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Reflection and non-reflection of particle wavepackets

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Abstract

Exact closed-form solutions of the time-dependent Schrödinger equation are obtained, describing the propagation of wavepackets in the neighbourhood of a potential. Examples given include zero reflection, total reflection and partial reflection of the wavepacket, for the $\mathrm{sech}^2\frac{x}{a}$, $1/x^2$ and $\delta(x)$ potentials, respectively. In the first two of these cases the results are obtained using the methods of elementary supersymmetric quantum mechanics. This gives an introduction to supersymmetry in its simplest form, suitable for graduate or advanced undergraduate students. Animations of wavepacket propagation are provided.

1. Introduction

An exact free-particle wavepacket solution of Schrödinger's time-dependent equation dates back to the early days of quantum mechanics [1, 2]. This is the Gaussian wavepacket

$$\Phi_0(x,t) = \frac{b}{\sqrt{b^2 + \frac{\mathrm{i}\hbar t}{m}}} \exp\left\{\mathrm{i}k_0\left(x - x_0 - \frac{1}{2}v_0 t\right) - \frac{(x - x_0 - v_0 t)^2}{2(b^2 + \mathrm{i}\hbar t/m)}\right\}. \tag{1}$$

Here m is the mass of the particle, x_0 is the position of maximal $|\Phi_0|^2$ at $t = 0$, k_0 is the dominant wavenumber and v_0 is the group speed $\hbar k_0/m$. The length b gives the spread of the wavepacket at $t = 0$. At earlier and later times the width of the packet is greater, namely $[b^2 + (\hbar t/mb)^2]^{\frac{1}{2}}$. Thus $x = x_0$ can be thought of as the centre of the focal region of the wavepacket, occupied at $t = 0$. As t increases towards zero the wavepacket converges to its most compact form, reaches it at $t = 0$ and then expands as it continues to propagate in the positive x-direction. Figure 1 shows its propagation through the focal region.

There are few known analytic solutions for wavepackets propagating in the presence of a potential, although exact solutions abound at one energy (see for example [3], especially the appendix). The potential well

$$U_\nu(x) = -\frac{\hbar^2}{2ma^2}\frac{\nu(\nu+1)}{\cosh^2\left(\frac{x}{a}\right)} \tag{2}$$

