

SWKB approach to confined isospectral potentials

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Recently we had formulated the supersymmetric Wentzel–Kramers–Brillouin (SWKB) quantization rule for one-dimensional confined quantum systems and applied the same to two trigonometric potentials, tangentially limited by infinite walls at $x = 0$ and $x = L$, viz., $V(x) = V_0 \cot^2(\pi x/L)$ and the Pöschl–Teller potential, $V(x) = V_{01} \operatorname{cosec}^2(\pi x/(2L)) + V_{02} \sec^2(\pi x/(2L))$. Both the potentials have received quite a lot of attention by various authors because of their importance in molecular physics. Though these potentials have been studied in the framework of WKB, BS (Bohr–Sommerfeld), mBS (matrix formulation of BS) formalisms, it was observed that the supersymmetric approach not only rendered the calculations simpler and more transparent, it also reproduced the exact analytical energies in both the cases.

In this study, we shall generate isospectral Hamiltonians of the above potentials with the help of a modified form of Darboux's theorem. We shall show that though the new potentials look different from the original ones, and have different eigenfunctions, they too, are confined in the same region of space, and share the same energy spectrum as their original counterparts. This may be of substantial importance in determining the energy spectrum of highly non-trivial systems.

KEY WORDS: supersymmetry, WKB quantization, spatial confinement, isospectral Hamiltonians, Darboux's theorem

1. Introduction

Confined quantum systems have captured the attention of scientists from far and wide for the last two decades. Since the beginning of 1980s, rapid progress in very accurate lithographic techniques have made it possible to confine electrons, atoms and molecules in microscopic cavities [1], thus giving birth to the so-called quantum wires (quasi-one-dimensional structure) [2,3], quantum wells (quasi-two-dimensional structure) [4–6] and quantum dots (quasi-zero-dimensional structure) [7–11]. Quantum wires are produced in the form of miniature strips, etched in a sample containing a quantum well. Their typical transverse dimensions are significantly larger than the depth of the quantum well, reaching 10–400 nm. Imposing strong confinement in all 3 spatial dimensions, i.e., complete quantization of the particle's free motion results in a quantum dot. Spatial confinement significantly alters the physical and chemical properties of the system [12–15]. It influences the bond formation and chemical reactivity inside the cavities

to a great extent. Even the optical properties (absorption and emission of light in the visible or far infra-red range, Raman scattering) and electrical properties (capacitance and transport studies) change radically. Hence this branch of science is extremely useful in the study of thermodynamic properties of non-ideal gases, investigation of atomic effects in solids, in atoms and molecules under high pressure, impurity binding energy in quantum wells, and even in the context of partially ionised plasmas.

Quantum dots absorb and emit light in a very narrow spectral range, which is controlled, for instance, by an applied magnetic field. Hence it is expected that they might be used to construct more precisely controlled semiconductor lasers. The strong quantization of the electron energy will probably allow quantum-dot lasers to be able to work at high temperature and at lower injection currents [1]. Their application in a new generation of computers is also very promising [16]. The extremely small dimension and possibility of dense packing of quantum-dot matrices could permit them to be used for memory media of huge capacity, further enhancing the importance of confined quantum systems.

Recently, we had studied spatial confinement in the framework of WKB [17] and SWKB (its supersymmetric version) [18] methods. In the present work we shall take up two one-dimensional trigonometric potentials (tangentially limited by infinite walls at $x = 0$ and $x = L$, where L is the dimension of the confining box) of tremendous importance in molecular spectroscopy, viz.,

$$V(x) = V_0 \cot^2 \frac{\pi x}{L} \quad (1)$$

and the Pöschl–Teller potential [19],

$$V(x) = V_{01} \operatorname{cosec}^2 \frac{\pi x}{2L} + V_{02} \operatorname{sec}^2 \frac{\pi x}{2L}. \quad (2)$$

(It may be mentioned here that though the first potential is a special case of the second one with the identification $V_{01} = V_{02} = V_0/4$, it has been discussed by various authors due to its importance in molecular physics [20]. Potential (1) represents a well symmetric around $x = L/2$. Unless $V_{01} = V_{02}$, potential (2) represents an asymmetric well. For small V_0, V_{01}, V_{02} , both the potentials represent perturbations on an infinite square well.) Though both the potentials are periodic in nature, we consider a single hole only as the barriers put by the singularities between the holes are impenetrable. Both the potentials have been studied in the framework of BS (Bohr–Sommerfeld), mBS (matrix formulation of Bohr–Sommerfeld), WKB (Wentzel–Kramers–Brillouin) [20] as well as the SWKB (supersymmetric version of WKB) [18] approximations, of which the last approach (viz. the SWKB quantization rule) reproduces the exact Schrödinger energies in both the cases.

