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1983 J. Phys. A: Math. Gen. 16 43

(http://iopscience.iop.org/0305-4470/16/1/013)

J. Phys. A: Math. Gen. 16 (1983) 43–48. Printed in Great Britain

Associated harmonic oscillator potential models for Schrödinger equations

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Received 22 June 1982

Abstract. By means of the Darboux transformation the associated harmonic oscillator potential problem is solved analytically. For properly chosen parameters the potentials appear as asymmetric double wells. The penetration problem is discussed for inverted potentials.

In Zheng (1982) we discussed the Darboux transformation (Darboux 1882, Ince 1956) and its application to solving the symmetric double-well potential problem. Here we shall use the transformation to solve the asymmetric double-well potential problem, and then discuss the penetration problem for inverted potentials.

The one-dimensional Schrödinger equation to be discussed is

$$d^2\psi/dx^2+[E-V(x)]\psi=0 \tag{1}$$

with

$$V(x)=\phi(x)\, d^2[1/\phi(x)]/dx^2, \tag{2}$$

where $\phi(x)$ is a solution of the Weber equation (Abramovitz and Stegun 1965)

$$d^2\phi/dx^2-(x^2/4+a)\phi=0. \tag{3}$$

In general, the function $\phi(x)$ can be written as a linear combination of the odd and even solutions to the Weber equation:

$$\phi(x)=y_1(a,x)+\beta y_2(a,x) \tag{4a}$$

$$=\exp(-\tfrac{1}{4}x^2)\,{}_1F_1(\tfrac{1}{2}a+\tfrac{1}{4},\tfrac{1}{2},\tfrac{1}{2}x^2)+\beta x\exp(-\tfrac{1}{4}x^2)\,{}_1F_1(\tfrac{1}{2}a+\tfrac{3}{4},\tfrac{3}{2},\tfrac{1}{2}x^2). \tag{4b}$$

The shape of the potential $V(x)$ for $\beta=0$ has been briefly discussed by Zheng (1982): $V(x)$ is

a single well	for $a\geqslant\frac{1}{2}$,
a double well	for $0\leqslant a<1/2\sqrt{2}$,
a multiple well	for $0>a>-1/2\sqrt{2}$.

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‡ Supported by the Robert A Welch Foundation.

For $0<a<1/2\sqrt{2}$ and $\beta \ll \beta_c=\sqrt{2}\,\Gamma(\frac{1}{2}a+\frac{3}{4})/\Gamma(\frac{1}{2}a+\frac{1}{4})$, $V(x)$ is an asymmetric double well. The typical curves of $V(x)$ for $a=-0.3$ and $\beta=-0.08$, 0, 0.04 are shown in figure 1.

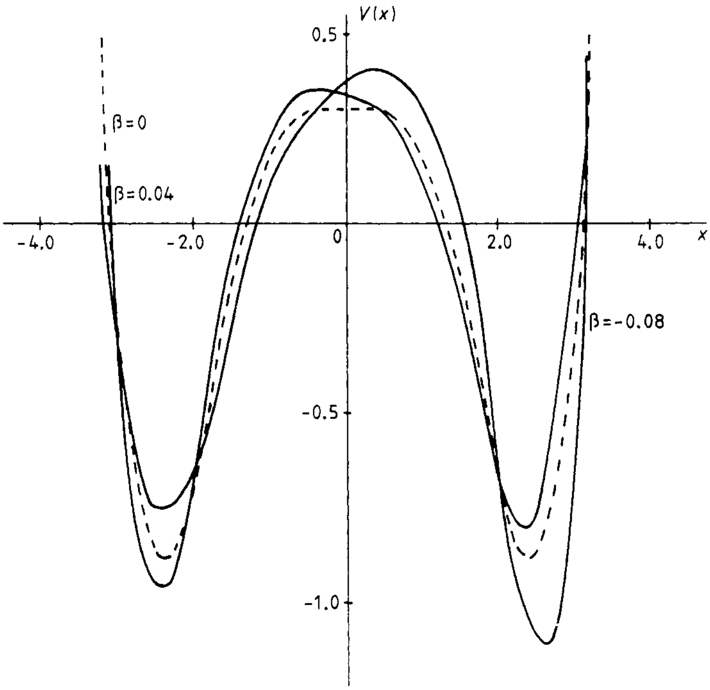

Figure 1.

