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Low momentum scattering in the Dirac equation

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Abstract

It is shown that the amplitude for reflection of a Dirac particle with arbitrarily low momentum incident on a potential of finite range is -1 and hence the transmission coefficient $T = 0$ in general. If, however, the potential supports a half-bound state at momentum $k = 0$ this result does not hold. In the case of an asymmetric potential the transmission coefficient T will be nonzero whilst for a symmetric potential $T = 1$. Therefore in some circumstances a Dirac particle of arbitrarily small momentum can tunnel without reflection through a potential barrier.

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1. Introduction

The results for scattering at arbitrary low energy E in one dimension in the Schrödinger equation are well known. If the potential $V(x)$ is sufficiently well behaved at infinity, then the reflection coefficient at zero energy is unity and the transmission coefficient is zero [1] unless the potential supports a zero energy resonance (a half-bound state). In that case the transmission coefficient is unity and there is no reflection provided that the potential is symmetric. Bohm calls this a transmission resonance [2]. These results have been generalized to asymmetric potentials [3, 4]. In this paper we repeat the analysis for the Dirac equation. To some extent this has already been done by Clemence [5] in the mathematical literature in his analysis of the Levinson theorem but we approach the problem as physicists. Our results show that transmission resonances will occur in the Dirac equation even for the case where the potential $V(x)$ is everywhere positive and thus represents a potential barrier.

The potentials $V(x)$ we shall consider are smooth and of finite range. In non-relativistic systems for such potentials, scattering states with continuum wavefunctions have $E \geqslant 0$ whereas bound states with normalizable wavefunctions have $E < 0$. A half-bound state [6] or zero energy resonance in non-relativistic scattering occurs when the potential supports a bound state of energy $E = -\kappa^2/2m$ in the limit $\kappa \to 0$: the corresponding wavefunction thus becomes a continuum wavefunction. An example of this is when a square well is sufficiently deep to just support the first odd bound state: the resulting wavefunction describes a non-normalizable half-bound state which corresponds both to a particle of arbitrarily low energy incident on the potential from the left and also to a particle of arbitarily low energy incident from the right.

In the relativistic Dirac equation, the notion of half-bound states is more subtle. For a free Dirac particle, there exists a gap $E \leqslant |m|$ which separates the positive and negative energy continuum states: the positive energy states correspond to particle states and the absence of negative energy states (hole states) describes anti-particles. On the introduction of a potential $V(x)$ this gap becomes distorted and bound states now occur between $E = -m$ and $E = m$. A potential which is attractive to particles and supports a half-bound state at $E = -m$ or a potential which is attractive to anti-particles and supports a half-bound state at $E = m$ is called a supercritical potential: thus the Dirac equation has half-bound states at both $E = -m$ and $E = m$ in contrast to the Schrödinger equation where these only exist at $E = 0$. It follows also that we should talk of zero momentum resonances in the relativistic case rather than zero energy resonances.

In the following sections we discuss the one-dimensional Dirac equation using a two-component approach and establish the formalism needed for the consideration of scattering and bound states. We will then prove that Dirac particles with energy $E > m$ and arbitrarily small momentum incident on a potential of finite range will be completely reflected unless the lower component of a particular wavefunction vanishes. If the potential supports a half-bound state at the threshold energy $E = m$ this condition is shown to be satisfied. In this case there will be a nonzero transmission coefficient in general whilst for a symmetric potential, there will be a transmission resonance: the particle will tunnel without reflection. In particular, we confirm our previous result [7] that solutions of the Dirac equation exist in which a particle of arbitrarily small momentum can tunnel completely through a potential barrier. In the appendix we illustrate our results by considering an asymmetric potential which is soluble analytically.

2. The two-component approach

Following an earlier paper [8] 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 $V(x)$ is

$$\left(\sigma_x \frac{\partial}{\partial x} - (E - V(x))\sigma_z + m\right)\psi = 0. \tag{1}$$

We write

$$\psi(x) = \begin{pmatrix} f(x) \\ g(x) \end{pmatrix} \tag{2}$$

to obtain the coupled differential equations

$$f'(x) = -(E - V(x) + m)g(x) \tag{3a}$$

$$g'(x) = (E - V(x) - m)f(x). \tag{3b}$$

For a free Dirac particle of momentum k the solution is $\psi = \binom{A}{B}\,\mathrm{e}^{\mathrm{i}kx}$ where $k^2 = E^2 - m^2$ and

$$A = \left(\frac{\mathrm{i}k}{E - m}\right) B = \mathrm{i}\sqrt{\frac{E + m}{E - m}} B = \left(\frac{E + m}{-\mathrm{i}k}\right) B. \tag{4}$$

Suitable choices for A and B will facilitate future calculations. For threshold problems where $E \to m$, choosing $B = -\mathrm{i}k$ leads to $A = E + m$ and the free particle wavefunction ψ can be written apart from a normalization factor as

$$\psi = \begin{pmatrix} E + m \\ -\mathrm{i}k \end{pmatrix} \mathrm{e}^{\mathrm{i}kx}. \tag{5}$$

It is clear that in this form the top and bottom components do not simultaneously tend to zero as $E \to m, k \to 0$. If on the other hand we were interested in threshold wavefunctions where $E \to -m$ then choosing $B = E - m$ leads to $A = \mathrm{i}k$ and the free wavefunction can now be written (again up to normalization) as

$$\psi = \begin{pmatrix} \mathrm{i}k \\ E - m \end{pmatrix} \mathrm{e}^{\mathrm{i}kx}. \tag{6}$$

3. S-matrix formalism for the one-dimensional Dirac equation

The S-matrix formalism for scattering in one dimension for the Schrödinger equation is well known and covered in a large number of texts (e.g. [1, 9]). The same arguments are applicable for the Dirac equation in one dimension [5, 10] and here we will summarize a number of the more important results in the context of a relativistic equation.