Here, we shall generate a series of exactly solvable isospectral supersymmetric (SUSY) Hamiltonians starting from a single exactly solvable SUSY Hamiltonian with the help of a modified version of the Darboux's theorem [21]. We shall show that though the new potentials have different shapes and different eigenfunctions, they share the same energy spectrum as the original one. Even the region of confinement of both the

old and new potentials remains the same. This enables one to determine the exact eigen-energies of highly non-trivial potentials.

The organization of the paper is as follows. To make the paper self-contained, we briefly describe the SWKB formalism in section 2, and a modified version of Darboux theorem in section 3. In section 4, we calculate the isospectral Hamiltonians for the confined potentials given above. The wave functions of the confined potentials and their isospectral counterparts are also compared. Section 5 is kept for discussions and conclusions.

Units used throughout are $\hbar = 2m = 1$.

2. SWKB formalism for confined quantum systems

The SWKB method follows from the ordinary WKB approximation by writing the potential $V(x)$ in terms of the superpotential $W_0(x)$ [21]

$$V(x) = W_0^2 + W_0'(x). \tag{3}$$

This modifies the WKB quantization condition, viz.,

$$\int_a^b [E - V(x)]^{1/2} dx = \left(n + \frac{1}{2}\right)\pi, \quad n = 0, 1, 2, \dots, \tag{4}$$

where a, b are the roots of the equation

$$E - V(x) = 0 \tag{5}$$

to the SWKB quantization condition

$$\int_c^d [E' - W_0^2(x)]^{1/2} dx = n\pi, \quad n = 0, 1, 2, \dots, \tag{6}$$

with c, d being the roots of the equation

$$E' - W_0^2(x) = 0, \tag{7}$$

E' being the supersymmetric energy. The ground state

$$\psi_0 = \exp\left(\int W_0(x) dx\right) \tag{8}$$

will be normalizable if $\int W_0(x) dx$ exists.

We had applied the above formalism to the two trigonometric potentials, given by equations (1) and (2), with impenetrable walls at $x = 0$ and $x = L$ [18]. The supersymmetric WKB approach yielded the exact Schrödinger energies as well as ground state eigenfunctions in both the cases [24,25].

Omitting the detailed calculations (with the help of formulae in [23]) for brevity, we quote the SWKB energy directly.

For the Pöschl–Teller potential given by

$$V(x) = V_{01} \operatorname{cosec}^2 \frac{\pi x}{2L} + V_{02} \sec^2 \frac{\pi x}{2L} \quad (9)$$

the energy is calculated to be

$$E_n^{\text{swkb}} = E_1^\infty \left\{ n - \frac{1}{2} + \sqrt{v_{01} + \frac{1}{16}} + \sqrt{v_{02} + \frac{1}{16}} \right\}^2, \quad n = 1, 2, 3, \dots, \quad (10)$$

and the ground state eigenfunction takes the form

$$\psi_0 = |N_0| \frac{\sin^{A_1} x}{\cos^{A_2} x}, \quad (11)$$

where $|N_0|$ is fixed by normalisation. In the above expressions, the symbols stand for

$$V_{01} = A_1^2 - A_1, \quad (12)$$

$$V_{02} = A_2^2 + A_2, \quad (13)$$

$$v_{01} = V_{01}/E_1^\infty, \quad v_{02} = V_{02}/E_1^\infty, \quad E_n = \varepsilon_n E_1^\infty,$$

where $E_1^\infty = \pi^2/L^2 = 4$, and the superpotential is taken as

$$W_0(x) = A_1 \cot x + A_2 \tan x. \quad (14)$$

Spatial confinement within the region $0 < x < L$ significantly alters the boundary conditions and imposes the following constraint on A_1 and A_2 :