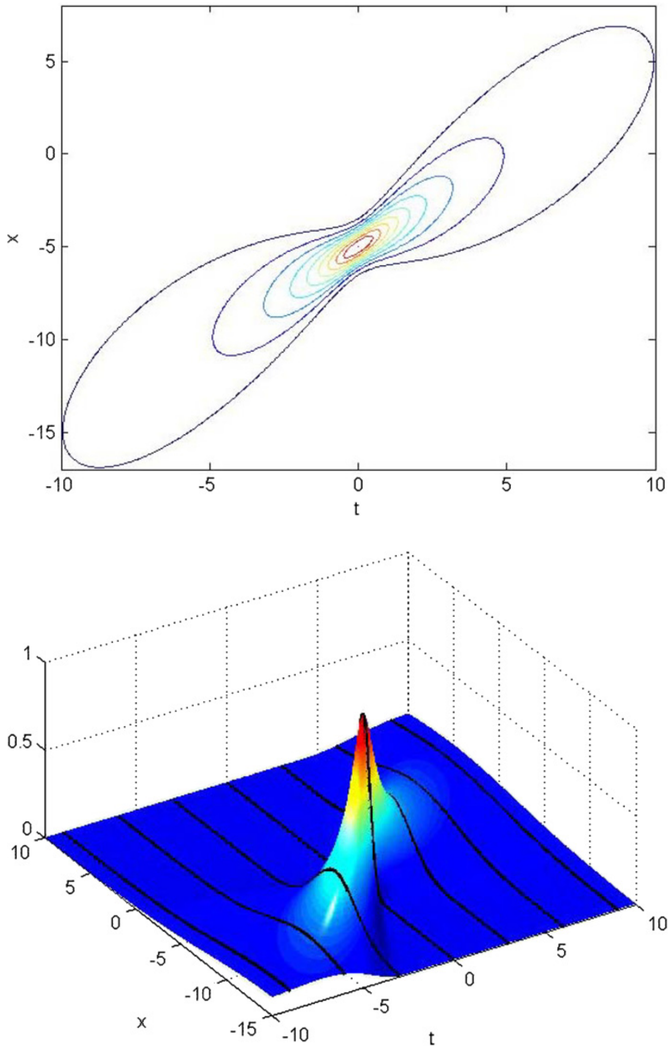

Figure 1. Motion of the free-particle Gaussian wavepacket $\Phi_0(x, t)$ through its focal region. The parameters used are $x_0 = -5b$, $k_0 b = 1$. The time varies from $t = -10b/v_0$ to $+10b/v_0$, where $v_0 = \hbar k_0/m$ is the group speed. The position varies from $x = -15b$ to $+10b$. The focal region is centred on $x_0 = -5b$ at $t = 0$. The plots show the probability density $|\Phi_0|^2$: the upper plot as contours, the lower plot as a surface. Snapshots of the probability density at times ranging from $-9b/v_0$ to $9b/v_0$ incrementing by $3b/v_0$ are shown as dark curves on the lower plot.

has the remarkable property that, for integer ν, it does not reflect, *at any energy*. For example, the $\nu = 1$ energy eigenstate (of eigenvalue $E_k = \hbar^2 k^2/2m$) propagating in the $+x$-direction can be written as [4–7]

$$\psi_1(k, x, t) = \left[1 + \frac{\mathrm{i}}{ka} \tanh \frac{x}{a}\right] \mathrm{e}^{\mathrm{i}kx - \mathrm{i}k^2\hbar t/2m}. \tag{3}$$

This has no reflected part, manifestly, and so *any* superposition of such eigenstates will not reflect either. One such superposition gives the wavepacket [5, 7]

$$\Phi_1(x, t) = \left[\frac{a(x - x_0 - \mathrm{i}k_0 b^2)}{b^2 + \mathrm{i}\hbar t/m} + \tanh \frac{x}{a}\right] \Phi_0(x, t) \tag{4}$$

