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# The Woods–Saxon potential in the Dirac equation

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**Abstract**
The two-component approach to the one-dimensional Dirac equation is applied to the Woods–Saxon potential. The scattering and bound state solutions are derived and the conditions for a transmission resonance (when the transmission coefficient is unity) and supercriticality (when the particle bound state is at $E = -m$) are then derived. The square potential limit is discussed. The recent result that a finite-range symmetric potential barrier will have a transmission resonance of zero momentum when the corresponding well supports a half-bound state at $E = -m$ is demonstrated.

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## Introduction

There is a well-known theorem for low-momentum scattering in the Schrödinger equation in one dimension by an even potential well [1, 2]: as momentum $k$ tends to zero, the reflection coefficient $L(k)$ tends to unity unless the potential $V(x)$ supports a zero-energy resonance [3]. In this case $L(k) \to 0$ and correspondingly the transmission coefficient $T(k) \to 1$. Bohm [4] calls this a transmission resonance. Recently we [5] have generalized this result to the Dirac equation. Since the Dirac equation covers anti-particle scattering as well as particle scattering, the generalization gives two distinct results since the $k \to 0$ limit in the Dirac equation corresponds both to particle states where the energy $E = m$ and anti-particle states where $E = -m$ and $m$ is the particle mass. The result that anti-particles can have transmission resonances when they scatter off potential wells is equivalent to particles having transmission resonances when scattering off potential barriers. This is itself related to the result on barrier penetration found by Klein [6] and now called the Klein paradox.

Our result [5] shows that transmission resonances at $k = 0$ in the Dirac equation occur for a potential barrier $V = U_c(x)$ when the corresponding potential well $V = -U_c(x)$ just supports a bound state at $E = -m$; this is called a supercritical state. While transmission resonances for a square barrier in the Dirac equation have been known for some time [7] and their relationship to supercritical states for a square well was pointed out more recently [8], we are not aware of any other analytic solution of the Dirac equation for which they can be demonstrated. Nevertheless, Dosch *et al* [9] showed in 1971 that a transmission resonance does exist for the Woods–Saxon potential, which is a smoothed out form of the square well/barrier. In this paper we take this example further. We solve the Dirac equation for the Woods–Saxon potential well to demonstrate the supercritical states and find complete solutions for the reflection and transmission amplitudes for scattering off a Woods–Saxon potential barrier. We then are able to demonstrate the correspondence between the supercritical states and the transmission resonances analytically. We also consider the limit where the Woods–Saxon potential becomes a square well/barrier.

## The one-particle Dirac equation in one dimension

In the one-dimensional Dirac equation, solutions can be greatly simplified by adopting a two-component approach; both the positive and negative energy solution states are retained without the added complication of spin. Starting with the relativistic free-particle Dirac equation ($\hbar = c = 1$):

$$\left(\mathrm{i}\gamma^{\mu}\frac{\partial}{\partial x^{\mu}} - m\right)\psi = 0. \tag{1}$$

In the presence of an external potential $V(x)$ and taking the gamma matrices $\gamma_x$ and $\gamma_0$ to be the Pauli matrices $\mathrm{i}\sigma_x$ and $\sigma_z$, respectively, the Dirac equation in one dimension can be written as

$$\left(\sigma_x\frac{\mathrm{d}}{\mathrm{d}x} - (E - V(x))\sigma_z + m\mathbf{1}\right)\psi(x) = 0. \tag{2}$$

The four-spinor, $\psi$, is decomposed into two spinors, $u_1$ and $u_2$, so that

$$\psi(x) = \begin{pmatrix} u_1(x) \\ u_2(x) \end{pmatrix}. \tag{3}$$

Thus the problem is to solve the coupled differential equations

$$\begin{aligned} u_1' &= -(m + E - V(x))u_2(x) \\ u_2' &= -(m - E + V(x))u_1(x). \end{aligned} \tag{4}$$

Following a similar procedure to that used by Flügge [10], introduce the following combinations:

$$\phi(x) = u_1(x) + \mathrm{i}u_2(x) \qquad \chi(x) = u_1(x) - \mathrm{i}u_2(x). \tag{5}$$

Substituting these into (4) and re-arranging gives

$$\phi'(x) = -\mathrm{i}m\chi(x) + \mathrm{i}(E - V(x))\phi(x) \tag{6}$$

$$\chi'(x) = \mathrm{i}m\phi(x) - \mathrm{i}(E - V(x))\chi(x). \tag{7}$$

The two components, $\phi(x)$ and $\chi(x)$, satisfy

$$\phi''(x) + [(E - V(x))^2 - m^2 + \mathrm{i}V'(x)]\phi(x) = 0 \tag{8}$$

$$\chi''(x) + [(E - V(x))^2 - m^2 - \mathrm{i}V'(x)]\chi(x) = 0. \tag{9}$$

In the following the full solutions for $\phi(x)$ will be presented. In order to establish $\chi(x)$, use will be made of (6).

