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A New Paradox in Relativistic Quantum Mechanics

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Abstract

In this article, we discuss a paradoxical result that exists for positive energy Klein-Gordon particles. It may be called “Klein paradox” of another kind. We have shown its existence in one, two and three dimensions. The paradox seems to indicate the limitations of the single particle Klein-Gordon equation in the presence of strong potentials.

Keywords: Binding Criteria in Quantum theory, Minimum coupling rule, Klein-Gordon equation.

1. Introduction

In non-relativistic quantum mechanics, the scattering of a particle by a potential barrier is one of the simplest solvable problems [1-3]. There is a finite probability of the particle passing through the barrier and some probability of its reflection from the barrier. However, a similar problem with a potential step or a barrier for an electron (Obeying Dirac relativistic equation) leads to a paradoxical result.

In the original work of Klein [4] in 1929, electrons incident on a large potential step was considered. It was shown that for large potentials ($V > E + mc^2$) the reflection coefficient exceeds unity while the transmission coefficient becomes negative. Such a puzzling result, contradicting the conventional wisdom of non-relativistic quantum mechanics has come to be known as Klein Paradox. Bjorken and Drell[5] have shown that when electrons are incident on electrostatic potential with a sharp boundary, the reflected current exceeds the incident current for a potential barrier ($V_0 > E + mc^2$) for positive energy electrons. They suggest that such a paradoxical result can be explained by understanding and

interpreting the negative energy solutions.

Similar results are found [6-8] for relativistic spin zero particles obeying the Klein-Gordon equation. In this article, we discuss the appearance of another kind of paradoxical result for relativistic spin zero particles (Obeying the Klein-Gordon wave equation).

2. The Klein-Gordon particle in a potential

The one-dimensional Klein-Gordon (K-G) wave equation for a free particle of mass m is given by

$$E^2\psi = -\hbar^2 c^2 \frac{d^2\psi}{dx^2} + m^2 c^4 \psi \quad (1)$$

In the presence of a potential field $V(x)$, the Klein-Gordon equation can be obtained by introducing the potential as the fourth component of a four-vector potential. This is the familiar canonical or minimal coupling rule. Hence, the K-G equation with potential $V(x)$, can be written as

$$(E - V(x))^2 \psi = -\hbar^2 c^2 \frac{d^2\psi}{dx^2} + m^2 c^4 \psi \quad (2)$$

This can be simplified to

$$\frac{d^2\psi}{dx^2} + \left\{ \frac{[E - V(x)]^2 - m^2 c^4}{\hbar^2 c^2} \right\} \psi = 0 \quad (3)$$

Let us compare this with the Schrodinger equation

for non-relativistic particles in the presence of a potential $V(x)$:

$$\frac{d^2 \psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \psi(x) = 0 \quad (4)$$

Equation (3) can be cast into the above form

$$\frac{d^2 \psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E_{eff} - V_{eff}(x)] \psi(x) = 0 \quad (5)$$

Where

$$E_{eff} = \frac{E^2 - m^2c^4}{2mc^2} \quad (6)$$

and

$$V_{eff}(x) = \frac{2EV(x) - V^2(x)}{2mc^2} \quad (7)$$

Taking over the results of non-relativistic quantum mechanics, the relativistic wave function will be oscillatory in the region where $E_{eff} > V_{eff}$ and will be exponentially growing or damped in regions where $E_{eff} < V_{eff}$.

Let us consider, as an example, the simple harmonic oscillator potential $V(x) = \frac{1}{2}Kx^2$.

$$\text{Then, } V_{eff}(x) = \frac{EKx^2 - \frac{1}{4}K^2x^4}{2mc^2} \quad (8)$$

A typical plot of $V_{eff}(x)$ for positive energies as a function of x is shown in figure (1).