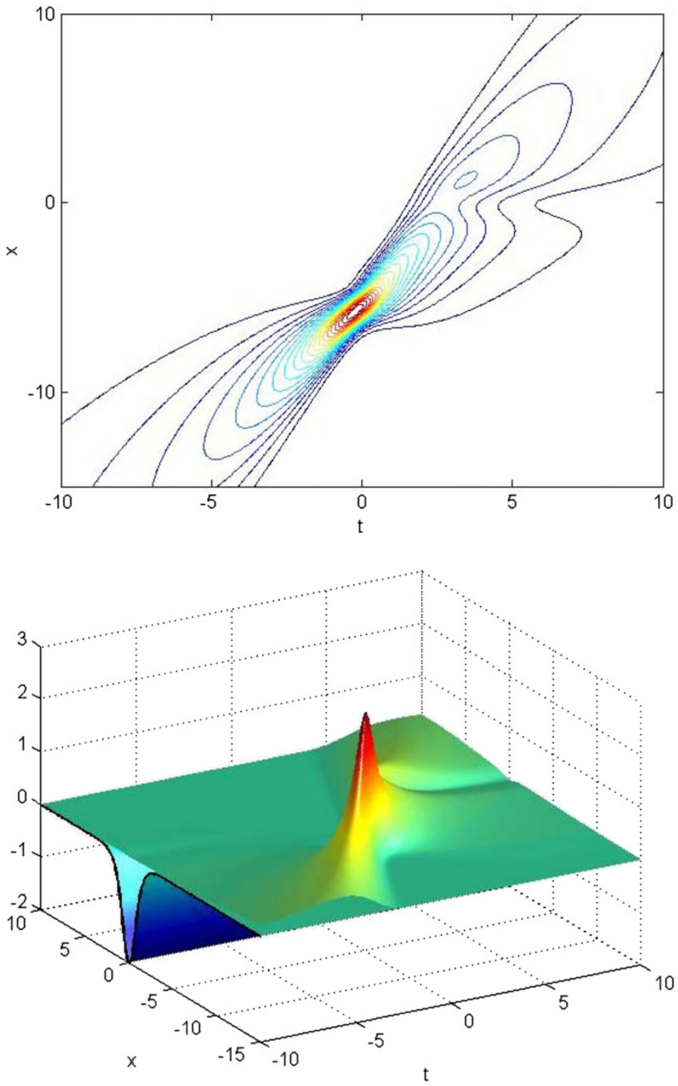

Figure 2. Motion of the non-reflecting wavepacket $\Phi_1(x, t)$ through the potential region; $|\Phi_1|^2$ is plotted. The parameters are as in figure 1, and $a = b$. The potential $U_1(x)$ is also shown. Note the constriction in the probability as the packet passes over the potential well, centred on $x = 0$.

where Φ_0 is the free-space Gaussian packet given in (1). Another, more complicated example of a non-reflecting wavepacket based on (3) is given in [7], where wavepacket properties such as group and phase speeds, width and local wavelength are discussed. Figure 2 shows how the non-reflecting wavepacket Φ_1 propagates through the potential well region.

In this paper we shall show how results such as (4) can be obtained in a much easier way, accessible to students. The methods we use are (mainly) based on the operational algebra of supersymmetric quantum mechanics [6, 8, 9], in its very simplest form. (What is now known as supersymmetry arose from the application of the Darboux transformation; see for example [5] and references therein.) The methods thus provide both a shortcut that avoids quite laborious calculus and an introduction to supersymmetry for students of quantum mechanics.

2. Application of supersymmetric algebra to sech^2 wavepackets

Supersymmetric quantum mechanics, in its simplest form, deals with relationships between the eigenstates of two related Hamiltonians [5, 6, 8, 9]:

$$H = \frac{-\hbar^2}{2m}\partial_x^2 + V(x), \qquad V(x) = W^2 - \frac{\hbar}{\sqrt{2m}}\partial_x W \tag{5}$$

$$\tilde{H} = \frac{-\hbar^2}{2m}\partial_x^2 + \tilde{V}(x), \qquad \tilde{V}(x) = W^2 + \frac{\hbar}{\sqrt{2m}}\partial_x W \tag{6}$$

where W is called the *superpotential*; an alternative name is *root potential*, since dimensionally W is the square root of a potential, and because it gives rise to the two potentials V and $\tilde{V}$. The two supersymmetric partner Hamiltonians may be written in terms of operators A and A^+:

$$A = \frac{\hbar}{\sqrt{2m}}\partial_x + W, \qquad A^+ = -\frac{\hbar}{\sqrt{2m}}\partial_x + W \tag{7}$$

$$H = A^+A, \qquad \tilde{H} = AA^+. \tag{8}$$

It is simple to verify that (5) and (6) are equivalent to (7) and (8). Also, if an energy eigenstate of $\tilde{H}$ is $\tilde{\psi}$, with eigenvalue $\tilde{E}$, $\tilde{H}\tilde{\psi} = \tilde{E}\tilde{\psi}$, operating with A^+ from the left gives $A^+A(A^+\tilde{\psi}) = \tilde{E}(A^+\tilde{\psi})$. Thus operating with A^+ on an eigenstate of $\tilde{H}$ gives an eigenstate of $H = A^+A$, with the eigenvalue $\tilde{E}$.

