SWKB Quantization Rules for Bound States in Quantum Wells

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Abstract

In a recent paper by M A F Gomes and S K Adhikari(J.Phys.(**B30**) **,5987.(1997)), a matrix formulation of the Bohr-Sommerfeld (mBS) quantization rule has been applied to the study of bound states in one-dimensional quantum wells. They have observed that the usual Bohr-Sommerfeld (BS) and the Wentzel-Kramers-Brillouin (WKB) quantization rules give poor estimates of the eigen energies of the two confined trigonometric potentials,** *viz.*, $V(x) = V_0 \, cot^{\,2} \, \frac{\pi \, x}{L}$ **, and the famous Pöschl-Teller potential,** $V(x) = V_{01} \, cosec^{\,2} \, \frac{\pi \, x}{2L} + V_{02} \, sec^{\,2} \, \frac{\pi \, x}{2L}$ **, the WKB approach being worse of the two, particularly for small values of** n**. They suggested a matrix formulation of the Bohr-Sommerfeld method (mBS). Though this technique improves the earlier results, it is not very accurate either. Here we study these potentials in the framework of supersymmetric Wentzel-Kramers-Brillouin (SWKB) approximation, and find that the SWKB quantization rule is superior to each one of the BS, mBS, and WKB approximations, as it reproduces the exact analytical results for the eigen energies. Its added advantage is that it gives the correct analytical ground state wave functions as well.**

Introduction :

The study of confined quantum systems is of considerable importance in modern times as spatial confinement significantly alters the physical and chemical properties of the system [1-4]. 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.

Various authors have emppployed different techniques to study such systems. Fairly recently, M A F Gomes and S K Adhikari [5] have suggested a matrix formulation of the Bohr-Sommerfeld (mBS) quantization rule to give an estimate of the eigen energies of the Schrödinger equation, for various one-dimensional quantum wells. They have compared the energies thus obtained with those by Wentzel-Kramers-Brillouin (WKB) and usual Bohr-Sommerfeld (BS) methods, as well as the exact analytical solution of the Schrödinger equation. They observed that in many cases the mBS quantization rule yields more precise energies than the WKB or BS quantization rules. For small n particularly, the WKB approximation gives the poorest estimates.

In this short comment, we study spatial confinement in the framework of SWKB (supersymmetric version of WKB) approximation. The motivation for the SWKB approach arises from the fact that this gives exact results in case of shape-invariant potentials. In this work, we deal with two trigonometric potentials, discussed in ref. [5], *viz.*,

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

and the famous Pöschl-Teller potential,

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

Both the potentials are tangentially limited by infinite walls at $x = 0$ and $x = L$, (L being the dimension of the confining box) and are of tremendous importance in molecular spectrocopy. We find that our SWKB energies are identical to the exact analytical results [6,7] in both the cases. It is worth noting 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. 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 represents perturbations on an infinite sqare well. Though both the potentials are periodic in nature, the barriers put by the singularities between the holes are impenetrable. So we consider a single hole only. The added advantage of the SWKB approximation is that it gives the exact analytical ground state wave functions as well.

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

Theory :

First we give a brief outline of the SWKB method, starting from the ordinary WKB approximation. Writing the potential $V(x)$ in terms of the superpotential $W(x)$ [8]

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

the WKB quantization condition , viz.,

$$\int_a^b [E - V(x)]^{1/2}\, dx = (n + 1/2)\pi \qquad n = 0, 1, 2, ... \tag{4}$$

where a, b are the roots of the equation

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

gets modified to the SWKB quantization condition

$$\int_c^d [E' - W^2(x)]^{1/2}\, dx - \frac{1}{2}\int_c^d \frac{W'}{[E' - W^2(x)]^{1/2}} dx = (n + 1/2)\pi \qquad n = 0, 1, 2, ... \tag{6}$$

where c, d are the roots of the equation

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

Since the second integral has the value $\pi/2$, the SWKB quantization rule reads

$$\int_c^d [E\ ' \ - \ W^2(x)]^{\ 1/2} \ dx \ = \ n \ \pi \qquad n = 1, 2, 3, ... \tag{8}$$