We adopt the usual formalism for a Dirac particle incident from the left scattering off the piecewise continuous potential $V(x)$ of finite range where $V = 0$ for $|x| \geqslant \xi$ where the asymptotic solution $\psi_l(x)$ of equations (3) for particles incident from the left with momentum k and energy E using equation (5) is

$$\psi_l \to \begin{pmatrix} E + m \\ -\mathrm{i}k \end{pmatrix} \mathrm{e}^{\mathrm{i}kx} + l(k) \begin{pmatrix} E + m \\ \mathrm{i}k \end{pmatrix} \mathrm{e}^{-\mathrm{i}kx} \qquad x \to -\infty \tag{7}$$

which defines the (left) reflection amplitude $l(k)$. We can also define the (left) transmission amplitude $t_l(k)$

$$\psi_l \to t_l(k) \begin{pmatrix} E + m \\ -\mathrm{i}k \end{pmatrix} \mathrm{e}^{\mathrm{i}kx} \qquad x \to \infty. \tag{8}$$

We can similarly define the asymptotic wavefunction for particles incident from the right as

$$\psi_r \to t_r(k) \begin{pmatrix} E + m \\ \mathrm{i}k \end{pmatrix} \mathrm{e}^{-\mathrm{i}kx} \qquad x \to -\infty \tag{9}$$

$$\psi_r \to \begin{pmatrix} E + m \\ \mathrm{i}k \end{pmatrix} \mathrm{e}^{-\mathrm{i}kx} + r(k) \begin{pmatrix} E + m \\ -\mathrm{i}k \end{pmatrix} \mathrm{e}^{\mathrm{i}kx} \qquad x \to \infty \tag{10}$$

thus defining the right reflection and transmission coefficients $r(k)$, $t_r(k)$.

The left scattering coefficients and the right coefficients can be simplified further. If we had two independent solutions of the Dirac equation,

$$\psi_1 = \begin{pmatrix} f_1(x) \\ g_1(x) \end{pmatrix} \qquad \psi_2 = \begin{pmatrix} f_2(x) \\ g_2(x) \end{pmatrix} \tag{11}$$

then the Wronskian of the solutions ψ_1, ψ_2 of the first-order linear differential equations of equations (3), defined as [11]

$$W[\psi_1, \psi_2](x) = f_1(x)g_2(x) - f_2(x)g_1(x) \tag{12}$$

would satisfy $W'(x) = 0$, with $W(x)$ is constant and nonzero. (When $k = 0$ it is easy to see that any two solutions are not independent and $W = 0$.) We can now evaluate the Wronskian $W(\psi_l, \psi_r)(x)$ as $x \to \pm\infty$ to give

$$t_l(k) = t_r(k) = t(k). \tag{13}$$

So there is only one transmission coefficient $t(k)$.

The general solution of the Dirac equation $\psi(x)$ can thus be written as a linear combination of ψ_l and ψ_r:

$$\psi = A\psi_l + B\psi_r. \tag{14}$$

The asymptotic solutions are now found to be

$$\psi \to A \begin{pmatrix} E+m \\ -\mathrm{i}k \end{pmatrix} \mathrm{e}^{\mathrm{i}kx} + \tilde{B} \begin{pmatrix} E+m \\ \mathrm{i}k \end{pmatrix} \mathrm{e}^{-\mathrm{i}kx} \qquad x \to -\infty \tag{15}$$

$$\psi \to \tilde{A} \begin{pmatrix} E+m \\ -\mathrm{i}k \end{pmatrix} \mathrm{e}^{\mathrm{i}kx} + B \begin{pmatrix} E+m \\ \mathrm{i}k \end{pmatrix} \mathrm{e}^{-\mathrm{i}kx} \qquad x \to \infty \tag{16}$$

where

$$\tilde{A}(k) = At(k) + Br(k) \qquad \tilde{B}(k) = Al(k) + Bt(k). \tag{17}$$

The coefficients A and B are the amplitudes of the incoming waves for particles arriving from $x \to -\infty$ and $x \to \infty$, respectively. Conversely, the coefficients $\tilde{A}$ and $\tilde{B}$ are the coefficients of the outgoing waves for the transmitted or reflected particles. We can now introduce the matrix $S(k)$ which allows us to calculate the outgoing amplitudes in terms of the incoming amplitudes

$$\begin{pmatrix} \tilde{A} \\ \tilde{B} \end{pmatrix} = S(k) \begin{pmatrix} A \\ B \end{pmatrix} \quad \Rightarrow \quad S(k) = \begin{pmatrix} t(k) & r(k) \\ l(k) & t(k) \end{pmatrix}. \tag{18}$$

The flux j is given by

$$j = \overline{\psi}(x)\gamma_x\psi(x) = \mathrm{i}\overline{\psi}(x)\sigma_x\psi = \mathrm{i}\overline{\psi}(x)\sigma_z\sigma_x\psi = -\psi^\dagger(x)\sigma_y\psi(x). \tag{19}$$