To illustrate the uses of these relations, we shall derive the exact energy eigenstate and wavepacket associated with the $\nu = 1$ potential (2), namely the results given in equations (3) and (4). Consider the root potential

$$W_\nu(x) = \frac{\hbar}{\sqrt{2m}}\frac{\nu}{a}\tanh\frac{x}{a}. \tag{9}$$

Then (5) and (6) give potentials related to (2):

$$V_\nu(x) = \frac{\hbar^2}{2ma^2}\left\{\nu^2 - \nu(\nu+1)\,\mathrm{sech}^2\frac{x}{a}\right\} \tag{10}$$

$$\tilde{V}_\nu(x) = \frac{\hbar^2}{2ma^2}\left\{\nu^2 - \nu(\nu-1)\,\mathrm{sech}^2\frac{x}{a}\right\}. \tag{11}$$

Since for $\nu = 1$ $\tilde{V}_1$ is the constant potential $\hbar^2/2ma^2$, $\tilde{H}_1$ has scattering eigenstates $\mathrm{e}^{\pm\mathrm{i}kx}$, with eigenvalue $\frac{\hbar^2}{2m}\left(k^2 + \frac{1}{a^2}\right)$, for any real k. Taking $\tilde{\psi} = \mathrm{e}^{\mathrm{i}kx}$, we obtain an eigenstate of H_1:

$$A_1^+\,\mathrm{e}^{\mathrm{i}kx} = \frac{\hbar}{\sqrt{2m}}\left(-\partial_x + \frac{1}{a}\tanh\frac{x}{a}\right)\mathrm{e}^{\mathrm{i}kx}. \tag{12}$$

This is proportional to the $t = 0$ value of ψ_1 given in (3). To get full correspondence with ψ_1 we subtract the constant term $\hbar^2/2ma^2$ from the $\nu = 1$ potentials in (10) and (11), so the energy eigenvalue $\tilde{E}$ becomes $\hbar^2k^2/2m$. The time dependence in (3) is then obtained from the fact that the solution of $H\psi = \mathrm{i}\hbar\partial_t\psi$ is formally $\psi(x,t) = \mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi(x,0)$, which becomes $\psi(x,t) = \mathrm{e}^{-\mathrm{i}Et/\hbar}\psi(x,0)$ for energy eigenstates.

It is obvious that a constant potential (here $\tilde{V}$ for $\nu = 1$) does not reflect; correspondingly the derived scattering eigenstate (3) of V has no reflected part. This is in accord with the general result that the reflection amplitudes of the partner potentials V and $\tilde{V}$ are proportional to each other ([9], p 21), so if one is zero the other one will also be zero.

To derive the $\nu = 1$ wavepacket given in (4), we consider the Fourier expansion of the free-space Gaussian packet:

$$\Phi_0(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}kx - \mathrm{i}k^2\hbar t/2m} F_0(k). \tag{13}$$

The explicit form of the Fourier amplitude $F_0(k)$ is used in [7] to obtain $\Phi_1(x,t)$, but it is not needed here. Consider

$$\begin{aligned} \frac{a\sqrt{2m}}{\hbar} A_1^+ \Phi_0(x,t) &= \left(-a\partial_x + \tanh\frac{x}{a}\right) \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}kx - \mathrm{i}k^2\hbar t/2m} F_0(k) \\ &= \int_{-\infty}^{\infty} \mathrm{d}k\, \mathrm{e}^{-\mathrm{i}k^2\hbar t/2m} F_0(k) \left(-a\partial_x + \tanh\frac{x}{a}\right) \mathrm{e}^{\mathrm{i}kx} \\ &= \int_{-\infty}^{\infty} \mathrm{d}k\, F_0(k)(-\mathrm{i}ka)\psi_1(k,x,t). \end{aligned} \tag{14}$$

This wavepacket is a superposition of exact non-reflecting energy eigenstates, and thus solves the time-dependent Schrödinger equation. Carrying out the differentiation implicit in $A_1^+\Phi_0(x,t)$ gives us (4).

