Supercriticality and Transmission Resonances in the Dirac Equation

Norman Dombey,[1,*] Piers Kennedy,[1,†] and A. Calogeracos[2,‡]
[1]*Centre for Theoretical Physics, University of Sussex, Brighton BN1 9QJ, United Kingdom*
[2]*NCA Research Consultants, P.O. Box 61147, Maroussi 151 22, Greece*
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It is shown that a Dirac particle of mass m and arbitrarily small momentum will tunnel without reflection through a potential barrier $V = U_c(x)$ of finite range provided that the potential well $V = -U_c(x)$ supports a bound state of energy $E = -m$. This is called a supercritical potential well.

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It is now over 70 years since the Dirac equation was written down. Yet new results have been discussed in recent years, even in the relatively simple cases of one [1] and two spatial dimensions [2] as well as in three dimensions [3–6]. In this Letter, we generalize a well known theorem of scattering off a one-dimensional potential well in the Schrödinger equation to the Dirac equation. This is not difficult, but the theorem has an unexpected twist. Since the Dirac equation covers antiparticle scattering as well as particle scattering, the generalization gives two distinct results. One of these results implies a remarkable property of tunneling through a potential barrier in the Dirac equation which is related to the result on barrier penetration found by Klein [7] and is now called the Klein paradox.

We begin by considering the scattering off a class of one-dimensional potential wells $V(x)$ where $V(x) = 0$ for $|x| \geq a$ and $V(x) = -U(x) \leq 0$ for $|x| < a$ where the piecewise continuous function $U(x) \geq 0$. The potential is also taken to be even so that $V(-x) = V(x)$. We first seek to generalize to the Dirac equation the nonrelativistic result that the reflection coefficient $R(k)$ for scattering off the potential well $V(x) = -U_0(x)$ which supports a zero energy resonance satisfies $R(0) = 0$, where k is the momentum of the particle. This theorem was known to Schiff [8] and Bohm [9] but a proof was published only relatively recently by Senn [10] and Sassoli de Bianchi [11]. The situation where $R(k) = 0$ and the transmission coefficient $T(k) = 1$ is called a transmission resonance [9]. In nonrelativistic systems a zero energy resonance (or half-bound state) [12] is the nontrivial limit where a bound state just emerges from the continuum, for example, when a square well potential is just strong enough to support a second bound state.

Following an earlier paper [13] we take the gamma matrices γ_x and γ_0 to be the Pauli matrices σ_x and σ_z, respectively. Then the Dirac equation for scattering of a particle of energy E and momentum k by the potential $V(x)$ can be written as the coupled equations

$$\frac{\partial f}{\partial x} + [E - V(x) + m]g = 0\,, \tag{1a}$$

$$\frac{\partial g}{\partial x} - [E - V(x) - m]f = 0\,, \tag{1b}$$

where the Dirac spinor $\psi = \binom{f}{g}$.

Equations (1) have simple solutions as $x \to \pm\infty$ where $V = 0$. In particular, the analog of a zero energy resonance in the Schrödinger equation is a zero momentum resonance in the Dirac equation [2] where a particle of zero momentum has $E = m$ or an antiparticle has $E = -m$. (The antiparticle is described by the hole wave function corresponding to the absence of the state with $E = -m$.) It is easy to see that the solution of Eq. (1) for $E = m$ and $V = 0$ appropriately normalized is $\psi = \binom{2m}{0}$ while the solution for $E = -m$ and $V = 0$ is $\binom{0}{2m}$. As in Ref. [13] we can now write down the solutions of Eq. (1) for a particle of momentum k as $x \to \pm\infty$ to obtain $\psi = \binom{E+m}{-ik}e^{ikx}$ while an antiparticle of momentum k will have $\psi = \binom{ik}{m-E}e^{-ikx}$.

We now set up the usual formalism for particle scattering by the potential $V(x)$ in the Dirac equation. We take the particle as incident from the left, so the amplitude for reflection $r(k)$ is defined through the spinor $\psi(x)$ as $x \to -\infty$:

$$\psi(x) = \begin{pmatrix} E + m \\ -ik \end{pmatrix} e^{ikx} + r(k) \begin{pmatrix} E + m \\ ik \end{pmatrix} e^{-ikx}, \tag{2}$$

while as $x \to \infty$

$$\psi(x) = t(k) \begin{pmatrix} E + m \\ -ik \end{pmatrix} e^{ikx}. \tag{3}$$

In the Dirac equation [14] as for the Schrödinger equation with symmetric potentials [11], unitarity implies that

$$|r|^2 + |t|^2 = 1; \qquad \mathrm{Im}(r^* t) = 0\,, \tag{4}$$

so $R + T = 1$ where the reflection and transmission coefficients are given by $R = |r|^2$, $T = |t|^2$.

