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Explicit solutions of the time-dependent Schrödinger equation

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Abstract. The Darboux transformation is used to generate explicit solutions of the time-dependent Schrödinger equation in one dimension. The potentials are a reflectionless potential and certain asymmetric double well potentials.

1. Introduction

If explicit solutions of a second-order ordinary differential equation are known, then the Darboux transformation generates explicit solutions of a related differential equation (Deift and Trubowitz 1979, Lamb 1980). When applied to the time-independent Schrödinger equation, this method gives a new equation with a different potential function. The purpose of this paper is to apply the procedure to the time-dependent Schrödinger equation in one dimension. A number of new explicit solutions are thereby obtained, given by closed formulae which do not require knowledge of the eigenfunctions.

In § 2 the application of the Darboux transformation to the time-independent Schrödinger equation is summarised, and then extended to give general results for the time-dependent equation. Section 3 discusses the case where the known (soluble) problem is the free particle in one dimension and the transformed problem has potential $-2\beta^2 \operatorname{sech}^2 \beta x$. This is a reflectionless potential. The s wave of the three-dimensional problem is also considered. The last section uses the one-dimensional harmonic oscillator as the known (soluble) problem. This leads to explicit time-dependent solutions for a particle moving, for example, in a double-well potential; the formulae contain the error function.

Time-dependent wavefunctions for motion in various potentials, which include $-2\beta^2 \operatorname{sech}^2 \beta x$, have been given by Gutschick and Nieto (1979). Their formulae are eigenfunction expansions, which are not easily computed, and represent wavepackets that oscillate within the potential well. The results in § 3 correspond to scattering states.

2. The Darboux method

Suppose $U(x)$ is a potential for which there are some known explicit solutions of the time-independent Schrödinger equation

$$H_0\psi = (-\mathrm{D}^2 + U)\psi = \lambda\psi \tag{2.1}$$

where $D = d/dx$. From some particular solution ϕ, with $\lambda = \mu$, define operators ($'$ denotes differentiation with respect to x)

$$B = D - (\phi'/\phi) \qquad C = -D - (\phi'/\phi) \tag{2.2}$$

$$H = H_0 - 2(\phi'/\phi)'. \tag{2.3}$$

Then

$$H_0 = CB + \mu \qquad H = BC + \mu \tag{2.4}$$

and

$$H_0\psi = \lambda\psi \Rightarrow H(B\psi) = \lambda(B\psi). \tag{2.5}$$

Thus from known eigenfunctions ψ with the potential U one obtains eigenfunctions $B\psi$ for the Schrödinger equation with potential $U - 2(\phi'/\phi)'$. A detailed discussion of the theory was given by Deift and Trubowitz (1979) and a useful summary of specific calculations was given by Sukumar (1985).

Since equation (2.5) relates any eigenfunctions of H to those of H_0, with the same eigenvalue, the transformation operator B can evidently be applied to a superposition of eigenfunctions. This means that the method also works for solutions of the time-dependent Schrödinger equation. For an arbitrary initial state $\chi(x)$, the solution of $H_0\psi = i(\partial\psi/\partial t)$ is $\exp(-iH_0t)\chi$. From (2.4)

$$BH_0 = HB \qquad B\exp(-iH_0t) = \exp(-iHt)B \tag{2.6}$$

and therefore

$$B[\exp(-iH_0t)\chi] = \exp(-iHt)(B\chi). \tag{2.7}$$

The work in this paper is based on this equation, which states that operating with B on the solution of $H_0\psi = i(\partial\psi/\partial t)$ emanating from χ gives the solution of $H\psi = i(\partial\psi/\partial t)$ emanating from $B\chi$.

