Extension of Dirac Equation with Harmonic Functions and Its Novel Features

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Abstract
In this work we present the solution of the Dirac equation with sine and cosine functions as extensions. In both cases, we find the same probability distribution which is a continuous spatial function with locally bound states. It is also observed that the particle has periodic momentum. It is expected from this work that the equation will have applications in condensed matter physics and nanophysics.
Keywords: Modified Dirac equation, Space dependent probability, periodic momentum, Gaussian probability.

I.   1 Introduction

The most elegant equation that combines quantum mechanics and special relativity, to give a more complete theory of electron, is Dirac equation. Solving this equation, we get plane wave solutions. Dirac equation for free particle has the form

$$(c\vec{\alpha} \cdot \vec{p} + \beta mc^2)\psi = E\psi. \tag{1}$$

Here, m is the rest mass of the particle,$\beta$is a constant, $\alpha$is a constant space vector and the momentum operator is$\vec{p} = -i\hbar\vec{\nabla}$. Solution to this equation is a bispinor which satisfies the relativistic energy condition and obey boundary conditions too. Eq.(1) has solutions as plane wave containing$\exp(i\vec{k} \cdot \vec{r})$ term which refers to an infinite wave train. But we cannot use wave trains suitably. Several authors addressed that relativistic wave packets create a challenge to theory[1, 2, 3, 4]. Many researchers includedδ-function potentials with Dirac equation[5, 6] in condensed matter physics. In nanophysics, the study of wave packets in the light of Dirac theory is an important piece of work[7, 8, 9, 10]. We wish to find localized states of Dirac equation and other forms of states that describe the physical reality of interest. Dirac equation can be extended by replacing$p$ by $-i\beta\omega\vec{r}$ to give oscillatory state which is now known as Dirac oscillator[11]. Dirac oscillator has already been realized experimentally[12]. Experimental realization of the Dirac oscillator allows us to implement other one-dimensional Dirac type equations. In the light of Dirac oscillator Faruque et al. used the modification $\vec{p} \to \vec{p} - iq\vec{r}$[13] and found localized wave packets as solutions. In the light of all these modifications, in this work, we modified Dirac equation by replacing $\vec{p}$ by$\vec{p} - ig \sin \vec{q} \cdot \vec{r}$ and obtained the following equation

$$[c\vec{\alpha} \cdot (\vec{p} - ig \sin \vec{q} \cdot \vec{r}) + \beta mc^2]\psi = E\psi. \tag{2}$$

In one dimension, say, for motion in z-direction, Eq.(2) reduces to

$$[c\alpha_z(p_z - ig \sin q\,z) + \beta mc^2]\psi = E\,\psi, \tag{3}$$

where we have assumed stationary states with energy$E$. In Eq.(3),$\alpha_z$is the Dirac matrix made with σ_z, $p_z$is the momentum in the z-direction, g and q are parameters. g has dimension of momentum and q has dimension of $length^{-1}$ i.e., it is wave number. It is noteworthy that Eq.(3) is PT-symmetric.

II.   Sine Function as Extension

We want to solve the eigenvalue problem$H\psi = E\psi$
for

$$H = [c\alpha_z(p_z - ig \sin q\,z) + \beta mc^2]. \tag{4}$$

Here we are assuming the particle to be in motion along z-direction with momentum p. For this reason we use α_z instead of α, and z in the place of $\vec{r}$.

Before solving the equation it's noteworthy to mention that the Hamiltonian H commutes with the z-component of spin, $\sum_z$, i.e. $[\sum_z, H] = 0$. And therefore, our solution will be simultaneous eigenstates of energy and spin. So, we write the solution in the following form:

$$\psi(z) = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}. \tag{5}$$

Substituting this in Eq.(3) we get the eigenvalue equation as

$$\begin{pmatrix} mc^2 & 0 & cp - icg\sin qz & 0 \\ 0 & mc^2 & 0 & -cp + icg\sin qz \\ cp - icg\sin qz & 0 & -mc^2 & 0 \\ 0 & -cp + icg\sin qz & 0 & -mc^2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = E \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}.$$

Solving this equation yields the following coupled equations:

$$(cp - icg\sin qz)u_3 = (E - mc^2)u_1, \tag{6}$$

$$(cp - icg\sin qz)u_1 = (E + mc^2)u_3, \tag{7}$$

and

$$(-cp + igc\sin qz)u_4 = (E - mc^2)u_2, \tag{8}$$

$$(-cp + igc\sin qz)u_2 = (E + mc^2)u_4. \tag{9}$$

Following traditional methods, let us assume $u_2 = u_4 = 0$ and from Eq.(6) and Eq.(7) we have

$$(cp - icg\sin qz)(cp - icg\sin qz)u_1 = (E^2 - m^2c^4)u_1 \tag{10}$$

$$(cp - icg\sin qz)(cp - icg\sin qz)u_3 = (E^2 - m^2c^4)u_3. \tag{11}$$

Since, u_1 and u_3 satisfy the same equation, we need to solve only one of them, say, Eq.(10). To solve this equation, we use $p = -i\hbar\frac{\delta}{\delta z}$. Then we obtain an equation of the form:

$$\frac{d^2}{dz^2}u_1 + \frac{2g}{\hbar}\sin qz\frac{du_1}{dz} + \frac{qg}{\hbar}\cos qz\, u_1 + \frac{g^2}{\hbar^2}\sin^2 qz\, u_1 = ku_1, \tag{12}$$

where, $k = \frac{E^2 - m^2c^4}{\hbar^2c^2}$.