$$A_1 > 0, \quad A_2 < 0.$$

Similarly, for the special case,

$$V_{01} = V_{02} = \frac{V_0}{4},$$

the Pöschl–Teller potential may be cast in the form

$$V(y) = V_0 \cot^2 y. \quad (15)$$

Taking the superpotential to be

$$W_0(y) = A \cot y \quad (16)$$

with

$$V_0 = A^2 - A, \quad (17)$$

$$E = E' + A, \quad (18)$$

the SWKB quantization condition (8) yields the energy

$$E_n^{\text{swkb}} = E_1^\infty \left\{ n^2 + \left(n - \frac{1}{2} \right) \sqrt{4v + 1} - 1 \right\}, \quad n = 1, 2, 3, \dots, \quad (19)$$

with the identification

$$V_0 = vE_1^\infty, \tag{20}$$

$$E_n^\infty = n^2, \tag{21}$$

and the ground state wave function takes the form

$$\psi_0(y) = |c_0| \exp\left(\int W_0(y) dy\right) = |c_0| \sin^A y, \tag{22}$$

where $|c_0|$ is the normalisation factor. Again, A must satisfy the condition

$$A > 0$$

because of spatial confinement.

3. Modified form of Darboux's theorem

Now we shall show how a modified form of Darboux theorem enables one to obtain a series of new exactly solvable isospectral Hamiltonians, i.e., Hamiltonians with the same eigenvalues [21]. Thus if one knows the energy spectrum of a certain potential, one can obtain a series of highly non-trivial potentials with the same energy spectrum.

We know that if the potential $V_-(x)$ can be written as

$$V_-(x) = W_0^2(x) - W_0'(x) \tag{23}$$

then it is isospectral with the potential $V_+(x)$ where

$$V_+(x) = W_0^2(x) + W_0'(x). \tag{24}$$

However, in the present case $V_-(x)$ and $V_+(x)$ are of the same nature. To find a non-trivial partner we notice that the Riccati equation

$$W_1^2(x) - W_1'(x) = W_0^2(x) - W_0'(x) \tag{25}$$

has a solution $W_1 \neq W_0$ which is given by [21]

$$W_1(x) = W_0(x) - u(x), \tag{26}$$

where u is given by

$$u' - 2uW_0 + u^2 = 0. \tag{27}$$

It is to be noted here that $W_1^2(x) + W_1'(x) \neq W_0^2(x) + W_0'(x)$.

But $V_1(x) = W_1^2(x) + W_1'(x)$ is isospectral with $W_1^2(x) - W_1'(x)$, and hence isospectral with $V_+(x) = W_0^2(x) + W_0'(x)$, with the possible exception of the ground state of $V_+(x)$. It is also phase-equivalent with $V_+(x)$ [26,27].

It can be found (after some calculations) that $u(x)$ is of the form

$$u(x) = \frac{\exp\{2 \int^x W_0(t) dt\}}{k + \int^x dr \exp\{2 \int^r W_0(t) dt\}}, \quad (28)$$

where k is an integral constant. In other words, $u(x)$ is of the form f'/f where f is given by

$$f = k + \int^x dr \exp\left\{2 \int^r W_0(t) dt\right\}. \quad (29)$$

Hence, the isospectral potential $V_1(x)$ can be explicitly written as

$$V_1(x) = W_0^2(x) + W_0'(x) + \frac{2f'^2}{f^2} - \frac{f'' + 2W_0 f'}{f}. \quad (30)$$

One can repeat this process and obtain a series of isospectral and phase-equivalent potentials. For example, one can write

$$W_2(x) = W_1(x) + g(x) \quad (31)$$

with

$$g(x) = \frac{\exp\{-2 \int^x W_1(t) dt\}}{k' + \int^x dr \exp\{-2 \int^r W_1(t) dt\}} \quad (32)$$

and k' another integral constant, and obtain another isospectral Hamiltonian (with superpotential $W_2(x)$) given by

$$H_2 = -\frac{d^2}{dx^2} + V_2(x), \quad (33)$$

where

$$V_2(x) = W_2^2 - W_2' \quad (34)$$

and so on.