From the Darboux theorem (Darboux 1882, Ince 1956), the physical solution to equation (1) for the eigenvalue $E_n=n+a+\frac{1}{2}$ is

$$\psi_n(x)=\phi(x)[D_n(x)/\phi(x)]' \tag{5a}$$

$$=D_n'(x)-(\phi'(x)/\phi(x))D_n(x), \tag{5b}$$

where we have used the boundary conditions at infinity, and the Weber function $D_n(x)$ with n an integer parameter is related to the Hermite polynomial $H_n(x)$ (Abramovitz and Stegun 1965)

$$D_n(x)=2^{-n/2}\exp(-\tfrac{1}{4}x^2)H_n(x/\sqrt{2}). \tag{6}$$

It is easy to verify that the function $[\phi(x)]^{-1}$ is a solution to equation (1) with the eigenvalue $E=0$. As long as a is not less than $-\frac{1}{2}$ and $\beta<\beta_c$, the function $[\phi(x)]^{-1}$ is positive definite without any node, so it is the ground state. We have thus found all the eigenvalues and eigenfunctions of equation (1).

The normalisation factors for the eigenfunction $\psi_n(x)$ can be calculated by using the two transformations discussed in Zheng (1982): Darboux's differential form and the integral one. The relation between the two transformations is (Zheng 1982)

$$\phi(x)\left(\frac{D_n(x)}{\phi(x)}\right)'=-\frac{E_n}{\phi(x)}\left(\int_0^x D_n(x)\phi(x)\,\mathrm{d}x-d_\beta\right) \tag{7}$$

with

$$d_\beta = \phi(0)\left(\frac{D_n(x)}{\phi(x)}\right)'\bigg|_{x=0} = D_n'(0) - \beta D_n(0). \tag{8}$$

Therefore,

$$\begin{aligned} C_n^2 &\equiv \int_{-\infty}^{+\infty} \psi_n^2(x)\,\mathrm{d}x \\ &= \int_{-\infty}^{+\infty} \phi(x)\left(\frac{D_n(x)}{\phi(x)}\right)'\left[-\frac{E_n}{\phi(x)}\left(\int_0^x D_n(x)\phi(x)\,\mathrm{d}x - d_\beta\right)\right] \\ &= E_n\left[-\frac{D_n(x)}{\phi(x)}\left(\int_0^x D_n(x)\phi(x)\,\mathrm{d}x - d_\beta\right)\bigg|_{-\infty}^{+\infty} + \int_{-\infty}^{+\infty} [D_n(x)]^2\,\mathrm{d}x\right] \\ &= \left[D_n(x)\phi(x)\left(\frac{D_n(x)}{\phi(x)}\right)'\right]\bigg|_{-\infty}^{+\infty} + E_n(2\pi)^{1/2} n!. \end{aligned} \tag{9}$$

In the last step of the above derivation we have used equation (7) once again and the formula (Gradshteyn and Ryzhik 1965)

$$\int_{-\infty}^{\infty} [D_n(x)]^2\,\mathrm{d}x = \sqrt{2\pi}\, n!. \tag{10}$$

According to Abramovitz and Stegun (1965), the function $\phi(x)$ can be written as a linear combination of the Weber functions $D_\nu(-x)$ and $D_\nu(x)$ with $\nu = -a - \frac{1}{2}$,

$$\phi(x) = \lambda_+ D_\nu(x) + \lambda_- D_\nu(-x), \tag{11}$$

where λ_+ and λ_- are some constants. By considering the asymptotic behaviour of $D_\nu(x)$ and $D_n(x)$ at infinity (Abramovitz and Stegun 1965), the first term on the RHS of equation (9) vanishes. Thus, we have finally

$$C_n^2 = (n + a + \tfrac{1}{2})\sqrt{2\pi}\, n!. \tag{12}$$

The normalisation factor for the ground state $[\phi(x)]^{-1}$ should be calculated separately. From the Darboux theorem we have an identity (Zheng 1982)

$$\frac{1}{\phi(x)} = \phi(x)\left(\frac{\lambda_1 y_1(a,x) + \lambda_2 y_2(a,x)}{\phi(x)}\right)', \tag{13}$$

where the constants λ_1 and λ_2 can be determined by taking $x \to \infty$ and $x = 0$ for equation (13) (Zheng and Hongler 1982). Finally, we find

$$1/\phi(x) = \phi(x)(y_2(a,x)/\phi(x))'$$

or

$$C_0^2 \equiv \int_{-\infty}^{+\infty} [\phi(x)]^{-2}\,\mathrm{d}x = \left(\frac{y_2(a,x)}{\phi(x)}\right)\bigg|_{-\infty}^{+\infty}. \tag{14}$$

Considering the asymptotic behaviour of the functions $y_1(a,x)$ and $y_2(a,x)$, from equation (14) we obtain finally

$$C_0^2 = 2\beta_c/(\beta_c^2 - \beta^2), \tag{15}$$

where

$$\beta_c = \sqrt{2}\,\Gamma(\tfrac{1}{2}a + \tfrac{3}{4})/\Gamma(\tfrac{1}{2}a + \tfrac{1}{4}) \tag{16}$$

is a quantity introduced for the discussion of the shapes of the potentials $V(x)$. As one can see from equation (15), only when $\beta < \beta_c$ is the expression (15) meaningful. In fact, when $\beta \to \beta_c$ the function $[\phi(x)]^{-1}$ touches the real axis, and then the integral (14) becomes divergent. For $\beta > \beta_c$ we obtain the same situation.