Since the potentials $V_\nu(x)$ and $\tilde{V}_{\nu+1}(x)$ differ by a constant, the corresponding Hamiltonians share the same energy eigenstates. For example ψ_1, given in (3), is an eigenstate of $\tilde{H}_2$, $\psi_1 = \tilde{\psi}_2$. We have also seen that $A_\nu^+\tilde{\psi}_\nu$ is an eigenstate of H_ν. Thus,

$$A_2^+\tilde{\psi}_2 = A_2^+\psi_1 = \frac{\hbar}{\sqrt{2m}}\left(-\partial_x + \frac{2}{a}\tanh\frac{x}{a}\right)\psi_1 \tag{15}$$

is an eigenstate of H_2. Carrying out the differentiation gives us, up to a constant factor,

$$\psi_2 = \left[1 + (ka)^2 - 3\tanh^2\frac{x}{a} + 3\mathrm{i}ka\tanh\frac{x}{a}\right]\mathrm{e}^{\mathrm{i}kx}. \tag{16}$$

This wavefunction was obtained in [7], by using identities for hypergeometric functions. The present route gives the result by a simple differentiation. Likewise $A_3^+\tilde{\psi}_3 = A_3^+\psi_2$ is an eigenstate of H_3 and so on.

The corresponding wavepackets follow: for example

$$\Phi_2(x,t) = A_2^+\Phi_1(x,t) \sim \left(-a\partial_x + 2\tanh\frac{x}{a}\right)\Phi_1(x,t) \tag{17}$$

is, by steps analogous to those in (14), a superposition of exact non-reflecting energy eigenstates $\psi_2(k,x,t)$, and is thus a non-reflecting wavepacket which exactly solves Schrödinger's equation for the U_2 potential.

3. Examples of the total reflection of wavepackets

We have seen that the choice (9) for the root potential gave partner potentials which both have a $\mathrm{sech}^2\frac{x}{a}$ shape. Can we choose $W(x)$ so that one potential (say $\tilde{V}$) is constant? Equation (6) then gives us the Riccati equation for $W(x)$:

$$\frac{\hbar}{\sqrt{2m}}\partial_x W + W^2 = \bar{W}^2. \tag{18}$$

This has the solution

$$W(x) = \bar{W}\coth\left[\frac{\sqrt{2m}}{\hbar}\bar{W}(x - \bar{x})\right]. \tag{19}$$

The partner potential to $\tilde{V} = \bar{W}^2$ is singular at $x = \bar{x}$:

$$V(x) = \bar{W}^2 \frac{\cosh^2 \frac{\sqrt{2m}}{\hbar} \bar{W}(x - \bar{x}) + 1}{\cosh^2 \frac{\sqrt{2m}}{\hbar} \bar{W}(x - \bar{x}) - 1}. \tag{20}$$

We shall examine the simplest case, $\bar{x} = 0$ and $\bar{W} \to 0$:

$$W_0(x) = \frac{\hbar}{\sqrt{2m}} \frac{1}{x}, \qquad V_0(x) = \frac{\hbar^2}{mx^2}, \qquad \tilde{V}_0 = 0. \tag{21}$$

The potential V_0 forms an impenetrable barrier centred on the origin. We shall consider wavepackets that come up to this barrier from $x = -\infty$ and are reflected, with zero probability amplitude at the $x = 0$ singularity. We thus build on the stationary wave $\tilde{\psi}_0 = \mathrm{e}^{\mathrm{i}kx} - \mathrm{e}^{-\mathrm{i}kx}$, which leads to the wavepacket

$$\tilde{\Phi}_0(x, t) = \Phi_0(x, t) - \Phi_0(-x, t) \tag{22}$$

for the free-particle case. Now we operate with A^+ on $\tilde{\psi}_0$, obtaining energy eigenstates of $H = -\frac{\hbar^2}{2m}\partial_x^2 + V_0(x)$. As before, the superposition of these eigenstates gives us a wavepacket solution of Schrödinger's equation. Omitting the factor $\hbar/\sqrt{2m}$, this is

$$\begin{aligned} \Phi(x, t) &= \left(-\partial_x + \frac{1}{x}\right)[\Phi_0(x, t) - \Phi_0(-x, t)] \\ &= \left[\frac{1}{x} + \frac{x - x_0 - \mathrm{i}k_0 b^2}{b^2 + \mathrm{i}\hbar t/m}\right]\Phi_0(x, t) - \left[\frac{1}{x} + \frac{x + x_0 + \mathrm{i}k_0 b^2}{b^2 + \mathrm{i}\hbar t/m}\right]\Phi_0(-x, t). \end{aligned} \tag{23}$$

There is no singularity at $x = 0$; in fact the leading term is $O(x^2)$. Figure 3 shows the propagation and total reflection of this wavepacket.

