# Klein paradox and the Dirac-Kronig-Penney model

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We analyze the barrier problem and the Kronig-Penney model for Dirac particles, paying attention to the Klein paradox and the nature of the potential. The ambiguities associated with the δ-function limit are examined and the physically reasonable way to include δ-function potentials in the Dirac-Kronig-Penney problem is identified.

Since the observation that relativistic effects play a significant role in determining the band structure of heavy metals,[1] a number of authors have discussed the generalization to Dirac electrons of the classic Kronig-Penney model[2] and its generalization to model surface states,[3,4] substitutional alloys,[5] and liquid metals.[6] It was natural for these authors to discuss an array of δ-function potentials. It was then noted that the method of obtaining the band equation for a square well (or square barrier) and taking the δ-function limit, and the method of directly solving the Dirac equation for a δ-function potential gave different results. However, it was noted that these results became identical when the strength of the δ-function potential was weak.

The conventional explanation of this discrepancy is due to Fairbairn, Glasser, and Steslicka,[3] and is based on the difficulty of localizing Dirac particles within a distance $\hbar/mc$ without coupling to negative energy states or producing pairs of particles.[7] This argument has been interpreted as leading to the Klein paradox[8] and as justifying the use of the results obtained by solving the Dirac equation for a δ-function potential.[3]

We have recently investigated the potential representation of quark confinement in the Dirac equation,[9] and the Dirac-Kronig-Penney model as a crude representation of the behavior of quarks in the nucleus.[10] In the course of these investigations we studied the manifestations of the Klein paradox in the relativistic barrier penetration problem and in the Dirac-Kronig-Penney model. We also obtained the general solution of the Dirac equation for a potential which approaches a δ-function limit. In all of these calculations we considered both potentials of the electrostatic type and potentials of the Lorentz scalar type. As a result of this we believe we have obtained some new insight into the question of how to take the δ-function limit in the Dirac-Kronig-Penney problem. We refer the reader to Ref. 10 for a detailed account of the calculations, and simply reproduce parts of that paper as they are necessary for the present discussion.

The classic example used to discuss the Klein paradox is the potential step.[11] When the potential is of the electrostatic type (i.e., the time component of a four-vector potential), and it exceeds $E$-$m$, the reflection coefficient exceeds unity and the transmission coefficient is negative. In the hole-theory interpretation[12] the strong potential raises the energy of the occupied negative energy levels to the point where the electrons tunnel through to the positive energy electron levels in the field-free region. These electrons are then repelled by the potential barrier, giving the large reflected current. The holes they leave behind are positrons which produce the negative transmitted current. As was demonstrated by Sauter[13] and emphasized by Pauli,[14] this effect depends only on the eventual strength of the potential and is quite independent of the rate of increase of the potential, or of its step nature.

After the introduction of the quark model of hadrons, and the desire to find models in which the light quarks are confined relativistically, it was realized by Bogoliubov[15] and others[16] that a Lorentz scalar potential did not exhibit the Klein paradox and did provide a relativistic potential model of confinement.

To see how the Klein paradox influences the barrier problem, note that the transmission coefficient $\mathcal{T}$ for a square barrier of width $a$ and height $V_e$ is

$$\mathcal{T}=\frac{1}{1+\frac{1}{4}\left[\frac{\Lambda}{\lambda}-\frac{\lambda}{\Lambda}\right]^2\sin^2(Ka)} \tag{1}$$

for electrostatic potentials, where $K$ is the wave number in the barrier region

$$K=[(E-V_e)^2-m^2]^{1/2} , \tag{2}$$

$k$ is the wave number in the field-free region,

$$\lambda=\frac{k}{E+m}, \quad \Lambda=\frac{K}{E-V_e+m} . \tag{3}$$

The form of $\mathcal{T}$ quoted in (1) is valid for real values of $K$, in particular, for $V_e > E-m$, and is appropriate for discussing the Klein paradox for the potential barrier. If we allow $V_e$ and hence $K$ to become very large, $\Lambda \rightarrow +1$ and $\mathcal{T}$ is bounded by

$$1 \geq \mathcal{T} \geq \frac{1}{1+\frac{1}{4}(\lambda^{-1}-\lambda)^2} . \tag{4}$$

Thus, $\mathcal{T}$ never approaches zero, no matter how strong the potential is. A strong electrostatic type of potential barrier is not able to confine the particle to one side of it. In the hole-theory picture this should be expected. The occupied negative energy states in the barrier region are able to tunnel to positive energy states on either side of the barrier, producing a finite transmitted current. To demonstrate that this result is independent of the steepness of the barrier, consider massless particles, for which (1) gives $\mathcal{T}=1$ for the square barrier.