We shall next discuss the penetration problem for the inverted potentials. Instead of $V(x)$ as given in equation (2), we should consider

$$\tilde{V}(x) = V_{ia}(e^{i\pi/4}x) = \tilde{\phi}(x)\, d^2(1/\tilde{\phi}(x))/dx^2 \tag{17}$$

with

$$\tilde{\phi}(x) = y_1(ia, e^{i\pi/4}x) + \beta y_2(ia, e^{i\pi/4}x). \tag{18}$$

Employing the recurrence relations (Abramovitz and Stegun 1965).

$$U'(a, x) - \tfrac{1}{2}xU(a, x) + U(a+1, x) = 0, \tag{19a}$$

$$[U(a, -x)]' - \tfrac{1}{2}xU(a, -x) + U(a-1, -x) = 0, \tag{19b}$$

and the formulae (Abramovitz and Stegun 1965)

$$U(a, x) = D_{-a-1/2}(x), \tag{20}$$

$$E(a, x) = \sqrt{2}\exp[\tfrac{1}{4}\pi a + \tfrac{1}{8}i\pi + \tfrac{1}{2}\arg\Gamma(\tfrac{1}{2} + ia)]U(ia, x\, e^{-i\pi/4}), \tag{21}$$

$$E(a, x) = (2/x)^{1/2}\exp[i(\tfrac{1}{4}x^2 - a\ln x + \tfrac{1}{2}\arg\Gamma(\tfrac{1}{2} + ia) + \tfrac{1}{4}\pi)](1 + O(x^{-1})) \qquad (x \to +\infty), \tag{22}$$

$$(1 + e^{2\pi a})^{1/2}E(a, x) = e^{\pi a}E^*(a, x) + iE^*(a, -x), \tag{23}$$

from equations (17), (18) and (11) we obtain

$$\tilde{V}(x) = -\tfrac{1}{4}x^2[1 + O(x^{-2})] \qquad (x \to \pm\infty). \tag{24}$$

Assume that for large values of positive x there are waves moving to the right only, so from equation (24) the wavefunctions should behave asymptotically like the complex solution $E(\gamma, x)$ to the Weber equation with γ being some constant.

From the Darboux theorem the general solutions to the Schrödinger equation with the inverted potential $\tilde{V}(x)$ given by equation (17) are

$$\tilde{\psi}(x) = \tilde{\phi}(x)\left(\frac{k_+E(\mu, x) + k_-E^*(\mu, -x)}{\tilde{\phi}(x)}\right)',$$

where k_+ and k_- are arbitrary constants. An analysis of the asymptotic behaviour of the above functions allows us to choose proper wavefunctions:

$$\tilde{\psi}(x) = \tilde{\phi}(x)(E(\mu, x)/\phi(x))', \tag{25}$$

where the parameter μ is closely related to the eigenvalue E of the Hamiltonian operator and is determined from the Darboux theorem (Zheng 1982) as

$$\mu = a - E. \tag{26}$$

Using formula (23) and equation (25), for large negative x we have

$$\begin{aligned}\tilde{\psi}(-|x|) = {} & (1 + e^{2\pi\mu})^{1/2}i\tilde{\phi}(x)(E^*(\mu, |x|)/\tilde{\phi}(x))' && \text{(incident wave)},\\ & -e^{\pi a}i\tilde{\phi}(x)(E(\mu, |x|)/\tilde{\phi}(x))' && \text{(reflected wave)}.\end{aligned} \tag{27}$$

Therefore, the transmission coefficient (Merzbacher 1970) is

$$T = 1 + e^{2\pi\mu} = 1 + e^{2\pi(a-E)} \tag{28}$$

which is the same as the result for the inverted harmonic oscillator potential (Hill and Wheeler 1953, Prakash 1976).

The Fokker–Planck equations are closely related to the Schrödinger equations (van Kampen 1977). The discussion on the corresponding Fokker–Planck equations is given elsewhere (Hongler and Zheng 1982).

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