The ground state

$$\psi_0 = exp\ (\int \ W(x) \ dx) \tag{9}$$

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

For the Pöschl-Teller potential

$$V(x) \ = \ V_{01} \ cosec^{\ 2} \ \frac{\pi \ x}{2L} \ + \ V_{02} \ sec^{\ 2} \ \frac{\pi \ x}{2L} \tag{10}$$

the superpotential can be taken as

$$W(x) \ = \ A_1 \ cot \ \alpha x \ + \ A_2 \ tan \ \alpha x \tag{11}$$

Now the Schrödinger equation

$$\left(\ - \ \frac{d^2}{dx^2} \ + \ V(x) \right) \ \psi \ = \ E \ \psi \tag{12}$$

can be written in the form

$$\left(\ - \ \frac{d^2}{dx^2} \ + \ (W^{\ 2} \ + \ W\ ') \right) \ \psi \ = \ E\ ' \ \psi \tag{13}$$

with

$$\alpha \ = \ \frac{\pi}{2L} \tag{14}$$

$$V_{01} \ = \ A_1^2 \ - \ A_1 \alpha \tag{15}$$

$$V_{02} \ = \ A_2^2 \ + \ A_2 \alpha \tag{16}$$

$$E\ ' \ = \ E \ - \ (A_1 \ - \ A_2)^2 \tag{17}$$

Hence the SWKB condition (8) takes the form

$$\int_{x_1}^{x_2} \left\{ E\ ' \ - \ A_1^2 \ cosec^{\ 2} \alpha x \ - \ A_2^2 \ sec^{\ 2} \alpha x \ + \ (A_1 \ - \ A_2)^2 \right\}^{\ 1/2} \ dx \ = \ n \ \pi \qquad n = 0, 1, 2, ... \tag{18}$$

which can be written as

$$\frac{1}{\alpha} \ \int_{z_1}^{z_2} \left\{ E \ - \ \frac{A_1^2}{z^2} \ - \ \frac{A_2^2}{1 \ - \ z^2} \right\}^{\ 1/2} \ \frac{dz}{(1 \ - \ z^2)^{\ 1/2}} \ = \ n \ \pi \qquad n = 0, 1, 2, ... \tag{19}$$

where

$$z \;=\; sin\;(\alpha x) \tag{20}$$

Putting

$$z^2 \;=\; t \tag{21}$$

(19) reduces to

$$\frac{1}{2\alpha}\int_{t_1}^{t_2}\left\{\frac{-\;A_1^2\;+\;(A_1^2\;-\;A_2^2\;+\;E)t\;-\;Et^2}{t(1\;-\;t)}\right\}dt\;=\;n\;\pi \qquad n=0,1,2,... \tag{22}$$

This can be evaluated with the help of formulae given in [9].

Omitting the detailed calculations for brevity, we quote the SWKB energy directly.

$$E_n^{swkb} = [2\;\alpha\;n\;+\;(A_1\;-\;A_2)]^2 \qquad n\;=\;0,1,2,... \tag{23}$$

Writing

$$V_{01}\;=\;v_1\;E_1^{\infty}$$

$$V_{02}\;=\;v_2\;E_1^{\infty}$$

$$E_n\;=\;\epsilon_n\;E_1^{\infty}$$

the SWKB energy can be reformulated as

$$E_p\;=\;E_1{}^{\infty}\;\left\{p\;+\;\frac{1}{2}\;+\;\sqrt{v_{01}\;+\;\frac{1}{16}}\;+\;\sqrt{v_{02}\;+\;\frac{1}{16}}\right\} \qquad p\;=\;1,2,3,... \tag{24}$$

which is identical to the exact analytical formula for the Schrödinger eigenenergies [6]. Thus our SWKB approach reproduces the exact eigenenergies of the Pöschl-Teller potential.

Also the ground state eigenfunction $\psi_0\;=\;|N_0|\;exp(\int W_0\;dx)$ **takes the form**

$$\psi_0\;=\;|N_0|\;\frac{sin\;^{A_1/\alpha}\;\alpha x}{cos\;^{A_2/\alpha}\;\alpha x} \tag{25}$$

where N_0 **is fixed by normalization. For** $\psi\;=\;0$ **at** $x=0$ **and** $x=L$**,** A_1 **and** A_2 **must satisfy the condition**

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

Thus the SWKB approach reproduces the exact ground state wave function of the system [6].