The ground state wave function $\psi_1^0(x)$ of the equivalent isospectral $V_1(x)$ is given by

$$\psi_1^0(x) = \exp\left(\int W_1(x) dx\right) \quad (35)$$

apart from a normalization factor. With $u(x) = f'/f$, equation (31) enables us to express $\psi_1^0(x)$ in terms of the original ground state wave function $\psi_0(x)$ as

$$\psi_1^0(x) = \frac{1}{f} \psi_0(x). \quad (36)$$

Whether the new ground state $\psi_1^0(x)$ is unphysical or physical, depends on the value of k .

4. Isospectral Hamiltonians

In this section we shall calculate the isospectral Hamiltonians for the potentials given in (1) and (2) above.

The Pöschl–Teller potential is given by

$$V(x) = V_{01} \operatorname{cosec}^2 x + V_{02} \sec^2 x.$$

If the original superpotential be

$$W_0(x) = A_1 \cot x + A_2 \tan x \tag{37}$$

then the equivalent superpotential is given by

$$W_1(x) = W_0(x) - u(x), \tag{38}$$

where $u(x)$ turns out to be (from equations (33) and (42))

$$u(x) = \frac{\sin^{\sigma_1} x / \cos^{\sigma_2} x}{k + \int dx \sin^{\sigma_1} x / \cos^{\sigma_2} x}. \tag{39}$$

In the above equation, σ_1 and σ_2 stand for,

$$\sigma_1 = 2A_1, \tag{40}$$

$$\sigma_2 = 2A_2. \tag{41}$$

For the existence of bound states, i.e., for the coefficients of $\operatorname{cosec}^2 x$ and $\sec^2 x$ to be positive, σ_1, σ_2 must be constrained to

$$\sigma_1 > 2, \quad \sigma_2 < -2.$$

We shall take a suitable choice for σ_1 and σ_2 . For the potential to be asymmetric, $V_{01} \neq V_{02}$, which in turn implies that $\sigma_1 \neq -\sigma_2$. Let us take $\sigma_1 = 4, \sigma_2 = -3$. This yields the value of $u(x)$ as

$$u(x) = \frac{\sin^4 x \cos^3 x}{k + \frac{\sin^3 x}{7} \left\{ \frac{2}{5} + \frac{3}{5} \cos^2 x - \cos^4 x \right\}}. \tag{42}$$

Thus the isospectral potential turns out to be

$$\begin{aligned} V_1(x) = & 2 \operatorname{cosec}^2 x + \frac{3}{4} \sec^2 x - \frac{49}{4} \\ & + \frac{2 \sin^8 x \cos^6 x}{\left[k + \frac{\sin^3 x}{7} \left\{ \frac{2}{5} + \frac{3}{5} \cos^2 x - \cos^4 x \right\} \right]^2} \\ & + \frac{2 \sin^3 x \cos^2 x \{ 3 \sin^2 x - 4 \cos^3 x \}}{k + \frac{\sin^3 x}{7} \left\{ \frac{2}{5} + \frac{3}{5} \cos^2 x - \cos^4 x \right\}}. \end{aligned} \tag{43}$$

$V_1(x)$ gives a new Hamiltonian (with superpotential W_1), which is isospectral with the supersymmetric (SUSY) Hamiltonian of the Pöschl–Teller potential (equation (2))

with superpotential W_0 . From equation (40), the *ground state wave function* of the Schrödinger equation with potential $V_1(x)$ (equation (48)) is given by

$$\psi_1^0(x) = |N_1| \frac{\sin^2 x \cos^{3/2} x}{\left[k + \frac{\sin^3 x}{7} \left\{ \frac{2}{5} + \frac{3}{5} \cos^2 x - \cos^4 x \right\} \right]} \quad (44)$$

while the ground state wave function of the original Schrödinger equation (equation (2)), is given by

$$\psi_0(x) = |N_0| \sin^2 x \cos^{3/2} x, \quad (45)$$

where N_0 and N_1 are normalization constants. It is easily observed that $\psi_0(x)$ vanishes at the boundaries $x = 0$ and $x = \pi/2$, the reason being the spatial confinement of the Pöschl–Teller potential (equation (2)) in the range $0 < x < \pi/2$. The range of the equivalent potential is determined by the choice of k . We shall choose k suitably such that there is no singularity in the range $0 < x < \pi/2$, and $\psi_1^0(x)$ is a physical solution. Hence both the original (equation (2)) as well as the equivalent (equation (48)) potentials are confined in the same spatial region $0 < x < \pi/2$.