Since the potentials we consider are even, parity is conserved. In our two-component approach, the transformation of a wave function under $x \to -x$ is given [13] by

$$\psi'(x, t) = \sigma_z \psi(-x, t)\,. \tag{5}$$

It follows that an even wave function ψ has an even top component f and an odd bottom component g. Similarly, for an odd wave function ψ, f will be odd and g will be even.

We first consider an even bound state in the potential $V(x)$. As $x \to \pm\infty$, its unnormalized wave function will be of the form

$$\psi(x) = \begin{pmatrix} m + E \\ -\kappa \end{pmatrix} e^{\kappa x} \qquad x \to -\infty\,, \tag{6a}$$

$$\psi(x) = \begin{pmatrix} m + E \\ \kappa \end{pmatrix} e^{-\kappa x} \qquad x \to \infty, \tag{6b}$$

where $E^2 = m^2 - \kappa^2$. We require the potential well $V = -U_0(x)$ to just bind this bound state with arbitrarily small κ. If this is the case, then the limit $\kappa \to 0$ exists, and $\psi(x)$ becomes a continuum wave function since it is no longer square integrable.

We can now compare Eqs. (6) with Eqs. (2) and (3) in the limit $k \to 0, \kappa \to 0$. We obtain $2m[1 + r(0)] = 2mt(0)$ or

$$1 + r(0) = t(0) \neq 0. \tag{7}$$

We have written $t(0) \neq 0$ since otherwise $\psi(x)$ would vanish in the limit $k \to 0$, $\kappa \to 0$, and we would not be considering a zero momentum resonance. [In Ref. [15] we adopt a more general approach to obtain the results of this Letter, thereby avoiding the use of $t(0) \neq 0$.]

The theorem now follows easily just as it does in the Schrödinger case [11]. Combining Eq. (7) with the unitarity condition $\mathrm{Im}(r^* t) = 0$ of Eq. (4), we get $\mathrm{Im}(r^*) = 0$ so that $r(0)$ and $t(0)$ are real. From $|r|^2 + |t|^2 = 1$ we obtain

$$2r^2 + 2r + 1 = 1 \tag{8}$$

so that $r(0) = 0$ or $r(0) = -1$. Since $t(0) \neq 0$, we obtain the result $r(0) = 0$, and so in terms of the reflection and transmission coefficients

$$R(0) = 0, \qquad T(0) = 1. \tag{9}$$

If instead we had considered an odd bound state, an additional minus sign must be introduced into either Eq. (6a) or Eq. (6b). Equation (7) must be modified to $1 + r(0) = -t(0)$ and the subsequent analysis and conclusions remain valid. Hence, just as in the Schrödinger equation, the scattering of a particle in the Dirac equation off a potential well $V = -U_0(x)$ which "binds" a zero momentum resonance corresponds to a transmission resonance with zero reflection.

We now increase the strength of the potential well from $U_0(x)$ to $U_c(x)$ so that $V = -U_c(x)$ supports a bound state of energy $E = -m$. This is called a supercritical potential and is associated with spontaneous positron production [16,17]. We can redo the analysis exactly as before by defining amplitudes r_-, t_- for the reflection and transmission of an antiparticle of momentum k incident from the left on a potential well $V(x)$: so in place of Eq. (2) we have as $x \to -\infty$

$$\psi(x) = \begin{pmatrix} ik \\ m - E \end{pmatrix} e^{-ikx} + r_-(k) \begin{pmatrix} -ik \\ m - E \end{pmatrix} e^{ikx}, \tag{10}$$

while as $x \to \infty$ we have

$$\psi(x) = t_-(k) \begin{pmatrix} ik \\ m - E \end{pmatrix} e^{-ikx}. \tag{11}$$

As before, unitarity gives

$$|r_-|^2 + |t_-|^2 = 1, \qquad \mathrm{Im}(r_-^* t_-) = 0, \tag{12}$$

and the near-supercritical even bound state for $x \to \pm\infty$ is now

$$\psi(x) = \begin{pmatrix} -\kappa \\ m - E \end{pmatrix} e^{\kappa x} \qquad x \to -\infty, \tag{13a}$$

$$\psi(x) = -\begin{pmatrix} \kappa \\ m - E \end{pmatrix} e^{-\kappa x} \qquad x \to \infty. \tag{13b}$$

Note again that for the odd bound state we must drop the minus sign in Eq. (13b).