Using equations (15) and (16) we consequently find that

$$\begin{aligned} j &= 2k(E+m)(|A|^2 - |\tilde{B}|^2) \qquad x \to -\infty \\ j &= 2k(E+m))(|\tilde{A}|^2 - |B|^2) \qquad x \to \infty. \end{aligned} \tag{20}$$

The conservation of flux gives us the condition

$$|A|^2 + |B|^2 = |\tilde{A}|^2 + |\tilde{B}|^2. \tag{21}$$

Also

$$|\tilde{A}|^2 + |\tilde{B}|^2 = (\tilde{A}^*\tilde{B}^*) \begin{pmatrix} \tilde{A} \\ \tilde{B} \end{pmatrix} = (A^*B^*)S(k)^\dagger S(k) \begin{pmatrix} A \\ B \end{pmatrix} = |A|^2 + |B|^2.$$

Hence $S(k)$ is a unitary 2×2 matrix. From equation (18), this imposes the following conditions on the matrix elements of $S(k)$:

$$T(k) + L(k) = T(k) + R(k) = 1 \tag{22}$$

$$t(k)r^*(k) + t^*(k)l(k) = t^*(k)r(k) + t(k)l^*(k) = 0 \tag{23}$$

where $T(k) = |t(k)|^2$ is the transmission coefficient, $L(k) = |l(k)|^2$ is the reflection coefficient for a particle incident from the left and $R(k) = |r(k)|^2$ is the reflection coefficient for a particle incident from the right. It also follows that

$$|l(k)| = |r(k)|. \tag{24}$$

Additionally, if the potential is symmetric, i.e. $V(x) = V(-x)$ (see section 4.4), then $\psi'(x) = \sigma_z\psi(-x)$ is also a solution (this is equation (57)). The asymptotic wavefunction $\psi'(x)$ can be found from $\psi(x)$ using equations (15) and (16) by the substitutions $A \leftrightarrow B$ and $\tilde{A} \leftrightarrow \tilde{B}$. This implies that $S(k)$ must also be symmetric and consequently

$$r(k) = l(k) \tag{25}$$

in this case.

The last property we wish to illustrate is the behaviour of the amplitudes $t(k)$, $l(k)$ and $r(k)$ at $k = 0$. By taking the complex conjugate of equations (2)–(5) with negative momentum $-k$, we see that $\psi^*_{l,r}(-k, x)$ has the same form as $\psi_{l,r}(k, x)$. This in turn implies that

$$t^*(-k) = t(k) \qquad l^*(-k) = l(k) \qquad r^*(-k) = r(k). \tag{26}$$

So we see from equation (26) that all the amplitudes $l(0)$, $r(0)$, $t(0)$ are real. This will be of importance for the next section. We also have from equation (23) that

$$r(0) = -l(0) \qquad \text{or} \qquad t(0) = 0. \tag{27}$$

It follows from equations (25) and (27) that for symmetric potentials

$$r(0) = l(0) = 0 \qquad \text{or} \qquad t(0) = 0. \tag{28}$$

We discuss this further in section 4.4.

4. Reflection and transmission properties at zero momentum

4.1. The general case

Our approach will follow that presented for the Schrödinger equation by Senn [12]. When a Dirac particle is incident from the left scattering on the potential $V(x)$ of finite range so that $V(x) = 0$ for $|x| \geqslant \xi$, the solution ψ^s of equations (3) in region I $x \leqslant -\xi$ for particles incident from the left with momentum k and energy E is just

$$\psi^s = \psi_l = \begin{pmatrix} E+m \\ -\mathrm{i}k \end{pmatrix} \mathrm{e}^{\mathrm{i}kx} + l(k) \begin{pmatrix} E+m \\ \mathrm{i}k \end{pmatrix} \mathrm{e}^{-\mathrm{i}kx} \qquad x \leqslant -\xi. \tag{29}$$

Similarly, in region III $x > \xi$

$$\psi^s = \psi_l = t(k) \begin{pmatrix} E+m \\ -\mathrm{i}k \end{pmatrix} \mathrm{e}^{\mathrm{i}kx} \qquad x \geqslant \xi. \tag{30}$$

For $k \neq 0$ we can define two independent solutions of equations (3) by, for example,

$$\psi^L = \begin{pmatrix} E+m \\ -\mathrm{i}k \end{pmatrix} \mathrm{e}^{\mathrm{i}kx} \qquad x \to -\infty \tag{31}$$

$$\psi^R = \begin{pmatrix} E+m \\ \mathrm{i}k \end{pmatrix} \mathrm{e}^{-\mathrm{i}kx} \qquad x \to \infty \tag{32}$$

which represent purely incoming particles from the left and right, respectively. By taking appropriate linear combinations of ψ^L, ψ^R and normalizing we can choose two new independent solutions of equations (3)

$$\psi_1 = \begin{pmatrix} f_1(x) \\ g_1(x) \end{pmatrix} \qquad \psi_2 = \begin{pmatrix} f_2(x) \\ g_2(x) \end{pmatrix} \tag{33}$$

with the properties

$$g_1(-\xi) = 0 \qquad g_2(-\xi) = 1 \qquad f_1(-\xi) = 1 \qquad f_2(-\xi) = 0. \tag{34}$$

Note that the solutions ψ_1 and ψ_2 which satisfy equation (34) are everywhere real provided that k is real. We can then express our solution ψ^s in terms of a linear combination of ψ_1 and ψ_2 for all x and in particular in region II $|x| \leqslant \xi$

$$\psi^s = b\begin{pmatrix} f_1(x) \\ g_1(x) \end{pmatrix} + c\begin{pmatrix} f_2(x) \\ g_2(x) \end{pmatrix} \qquad -\xi \leqslant x \leqslant \xi. \tag{35}$$

We can evaluate the Wronskian of the solutions ψ_1, ψ_2, which is constant at the point $x = -\xi$, to give

$$W[\psi_1, \psi_2] = W(-\xi) = f_1(-\xi)g_2(-\xi) - f_2(-\xi)g(-\xi) = 1$$

thus confirming that the solutions ψ_1, ψ_2 are independent for $k \neq 0$.