From (2.2), C is the adjoint of B in this application. Then, using (2.4),

$$\langle B\chi, B\chi\rangle = \langle\chi, CB\chi\rangle = \langle\chi, (H_0 - \mu)\chi\rangle. \tag{2.8}$$

This allows the normalisation of χ to be chosen so that $B\chi$ is normalised. The same manipulation shows that the average energy is generally raised by the transformation. Using (2.4)

$$\langle H\rangle = \frac{\langle B\chi, HB\chi\rangle}{\langle B\chi, B\chi\rangle} = \frac{\langle\chi, (H_0 - \mu)H_0\chi\rangle}{\langle\chi, (H_0 - \mu)\chi\rangle}. \tag{2.9}$$

Then the Schwartz inequality $\langle H_0\chi, H_0\chi\rangle\langle\chi, \chi\rangle \geq \langle\chi, H_0\chi\rangle^2$ gives

$$\langle H\rangle \geq \frac{\langle\chi, H_0\chi\rangle}{\langle\chi, \chi\rangle} = \langle H_0\rangle \tag{2.10}$$

where the equality occurs only if χ is an eigenfunction of H_0.

Next consider the conditions on a given initial function $\psi(x, 0)$ in order for the resulting solution of $H\psi = i(\partial\psi/\partial t)$ to be obtained using (2.7). A normalisable χ satisfying $B\chi = \psi(x, 0)$ is required. This is not possible if $\psi(x, 0) = 1/\phi(x)$, because $C(1/\phi) = 0$, and the numbers in equation (2.8) would all be zero. The initial function must be orthogonal to $1/\phi$. Then define F by

$$F(x) = \int_{-\infty}^{x} dy\, \psi(y, 0)/\phi(y) \tag{2.11}$$

with $F(\infty)=0$ from the orthogonality assumption. It is easy to verify that

$$\chi(x)=\phi(x)F(x) \tag{2.12}$$

satisfies

$$B\chi=[\mathrm{D}-(\phi'/\phi)]\chi=\psi(x,0). \tag{2.13}$$

The above orthogonality condition is a trivial deficiency, because if μ is less than the ground-state eigenvalue of H_0, then μ is the ground-state eigenvalue of H, and $1/\phi$ is normalisable and is the ground-state eigenfunction. (This follows from (2.4) and $C(1/\phi)=0$.) This eigenfunction can be projected out of a given initial state and recombined after the time dependence has been obtained. Because $(1/\phi)$ is an eigenfunction, initial orthogonality to $\psi(x,0)$ persists for all t. Also $1/\phi$ is non-zero and located near the minimum of the new potential, so the real and imaginary parts of $\psi(x,t)$ must have zeros in the region to effect the orthogonality. When the zeros in the real and imaginary parts are near each other, $|\psi(x,t)|^2$ will have a minimum (as in figures 1 and 4).

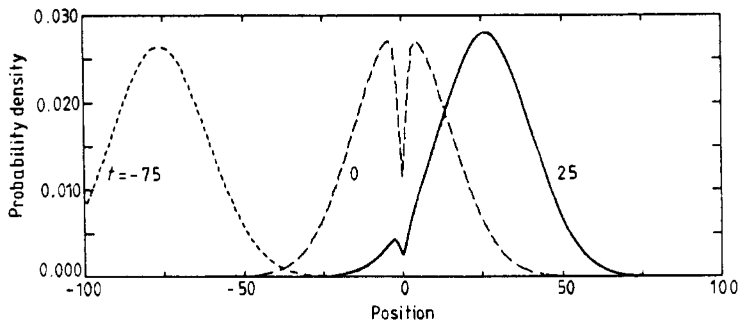

Figure 1. Wavepacket moving through a potential $V(x)=-0.72\,\mathrm{sech}^2(0.6x)$. The centre moves with speed 1.005.

Note that if ϕ is the ground-state eigenfunction of H_0, then $B\phi=0$, $1/\phi$ is not normalisable and μ is not an eigenvalue of H.

This section has assumed that $\phi(x)$ has no zero; otherwise the results can only be applied in restricted regions in which ϕ does not vanish (Lamb 1980, p 94).

3. Transformation of free-particle wavefunctions

Take

$$H_0=-\mathrm{D}^2 \qquad U(x)=0 \qquad \phi(x)=\cosh\beta x \qquad \mu=-\beta^2 \tag{3.1}$$

to obtain

$$B=\mathrm{D}-\beta\tanh\beta x \tag{3.2}$$

and

$$H=-\mathrm{D}^2-2\beta^2\,\mathrm{sech}^2\,\beta x. \tag{3.3}$$

The resulting derivation of the time-independent eigenfunctions of H is well known (Lamb 1980).