Repeating the analysis of Eqs. (7)–(9) we find in the limit $k \to 0$, $\kappa \to 0$ when the antiparticle is incident on the potential well $V = -U_c(x)$ with arbitrarily small momentum that

$$R_-(0) = 0, \qquad T_-(0) = 1, \tag{14}$$

where $R_- = |r_-|^2$, $T_- = |t_-|^2$.

So we see that in the Dirac equation there are two analogs of the Schrödinger result: one for zero momentum particles incident on a potential well which supports a zero momentum resonance and one for zero momentum antiparticles incident on a supercritical potential well.

We now can obtain our main result. The Dirac equation (1) is invariant under charge conjugation, that is to say under the transformation

$$E \to -E, \qquad V \to -V, \qquad f \to g, \qquad g \to f. \tag{15}$$

From Eq. (14) we know that an antiparticle of energy $E = -\sqrt{m^2 + k^2}$ incident on the supercritical potential well $V_c(x) = -U_c(x)$ will satisfy $T_-(0) = 1$; that is to say at arbitrarily small momentum it will have a vanishingly small reflection coefficient. Equation (14) then shows that if we replace the antiparticle of energy $E = -\sqrt{m^2 + k^2}$ incident on the supercritical potential well by a particle of energy $E = \sqrt{m^2 + k^2}$ incident on the corresponding potential barrier $V(x) = +U_c(x)$ the particle will still have a transmission resonance at zero momentum, even though now the potential well has been replaced by a potential barrier.We thus obtain the theorem that where an even potential well of finite range is strong enough to contain a supercritical state, then a particle of arbitrarily small momentum will be able to tunnel right through the potential barrier created by inverting the well without reflection. This result was noticed a few years ago for the particular case of square barriers [13], and one of us (P. K.) has shown numerically that it was also true for Gaussian and Saxon-Woods potential barriers [18]. In the Appendix we show the behavior of the upper and lower components of the wave function for particle scattering at zero momentum by a square and Gaussian barrier when the corresponding potential wells are supercritical.

Conclusions.—In his original work Klein [7] discovered that a Dirac particle could tunnel through an arbitrarily high potential. The generic phenomenon whereby fermions can tunnel through barriers without exponential

suppression we have called "Klein tunneling" [19]. The result of this Letter shows that Klein tunneling is a general feature of the Dirac equation: any potential well strong enough to support a supercritical state when inverted becomes a potential barrier which a fermion of arbitrarily low momentum can tunnel through without reflection. We do not claim here that any transmission resonance at zero momentum must correspond to supercriticality, only that supercriticality leads to a transmission resonance through a potential barrier at zero momentum. In another paper [15] we shall consider the question of the conditions on a potential for it to possess a zero momentum transmission resonance more generally. In three dimensions Hall and one of us (N. D.) [20] have recently demonstrated that maximal Klein tunneling is also associated with supercriticality.

The potential step that Klein considered has pathological properties [19]. Nevertheless, our result confirms that according to the Dirac equation a particle of low momentum can tunnel through an arbitrarily high smooth potential of finite range. The reason is straightforward: hole states can propagate under the potential barrier. In terms of the particle kinetic energy T under the barrier $T = E - V - m = -m - \sqrt{m^2 + q^2}$, where q is the momentum of the hole, so if $T \leq -2m$, hole states can propagate without exponential suppression. $T \leq -2m$ thus corresponds to penetrating under the barrier to distances $|x| < |x_K|$ where $V(x_K) = E + m \geq 2m$ [20].