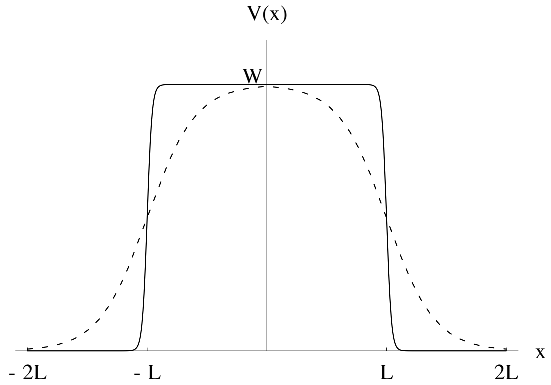


**Figure 1.** The Woods–Saxon potential barrier for $L = 10$ with $a = 5$ (solid line) and $a = 0.5$ (dotted line).

## The Woods–Saxon potential

The Woods–Saxon potential is defined as

$$V(x) = W\left(\frac{\theta(-x)}{1 + \mathrm{e}^{-a(x+L)}} + \frac{\theta(x)}{1 + \mathrm{e}^{a(x-L)}}\right) \tag{10}$$

with $W$ real and positive for a barrier or negative for a well; $a$ and $L$ are real and positive. $\theta(x)$ is the Heaviside step function.

At this stage it is worth mentioning that we will be interested in potentials where $aL \gg 1$; from figure 1 it can be seen that, for this condition, the potential has a less pronounced cusp at $x = 0$—the potential now closely resembles a square barrier with smooth walls. As stated in [9] this does not introduce any essential physical restriction on the problem and is significant only in that it allows exact solutions to be established (albeit in an approximation).

## Scattering states

First, consider the scattering solutions for $x < 0$ with $|E| > m$. On making the substitution $y = -\mathrm{e}^{-a(x+L)}$, equation (8) becomes

$$a^2 y \frac{\mathrm{d}}{\mathrm{d}y}\left[y \frac{\mathrm{d}\phi_{\mathrm{L}}}{\mathrm{d}y}\right] + \left[\left(E - \frac{W}{1-y}\right)^2 - m^2 - \frac{\mathrm{i}ayW}{(1-y)^2}\right]\phi_L = 0. \tag{11}$$

Splitting off fitting powers of $y$ and $(1 - y)$ by setting $\phi_{\mathrm{L}} = y^{\mu}(1 - y)^{-\lambda} f(y)$ and substituting into the above equation reduces it to the hypergeometrical equation

$$y(1-y)f''(y) + [(1+2\mu) - y(1+2\mu-2\lambda)]f'(y) - [(\mu-\nu-\lambda)(\mu+\nu-\lambda)]f(y) = 0 \tag{12}$$

where the primes denote derivatives with respect to $y$ and the following abbreviations have been used

$$\begin{aligned} &\mu = \frac{\mathrm{i}p}{a} \qquad \nu = \frac{\mathrm{i}k}{a} \qquad \lambda = \frac{\mathrm{i}W}{a} \\ &p^2 = (E-W)^2 - m^2 \qquad k^2 = E^2 - m^2. \end{aligned} \tag{13}$$

Note that as we are considering scattering states, $|E| > m$ which ensures that $k$ is real, and $W$ is real and positive. $p$ is real for $m < E < W - m$ (the Klein range) and $E > W + m$ and imaginary for $W - m < E < W + m$. Of principal interest are the energies which lie in the Klein range and potentially lead to Klein tunnelling—where fermions can tunnel through strong potentials without exponential suppression [11]. Equation (12) has the general solution

$$f(y) = D_1 y^{-2\mu} {}_2F_1(-\mu - \nu - \lambda, -\mu + \nu - \lambda, 1 - 2\mu; y) + D_2 {}_2F_1(\mu - \nu - \lambda, \mu + \nu - \lambda, 1 + 2\mu; y). \tag{14}$$

So

$$\phi_L(y) = D_1 y^{-\mu}(1 - y)^{-\lambda} {}_2F_1(-\mu - \nu - \lambda, -\mu + \nu - \lambda, 1 - 2\mu; y) + D_2 y^{\mu}(1 - y)^{-\lambda} {}_2F_1(\mu - \nu - \lambda, \mu + \nu - \lambda, 1 + 2\mu; y). \tag{15}$$