For massless particles the one-dimensional time-independent Dirac equation may be written as

$$i\frac{\partial\psi}{\partial x} = -\alpha_x[E-V_e(x)]\psi . \tag{5}$$

It is convenient to work in a representation in which $\alpha_x$ is diagonal, since observables such as transmission coefficients are independent of the representation.[10,17] This choice of representation is called the (1 + 1)-dimensional Weyl representation[17] with $\alpha_x=\sigma_z$ (and $\beta=\sigma_x$). The solutions in the potential-free region are

$$\psi_+ = \begin{bmatrix} e^{iEx} \\ 0 \end{bmatrix}, \quad \psi_- = \begin{bmatrix} 0 \\ e^{-iEx} \end{bmatrix} . \tag{6}$$

Whatever the electrostatic potential function $V_e(x)$ is, it cannot mix these components since (5) is diagonal even in the region of finite potential. Thus, as long as $V_e(x)\to 0$ as $|x|\to\infty$, the massless one-dimensional Dirac equation has a transmission coefficient of unity. Once again we see that the Klein paradox is independent of the shape of the potential.

It is straightforward to verify that the transmission coefficient for a scalar potential barrier vanishes like $e^{-2K_1 a}$, where $iK_1$ is the wave number in the barrier region and $K_1=[(m+V_s)^2-E^2]^{1/2}$ is real. The Klein paradox does not apply to scalar potentials.

The discrepancy between the two methods of treating the δ-function potential can be exhibited by quoting the relationship between the two- or four-component wave function on each side of the potential. Solving the Dirac equation for a *general* sharply peaked potential and then taking the δ-function limit of the potential, we obtain[18]

$$\psi(0+)=e^{-iS_e\alpha_x}\psi(0-) \tag{7}$$

for electrostatic type potentials, and

$$\psi(0+)=e^{-iS_s\alpha_x\beta}\psi(0-) \tag{8}$$

for Lorentz scalar potentials. The parameter $S_{e(s)}$ is the strength of the δ-function potential after the limit is taken:

$$V_{e(s)}\to S_{e(s)}\delta(x) . \tag{9}$$

These results are obtained by writing the one-dimensional Dirac equation in the form $\partial\psi/\partial x = G(x)\psi(x)$ and noting (by analogy with the time-dependent Schrödinger equation) that it has the formal solution

$$\psi(x) = \left[1+\int_{x_0}^{x} G(x')dx' + \int_{x_0}^{x} dx' \int_{x_0}^{x'} dx'' G(x')G(x'') + \cdots \right]\psi(x_0)$$
$$= P_x \exp\left[\int_{x_0}^{x} G(x')dx'\right]\psi(x_0) , \tag{10}$$

where $P_x$ is the spatial ordering operator defined by

$$P_x[A(x)B(y)] = A(x)B(y)\theta(x-y) + B(y)A(x)\theta(y-x) . \tag{11}$$

Now suppose that either the electrostatic potential or the scalar potential (but not both) is very sharply peaked in the region $(-\epsilon,\epsilon)$ around $x=0$, and apply (10) to $x=+\epsilon$, $x_0=-\epsilon$ to obtain

$$\psi(\epsilon) = P_x \exp\left[\int_{-\epsilon}^{\epsilon} G(x')dx'\right]\psi(-\epsilon) . \tag{12}$$

For small $\epsilon$, only the strongly peaked potential contributes significantly to the integral in (12), and this gives a term proportional to either $\alpha_x$ or $\alpha_x\beta$ according to the type of potential that is large. This dominant term commutes at spatially separated points, so we may set $P_x=1$ for this term and, after taking the limits that $\epsilon$ goes to zero and the potential magnitude becomes infinite, we obtain the results given in (7) and (8).