The wavefunction $\psi^s(x)$ must be continuous at $x = -\xi$ and $x = \xi$. The overlaps between regions I and II and between II and III then give the following boundary conditions:

$$(E+m)(\mathrm{e}^{-\mathrm{i}k\xi} + l(k)\,\mathrm{e}^{\mathrm{i}k\xi}) = b \tag{36a}$$

$$-\mathrm{i}k(\mathrm{e}^{-\mathrm{i}k\xi} - l(k)\,\mathrm{e}^{\mathrm{i}k\xi}) = c \tag{36b}$$

$$(E+m)t(k)\,\mathrm{e}^{\mathrm{i}k\xi} = bf_1(\xi) + cf_2(\xi) \tag{36c}$$

$$-\mathrm{i}kt(k)\,\mathrm{e}^{\mathrm{i}k\xi} = bg_1(\xi) + cg_2(\xi). \tag{36d}$$

For simplicity, write $\alpha_i = f_i(\xi)$ and $\beta_i = g_i(\xi)$, so that the last two equations become

$$(E+m)t(k)\,\mathrm{e}^{\mathrm{i}k\xi} = b\alpha_1 + c\alpha_2 \tag{37a}$$

$$-\mathrm{i}kt(k)\,\mathrm{e}^{\mathrm{i}k\xi} = b\beta_1 + c\beta_2. \tag{37b}$$

Note that b and c are dependent on k as are α_i and β_i. Eliminating t, b and c and then rearranging to solve for l give

$$l(k) = \left(\frac{k^2\alpha_2 + (E+m)^2\beta_1 + \mathrm{i}k(E+m)(\alpha_1 - \beta_2)}{k^2\alpha_2 - (E+m)^2\beta_1 - \mathrm{i}k(E+m)(\alpha_1 + \beta_2)}\right)\mathrm{e}^{-2\mathrm{i}k\xi}. \tag{38}$$

Similarly, t can be found to be

$$t(k) = \frac{-2\mathrm{i}k(E+m)(\alpha_1\beta_2 - \alpha_2\beta_1)}{k^2\alpha_2 - (E+m)^2\beta_1 - \mathrm{i}k(E+m)(\alpha_1 + \beta_2)}\,\mathrm{e}^{-2\mathrm{i}k\xi}. \tag{39}$$

We can then use the relation

$$W(\xi) = f_1(\xi)g_2(\xi) - f_2(\xi)g_1(\xi) = \alpha_1\beta_2 - \alpha_2\beta_1 = 1 \tag{40}$$

to simplify equation (39). It is a straightforward exercise to verify that equations (38) and (39) satisfy the unitarity condition (22).

We can now discuss the limit as $k \to 0$. It is apparent from equations (38) and (39) that provided $\beta_1(0) \neq 0$ the limit $E \to m$, $k \to 0$ gives

$$l(0) = r(0) = -1 \qquad t(0) = 0 \tag{41}$$

so that the reflection coefficients $L(0) = R(0) = 1$ and the transmission coefficient $T(0) = 0$. These results in the general case agree with those for the Schrödinger equation [3, 4].

Using equations (33a) and (33b) it can be seen that $b(0) = c(0) = 0$ in the $k = 0$ limit and therefore from equation (35) the wavefunction vanishes identically for all x. Thus the only physical solution of the Dirac equation (1) for $k = 0$ is the solution

$$\psi(x, k=0) = 0 \tag{42}$$

unless the potential has special properties which we investigate in the next section.

It should also be noted that as $f_i(x)$ and $g_i(x)$ are real at $x = \xi$, the quantities $\alpha_i(k)$ and $\beta_i(k)$ are also real. Hence from equation (39) as $k \to 0$, $t(k)$ is purely imaginary as it approaches zero in agreement with the Levinson theorem [5] for the Dirac equation provided $\beta_1(0) \neq 0$.

4.2. The special case $\beta_1(0) = 0$

If we return to equations (33*b*) and (34*b*) we see that as $k \to 0$ we must have

$$c(0) = 0 \qquad b(0)\beta_1(0) + c(0)\beta_2(0) = 0$$

so

$$b(0)\beta_1(0) = 0. \tag{43}$$

Furthermore since $c(0) = 0$, we must have from equation (34*a*)

$$2mt(0) = b(0)\alpha_1(0). \tag{44}$$

When $b(0) = 0$ as well as $c(0) = 0$ we obtain the general case already discussed. If $\beta_1(0) = 0$, however, then as we approach the limit $E \to m$, $k \to 0$ the reflection amplitude $l(k)$ does not satisfy $l(0) = -1$ and so the wavefunction $\psi(x, k = 0) \neq 0$. In this case we therefore have non-trivial solutions of the Dirac equation at $k = 0$. This implies that transmission coefficient $t(0)$ will be nonzero in this limit as will $\alpha_1(0)$.