For this to be a physically acceptable solution to the problem, it must satisfy the appropriate boundary conditions as $x \to -\infty$. The solutions as $x \to -\infty \Rightarrow y \to -\infty$ can be determined using the following formula for the asymptotic behaviour of the hypergeometric function [12]:

$${}_2F_1(a, b, c; y) = \frac{\Gamma(c)\Gamma(b - a)}{\Gamma(b)\Gamma(c - a)}(-y)^{-a} + \frac{\Gamma(c)\Gamma(a - b)}{\Gamma(a)\Gamma(c - b)}(-y)^{-b} \tag{16}$$

and noting that in the limit $x \to -\infty$, $(-y)^{\mp\nu} \to \mathrm{e}^{\pm \mathrm{i}k(x+L)}$. Therefore in this limit, $\phi_L(x)$ can be written as

$$\lim_{x\to-\infty} \phi_L(x) = A\mathrm{e}^{\mathrm{i}k(x+L)} + B\mathrm{e}^{-\mathrm{i}k(x+L)}. \tag{17}$$

From equation (6) the other component $\chi(x)$ is

$$\chi(x) = \frac{1}{\mathrm{i}m}[\mathrm{i}(E - V(x))\phi(x) - \phi'(x)]. \tag{18}$$

Substituting equation (17) into the above gives us

$$\lim_{x\to-\infty} \chi_L(x) = A\left(\frac{E - k}{m}\right)\mathrm{e}^{\mathrm{i}k(x+L)} + B\left(\frac{E + k}{m}\right)\mathrm{e}^{-\mathrm{i}k(x+L)} \tag{19}$$

where in both cases

$$A = D_1 \frac{\Gamma(1 - 2\mu)\Gamma(-2\nu)}{\Gamma(-\mu - \nu - \lambda)\Gamma(1 - \mu - \nu + \lambda)}\mathrm{e}^{-\mathrm{i}\pi\mu} + D_2 \frac{\Gamma(1 + 2\mu)\Gamma(-2\nu)}{\Gamma(\mu - \nu - \lambda)\Gamma(1 + \mu - \nu + \lambda)}\mathrm{e}^{\mathrm{i}\pi\mu} \tag{20}$$

and

$$B = D_1 \frac{\Gamma(1 - 2\mu)\Gamma(2\nu)}{\Gamma(-\mu + \nu - \lambda)\Gamma(1 - \mu + \nu + \lambda)}\mathrm{e}^{-\mathrm{i}\pi\mu} + D_2 \frac{\Gamma(1 + 2\mu)\Gamma(2\nu)}{\Gamma(\mu + \nu - \lambda)\Gamma(1 + \mu + \nu + \lambda)}\mathrm{e}^{\mathrm{i}\pi\mu}. \tag{21}$$

The choice of combinations of the wavefunction components (5) can be re-written as

$$u_1(x) = \frac{1}{2}(\phi(x) + \chi(x)) \qquad u_2(x) = \frac{1}{2\mathrm{i}}(\phi(x) - \chi(x)). \tag{22}$$

Upon substitution of equations (17) and (19) into the above it can be seen that the wavefunction, $\psi(x)$, comprises an incident and a reflected wave far to the left of the barrier which is the desired form to establish reflection and transmission amplitudes.

Now consider the solutions for $x > 0$. The analysis will differ slightly from [9] by making a more appropriate substitution to lead to the desired transmitted wavefunction far to the right of the barrier. This substitution will also lead to the correct wavefunctions when the bound state solutions are considered. On choosing $z^{-1} = 1 + \mathrm{e}^{a(x-L)}$, equation (8) becomes

$$a^2 z(1 - z)\frac{\mathrm{d}}{\mathrm{d}z}\left[z(1 - z)\frac{\mathrm{d}\phi_\mathrm{R}}{\mathrm{d}z}\right] + [(E - Wz)^2 - m^2 - \mathrm{i}az(1 - z)W]\phi_\mathrm{R} = 0. \tag{23}$$

Putting $\phi_R = z^{-\nu}(1-z)^{-\mu} g(z)$ and substituting into the above gives the hypergeometrical equation

$$z(1-z)g''(z) + [(1-2\nu) - z(2-2\mu-2\nu)]g'(z) \\ -[(1-\mu-\nu-\lambda)(-\mu-\nu+\lambda)]g(z) = 0. \tag{24}$$

