that

$$\gamma^\lambda p_\lambda - m = 0. \tag{28}$$

After the substitution of $p_\mu \to i\partial_\mu$, we find that

$$(i\gamma^\mu \partial_\mu - m)\psi = 0, \tag{29}$$

and we will introduce the Feynman slash notation $\not{\partial}_\mu = \gamma^\mu \partial_\mu$ so that

$$(i\not{\partial}_\mu - m)\psi = 0 \tag{30}$$

which is known as the Dirac equation.