Figure 1 shows the plot of $V(x)$ against x for the Pöschl–Teller potential given by equation (2), viz., $V(x) = V_{01} \operatorname{cosec}^2 x + V_{02} \sec^2 x$ (shown by the broken curve) and its equivalent isospectral form $V_1(x)$ given in equation (43) (shown by the solid line) for $k = -0.13$.

Figure 2 shows the plot of the ground state wave function $\psi_0(x)$ (equation (45)) for the potential given in equation (2) (shown by the broken curve) and $\psi_1^0(x)$ (equa-

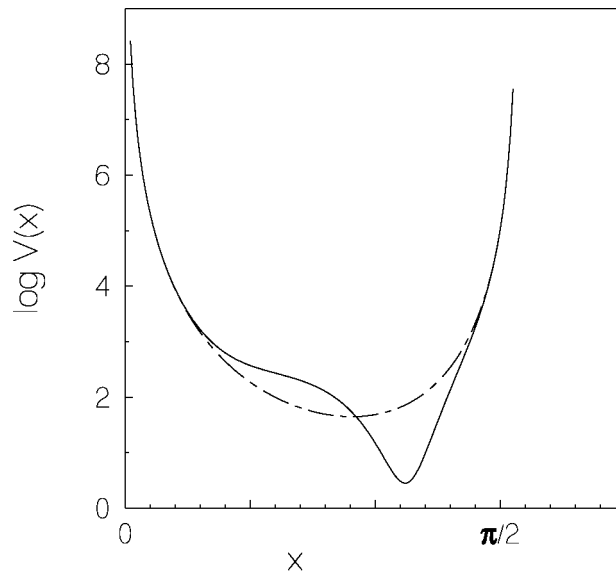


Figure 1. Plot of $\log V(x)$ against x . Broken curve: $\log V(x)$ from equation (2) (original potential). Solid curve: $\log V_1(x)$ from equation (43) (equivalent potential).

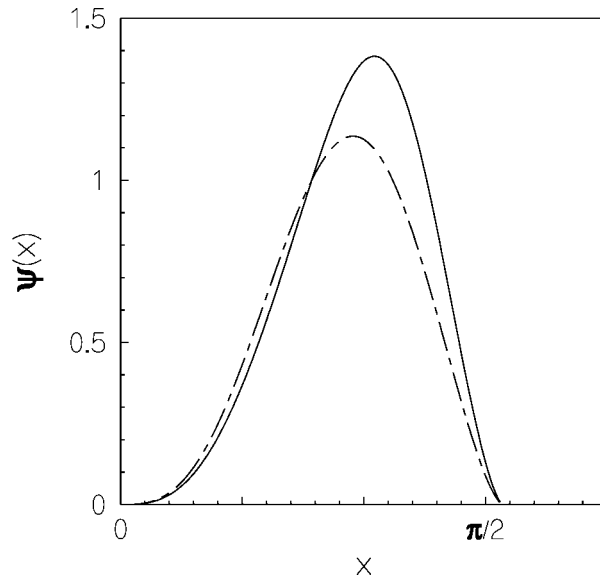


Figure 2. Plot of ground state wave function $\psi(x)$ against x . Broken curve: $\psi_0(x)$ from equation (45) (original wave function). Solid curve: $\psi_1^0(x)$ from equation (44) (equivalent wave function).

tion (44)) for the equivalent potential in equation (43) (shown by the solid curve) for $k = -0.13$.

Similarly for equation (1), viz.,

$$V(y) = V_0 \cot^2 y, \quad u(y) = \frac{\sin^\sigma y}{p + \int dy \sin^\sigma y}, \tag{46}$$

where

$$\sigma = 2A. \tag{47}$$

For bound states to exist, the coefficient of $\cot^2 y$ must be positive. Hence, σ must be constrained in the range $\sigma > 2$.