The term proportional to $\Phi_0(x, t)$ in (23) has maximum probability at $x \approx x_0 + v_0 t$ and will be dominant at negative times, while the term proportional to $\Phi_0(-x, t)$ has maximum probability at $-x \approx x_0 + v_0 t$ and will be dominant at positive times (assuming that $|x_0|$ is small).

4. Reflection and transmission by the delta function potential

We characterize the delta function potential by the reciprocal length κ (the magnitude of κ gives the strength, and the sign determines whether the potential is repulsive or attractive):

$$V(x) = \frac{\hbar^2 \kappa}{m}\delta(x). \tag{24}$$

The delta function causes a discontinuity in the gradient of ψ at $x = 0$: setting $E = \hbar^2 k^2/2m$ the time-independent Schrödinger equation becomes

$$\left(-\partial_x^2 + 2\kappa\delta(x)\right)\psi = k^2\psi. \tag{25}$$

Integration across the origin from $-\varepsilon$ to $+\varepsilon$ and letting $\varepsilon \to 0$ gives

$$\psi'(0-) - \psi'(0+) + 2\kappa\psi(0) = 0. \tag{26}$$

Let ρ and τ be the reflection and transmission amplitudes, so that

$$\psi(k, x) = \begin{cases} \mathrm{e}^{\mathrm{i}kx} + \rho\,\mathrm{e}^{-\mathrm{i}kx} & (x < 0) \\ \tau\,\mathrm{e}^{\mathrm{i}kx} & (x > 0). \end{cases} \tag{27}$$

Continuity of ψ at $x = 0$ implies $1 + \rho = \tau$, and the discontinuity in the derivative at $x = 0$ (equation (26)) gives $\mathrm{i}k(1 - \rho) - \mathrm{i}k\tau + 2\kappa\tau = 0$, so that (compare [10], equation (2.119))

$$\rho = \frac{-\mathrm{i}\kappa}{k + \mathrm{i}\kappa}, \qquad \tau = \frac{k}{k + \mathrm{i}\kappa}. \tag{28}$$