For the special case

$$V_{01} \ = \ V_{02} \ = \ V_0/4$$

the Pöschl-Teller potential may be cast in the form

$$V(x) \ = \ V_0 \ cot^{\ 2} \ \frac{\pi \ x}{L} \tag{26}$$

The superpotential can be taken to be

$$W(x) \ = \ A \ cot \ \alpha x \tag{27}$$

with

$$\alpha \ = \ \frac{\pi}{L} \tag{28}$$

$$V_0 \ = \ A^2 \ - \ A\alpha \tag{29}$$

$$E \ = \ E^{\ \prime} \ + \ A\alpha \tag{30}$$

so that the SWKB quantization condition (8) gives

$$\int_c^d [E^{\ \prime} \ - A^{\ 2} \ cot^{\ 2}(\frac{\pi x}{L})]^{\ 1/2} \ dx \ = \ n \ \pi \qquad n = 0, 1, 2, ... \tag{31}$$

Putting

$$z = A \ cot \ (\frac{\pi x}{L}) \tag{32}$$

(31) can be written as

$$- \ \frac{L}{A\pi} \ \int_{z_1}^{z_2} \frac{[E \ - z^{\ 2}]^{\ 1/2}}{1 \ + \ \frac{z^2}{A^2}} \ dz \ = \ n \ \pi \qquad n = 0, 1, 2, ... \tag{33}$$

Further substituting

$$\rho \ = \ \frac{z}{(E \ - \ z^2)^{\ 1/2}} \tag{34}$$

(33) reduces to, after some algebra,

$$\frac{2AL}{\pi} \ \int_0^\infty \left\{ \frac{1}{1 \ + \ \rho^2} \ - \ \frac{E \ + \ A^2}{\rho^2 \ (E \ + \ A^2) \ + \ A^2} \right\} \ d\rho \ = \ n \ \pi \qquad n = 0, 1, 2, ... \tag{35}$$

Once again omitting the lengthy calculations, it is found that the energy turns out to be

$$E_n^{\ swkb} \ = \ \frac{\pi^2}{2m \ L^2} \ \left\{ \sqrt{\frac{2m \ L^2 \ A^2}{\pi^2}} \ + \ n \right\}^2 \ - \ A^2 \ + \ \frac{A\pi}{L} \qquad n \ = 0, 1, 2, 3, ... \tag{36}$$

Using eqns. (28) and (29), eqn.(36) can be cast in the form of the exact Schrödinger energy for the potential under consideration [7]

$$E_p \; = \; E_1{}^{\infty} \left\{ p^2 \; + \; (p \; - \; \frac{1}{2}) \; \sqrt{4v \; + \; 1} \; - 1 \right\} \qquad\qquad p = 1, 2, 3, ... \tag{37}$$

with the identification

$$V_0 \; = \; v \; E_1{}^{\infty} \tag{38}$$

$$E_n^{\infty} \; = \; \frac{\pi^2 \; n^2}{L^2} \tag{39}$$

Similarly the ground state wave function

$$\psi_0 \; = \; |c_0| \; exp(\int W_0 \; dx)$$

$$= \; |c_0| \; sin \; ^{A/\alpha} \; \alpha x \tag{40}$$

coincides with the exact formula for the system [7], where c_0 is the normalization factor. For $\psi \; = \; 0$ at $x = 0$ and $x = L$, A must satisfy the condition

$$A \; > \; 0$$

Conclusions :

In this short comment, we have studied spatial confinement in the framework of SWKB (supersymmetric version of WKB) approximation. In particular, we have dealt with two trigonometric potentials, discussed in ref. [5], *viz.* ,

$$V(x) \; = \; V_0 \; cot \; ^2 \; \frac{\pi \; x}{L} \tag{41}$$

and the famous Pöschl-Teller potential,

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Both the potentials are tangentially limited by infinite walls at $x \; = \; 0$ and $x = L$, (L being the dimension of the confining box) and are of tremendous importance in molecular spectrocopy. It had been observed in ref. [5] that mBS eigenenergies are somewhat better than BS and / or WKB ones , the WKB approximation giving the worst results for small values of n. We find

that our SWKB quantization rule is far better than each one of the BS, mBS, and WKB approximations , as it reproduces the exact analytical eigenenergies for both the potentials. Also in the SWKB approach, we obtain the exact analytical ground state eigenfunction.

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