A textbook example of a solution of the time-dependent free particle equation is obtained from

$$\chi(x)=\exp(-\tfrac{1}{2}\alpha^2x^2+\mathrm{i}kx) \tag{3.4}$$

as

$$\exp(-\mathrm{i}H_0t)\chi(x)=\tau^{1/2}\exp(-\tfrac{1}{2}\alpha^2x^2\tau+\mathrm{i}k\tau x-\mathrm{i}t\tau k^2) \tag{3.5}$$

with

$$\tau=(1+2\mathrm{i}\alpha^2t)^{-1}. \tag{3.6}$$

Applying the operator B to the function in (3.5) gives

$$\psi(x,t)=\tau^{1/2}(-\alpha^2x\tau+\mathrm{i}k\tau-\beta\tanh\beta x)\exp(-\tfrac{1}{2}\alpha^2x^2\tau+\mathrm{i}k\tau x-\mathrm{i}t\tau k^2) \tag{3.7}$$

as a solution of

$$\mathrm{i}\partial\psi/\partial t=H\psi=(-\mathrm{D}^2-2\beta^2\operatorname{sech}^2\beta x)\psi \tag{3.8}$$

emanating from the initial state

$$\psi(x,0)=B\chi=(-\alpha^2x+\mathrm{i}k-\beta\tanh\beta x)\exp(-\tfrac{1}{2}\alpha^2x^2+\mathrm{i}kx). \tag{3.9}$$

To obtain normalised solutions, (3.4) is multiplied by the familiar factor $(\alpha/\sqrt{\pi})^{1/2}$; also (3.4) and (2.8) give

$$\langle B\chi,B\chi\rangle=\langle\chi,(-\mathrm{D}^2+\beta^2)\chi\rangle=(\sqrt{\pi}/\alpha)(k^2+\tfrac{1}{2}\alpha^2+\beta^2).$$

Thus a normalised solution of (3.8) is obtained by multiplying (3.7) by $[\alpha/(k^2+\frac{1}{2}\alpha^2+\beta^2)\sqrt{\pi}]^{1/2}$. Using integration by parts this may also be verified directly.

The position probability resulting from (3.7) is

$$|\psi(x,t)|^2=|\tau|^3[(\alpha^2x+\beta\tanh\beta x)^2+(k-2\alpha^2\beta t\tanh\beta x)^2]\exp\{-\alpha^2|\tau|^2(x-2kt)^2\} \tag{3.10}$$

$$=|\psi(-x,-t)|^2. \tag{3.11}$$

Figure 1 shows (3.10) (after normalisation) with $\alpha=0.05$, $\beta=0.6$, $k=0.5$, and $t=-75$, 0, 25. The minimum near $x=0$ is due to orthogonality to the ground state, as discussed at the end of the previous section. Note that (3.11) immediately gives (3.10) also at $t=-25$ and $t=75$.

The Gaussian part of (3.10) ensures that $|\psi|^2$ is negligible outside some region centred on $x=2kt$, as in figure 1. Then for sufficiently large $|t|$, $\tanh\beta x$ can be replaced by ±1, the sign being that of t. This permits analytic evaluation of expectation values:

$$v=\langle-2\mathrm{i}\partial/\partial x\rangle=2k[1+\alpha^2/(\beta^2+\tfrac{1}{2}\alpha^2+k^2)] \tag{3.12}$$

$$\langle x\rangle=vt\pm\beta/(\beta^2+\tfrac{1}{2}\alpha^2+k^2). \tag{3.13}$$

These equations hold provided $\psi(x,t)$ is negligible near $x=0$, for example if $|t|>50$ for the case considered in figure 1.