For $k \to 0$ with $\beta_1(0) = 0$ we can write $\beta_1(k) = k\beta_1'(0)$. So from equation (38)

$$l(0) = \lim_{k\to 0} \frac{\beta_2 - \alpha_1 + 2m\beta_1'(0)\mathrm{i}}{\beta_2 + \alpha_1 + 2m\beta_1'(0)\mathrm{i}}. \tag{45}$$

As k is arbitrarily small (and not actually equal to zero), the Wronskian $W = \alpha_1\beta_2 = 1 + O(k)$, so $\beta_2 = 1/\alpha_1 + O(k)$ and in the limit $k \to 0$ we have

$$l(0) = \frac{1 - \alpha_1^2(0) + 2m\mathrm{i}\alpha_1(0)\beta_1'(0)}{1 + \alpha_1^2(0) - 2m\mathrm{i}\alpha_1(0)\beta_1'(0)}. \tag{46}$$

We know however from equation (26) that $l(0)$ must be real. From equation (46) this means that either $\beta_1'(0) = 0$ or $\alpha_1(0) = 0$. But since we are considering the non-trivial case where $\psi(x, k = 0) \neq 0$ (and hence we expect that $t(0) \neq 0$) we do not want $\alpha_1(0) = 0$ since from equation (44) this would imply that $t(0) = 0$. Thus we would like to be able to show that

$$\beta_1'(0) = 0 \tag{47}$$

and $\beta_1(k) = O(k^2)$. This is not difficult to demonstrate using an argument of Lin [13]: the wavefunction ψ_1 of equation (11) is a solution of equations (3) subject to the k-independent boundary conditions given by equation (34). So its lower component

$$g_1(x, k) = g_1(x, E) \tag{48}$$

since the Dirac equation (3) involves E explicitly, not k. It follows that

$$\beta_1 = \beta_1(E) \tag{49}$$

which requires β_1 to be an even function of k and in particular that as $E = \sqrt{m^2 + k^2}$

$$\frac{\mathrm{d}\beta_1(k)}{\mathrm{d}k} = \frac{\mathrm{d}\beta_1(E)}{\mathrm{d}E}\frac{\mathrm{d}E}{\mathrm{d}k} = \frac{k}{E}\frac{\mathrm{d}\beta_1(E)}{\mathrm{d}E} = 0 \tag{50}$$

at $k = 0$ in agreement with equation (47).

This gives the final result for the reflection amplitudes in the special case when $\beta_1(0) = 0$:

$$l(0) = -r(0) = \frac{1 - \alpha_1^2(0)}{1 + \alpha_1^2(0)} \tag{51}$$

and for the corresponding transmission amplitude from equation (39):

$$t(0) = \frac{2\alpha_1(0)}{1 + \alpha_1^2(0)}. \tag{52}$$

These results agree with those obtained by Clemence [5].

4.3. Half-bound state

We will now show that if the potential were to support a bound state in the limit $E = m$ then $\beta_1(0) = 0$ so the scattering wavefunction will not vanish in the limit $k \to 0$. For an asymmetric potential the following bound state wavefunction is appropriate for $|x| \geqslant \xi$:

$$\begin{array}{lll} \text{region I} & \psi^b = s\begin{pmatrix} E+m \\ -\kappa \end{pmatrix} \mathrm{e}^{\kappa x} & x \leqslant -\xi \\ \text{region III} & \psi^b = s'\begin{pmatrix} E+m \\ \kappa \end{pmatrix} \mathrm{e}^{-\kappa x} & x \geqslant \xi. \end{array} \tag{53}$$

If the potential is such that the wavefunction ψ^b possesses a well-defined nonzero limit as $E \to m, \kappa \to 0$, then the wavefunction for $|x| \geqslant \xi$ in this limit is just proportional to

$$\begin{pmatrix} 2m \\ 0 \end{pmatrix} \tag{54}$$

albeit with different constants of proportionality s, s' on the left and right. It is clear that a wavefunction of this form is non-normalizable and forms part of the continuum.

The scattering solutions ψ^s which tend to the solutions (54) in the zero-momentum limit will therefore have a lower component which vanishes for sufficiently large $|x|$. From equation (35) this implies that at $x = \xi$

$$b(0)\beta_1(0) + c(0)\beta_2(0) = 0 \tag{55}$$

while at $x = -\xi$ using equation (34) we have $c(0) = 0$. Since $\psi^s(k = 0)$ is not zero for a half-bound state, $b(0) \neq 0$ and hence

$$\beta_1(0) = 0. \tag{56}$$

An example of a half-bound state in an asymmetric potential is given in the appendix together with an explicit demonstration that $\beta_1(k)$ is of order k^2 for small k when the condition $\beta_1(0) = 0$ holds.

4.4. Symmetric potentials

When the potential is symmetric so that $V(x) = V(-x)$ we can find more stringent conditions on $l(0)$, $r(0)$ and $t(0)$. In the two-component approach, the behaviour of the wavefunction under the parity transformation $x \to -x$ is given by

$$\psi'(-x, t) = \sigma_z \psi(x, t). \tag{57}$$

It follows that we can define an even wavefunction $\psi_+(x)$ under parity as one with an even top component and an odd bottom component whereas an odd wavefunction $\psi_-(x)$ has an odd top component and an even bottom component. The wavefunction ψ^b for the bound state given in equation (53) must now be either an even solution ψ_+ or an odd solution ψ_-. First let us assume that it is even.