To directly solve the Dirac equation for a δ-function potential it is necessary to define the value of the wave function at a point at which it is discontinuous, or equivalently to define the product $\delta(x)\theta(x)$. The definition[19]

$$\delta(x)\theta(x) = \tfrac{1}{2}\delta(x) , \tag{13}$$

or its equivalent integral form,

$$\int \delta(x) f(x) dx = \tfrac{1}{2}[f(0+)+f(0-)] , \tag{14}$$

has been employed by all writers on this subject. One then obtains

$$\psi(0+)=e^{-i\Sigma_e\alpha_x}\psi(0-) , \tag{15}$$

where

$$\Sigma_e = 2\tan^{-1}(S_e/2) \tag{16}$$

in the electrostatic case,[20] and

$$\psi(0+)=e^{-i\Sigma_s\alpha_x\beta}\psi(0-) , \tag{17}$$

where

$$\Sigma_s = 2\tanh^{-1}(S_s/2) \tag{18}$$

in the Lorentz scalar case.

Looking at the scalar potential result in Eqs. (17) and (18), we are immediately struck by the singularity which occurs at $S_s=2$, at which point $\Sigma_s\to\infty$ and the transmission coefficient [which from (17) is $(\cosh\Sigma_s)^{-2}$] vanishes. For larger values of $S_s$, $\Sigma_s$ becomes complex and the transmission coefficient remains finite as the strength of the δ-function potential becomes infinite.

Our previous experience has not prepared us for this Klein paradox type of behavior with a scalar potential. Moreover, we know of no physical reason for a singularity in the solution at $S_s=2$. Certainly there is no such singularity when we solve the Dirac equation for a peaked potential and then take the δ-function limit.

The connection formulas for the wave functions allow us to obtain the eigenvalue conditions for the Dirac-Kronig-Penney problem with δ-function potentials. For electrostatic types of potentials these relations are well known.[20] They are

$$\cos(\kappa l)=\cos(kl)\cos S_e+\frac{E}{k}\sin(kl)\sin S_e \ . \tag{19}$$

The equivalent condition in the Lorentz scalar case is

$$\cos(\kappa l)=\cos(kl)\cosh S_s+\frac{m}{k}\sin(kl)\sinh S_s \ . \tag{20}$$

In deriving (19) and (20) Eqs. (7) and (8) were used. To obtain the Dirac-Kronig-Penney band conditions for Eqs. (15) and (17), simply replace $S_{e(s)}$ by $\Sigma_{e(s)}$ in Eqs. (19) and (20). We will refer to the resulting equations as (19′) and (21′).

First we note that as $S_e\rightarrow 0$ and $S_s\rightarrow 0$, and $E\rightarrow m$, both Eqs. (19) and (20) approach the classic Kronig-Penney result as they should. So do (19′) and (20′).

However, for large $S$ the band structure described by these equations is quite different. For massless particles, Eqs. (19) and (19′) do not have forbidden bands, whereas Eq. (20) has narrow allowed bands centered on $k=(2n+1)(\pi/2l)$ which collapse to the central points as $S_s\rightarrow\infty$. This difference between Eqs. (19) and (20) is another manifestation of the Klein paradox—the electrostatic potential does not confine the particles even when the δ function has infinite strength, whereas the very strong scalar potential confines the particles to individual cells in the lattice. Equation (20′) exhibits quite anomalous behavior. For massless particles, at $S_s=2$ the allowed bands become degenerate at the points $k=(2n+1)(\pi/2l)$, but for $S_s>2$ the band equation (20′) becomes

$$\cos(\kappa l)=-\cos(kl)\cosh\left[\ln\left[\frac{S_s+2}{S_s-2}\right]\right] , \tag{21}$$

and the allowed bands widen as $S_s$ increases, there being no forbidden bands in the limit $S_s\rightarrow\infty$.

We are now faced with the situation that the results obtained by the direct solution of the Dirac equation for the δ-function scalar potential exhibit anomalies, and are qualitatively different from those obtained by taking the δ-function limit of a sharply peaked potential. The difference in the results for electrostatic potentials is not as dramatic, but it still exists. We must therefore decide which of these methods describes the physical situation correctly.

Fairbairn, Glasser, and Steslicka[3] argued that the solution obtained by solving the Dirac equation with an explicit δ function is to be preferred on the grounds that the amplitude of negative energy components in the wave function is of order $(ma_0)^{-1}$ where $a_0$ is the distance in which the particle is localized. They argued that when solving the Dirac equation for a well (or barrier) of width $b$ the particle is localized within $b$, and if $b$ becomes smaller than $m^{-1}$, pairs will be created. They then asserted that if the Dirac equation is solved for the explicit δ-function potential no localization is implied. However, it can be readily seen that both Eqs. (19) and (19′) yield the Klein-paradox result that there are no forbidden bands. Thus the Klein paradox is not avoided by the device advocated in Ref. 3 and this argument does not provide a reason for preferring one method of handling the δ function to the other.