The general solution to the above is

$$g(z) = d_1\, {}_2F_1(1-\mu-\nu-\lambda, -\mu-\nu+\lambda, 1-2\nu; z) \\ + d_2\, z^{2\nu}\, {}_2F_1(1-\mu+\nu-\lambda, -\mu+\nu+\lambda, 1+2\nu; z). \tag{25}$$

So

$$\phi_R = d_1\, z^{-\nu}(1-z)^{-\mu}\, {}_2F_1(1-\mu-\nu-\lambda, -\mu-\nu+\lambda, 1-2\nu; z) \\ + d_2\, z^{\nu}(1-z)^{-\mu}\, {}_2F_1(1-\mu+\nu-\lambda, -\mu+\nu+\lambda, 1+2\nu; z). \tag{26}$$

Also as $x \to \infty$, $z \to 0$ and $z^{-\nu} \to \mathrm{e}^{\mathrm{i}k(x-L)}$. Therefore in order to have a plane wave travelling to the right as $x \to \infty$, $d_2 = 0$. So

$$\phi_R = d_1\, z^{-\nu}(1-z)^{-\mu}\, {}_2F_1(1-\mu-\nu-\lambda, -\mu-\nu+\lambda, 1-2\nu; z) \tag{27}$$

and

$$\lim_{x\to\infty} \phi_R = d_1 \mathrm{e}^{-\mathrm{i}kL}\mathrm{e}^{\mathrm{i}kx} \tag{28}$$

whilst the other component

$$\lim_{x\to\infty} \chi_R = d_1 \left(\frac{E-k}{m}\right) \mathrm{e}^{-\mathrm{i}kL}\mathrm{e}^{\mathrm{i}kx}. \tag{29}$$

In order to find the energy eigenvalues, the wavefunctions $\phi_L$ and $\phi_R$ must be matched at $x = 0$. As $x \to 0$, $y \to 0$ and $z \to 1$ ($aL \gg 1$), so

$$\phi_L \to D_1 \mathrm{e}^{-\mathrm{i}\pi\mu}\mathrm{e}^{aL\mu}\mathrm{e}^{a\mu x} + D_2 \mathrm{e}^{\mathrm{i}\pi\mu}\mathrm{e}^{-aL\mu}\mathrm{e}^{-a\mu x} \tag{30}$$

and

$$\phi_R \to d_1 \mathrm{e}^{-a\mu x}\mathrm{e}^{aL\mu} \frac{\Gamma(2\mu)\Gamma(1-2\nu)}{\Gamma(1+\mu-\nu-\lambda)\Gamma(\mu-\nu+\lambda)} \\ + d_1 \mathrm{e}^{a\mu x}\mathrm{e}^{-aL\mu} \frac{\Gamma(-2\mu)\Gamma(1-2\nu)}{\Gamma(1-\mu-\nu-\lambda)\Gamma(-\mu-\nu+\lambda)} \tag{31}$$

where use has been made of the following continuation identity for the hypergeometric function in $\phi_R$:

$${}_2F_1(a, b, c; z) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\, {}_2F_1(a, b, a+b-c+1; 1-z) \\ + (1-z)^{c-a-b} \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}\, {}_2F_1(c-a, c-b, c-a-b+1; 1-z). \tag{32}$$

Comparing the coefficients of $\mathrm{e}^{\pm a\mu x}$ and eliminating $d_1$ gives

$$\frac{D_2}{D_1} = \mathrm{e}^{-2\mathrm{i}\pi\mu}\mathrm{e}^{4aL\mu} \frac{\Gamma(2\mu)\Gamma(1-\mu-\nu-\lambda)\Gamma(-\mu-\nu+\lambda)}{\Gamma(-2\mu)\Gamma(1+\mu-\nu-\lambda)\Gamma(\mu-\nu+\lambda)}. \tag{33}$$

The electrical current density for the one-dimensional equation (2) is defined as

$$j = \bar{\psi}(x)\gamma_x\psi(x) = -\psi(x)^\dagger\sigma_2\psi(x) = \mathrm{i}(u_1^* u_2 - u_2^* u_1) = \tfrac{1}{2}(|\phi(x)|^2 - |\chi(x)|^2) \tag{34}$$

where use has been made of the choice of combinations for the wavefunctions (5). The current as $x \to -\infty$ is $j_L = j_{in} - j_{refl}$ where $j_{in}$ is the incident current and $j_{refl}$ is the reflected current.