Then in the limit of a half-bound state at $E = m$ ($\kappa \to 0$) the solution remains even. As $k \to 0$ the scattering solution ψ^s will also be even. Thus from equations (7) and (8) we have

$$1 + l(0) = t(0). \tag{58}$$

From the unitarity relation we also know that

$$l(0)^2 + t(0)^2 = 1 = l(0)^2 + (1 + l(0))^2$$

therefore

$$l(0)^2 + l(0) = 0. \tag{59}$$

So either $l(0) = 0$ or $l(0) = -1$ in agreement with equation (28). We know that $l(0) \neq -1$ as $\psi^s(k = 0) \neq 0$. Hence

$$l(0) = 0 \tag{60}$$

and the transmission coefficient

$$T(0) = 1. \tag{61}$$

Using equation (52) we see that for an even half-bound state we must have $\alpha_1(0) = 1$ while for an odd half-bound state we have $\alpha_1(0) = -1$.

So we obtain the result that when a symmetric potential supports a half-bound state, a transmission resonance $T = 1$ occurs for an incident particle with arbitrarily small momentum. This agrees with our previous result for reflectionless scattering by a repulsive potential $V(x)$ where its attractive counterpart $U(x) = -V(x)$ is supercritical [7], that is to say $U(x)$ has a half-bound state at $E = -m$. To see this note that equations (3) are invariant under the (charge conjugation) transformation

$$E \to -E \qquad V \to -V \qquad f \to g \qquad g \to f \tag{62}$$

so it follows that $V(x)$ has a half-bound state at $E = m$ when $U(x)$ has a half-bound state at $E = -m$.

5. Discussion

We have now generalized the results for scattering in one dimension in the Schrödinger equation to the Dirac equation as we intended. But we are physicists not mathematicians: consequently our results are not yet as complete as those proved for the Schrödinger equation. Clemence [5], however, has shown that the class of potentials for which our results are true in the Dirac equation can be extended to include potentials which do not vanish for $|x| \geqslant \xi$. His results require the potentials $V(x)$ to satisfy

$$\int_{-\infty}^{\infty} (1 + |x|)|V(x)|\,\mathrm{d}x < \infty. \tag{63}$$

As stated in the introduction a half-bound state at $E = m$ can arise in two ways in the Dirac equation. These can most easily be distinguished by the examples of an attractive well for which $V(x) \leqslant 0$ and a repulsive barrier for which $V(x) \geqslant 0$, although it may be more difficult to characterize which is which for a complicated potential. In the case of an attractive potential a half-bound state with $E = m$ corresponds to a non-relativistic zero energy resonance. For example in the case of a square well $V(x) = -V_0$, $|x| \leqslant a$, $V(x) = 0$ elsewhere, one occurs at the threshold for the first odd state $V_0 = \pi^2/2ma^2$. In the case of a repulsive potential a half-bound state occurs as we have just seen when the corresponding attractive potential $U(x) = -V(x)$ is supercritical. For the square barrier $V(x) = V_0$, $|x| \leqslant a$, $V(x) = 0$ elsewhere, supercriticality first occurs when $V_0 = m + \sqrt{m^2 + \pi^2/4a^2}$ [8]. Note that $V_0 > 2m$ before supercriticality can occur.

Over 70 years ago Klein [14] discovered that a Dirac particle could tunnel through a potential barrier V with $V > 2m$. In this paper we have confirmed that tunnelling will always occur in the Dirac equation if a potential barrier $V(x)$ of short range is strong enough so that $U(x) = -V(x)$ is supercritical. The generic phenomenon whereby fermions can tunnel through barriers without exponential suppression we have called 'Klein tunnelling' [15]. Even strong long range repulsive potentials in the Dirac equation seem to have this property: in three dimensions Hall and one of us (ND) [16] have shown that Klein tunnelling is also associated with supercriticality for Coulomb potentials.

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Appendix

In order to illustrate scattering off an asymmetric potential we shall consider one of the few examples which can be solved analytically. We shall use a double delta potential barrier which comprises two unequal Dirac delta functions:

$$V(x) = \lambda\delta(x) + \mu\delta(x-a) \tag{64}$$

where $\lambda \neq \mu$ and $\lambda, \mu > 0$.

A.1. Scattering coefficients

The wavefunction for $x < 0$ is

$$\psi(x) = \begin{pmatrix} E+m \\ -\mathrm{i}k \end{pmatrix} \mathrm{e}^{\mathrm{i}kx} + l \begin{pmatrix} E+m \\ \mathrm{i}k \end{pmatrix} \mathrm{e}^{-\mathrm{i}kx} \tag{65}$$

while for $0 < x < a$ it is

$$\psi(x) = \alpha \begin{pmatrix} E+m \\ -\mathrm{i}k \end{pmatrix} \mathrm{e}^{\mathrm{i}kx} + \beta \begin{pmatrix} E+m \\ \mathrm{i}k \end{pmatrix} \mathrm{e}^{-\mathrm{i}kx} \tag{66}$$

and for $x > a$

$$\psi(x) = t \begin{pmatrix} E+m \\ -\mathrm{i}k \end{pmatrix} \mathrm{e}^{\mathrm{i}kx}. \tag{67}$$

The discontinuity condition on $\psi(x)$ at the first barrier at $x = 0_\pm$ is [8]

$$\psi(0_+) = \mathrm{e}^{\mathrm{i}\lambda\sigma_2}\psi(0_-) = \begin{pmatrix} \cos\lambda & \sin\lambda \\ -\sin\lambda & \cos\lambda \end{pmatrix} \psi(0_-). \tag{68}$$

The second discontinuity condition at $x = a_\pm$ is derived by replacing $0_\pm$ with $a_\pm$ and λ with μ.