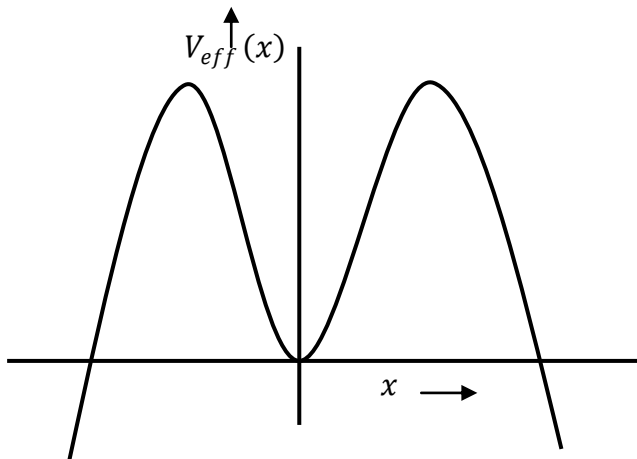


Figure (1).

For large values of $|x|$ we find $E_{eff} > V_{eff}$. Hence the particle cannot be confined in such a potential. This also follows from the fact that $V_{eff}(x)$ does not have a lower bound. Hence, genuine bound states do not exist.

3. The Klein-Gordon particle in a square potential well

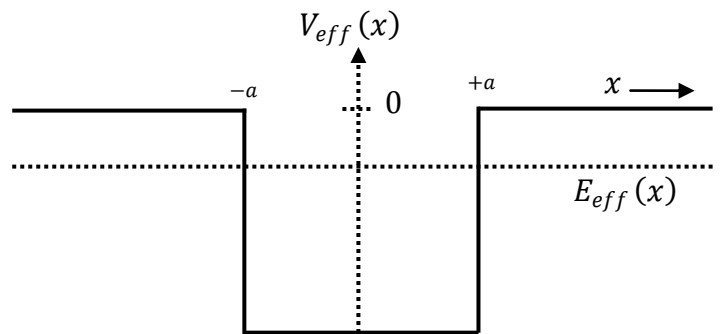
Let us consider a square potential well defined by

$$V(x) = \begin{cases} -V_0 & \text{for } |x| \leq a \\ 0 & \text{for } |x| > a \end{cases} \quad (9)$$

Then the effective potential for positive energy K-G particle is

$$V_{eff}(x) = \begin{cases} -\frac{2EV_0 - V_0^2}{2mc^2} & \text{for } |x| \leq a \\ 0 & \text{for } |x| > a \end{cases} \quad (10)$$

Hence, $V_{eff}(x)$ also corresponds to another square well of depth $(2EV_0 + V_0^2)/2mc^2$ in place of V_0 that has the same range as before (see figure (2)). Therefore, genuine bound states can exist for some values of positive energies such that $E < mc^2$.



Figure(2).

Since the energy of the K-G particle is positive the probability density takes only non-negative values as in the non-relativistic case.

4. The Klein-Gordon particle in the presence of a square potential barrier.

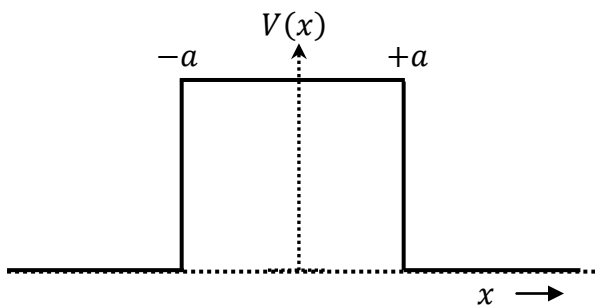
Let us consider a square potential barrier (for mathematical simplicity) given by

$$V(x) = \begin{cases} +V_0 & \text{for } |x| \leq a \\ 0 & \text{for } |x| > a \end{cases} \quad (11)$$

Then the effective potential for this case is

$$V_{eff}(x) = \begin{cases} \frac{2EV_0 - V_0^2}{2mc^2} & \text{for } |x| \leq a \\ 0 & \text{for } |x| > a \end{cases} \quad (12)$$

(A) For “weak” potentials, i.e, when $V_0 \ll mc^2$ and for positive energy particles $V_{eff}(x)$ leads to another square potential barrier as shown in figure(3).