We need to solve this 2nd order differential equation and by intelligent guess we suppose

$$u_1 = \frac{g}{q\hbar}\cos qz,$$

and solve the above equation by inserting the value of u_1 in Eq.(12).
And thus, at last we have

$$u_1 = \frac{\frac{g^2}{\hbar^2} - 3\frac{g^2}{\hbar^2}\sin^2 qz}{k + q^2 - \frac{g^2}{\hbar^2}\sin^2 qz}.$$

Similarly, we can have

$$u_3 = \frac{\frac{g^2}{\hbar^2} - 3\frac{g^2}{\hbar^2}\sin^2 qz}{k + q^2 - \frac{g^2}{\hbar^2}\sin^2 qz}.$$

If we assume $u_1 = u_3 = 0$ and then solve for u_2 and u_4 following the similar procedure we get the same solution for u_2 and u_4 as well.

As we know a spinor has two independent forms for spin up and down, we can write our results as follows:

$$\psi_{up}(z) = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} \frac{\frac{g^2}{\hbar^2} - 3\frac{g^2}{\hbar^2}\sin^2 qz}{k + q^2 - \frac{g^2}{\hbar^2}\sin^2 qz},$$

$$\psi_{down}(z) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} \frac{\frac{g^2}{\hbar^2} - 3\frac{g^2}{\hbar^2}\sin^2 qz}{k + q^2 - \frac{g^2}{\hbar^2}\sin^2 qz}.$$

Hence, the probability of the electron to be at the position z is

$$p = |\psi|^2 = \psi^*\psi = |u_1|^2 + |u_3|^2 = 2|u_1|^2$$

$$\therefore |\psi|^2 = 2\left(\frac{\frac{g^2}{\hbar^2} - 3\frac{g^2}{\hbar^2}\sin^2 qz}{k + q^2 - \frac{g^2}{\hbar^2}\sin^2 qz}\right)^2. \tag{13}$$

III. Cosine Function as Extension

When we modify the Dirac equation with cosine function as an extension, we have

$$[c\alpha_z(p_z - ig\cos q\, z)]\psi = E\psi, \tag{14}$$

for one dimensional motion of the particle. After following the same procedure as section 2 we gain the solutions as

$$\psi_{up} = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} \frac{\frac{g^2}{\hbar^2} - 3\frac{g^2}{\hbar^2}\cos^2 qz}{-q^2 - k + \frac{g^2}{\hbar^2}\cos^2 qz},$$

and

$$\psi_{down} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} \frac{\frac{g^2}{\hbar^2} - 3\frac{g^2}{\hbar^2}\cos^2 qz}{-q^2 - k + \frac{g^2}{\hbar^2}\cos^2 qz}.$$

Hence, the probability is

$$|\psi|^2 = 2\left(\frac{\frac{g^2}{\hbar^2} - 3\frac{g^2}{\hbar^2}\cos^2 qz}{-q^2 - k + \frac{g^2}{\hbar^2}\cos^2 qz}\right)^2. \tag{15}$$

IV. Results
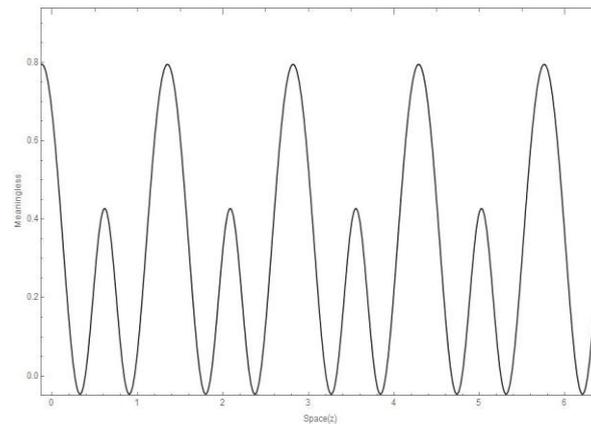
Figure 1: Graphical rendering of probability (Eq.13 and Eq.15).

$$\text{Where,} \frac{g}{\hbar} = 0.5, q = \sqrt{5}, k = -5.5$$

The graphical representation gives a periodic probability distribution. In the classical approximation,

$$dp \propto \frac{dx}{v_{cl}}. \tag{16}$$

Where, v_{cl} is the classical velocity, $dp \propto |\psi(r)|^2 d^3 r$ is the probability of the particle to be found at the position r in the range $d^3 r$. In the case of one-dimensional movement of the particle, the probability is

$$dp \propto |\psi(x)|^2 dx. \tag{17}$$

So, it is obvious that in the region where $|\psi|^2$ is less, the particle is moving fast there. In the region where $|\psi|^2$ is large, the particle is slow. If $|\psi|^2$ shows a periodic pattern with highs and lows alternatively, we can say that the particle is moving with periodic momentum. Periodic momentum is observed in the case of harmonic oscillators but there the periodicity is time dependent, whereas here we have space dependent periodic momentum. Periodicity in space is observed in the case of lattice structure. Figure-1 also shows that the wave function is not bounded in a region so the outcome can be realized only in a one-dimensional lattice which is virtually infinite. There are forbidden regions where the particle cannot be found hence the particles are bounded between two forbidden regions. And hence the probability is Gaussian.

V. Summary and Conclusion

We have introduced two extensions of Dirac equation in this paper, given by Eq.1 and another by Eq.14 and in both cases, we have found the same probability distribution. Our results give periodic momentum in one dimensional lattice. Since the study of particles in periodic potentials is in the heart of condensed matter physics, this work can play a very important role in this arena. The widely used Kronig-Penny model describes an electron in one dimensional potential but it hardly describes relativistic effects of the electron. Our work is conducted from a relativistic point of view and it is expected to be useful to explain various relativistic effects of electrons in one dimensional potential. It can be useful to study relativistic effects in the band structure too.

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