Similarly, as $x \to \infty$ we have that the current $j_\mathrm{R} = j_\mathrm{trans}$ where $j_\mathrm{trans}$ is the transmitted current. Substituting equations (17), (19), (28) and (29) into (34) we find that

$$\begin{aligned} j_\mathrm{L} &= |A|^2 \frac{k}{m^2}(E-k) - |B|^2 \frac{k}{m^2}(E+k) \\ j_\mathrm{R} &= |d_1|^2 \frac{k}{m^2}(E-k). \end{aligned} \tag{35}$$

From the conservation of charge we have that $j_\mathrm{L} = j_\mathrm{R}$ which together with the reflection coefficient, $R$, and the transmission coefficient, $T$

$$R = \frac{j_\mathrm{refl}}{j_\mathrm{in}} = \frac{|B|^2}{|A|^2}\left(\frac{E+k}{E-k}\right) \qquad T = \frac{j_\mathrm{trans}}{j_\mathrm{in}} = \frac{|d_1|^2}{|A|^2} \tag{36}$$

we obtain the unitarity condition

$$R + T = 1. \tag{37}$$

For the purpose of comparison with [9] the following expressions for the reflection and transmission amplitudes are useful:

$$r = \left(\frac{m+E+k}{m+E-k}\right) \mathrm{e}^{-2\mathrm{i}kL} \frac{B}{A} \qquad t = \mathrm{e}^{-2\mathrm{i}kL} \frac{d_1}{A}. \tag{38}$$

The reflection amplitude is found to be

$$\begin{aligned} r = {} & \frac{\mathrm{e}^{-2\mathrm{i}kL}}{\Omega} \frac{(m+E+k)B(2\nu, -\mu-\nu-\lambda)}{(m+E-k)B(-2\nu, 1-\mu+\nu+\lambda)} \\ & \times \left[1 - \mathrm{e}^{4\mathrm{i}pL} \frac{B(2\mu, -\mu-\nu+\lambda)B(2\mu, -\mu+\nu+\lambda)}{B(-2\mu, \mu+\nu-\lambda)B(-2\mu, \mu-\nu-\lambda)}\right] \end{aligned} \tag{39}$$

where

$$\Omega = 1 - \mathrm{e}^{4aL\mu} \left[\frac{(\mu+\nu)^2 - \lambda^2}{(\mu-\nu)^2 - \lambda^2}\right] \frac{B^2(2\mu, -\mu-\nu+\lambda)}{B^2(-2\mu, \mu-\nu-\lambda)} \tag{40}$$

and $B(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$ is the beta function. Note that this equation yields identical results to the $r$ given in [9]. The transmission amplitude is found to be

$$t = \frac{\mathrm{e}^{-2\mathrm{i}kL+2a\mu L}}{\Omega} \left(\frac{(\mu+\nu)^2 - \lambda^2}{4\mu\nu}\right) \frac{\Gamma^2(-\mu-\nu-\lambda)\Gamma^2(-\mu-\nu+\lambda)}{\Gamma^2(-2\mu)\Gamma^2(-2\nu)}. \tag{41}$$

Using equations (39) and (41), the unitary condition (37) can be established; the algebra is quite involved and some care must be taken for the two cases where $p$ is real and imaginary.

In order to establish the condition for a transmission resonance, $T = 1$, to occur, it is more convenient to look at the reflection amplitude for $r = 0$. In this instance, only the square-bracketed term on the right of (41) needs to be considered; although poles of the gamma-functions could make $r$ zero, $\mu$, $\nu$ and $\lambda$ are all purely imaginary for energies in the Klein range and do not give the negative integer required for this to happen (figure 2). Consequently, transmission resonances occur when

$$1 - \mathrm{e}^{4\mathrm{i}pL} \frac{B(2\mu, -\mu-\nu+\lambda)B(2\mu, -\mu+\nu+\lambda)}{B(-2\mu, \mu+\nu-\lambda)B(-2\mu, \mu-\nu-\lambda)} = 0. \tag{42}$$