Figure(3).

Therefore, non-trivial solutions of equation (5) are very much like those of the non-relativistic case. Note that non-trivial (scattering) solutions exist for all values of energy greater than mc^2 . No solutions exist for $E < mc^2$.

(B) Let us consider case of “strong” potentials. For potential barrier heights $V_0 > 2mc^2$ and staying with positive energies the effective potential takes the unusual form of a potential well as shown in figure (4) with a depth

$$V'_0 = \frac{V_0^2 - 2EV_0}{2mc^2}.$$

The effective energy E_{eff} can be positive or negative depending on $E > mc^2$ or $E < mc^2$.

If $E > mc^2$, we get the usual scattering state solution. However, if $E < mc^2$, then E_{eff} will be negative, leading to a situation like the states of a particle bound in a square well potential. This is indeed a paradoxical result. Here, we are getting genuine bound states for a positive energy K-G particle ($mc^2 > E > 0$) that forms a bound state in a strong square potential barrier. This may be called Klein’s Paradox of another kind.

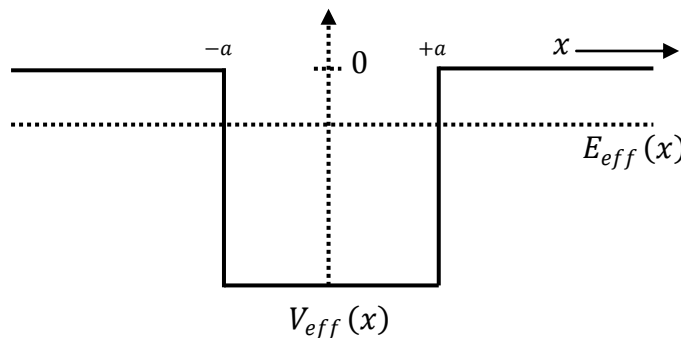


Figure (4).

It is to be noted that, our choice of a square potential barrier is only for mathematical simplicity and that genuine bound states can exist for a strong potential ($V_{peak} > 2mc^2$) of any shape.

Since we are considering only positive energy solutions of the K-G equation, the probability density remains non-negative throughout our physical region.

5. Paradoxical bound states in higher dimensions

Let us consider a K-G particle in a two-dimensional central potential $V(\rho)$. The two-dimensional equivalent of equation (4) will be given by

$$\left[\frac{d^2}{d\rho^2} + \frac{1}{\rho} \frac{d}{d\rho} - \frac{n^2}{\rho^2} + \frac{E^2 - m^2c^4}{\hbar^2c^2} + \frac{V^2 - 2EV}{\hbar^2c^2} \right] \psi(\rho) = 0 \quad (13)$$

Where $n = 0, 1, 2, \dots$ being the angular quantum number.

Considering a square barrier(hill) potential of height V_0 defined by

$$V(\rho) = \begin{cases} +V_0 & \text{for } |\rho| \leq a \\ 0 & \text{for } |\rho| > a \end{cases} \quad (14)$$

We can see that for “strong” potential barriers, such that $V_0 \geq mc^2$

$$\frac{2m}{\hbar^2} [E_{eff} - V_{eff}] = \frac{E^2 - m^2c^4 - 2EV_0 + V_0^2}{\hbar^2c^2} \quad (15)$$

And takes positive values for $\rho \leq a$ and negative values for $\rho > a$.

Hence the radial wave function (equation (13)) takes the general form

$$\left\{ \frac{d^2}{d\rho^2} + \frac{1}{\rho} \frac{d}{d\rho} + \left[K^2 - \frac{n^2}{\rho^2} \right] \right\} \psi(\rho) = 0 \quad (16)$$

It is nothing but familiar Bessel equation [9-10] whose solutions for $\rho \leq a$ are the Bessel function $J_n(K\rho)$ of order n .