Suitably taking $\sigma = 3$,

$$u(y) = \frac{\sin^3 y}{k' + \frac{\cos^3 y}{3} - \cos y}. \tag{48}$$

Working in an analogous manner, the isospectral partner turns out to be

$$V_1(y) = \frac{3}{4} \cot^2 y - \frac{6}{4} + \frac{2 \sin^6 y}{\left\{k' + \frac{\cos^3 y}{3} - \cos y\right\}^2} - \frac{6 \sin^2 y \cos y}{k' + \frac{\cos^3 y}{3} - \cos y}. \tag{49}$$

This potential is quite different from the original potential $V(y) = V_0 \cot^2 y$ (equation (1)). Choosing k' suitably, one can ensure that there is no singularity in the range $0 < y < \pi$, so that the spatial range of both the original and equivalent potential remains

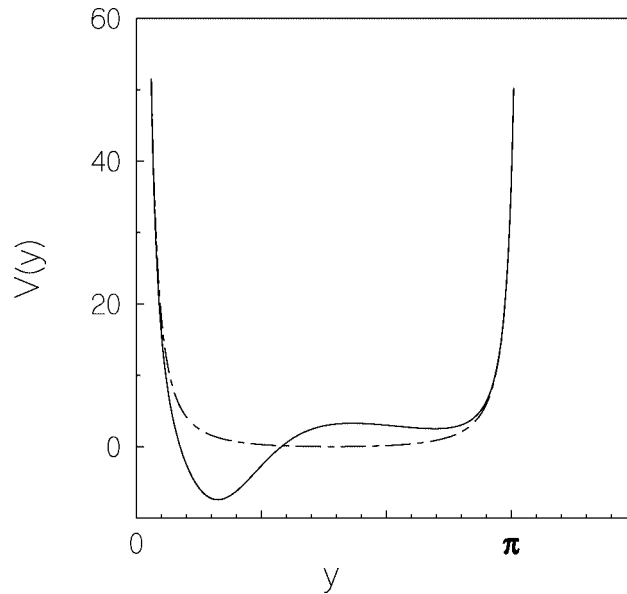


Figure 3. Plot of $V(y)$ against y . Broken curve: $V(y)$ from equation (1) (original potential). Solid curve: $V_1(y)$ from equation (49) (equivalent potential).

unchanged. This fact is clear from the plots of the original (equation (1)) and equivalent (equation (54)) potentials presented in figure 3 for $k' = 0.8$.

The *ground state wave function* of the isospectral potential (equation (49)) is calculated in an analogous way and turns out to be

$$\psi_1^0(y) = |c_1| \frac{\sin^{3/2} y}{k' + \frac{\cos^3 y}{3} - \cos y} \quad (50)$$

while the ground state wave function for the potential in equation (1) is

$$\psi_0(y) = |c_0| \sin^{3/2} y, \quad (51)$$

where c_0 and c_1 are obtained from the normalization condition.

Figure 4 shows the plot of the ground state wave function $\psi_0(y)$ (equation (51)) for the potential given in equation (1), (shown by the broken curve) and $\psi_1^0(y)$ (equation (50)) for the equivalent potential in equation (49) (shown by the solid curve) for $k' = 0.8$.

Though the SWKB approach reproduces the exact analytical eigen energies as well as the ground state wave functions in both the cases, it is interesting to study the behaviour of the *excited state wave functions*. For the excited states, however, the SWKB wave functions have to be evaluated numerically. For this purpose we shall deal with potential (1) only. The other potential follows in a similar manner.

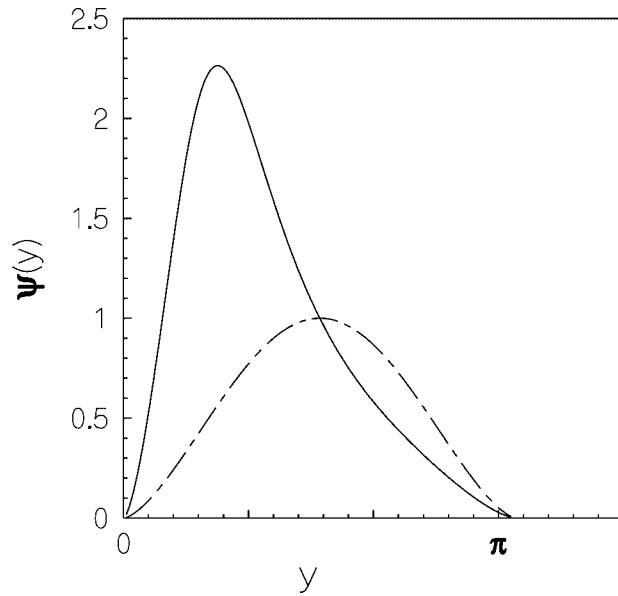


Figure 4. Plot of ground state wave function $\psi(y)$ against y . Broken curve: $\psi_0(y)$ from equation (51) (original wave function). Solid curve: $\psi_1^0(y)$ from equation (50) (equivalent potential).