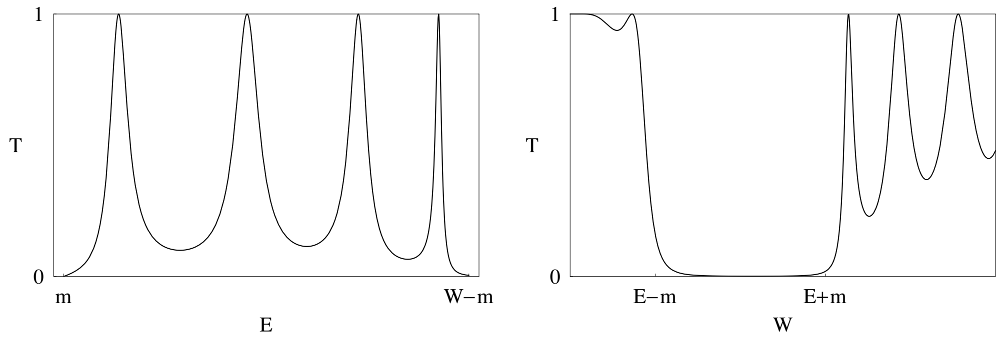


**Figure 2.** The transmission coefficient for the relativistic Woods–Saxon potential barrier. The left-hand plot illustrates $T$ for varying energy, $E$, with $L = 10$, $a = 5$, $m = 0.4$ and $W = 1.2$. The right-hand plot is for varying barrier height, $W$, with $L = 10$, $a = 5$, $m = 0.2$ and $E = 2m$. Both plots illustrate the tunnelling without reflection predicted by Dosch, Jensen and Müller.

## Bound states

In order to study the bound states, use can be made of the wavefunction derived for $x > 0$, but the analysis can be simplified for $x < 0$ by making the substitution $y^{-1} = 1 + \mathrm{e}^{-a(x+L)}$ which leads to the following equation:

$$a^2 y(1-y)\frac{\mathrm{d}}{\mathrm{d}y}\left[y(1-y)\frac{\mathrm{d}\phi_\mathrm{L}}{\mathrm{d}y}\right] + [(E+Wy)^2 - m^2 - \mathrm{i}ay(1-y)W]\phi_\mathrm{L} = 0 \tag{43}$$

where $W \to -W$ in equation (10) for potential wells. Putting $\phi_\mathrm{L} = y^\sigma(1-y)^\gamma h(y)$ leads to the hypergeometric equation

$$y(1-y)h''(y) + [(1+2\sigma) - y(2+2\sigma+2\gamma)]h'(y) - [(1+\sigma+\gamma-\lambda)(\sigma+\gamma+\lambda)]h(y) = 0 \tag{44}$$

where

$$\sigma = \frac{\kappa}{a} \qquad \kappa = m^2 - E^2 \qquad \gamma = \frac{\mathrm{i}p'}{a} \qquad p'^2 = (E+W)^2 - m^2. \tag{45}$$

As $x \to -\infty$, $y \to 0$ so choose the solution

$$h(y) = {}_2F_1(1+\sigma+\gamma-\lambda, \sigma+\gamma+\lambda, 1+2\sigma; y) \tag{46}$$

and therefore

$$\phi_\mathrm{L} = A' y^\sigma (1-y)^\gamma {}_2F_1(1+\sigma+\gamma-\lambda, \sigma+\gamma+\lambda, 1+2\sigma; y). \tag{47}$$

For $x > 0$, use equation (26) with $W \to -W$ so $\lambda \to -\lambda$ and $\mu \to \gamma$ and also $k \to \mathrm{i}\kappa$ so $\nu \to -\sigma$, then choose the solution

$$\phi_\mathrm{R} = B' z^\sigma (1-z)^{-\gamma} {}_2F_1(1+\sigma-\gamma+\lambda, \sigma-\gamma-\lambda, 1+2\sigma; z). \tag{48}$$

Once again, in order to find the energy eigenvalues these two wavefunctions must be matched at $x = 0$ where both $y, z \to 1$ ($aL \gg 1$). By making use of the continuation formula (32) the component $\phi$ can be written as

$$\begin{aligned}\phi_\mathrm{L} \to\ & A'\mathrm{e}^{-\gamma ax}\mathrm{e}^{-\gamma aL}\frac{\Gamma(-2\gamma)\Gamma(1+2\sigma)}{\Gamma(1-\gamma+\sigma-\lambda)\Gamma(-\gamma+\sigma+\lambda)} \\ & + A'\mathrm{e}^{\gamma ax}\mathrm{e}^{\gamma aL}\frac{\Gamma(2\gamma)\Gamma(1+2\sigma)}{\Gamma(1+\gamma+\sigma-\lambda)\Gamma(\gamma+\sigma+\lambda)}\end{aligned} \tag{49}$$