For $\rho > a$, we get damped solutions proportional to the modified Bessel function $K_n(q\rho)$, where $q^2 = m^2c^4 - E^2$.

The numerical values of bound state energies can be obtained by usual procedure of matching the wave functions and their derivatives at the radial value $\rho = a$. Therefore we conclude that genuine bound states are possible for a two-dimensional potential barrier when the barrier height is greater than $2mc^2$. Hence the paradox exists in two dimensions also.

Let us, finally consider a three-dimensional central potential $V(r)$ having the form

$$V(r) = \begin{cases} +V_0 & \text{for } |r| \leq a \\ 0 & \text{for } |r| > a \end{cases} \quad (17)$$

The equation for the radial part of the wave function can be written as

$$\left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) - \frac{l(l+1)}{r^2} + \frac{E^2 - m^2c^4}{\hbar^2c^2} + \frac{V^2 - 2EV}{\hbar^2c^2} \right] \psi(r) = 0 \quad (18)$$

Where $l = 0, 1, 2, \dots$ being the angular momentum quantum number.

Putting $\psi(r) = \frac{u(r)}{r}$, we get the following equation for $u(r)$:

$$\left[\frac{d^2}{dr^2} + \frac{E^2 - m^2c^4}{\hbar^2c^2} + \frac{V^2 - 2EV}{\hbar^2c^2} - \frac{l(l+1)}{r^2} \right] u(r) = 0 \quad (19)$$

Now, specialize to the case of a square potential

barrier defined by

$$V(r) = \begin{cases} V_0 & \text{for } |r| \leq a \\ 0 & \text{for } |r| > a \end{cases} \quad (20)$$

Let

$$\frac{E^2 - m^2c^4 + V_0^2 - 2EV_0}{\hbar^2c^2} = K^2 \quad (21)$$

For $V_0 \geq E + mc^2$ and $E \leq mc^2$, K^2 will be positive. Then the equation for $u(r)$ becomes

$$\left\{ \frac{d^2}{dr^2} + \left[K^2 - \frac{\left(l + \frac{1}{2}\right)^2}{r^2} \right] \right\} u(r) = 0 \quad (22)$$

Substituting $\chi(r) = \frac{u(r)}{\sqrt{r}}$, we get the reduced equation

$$\left\{ \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} + \left[K^2 - \frac{\left(l + \frac{1}{2}\right)^2}{r^2} \right] \right\} \chi(r) = 0 \quad (23)$$

This can be easily identified as the modified Bessel equation whose solutions are given by Spherical Bessel functions $\chi_{in}(r) \propto J_{l+\frac{1}{2}}(Kr)$ in the region $r \leq a$.

Outside the potential barrier (hill) region we get the equation

$$\left\{ \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \left[q^2 - \frac{\left(l + \frac{1}{2}\right)^2}{r^2} \right] \right\} \chi_{out}(r) = 0 \quad (24)$$

Physical $\chi_{out}(r)$ is exponentially damped solution which is proportional to spherical Hankel functions. Therefore, we come to the conclusion that for "strong" potentials ($V_0 > 2mc^2$) genuine bound states are possible for the K-G particle with positive energy. This, again, is a paradoxical result. The actual values of the bound states can be obtained by the well-known procedure of matching the wave functions and their derivatives at the boundary $r = a$.

6. Results and Discussion

Genuine bound states for strong potential barriers

(with $V_0 > 2mc^2$) are possible for K-G particles having positive energies ($0 < E < mc^2$) in one, two and three spatial dimensions. As the choice of the square potential barriers is only for mathematical convenience, we can expect to find bound states as long as the potential is “strong” ($V > 2mc^2$) in some region of its definition.

This paradoxical result seems to indicate the shortcomings of the single particle Klein-Gordon equation as the strong particles may lead to the production of particles and antiparticles. Further, we may expect to find similar paradoxical results for spin-half particles obeying the Dirac equation, even though we are led to face coupled equations in that case.

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