The energy expectation values, given by (2.9), are

$$\langle\chi,H_0\chi\rangle=k^2+\tfrac{1}{2}\alpha^2$$

$$\langle\psi,H\psi\rangle=\langle\chi,H_0\chi\rangle+\tfrac{1}{2}\alpha^2(\alpha^2+4k^2)(\beta^2+\tfrac{1}{2}\alpha^2+k^2)^{-1}.$$

Another initial state (Glasser 1980) for which the free-particle problem is soluble is $\chi(x)=\exp(\mathrm{i}kx)\operatorname{sech}\alpha x$. Then

$$\psi(x,0)=B\chi=(\mathrm{i}k-\alpha\tanh\alpha x-\beta\tanh\beta x)\operatorname{sech}\alpha x. \tag{3.14}$$

The free-particle solution was given as a series, which can be summed explicitly for certain values of t. Applying B to such closed form expressions gives, for example,

$$\psi(x, t=\pi/4\alpha^2) = [(ik-\alpha\tanh y - \beta\tanh\beta x)\exp(i\pi/4 + ikx - ik^2\pi/4\alpha^2) - i(2i\alpha^2 x/\pi - \alpha\tanh y - \beta\tanh\beta x)\exp(i\alpha^2x^2/\pi)]\operatorname{sech} y \qquad (3.15)$$

where $y = \alpha x - k\pi/2\alpha$. Again $|\psi(-x,-t)|^2 = |\psi(x,t)|^2$; computer plots of $|\psi|^2$ using (3.14) and (3.15) give pictures like those in figure 1.

For a given $\psi(x,0)$, the required procedure is to project out the bound-state component ($1/\phi = \operatorname{sech}\beta x$) and then evaluate

$$\chi(x) = \phi(x)\int_{-\infty}^{x}\psi(y,0)\cosh\beta y\,dy$$

as given by (2.11) and (2.12). If $\chi(x)$ can be thus obtained explicitly, and also $\exp(-iH_0t)\chi(x)$ in closed form, then $\psi(x,t)$ can be given in closed form. Otherwise this method has no advantage over the direct use of the propagator (Crandall 1983a).

The s wave of a three-dimensional system is equivalent to the one-dimensional system restricted to odd parity states. Since H commutes with parity, an odd initial state gives an odd state at any other time, so any odd solution of the one-dimensional problem gives an s-wave solution for the central potential $V(r) = -2\beta^2\operatorname{sech}^2\beta r$. In analogy with (3.4), take $\chi(r) = -\exp(-\frac{1}{2}\alpha^2r^2)\cos kr$ to obtain

$$u(r,0) = [(\alpha^2 r + \beta\tanh\beta r)\cos kr + k\sin kr]\exp(-\tfrac{1}{2}\alpha^2r^2)$$

and

$$u(r,t) = \tau^{1/2}[(\alpha^2 r\tau + \beta\tanh\beta r)\cos(kr\tau) + k\tau\sin(kr\tau)]\exp(-\tfrac{1}{2}\alpha^2r^2\tau - it\tau k^2) \qquad (3.16)$$

with $\tau = (1+2i\alpha^2 t)^{-1}$. Figure 2 shows $|u(r,t)|^2$ from (3.16) with $k=0.5$, $\alpha=0.05$, $\beta=0.6$, $t=-40$, 0, 60. Note that in order for $u(r,t)$ to be an odd function (zero at $r=0$) one must choose an (unphysical) even function for $\chi(r)$.

4. Transformation of oscillator wavefunctions

Let

$$f(x) = \gamma + \tfrac{1}{2}(\pi/\beta)^{1/2}\operatorname{erf}(x\sqrt{\beta}) \qquad (4.1)$$

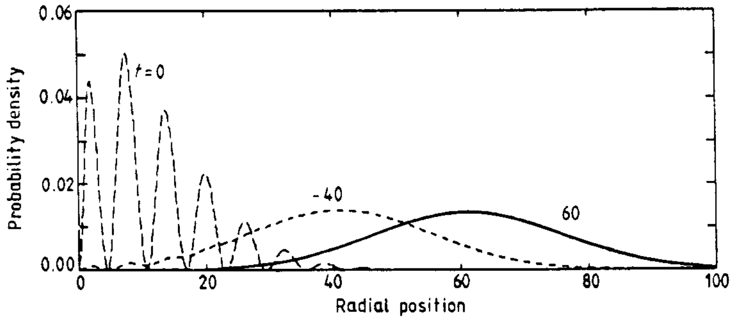

Figure 2. Spherically symmetric s wave interacting with a central potential $V(r) = -0.72\operatorname{sech}^2(0.6r)$. At $t=-40$ the wave is moving inwards (to the left); at $t=60$ it moves outwards.