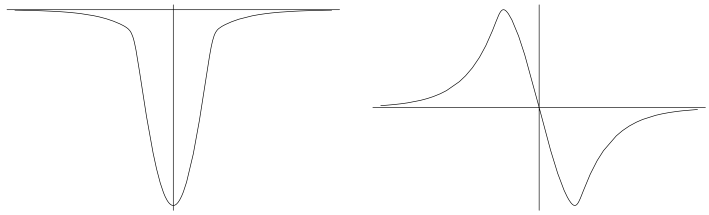

**Figure 3.** The upper (left) and lower (right) components of the first even bound state wavefunction for the sub-critical Woods–Saxon potential well where $a = 10$, $L = 2$, $m = 1$ and $W = 2$. The energy of the bound state is $E = 0.759$.

and

$$\phi_{\mathrm{R}} \to B' \mathrm{e}^{-\gamma a x} \mathrm{e}^{\gamma a L} \frac{\Gamma(2\gamma)\Gamma(1+2\sigma)}{\Gamma(1+\gamma+\sigma+\lambda)\Gamma(\gamma+\sigma-\lambda)} + B' \mathrm{e}^{\gamma a x} \mathrm{e}^{-\gamma a L} \frac{\Gamma(-2\gamma)\Gamma(1+2\sigma)}{\Gamma(1-\gamma+\sigma-\lambda)\Gamma(-\gamma+\sigma-\lambda)}. \tag{50}$$

Comparing terms in $\mathrm{e}^{\pm\gamma a x}$ and eliminating $A'$ and $B'$ ultimately leads to

$$\frac{B(-2\gamma, \gamma+\sigma-\lambda)^2}{B(2\gamma, -\gamma+\sigma+\lambda)^2} = \mathrm{e}^{4\gamma a L} \frac{(\sigma-\gamma)^2 - \lambda^2}{(\sigma+\gamma)^2 - \lambda^2}. \tag{51}$$

So

$$\frac{B(-2\gamma, \gamma+\sigma-\lambda)}{B(2\gamma, -\gamma+\sigma+\lambda)} = \pm \mathrm{e}^{2\gamma a L} \sqrt{\frac{(\sigma-\gamma)^2 - \lambda^2}{(\sigma+\gamma)^2 - \lambda^2}} \tag{52}$$

where the even solutions are determined by the positive square root and the odd solutions by the negative square root. These equations need to be solved numerically to find the energy eigenvalues for the bound states. It is also possible to plot the upper and lower components of the bound state wavefunction $\psi(x)$ (figure 3).

**Supercriticality**

As the potential well deepens for increasing $W$, the energy eigenvalue of any given bound state will also decrease. When this energy reaches $E = -m$, the bound state merges with the negative energy continuum and the potential is said to be supercritical. When $E \to -m$, $\kappa \to 0$ and consequently $\sigma \to 0$. Writing

$$\gamma_{\mathrm{c}} = \frac{\mathrm{i}}{a} p_{\mathrm{c}} \qquad p_{\mathrm{c}}^2 = W^2 - 2mW \tag{53}$$

the energy eigenvalue equation (51) becomes

$$\frac{B(-2\gamma_{\mathrm{c}}, \gamma_{\mathrm{c}}-\lambda)^2}{B(2\gamma_{\mathrm{c}}, -\gamma_{\mathrm{c}}+\lambda)^2} = \mathrm{e}^{4\gamma_{\mathrm{c}} a L}. \tag{54}$$

Once again the even and odd supercritical energy eigenvalues can be determined by taking the positive and negative square roots, respectively.

**Square well limit: bound states**

Using

$$B(a, b) = \left(\frac{a+b}{b}\right)\left(\frac{a+b+1}{a}\right) B(a+1, b+1) \tag{55}$$

we find that

$$B(\mp 2\gamma, \pm\gamma + \sigma \mp \lambda) = \mp \frac{(\mp\gamma + \sigma \mp \lambda)(1 \mp \gamma + \sigma \mp \lambda)}{2\gamma(\pm\gamma + \sigma \mp \lambda)} B(1 \mp 2\gamma, 1 \pm \gamma + \sigma \mp \lambda). \tag{56}$$

Therefore in the square well limit $a \to \infty, \gamma, \sigma, \lambda \to 0$ and

$$\frac{B(-2\gamma, \gamma + \sigma - \lambda)}{B(2\gamma, -\gamma + \sigma + \lambda)} \to -\frac{(-\gamma + \sigma - \lambda)(-\gamma + \sigma + \lambda)}{(\gamma + \sigma - \lambda)(\gamma + \sigma + \lambda)} \tag{57}$$

where we have used $B(1, 1) = 1$. Substituting this into (51) we obtain

$$\mathrm{e}^{4\mathrm{i}p'L} = \frac{(\sigma - \gamma)^2 - \lambda^2}{(\sigma + \gamma)^2 - \lambda^2} = \frac{(\kappa - \mathrm{i}p')^2 + W^2}{(\kappa + \mathrm{i}p')^2 + W^2}. \tag{58}$$