The reflection and transmission amplitudes l and t can then be calculated to give

$$l = -\frac{\mathrm{i}mk(\cos\mu\sin\lambda + \mathrm{e}^{2\mathrm{i}ak}\cos\lambda\sin\mu) + mE(\mathrm{e}^{2\mathrm{i}ak}-1)\sin\lambda\sin\mu}{m^2(\mathrm{e}^{2\mathrm{i}ak}-1)\sin\lambda\sin\mu + k^2\cos(\lambda+\mu) + \mathrm{i}Ek\sin(\lambda+\mu)} \tag{69}$$

and

$$t = \frac{k^2}{m^2(\mathrm{e}^{2\mathrm{i}ak}-1)\sin\lambda\sin\mu + k^2\cos(\lambda+\mu) + \mathrm{i}Ek\sin(\lambda+\mu)}. \tag{70}$$

Using $E = \sqrt{k^2+m^2}$ we can write for small k

$$l = \frac{-\mathrm{i}m(\sin(\lambda+\mu) + 2ma\sin\lambda\sin\mu) + 2amk(am\sin\lambda\sin\mu + \cos\lambda\sin\mu) + O(k^2)}{\mathrm{i}m(\sin(\lambda+\mu) + 2ma\sin\lambda\sin\mu) + k(\cos(\lambda+\mu) - 2a^2m^2\sin\lambda\sin\mu) + O(k^2)} \tag{71}$$

$$t = \frac{k}{\mathrm{i}m(\sin(\lambda+\mu) + 2ma\sin\lambda\sin\mu) + k(\cos(\lambda+\mu) - 2a^2m^2\sin\lambda\sin\mu) + O(k^2)}. \tag{72}$$

From equations (71) and (72) it is easy to see that in general as $k \to 0$

$$l \to -1 \qquad t \to 0 \tag{73}$$

in agreement with equation (41). If however

$$\sin(\lambda+\mu)+2ma\sin\lambda\sin\mu=0 \tag{74}$$

then

$$l \to -\frac{am\sin(\lambda-\mu)}{\cos(\lambda+\mu)+am\sin(\lambda+\mu)} \tag{75}$$

and

$$t \to \frac{1}{\cos(\lambda+\mu)-2a^2m^2\sin\lambda\sin\mu}. \tag{76}$$

It is easy to show that l and t given above do indeed satisfy

$$|l|^2+|t|^2=1$$

provided that $\sin(\lambda+\mu)+2ma\sin\lambda\sin\mu=0$.

A.2. Exceptional case

The exceptional case in the proof above occurs when $\beta_1(0)=0$. We shall therefore calculate $\alpha_1(0)$ and $\beta_1(0)$ for the double delta potential. From equation (34) we consider the solution of the Dirac equation which takes the values $\binom{1}{0}$ at $x=-\xi$. The wavefunction $\psi(x)$ for $x<0$ thus has the form

$$(E+m)\psi(x)=\begin{pmatrix}(E+m)\cos k(x+\xi)\\ k\sin k(x+\xi)\end{pmatrix} \tag{77}$$

while for $0<x<a$ it is

$$(E+m)\psi(x)=\gamma\begin{pmatrix}(E+m)\cos kx\\ k\sin kx\end{pmatrix}+\delta\begin{pmatrix}(E+m)\sin kx\\ -k\cos kx\end{pmatrix} \tag{78}$$

and for $x>a$ we can write

$$(E+m)\psi(x)=\sigma\begin{pmatrix}(E+m)\cos k(x-\xi)\\ k\sin k(x-\xi)\end{pmatrix}+\tau\begin{pmatrix}(E+m)\sin k(x-\xi)\\ -k\cos k(x-\xi)\end{pmatrix}. \tag{79}$$

So at $x=\xi$ we see that

$$\alpha_1(k)=\sigma \qquad \beta_1(k)=-k\tau/(E+m). \tag{80}$$

For small k we calculate from the discontinuity conditions that

$$\sigma=[\cos(\lambda+\mu)+2m\xi\sin(\lambda+\mu)-2ma\sin\mu\cos\lambda+4am^2(\xi-a)\sin\mu\sin\lambda]+O(k^2) \tag{81}$$

and

$$k\tau=2m[(\sin(\lambda+\mu)+2am\sin\lambda\sin\mu)]+O(k^2). \tag{82}$$

Note that neither σ nor $k\tau$ has any term of order k. As $k\to 0$ we obtain

$$\beta_1(0)=-[(\sin(\lambda+\mu)+2am\sin\lambda\sin\mu)] \qquad \beta_1'(0)=0$$

so the exceptional case given by equation (74) above indeed satisfies $\beta_1(0)=0$. Furthermore when $\beta_1(0)=0$ it is easy to see that

$$\alpha_1(0)=\cos(\lambda+\mu)-2am\sin\mu(\cos\lambda+2am\sin\lambda). \tag{83}$$