where $\gamma^2 > \pi/4\beta$. Taking

$$H_0 = -\mathrm{D}^2 + \beta^2 x^2 + 2\beta \qquad \phi(x) = f(x)\exp(\tfrac{1}{2}\beta x^2) \qquad \mu = \beta \tag{4.2}$$

gives

$$B = \mathrm{D} + A(x) = \mathrm{D} - \beta x - \exp(-\beta x^2)/f(x). \tag{4.3}$$

The new potential $-\beta^2 x^2 + 2A^2(x)$ is shown in figure 3 for $\beta = 0.97$ and $\gamma = 0.9$. Other examples (with $\beta = 1$, $\alpha = 1/\gamma$) are shown in figure 3 of Sukumar (1985).

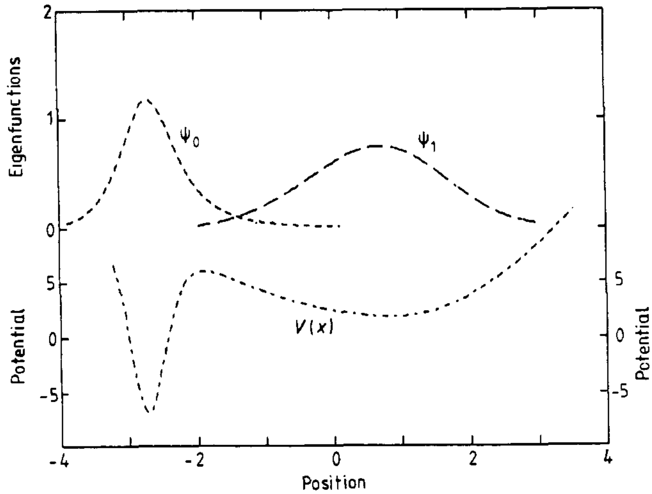

Figure 3. An asymmetric double well potential and its lowest two normalised eigenfunctions; the eigenvalues are 0.97 and 2.91.

These potentials were first considered by Mielnik (1984), who showed that the spectrum coincided with that of the harmonic oscillator, the eigenvalues being $\beta, 3\beta, 5\beta, \ldots$. The method was essentially that of the Darboux transformation, although not called such as it was obtained by considering factorisations of H_0 and H. Mielnik did not normalise the eigenfunctions, but the required constants can be found using the method given by Zheng (1983), or by direct integration after noting that $A(x)$ in (4.3) has the form $A(x) = -\beta x - f'(x)/f(x)$. The first two normalised eigenfunctions

$$\psi_0(x) = (\gamma^2 - \pi/4\beta)^{1/2}(\beta/\pi)^{1/4}\exp(-\tfrac{1}{2}\beta x^2)/f(x) \tag{4.4}$$

$$\psi_1(x) = (4\beta\pi)^{-1/4}(\beta x - A(x))\exp(-\tfrac{1}{2}\beta x^2) \tag{4.5}$$

are also shown in figure 3. The function ψ_1 is actually negative in the region of the potential minimum, as required to obtain orthogonality to ψ_0.