To clarify the relationship between the two methods of handling the δ-function potential, we consider a simple example, the one-component, one-dimensional equation generated by the electrostatic potential in the massless case

$$\frac{\partial\psi}{\partial x}=i[E-V_e(x)]\psi \ . \tag{22}$$

We write $\psi(x)=e^{iEx}\phi(x)$ so that $\phi(x)$ satisfies

$$\frac{\partial\phi}{\partial x}=-iV_e(x)\phi(x) \ . \tag{23}$$

We eventually want to solve Eq. (23) for the case

$$V_e(x)=S_e\delta(x) , \tag{24}$$

but as a first step we convert it to an integral equation

$$\phi(x)=\phi(x_0)-i\int_{x_0}^{x}dx'V_e(x')\phi(x') , \tag{25}$$

which has the Neumann series solution

$$\phi(x)=\exp\left[-i\int_{x_0}^{x}V_e(x')dx'\right]\phi(x_0) \ . \tag{26}$$

Now we can substitute (24) in (26) without having to invoke (13) or (14) to define $\delta(x)\theta(x)$, to obtain

$$\phi(x)=e^{-iS_e\theta(x)}\phi(-\infty) , \tag{27}$$

which is readily shown by substitution to satisfy (23).

It is easily seen that Eq. (27) reproduces the massless limit of Eq. (7), but its importance lies in the fact that it is a formal solution to the differential equation (23) for the δ-function potential which does not depend on the suspect definition of $\delta(x)\theta(x)$.

However, we could expand the exponential in (27) and use the relation

$$\theta^n(x)=\theta(x), \quad \text{for any integer } n>0 , \tag{28}$$

to rewrite (27) as

$$\phi(x)=[1+(e^{-iS_e}-1)\theta(x)]\phi(-\infty) \ . \tag{29}$$

If we now use (13) we see that (29) does not satisfy (23), but that if we replace $S_e$ by $\Sigma_e$ in (29) it does satisfy the differential equation (23). We call this new solution Eq. (29′).

Clearly the assumptions of (13) [or, equivalently, the assumption of the validity of differentiation of (28)] are the critical step which generates the discrepancy between (27) and (29′), both of which purport to be solutions of the fundamental equation (23). The difficulty lies in the attempt to define $\delta(x)\theta(x)$, which does not exist in a strict distribution-theory sense.[21] While (13) or (14) seem plausible, consider the effect of using them when solving the initial-value problem posed by Eq. (23) starting from $x = x_0 < 0$. We could imagine doing this on a computer in such a way that one mesh point is at $0-\epsilon$, and the next at $0+\epsilon$. To generate $\phi(0+\epsilon)$ the differential equation tells us to add $S_e\phi(0)$ to the value $\phi(0-\epsilon)$. This destroys the initial-value character of the solution, in that $\phi(0)$ depends on both $\phi(0-\epsilon)$ and $\phi(0+\epsilon)$.

To summarize, we have shown that the use of (13) changes the character of the Dirac equation, that (13) is not well established in distribution theory, that (13) is not needed to generate a solution of the Dirac equation [given in (7) and (8)] for a δ function which is manifestly independent of the representation of the δ function, and that the results obtained by using (13) are counterinitiative, especially for scalar potentials. To us, this is overwhelming evidence that the solutions (15) and (17) for the Dirac equation, and (19′) and (20′) for the Dirac-Kronig-Penney problem, which are based on (13), should be discarded as unphysical, and that the correct solutions are (7) and (8) for the δ-function barrier and (19) and (20) for the Dirac-Kronig-Penney problem.

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[18]Equation (7) or its equivalent may be found in a number of the papers in Refs. 2–6, in a form which depends on the particular choice of representation for the Dirac matrices.

[19]A simple "derivation" of (10) is

$$\delta(x)\theta(x)=\frac{1}{2}\frac{d}{dx}[\theta^2(x)]=\frac{1}{2}\frac{d}{dx}[\theta(x)]=\tfrac{1}{2}\delta(x)\ ,$$

although it should be noted that $\delta(x)\theta(x)$ is not well defined in a distribution-theory sense, and that if one tries to carry through this derivation in a rigorous way it breaks down.

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