The SWKB solution to the 1-dimensional Schrödinger equation (with a confined potential)

$$\left(\frac{d^2}{dx^2} + \Gamma^2(x) \right) \psi_n(x) = 0, \tag{52}$$

where

$$\Gamma = (E'_n - V)^{1/2} = (E'_n - W^2)^{1/2} + \frac{1}{2} \frac{W'}{(E'_n - W^2)^{1/2}} + \dots \tag{53}$$

can be obtained just like the confined WKB solutions [17]. We simply quote the results here.

$$\psi_n(x) = \frac{N}{\sqrt{\Gamma}} \sin \left(\int_0^x (E'_n - W^2)^{1/2} dx + \frac{1}{2} \sin^{-1} \frac{W(x)}{\sqrt{E'_n}} \right), \quad 0 < x < x_1, \tag{54}$$

$$\psi_n(x) = \frac{N}{\sqrt{\kappa}} \left[\frac{1}{2} \sin \theta e^{-(\beta(x) - \lambda(x))} + \cos \theta e^{(\beta(x) - \lambda(x))} \right], \quad x_1 < x < x_2, \tag{55}$$

$$\psi_n(x) = \frac{N}{\sqrt{\Gamma}} \sin \left(\theta + \int_{x_2}^x (E'_n - W^2)^{1/2} dx + \frac{1}{2} \sin^{-1} \frac{W(x)}{\sqrt{E'_n}} \right), \quad x_2 < x < L, \tag{56}$$

where x_1, x_2 are the roots of the equation

$$E'_n - W^2 = 0$$

and

$$\theta = \frac{1}{2} \int_{x_1}^{x_2} (E'_n - W^2)^{1/2} dx, \quad (57)$$

$$\beta = \int_{x_1}^x (W^2 - E'_n)^{1/2} dx, \quad (58)$$

$$\lambda = \frac{1}{2} \ln \frac{W(x) + (W^2 - E'_n)^{1/2}}{\sqrt{E'_n}}. \quad (59)$$

The analytical eigenfunctions of the system with potential (1) are given by [25]

$$\psi_n(x) = c_n (\sin x)^{-2\rho} F\left(-\frac{n}{2} - 2\rho, \frac{n}{2}, \frac{1}{2}, \cos^2 x\right), \quad (60)$$

where

$$\rho = \frac{1}{4} (\sqrt{4V_0 + 1} - 1). \quad (61)$$

5. Results and discussions

We had shown earlier [18] that the SWKB approach reproduces the exact analytical eigenenergies as well as the ground state eigenfunctions for both the potentials under study, though the WKB, BS or mBS energies [20] are far away from the exact results. In this study we have generated the equivalent potentials of both (1) and (2) by a modified form of Darboux's theorem. Though quite different from the original potentials, the respective equivalent counterparts (equations (49) and (43)) have the same energy spectrum and spatial boundary, with the possible exception of the ground state. However, the choice of k determines whether the solutions are physical or unphysical. Thus this approach may be used to determine the energy eigenvalues of highly non-trivial confined potentials. The original potentials, along with their respective isospectral forms, are shown in figures 1 and 3.

Using the fact that the SWKB approach reproduces the exact analytical ground state eigenfunctions, we have evaluated the ground state wave functions (equations (51) and (45)) of the potentials (equations (1) and (2)), as well as those (equations (50) and (44)) of their respective equivalent forms (equations (49) and (43)). These are depicted graphically in figures 2 and 4, respectively. The wave functions have been normalised somewhat differently, by dividing by their value at $\pi/2$. It is easy to observe from the figures that the ground state is shared by both the original as well as the equivalent potentials in these particular cases. However, the SWKB eigenfunctions in the excited states have to be evaluated numerically.

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