A textbook example (Schrödinger, 1926) of a solution of the time-dependent harmonic oscillator equation $H_0\phi = \mathrm{i}\partial\phi/t$ is obtained from

$$\chi(x) = \exp[-\tfrac{1}{2}\beta(x-c)^2] \tag{4.6}$$

as

$$\Phi(x,t) = \exp[-\tfrac{1}{2}\beta x^2 + \beta c x \exp(-2\mathrm{i}\beta t) - \tfrac{1}{4}\beta c^2 \exp(-4\mathrm{i}\beta t) - \tfrac{1}{4}\beta c^2 - 3\mathrm{i}\beta t]. \tag{4.7}$$

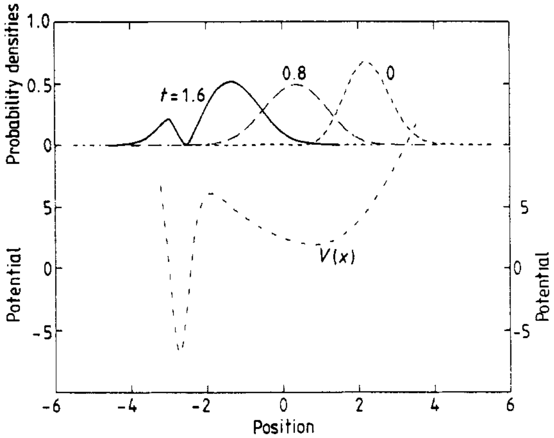

Figure 4. Oscillation of a wavepacket in a double well potential with period 3.24. The energy $\langle H\rangle = 4.016$ is below the potential maximum.

Applying the operator B of equation (4.3) gives

$$\psi(x, t) = [-\beta x + \beta c \exp(-2i\beta t) + A(x)]\Phi(x, t) \tag{4.8}$$

as a solution of $i\partial\psi/\partial t = H\psi = (-D^2 - \beta^2 x^2 + 2A^2)\psi.$ (4.9)

This solution has the same period π/β as $\Phi(x, t)$ and

$$|\psi|^2 = [-2A\beta x + \beta^2 x^2 + A^2 + \beta^2 c^2 + 2\beta c(A - \beta x)\cos 2\beta t] \exp[-\beta(x - c\cos 2\beta t)^2]. \tag{4.10}$$

From (4.6) and (2.8), the position probability is obtained by dividing (4.10) by

$$\langle B\chi, B\chi\rangle = \langle \chi, (-D^2 + \beta^2 x^2 + \beta)\chi\rangle = (2 + \beta c^2)(\beta\pi)^{1/2}.$$

The expectation value for the energy is evaluated from (2.9) as

$$\langle H\rangle = 3\beta + \beta^3 c^4/(2 + \beta c^2).$$

When $c = 0$, (4.8) is the stationary state (4.5). For small values of c, (4.8) and (4.10) represent what is essentially a wavepacket oscillating about the secondary minimum of the potential, although there is a small (negative) part overlapping ψ_0 to produce orthogonality. For larger c the wavepacket passes periodically into the region of the minimum; and at these times (4.10) has a distinctive minimum, as expected from the discussion in § 2. Figure 4 shows $|\psi|^2$ at quarter- and half-period times, taking $c = 1.5$; since $\langle H\rangle$ is less than the potential maximum, this is an illustration of tunnelling.

5. Conclusion

The Darboux transformation has been applied to the time-dependent Schrödinger equation, giving analytic solutions from which it is easy to obtain expectation values or position probabilities. The wavefunctions give explicit examples of the following results.

Firstly Crandall (1983b) has shown that a wavepacket incident on a reflectionless potential is transmitted without change of shape and with a time advance in comparison with free-particle motion. Equation (3.11) is an example of the preservation of shape and equation (3.13) shows the time advance.

Secondly Nieto *et al* (1985) have discussed tunnelling in double-well potentials from the secondary minimum to the actual minimum. Their $U=1$ potential has very similar properties to the potential shown in figure 3: the eigenvalues are equally spaced in integer steps and the first two eigenfunctions have little overlap. For small values of c, equation (4.10) represents a wavefunction that does not tunnel, looking very similar to the Gaussian packet in the $U=1$ potential. When tunnelling is obtained from (4.10) by increasing the energy, as in figure 4, the packet splits into two humps. This is similar to the evolution of a Gaussian packet in the $U=2$ potential of Nieto *et al* (their figure 5).

Note added in proof. In a recent paper by Gaveau and Schulman (1986) the propagator for the potential $-2\lambda^2 \operatorname{sech}^2 x$ is derived using the Darboux transformation.

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