Rationalizing we find that

$$\mathrm{e}^{4\mathrm{i}p'L} = \left(\frac{\kappa^2 - p'^2 + W^2}{2mW} - \frac{\mathrm{i}\kappa p'}{mW}\right)^2. \tag{59}$$

Choosing the positive root and solving for the real and imaginary parts one eventually obtains

$$\tan 2p'L = \frac{2\kappa p'}{p'^2 - \kappa^2 - W^2} \tag{60}$$

which after much laborious algebra gives for the even solutions

$$\tan p'L = \frac{mW + \kappa^2 - EW}{\kappa p'} = \sqrt{\frac{(m - E)(E + W + m)}{(m + E)(E + W - m)}} \tag{61}$$

and for the odd solutions

$$\tan p'L = -\frac{mW - \kappa^2 + EW}{\kappa p'} = -\sqrt{\frac{(m + E)(E + W - m)}{(m - E)(E + W + m)}} \tag{62}$$

(these are precisely the equations for even and odd bound states in the square well [8] with $W = V$).

## Zero-momentum resonances and supercriticality

It was first pointed out in [13] that the conditions for supercriticality and zero-momentum resonances were the same for the square, Gaussian and Woods–Saxon potentials. Indeed, for the square potential well, $V(x)$, where $V(x) = 0$ for $|x| \geqslant a$ and $V(x) = -U \leqslant 0$ for $|x| < a$, the condition for supercriticality is $2p'a = N\pi$ where $p'^2 = U^2 - 2mU$ [11]. The Dirac equation (4) is invariant under charge conjugation, that is to say under the transformation

$$E \to -E \qquad U \to -U \qquad u_1 \to u_2 \qquad u_2 \to u_1. \tag{63}$$

Consequently, the condition for a supercritical particle at $E = -m$ in a square well is the same as that for a supercritical antiparticle at $E = m$ in a square barrier. It can also be shown that for a transmission resonance to occur, $2pa = N\pi$ where $p^2 = (E - V)^2 - m^2 = k^2 + V^2 - 2VE$. In the zero-momentum limit, $k \to 0$, this is seen to be identical to the condition for a supercritical antiparticle. In other words, when a 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 [5]. From (42) the condition for a transmission resonance to occur for the Woods–Saxon potential is

$$\mathrm{e}^{4\mathrm{i}pL} = \frac{B(-2\mu, \mu + \nu - \lambda)B(-2\mu, \mu - \nu - \lambda)}{B(2\mu, -\mu - \nu + \lambda)B(2\mu, -\mu + \nu + \lambda)}. \tag{64}$$

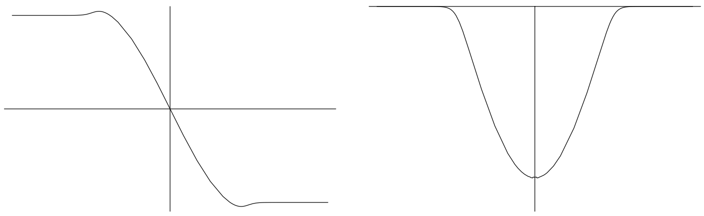

**Figure 4.** The upper (left) and lower (right) components of the first zero-momentum wavefunction for the supercritical Woods–Saxon potential barrier where $a = 10$, $L = 2$, $m = 1$ and $W = 2.274$.

When $E \to m$ (for a low-momentum particle), we find that $p^2 \to W^2 - 2mW = p_c$ so that $\mu \to \gamma_c$ and also $k \to 0 \Rightarrow \nu \to 0$. So (64) becomes

$$e^{4ip_cL} = \frac{B(-2\gamma_c, \gamma_c - \lambda)^2}{B(2\gamma_c, -\gamma_c + \lambda)^2}. \tag{65}$$

As expected, this is precisely the condition required for the potential barrier to be supercritical (54) once the 'flipping' procedure on the potential well as described above is considered. The components of the zero-momentum resonance/half-bound state wavefunction, $\psi(x)$, can be plotted and have the appearance shown in figure 4:

Comparison with the zero-momentum wavefunctions for the square and Gaussian barriers [5] highlights the existence of two turning points which occur in the top component of the wavefunction for the smooth Gaussian potential only. Once again these correspond to the points $\pm x_K$ where $V(\pm x_K) = E + m = 2m$ at zero momentum and are not manifest for the square barrier whose walls are discontinuous.

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