Appendix.—We illustrate the result above for the special cases of (i) a square barrier and (ii) a Gaussian barrier. First consider the square well potential $V = -U(x)$ where $U(x) = U$ for $|x| < a$ and $U(x) = 0$ for $|x| > a$. Then an unnormalized even wave function inside the well [13] has the form

$$\psi(x) = \begin{pmatrix} (E + U + m)\cos px \\ p \sin px \end{pmatrix} \qquad |x| \leq a\,, \quad (16)$$

where the internal momentum p is given by $(E + U)^2 = m^2 + p^2$. For supercriticality where $E = -m$ we require the phase condition $pa = N\pi/2$ where N is an integer [13]. The first supercritical state is thus given by $p = p_c = \pi/2a$ and correspondingly the critical potential is $V(x) = -U_c$, $|x| \leq a$, where $U_c = m + \sqrt{m^2 + \pi^2/4a^2}$. At supercriticality the wave function is thus given by

$$\psi(x) = \begin{pmatrix} 0 \\ 2m \end{pmatrix}, \qquad x < -a\,, \quad (17a)$$

$$\psi(x) = -2m\begin{pmatrix} b\cos(\pi x/2a) \\ \sin(\pi x/2a) \end{pmatrix}, \qquad |x| \leq a\,, \quad (17b)$$

$$\psi(x) = -\begin{pmatrix} 0 \\ 2m \end{pmatrix}, \qquad x > a\,, \quad (17c)$$

where $b = 2aU_c/\pi$.

Now consider a particle of arbitrarily small momentum incident on the square barrier $V(x) = U_c$, $|x| < a$; $V(x) = 0$, $|x| > a$. Equation (15) shows that the wave function is obtained by interchanging the top and bottom components of Eq. (17), thereby giving the transmission resonance

$$\psi(x) = \begin{pmatrix} 2m \\ 0 \end{pmatrix}, \qquad x < -a\,, \quad (18a)$$

$$\psi(x) = -2m\begin{pmatrix} \sin(\pi x/2a) \\ b\cos(\pi x/2a) \end{pmatrix}, \qquad |x| \leq a\,, \quad (18b)$$

$$\psi(x) = -\begin{pmatrix} 2m \\ 0 \end{pmatrix}, \qquad x > a\,, \quad (18c)$$

and the components of the wave function are shown in Fig. 1.

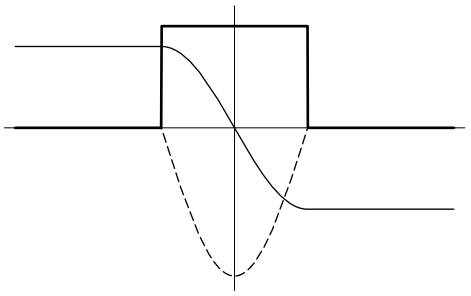

FIG. 1. The zero momentum wave function for the square barrier $V = U_c(x)$, depicted by the heavy line. The solid line is the upper component, and the dashed line is the lower component.

One of us (P. K.) has also solved the Dirac equation numerically for a Gaussian potential well and barrier where $U(x) = U\exp(-x^2/a^2)$ [18]. In Fig. 2 we show the components of the wave function for a particle of arbitrarily small momentum incident on a supercritical Gaussian barrier where $U = U_c = 3.26m$ for $ma = 1$ (cf. $U_c = m + \sqrt{m^2 + \pi^2/4a^2} = 2.86m$ for $ma = 1$ for a square barrier). Again there is a transmission resonance demonstrating complete penetration of the barrier.

While the wave functions in this case have a similar form to those for the square barrier, note the two turning points which occur in the top component of the Gaussian wave function. These correspond to the points $\pm x_K$ where $V(x_K) = E + m = 2m$ at zero momentum. Hole states can propagate under the potential without exponential

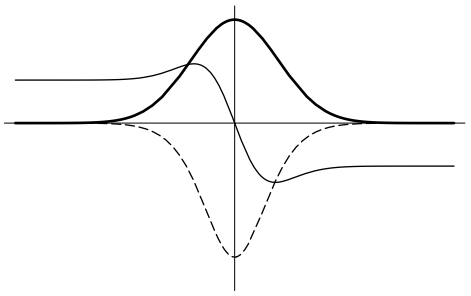

FIG. 2. The zero momentum wave function for the Gaussian barrier $V = U_c\exp(-m^2x^2)$, depicted by the heavy line. The solid line is the upper component, and the dashed line is the lower component.

suppression from $-x_K$ to $+x_K$ thus demonstrating Klein tunneling. Note also that the condition for hole states to propagate under a potential of finite range is $V > 2m$ which will in general not be sufficient for supercriticality (we have seen for a square barrier of range a with $ma = 1$ that $V_c = 2.86m$). So Klein tunneling should exist even for subcritical potentials as was pointed out by Dosch *et al.* [21].

*Email address: normand@sussex.ac.uk
†Email address: kapv4@pcss.maps.susx.ac.uk
‡Email address: acal@hol.gr

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