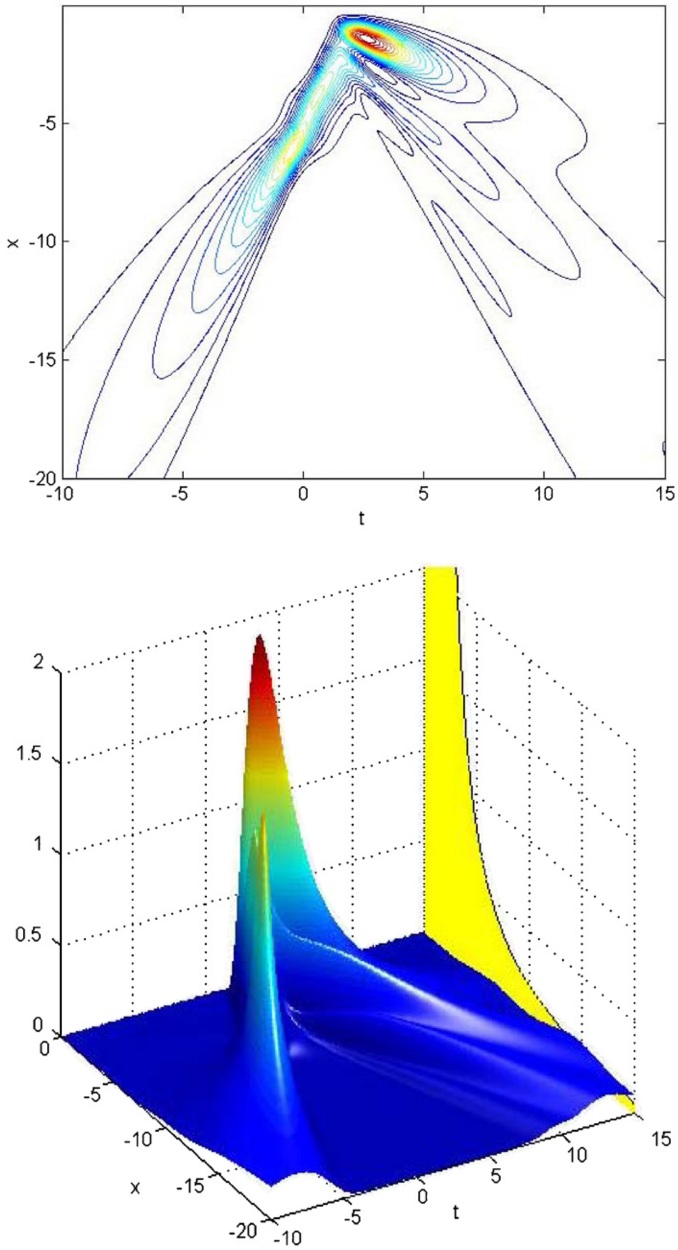

Figure 3. Total reflection of the wavepacket given in (23) by the potential $\hbar/mx^2$; the parameters are as in figure 1. Note the large probability $|\Phi|^2$ near $x = 0$ at $t \approx 2.5b/v_0$, and the interference fringes in the reflected part. The potential is shown on the right in the lower plot.

To construct a wavepacket we shall superpose the energy eigenstates (27). Note that the supersymmetric formalism connects the attractive and repulsive delta function potentials, with just a sign change in κ: setting $\nu = \kappa a$ in (10) and (11) and letting $\kappa a \to 0$ gives us the supersymmetric pairs