From equation (52) the transmission coefficient in the exceptional case when

$$\beta_1(0)=-[(\sin(\lambda+\mu)+2am\sin\lambda\sin\mu)]=0$$

can be expressed in terms of $\alpha_1(0)$:

$$t = \frac{2\alpha_1(0)}{1 + \alpha_1^2(0)}. \tag{84}$$

After some tedious manipulation we find that

$$\begin{aligned}1 + [\alpha_1(0)]^2 &= 2(1 + 2am\sin\lambda\cos\lambda + 2a^2m^2\sin^2\lambda)\\ &= 2(\cos(\lambda+\mu) + 2am\sin\lambda\cos\mu)(\cos(\lambda+\mu) - 2a^2m^2\sin\lambda\sin\mu)\\ &= 2\alpha_1(0)(\cos(\lambda+\mu) - 2a^2m^2\sin\lambda\sin\mu).\end{aligned} \tag{85}$$

So

$$t = \frac{2\alpha_1(0)}{2\alpha_1(0)[\cos(\lambda+\mu) - 2a^2m^2\sin\lambda\sin\mu]} \tag{86}$$

in agreement with equation (76). Similarly it can be shown that equation (75) for the reflection coefficient agrees with equation (51).

A.3. Bound states

Let us now consider the asymmetric potential well

$$U(x) = -V(x) = -\lambda\delta(x) - \mu\delta(x-a). \tag{87}$$

This will have bound states with a wavefunction for $x < 0$ of the form

$$\psi(x) = \begin{pmatrix} -\kappa \\ m-E \end{pmatrix} \mathrm{e}^{\kappa x} \tag{88}$$

while for $0 < x < a$

$$\psi(x) = \gamma\begin{pmatrix} -\kappa \\ m-E \end{pmatrix} \mathrm{e}^{\kappa x} + \delta\begin{pmatrix} \kappa \\ m-E \end{pmatrix} \mathrm{e}^{-\kappa x} \tag{89}$$

and for $x > a$

$$\psi(x) = s\begin{pmatrix} \kappa \\ m-E \end{pmatrix} \mathrm{e}^{-\kappa x}. \tag{90}$$

The discontinuity condition for the first delta well is

$$\psi(0_+) = \mathrm{e}^{-\mathrm{i}\sigma_2\lambda}\psi(0_-) = \begin{pmatrix} \cos\lambda & -\sin\lambda \\ \sin\lambda & \cos\lambda \end{pmatrix}\psi(0_-). \tag{91}$$

Note that this differs from the condition for barriers only in that $\lambda \to -\lambda$. The second discontinuity condition follows with $0_\pm \to a_\pm$ and $\lambda \to \mu$. This leads to the following four equations:

$$\kappa(-\gamma+\delta)\cos\lambda + (m-E)(\gamma+\delta)\sin\lambda = -\kappa \tag{92a}$$

$$-(m-E)(\gamma+\delta)\cos\lambda - \kappa(-\gamma+\delta)\sin\lambda = m-E \tag{92b}$$

$$\kappa(-\gamma\mathrm{e}^{a\kappa} + \delta\,\mathrm{e}^{-a\kappa})\cos\mu + (m-E)(\gamma\mathrm{e}^{a\kappa} + \delta\,\mathrm{e}^{-a\kappa})\sin\mu = s\kappa\,\mathrm{e}^{-a\kappa} \tag{92c}$$

$$(m-E)(\gamma\,\mathrm{e}^{a\kappa} + \delta\,\mathrm{e}^{-a\kappa})\cos\mu + \kappa(-\gamma\mathrm{e}^{a\kappa} + \delta\,\mathrm{e}^{-a\kappa})\sin\mu = s(m-E)\,\mathrm{e}^{-a\kappa} \tag{92d}$$

where γ and δ can be found from the first two equations (88*a*) and (88*b*) to be

$$\begin{aligned}\gamma &= -\frac{E\sin\lambda - \kappa\cos\lambda}{\kappa}\\ \delta &= -\frac{m\sin\lambda}{\kappa}.\end{aligned} \tag{93}$$

Eliminating s from (88c) and (88d) leads to

$$\gamma\, e^{2a\kappa}(\kappa\cos\mu - E\sin\mu) + \delta m\sin\mu = 0. \tag{94}$$

We thus obtain

$$e^{2a\kappa}(\kappa\cos\lambda - E\sin\lambda)(\kappa\cos\mu - E\sin\mu) - m^2\sin\lambda\sin\mu = 0. \tag{95}$$

Rearranging gives

$$\sin(\lambda+\mu) = \frac{\kappa^2 e^{2a\kappa}\cos\lambda\cos\mu + (e^{2a\kappa}E^2 - m^2)\sin\lambda\sin\mu}{E\kappa\, e^{2a\kappa}}. \tag{96}$$

At supercriticality $E = -m$, $\kappa = 0$ giving

$$\sin(\lambda+\mu) + 2ma\sin\lambda\sin\mu = 0 \tag{97}$$

in agreement with the exceptional condition $\beta_1(0) = 0$.

When $\lambda = \mu$ we obtain a symmetric potential. If $\sin(\lambda+\mu) + 2ma\sin\lambda\sin\mu = 0$ then either $\sin\lambda = 0$ and $\alpha_1(0) = 1$ or $\tan\lambda = -1/ma$ and $\alpha_1(0) = -1$. In both cases the transmission coefficient $T = 1$ in agreement with our previous result [7] for supercritical symmetric potentials.

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