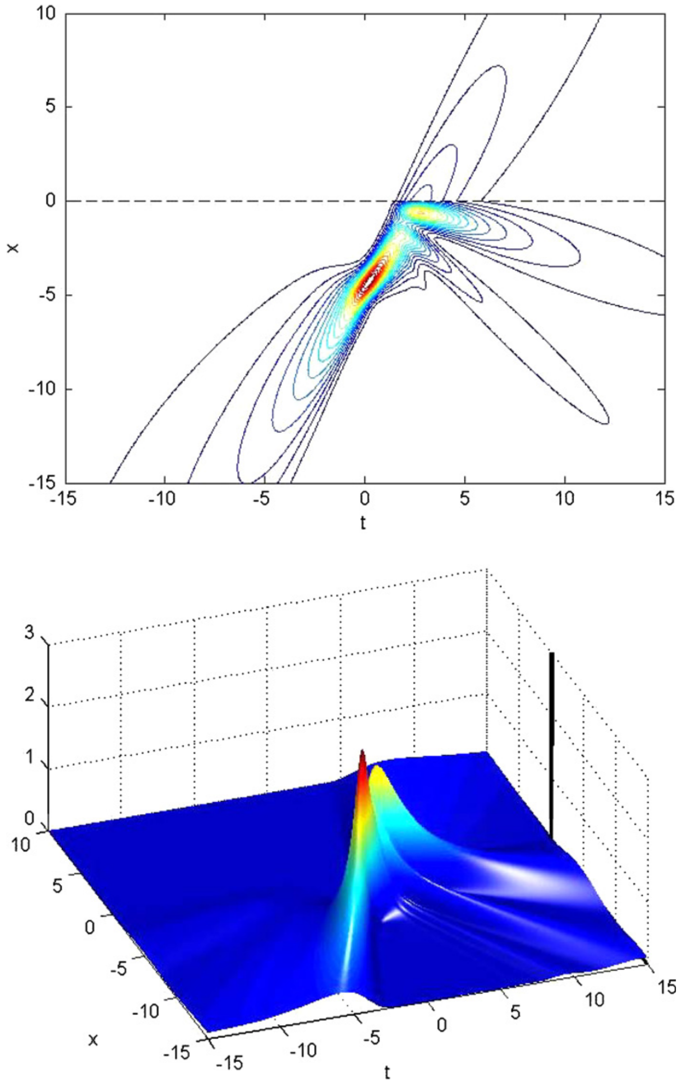

Figure 4. Partial reflection of a wavepacket by the delta function repulsive potential. The parameters are $x_0 = -5b$, $k_0b = 1$ and $\kappa b = 1$. Note the interference fringes in $|\Phi|^2$ after reflection. The potential (at zero x) is indicated by the dashed line in the upper plot, and by a spike in the lower plot.

$$V \to -\frac{\hbar^2\kappa}{m}\delta(x), \qquad \tilde{V} \to +\frac{\hbar^2\kappa}{m}\delta(x). \tag{29}$$

In superposing the energy eigenstates we can obtain simple results if (as suggested by the form of (28)) we use the Fourier amplitude

$$F(k) = (k + \mathrm{i}\kappa)F_0(k), \qquad F_0(k) = b\,\mathrm{e}^{-\mathrm{i}kx_0 - \frac{1}{2}(k-k_0)^2b^2}. \tag{30}$$

Then we have (with Φ_0 the free-space Gaussian, as before)

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}k\,\mathrm{e}^{\mathrm{i}kx - \mathrm{i}k^2\hbar t/2m}F_0(k) = \Phi_0(x,t) \tag{31}$$

and, by differentiation of (31) with respect to x,

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}k\ \mathrm{e}^{\mathrm{i}kx-\mathrm{i}k^2\hbar t/2m}\ \mathrm{i}kF_0(k) = \partial_x\Phi_0 = -\frac{x-x_0-\mathrm{i}k_0b^2}{b^2+\mathrm{i}\hbar t/m}\Phi_0. \tag{32}$$

Thus the superposition of $\psi(k,x)$ given by (27), with Fourier amplitude $(k+\mathrm{i}\kappa)F_0(k)$, gives the wavepackets (we remove a factor i)

$$\Phi(x,t) = \begin{cases} (-\partial_x+\kappa)\Phi_0(x,t) - \kappa\Phi_0(-x,t) & x<0 \\ -\partial_x\Phi_0(x,t) & x>0. \end{cases} \tag{33}$$

Note that one part of the wavepacket, namely $-\partial_x\Phi_0(x,t)$, is the same on the left and the right of the delta function potential. This part propagates straight through the potential. The other parts on the left, proportional to the potential strength κ, are the incident packet $\Phi_0(x,t)$ and the reflected packet $\Phi_0(-x,t)$. The three parts on the left overlap when near $x=0$, producing interference fringes, whereas the single transmitted part remains smooth on the right. Figure 4 illustrates the process.

5. Discussion

We have seen that the simplest version of supersymmetric algebra can reproduce the recently obtained results for wavepacket propagation in the presence of the non-reflecting potential well (2) (for integer ν). The same approach works for total reflection, again producing exact wavepacket solutions of the time-dependent Schrödinger equation in the presence of the repulsive $1/x^2$ potential. Finally, an exact solution was given for wavepacket reflection and transmission by a delta function potential, repulsive or attractive. In all cases the wavepackets are constructed from the free-space Gaussian wavepacket, by differentiation and simple algebraic manipulation. These analytic results complement numerical studies (see for example [11] and references therein), and at the same time show the workings of supersymmetric quantum mechanics at the most elementary level.

Animations of propagation of the wavepackets discussed here can be viewed at http://www.victoria.ac.nz/scps/staff/johnlekner/animations.aspx.

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