ISSN 1330–0016
CODEN FIZBE7

COMPARISON OF THE SWKB AND WKB APPROXIMATIONS FOR THE FINITE SQUARE WELL

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Received 31 December 1997; accepted 1 June 1998

Both the WKB and the supersymmetric WKB (SWKB) approximations have been applied to the finite square-well potential and compared with the corresponding exact results. Even though this potential is not shape-invariant, an analytic expression for the superpotential is possible and it is seen that the SWKB is better than the WKB for almost all states.

PACS numbers: 03.65.Ge UDC 539.144

Keywords: supersymmetric Wentzel-Kramers-Brillouin approximation (SWKB), finite square-well potential

1. Introduction

A large variety of potentials are encountered in various branches of physics. In many cases, exact analytic solutions of the Schrödinger equation for these potentials are not possible. One then has to resort to one or another of the approximation methods like the perturbation, variation or Wentzel-Kramers-Brillouin (WKB) methods. Among these, the WKB method is generally the most useful, since it can be applied to solve a one-dimensional (or multi-dimensional, if it can be reduced to an effective one-dimensional) Schrödinger equation with any smoothly varying potential. On the other hand, the success of the perturbation method depends on the possibility of splitting the Hamiltonian into an unperturbed Hamiltonian, for which exact solutions are known, and the remaining perturbation part, which should be small. In the case of the variational method, the success and accuracy of the approximate solution depend completely on the choice of a suitable trial wave function. Hence, both the perturbation and the variational methods depend on the potential, while the WKB method is general enough to be used for any smoothly varying potential. However, except for the harmonic oscillator, the WKB method fails to produce exact results even for potentials for which exact analytic solutions exist. Comtet et al. [1] applied the concept of supersymmetric quantum mechanics (SSQM) to the WKB method and proposed a modified semi-classical quantization condition, known as the supersymmetric WKB (SWKB) condition. Using this modified condition, Dutt et al. [2] have shown that the lowest order SWKB provides exact eigenvalues for all states, including the ground state, for one- and three-dimensional harmonic oscillator, Morse, Coulomb, Rosen-Morse, etc. potentials. It was further shown [3–5] that all the higher-order corrections vanish. All these potentials are analytically solvable and the energy is given in closed analytic expressions. It was shown in SSQM that potentials which are shape-invariant (either through translation or scaling of parameters appearing in the potential) are also analytically solvable, resulting in a closed expression for the energy eigenvalues [6]. All the above mentioned potentials are shape-invariant potentials (SIP) through translation of one or more parameters [6]. It was shown in general by Barclay and Maxwell [5] that the SWKB quantization condition gives the exact energy values for all states including the ground state for all SIP obtained by translation of parameters. Later, it was seen [7] that for SIP's obtained through scaling of parameters, the SWKB results are not exact. The SWKB is also not exact for potentials that are not shape-invariant. It is interesting to see how SWKB fares in comparison with WKB for potentials which are not SIP, but exact analytic treatment is possible. For such potentials, although the energy is not given in a closed expression, it can be obtained by solving transcendental equations. A simple and well-known example of such a potential is the one-dimensional finite square-well potential. In this communication, we investigate both the WKB and SWKB results for the finite square well and compare them with the exact results, obtained by solving the transcendental energy equation numerically.

In Section 2, we give a brief review of the SWKB quantization condition. In Section 3, we present the exact WKB and SWKB calculations for the finite square well. Numerical results are given in Section 4 and finally, in Section 5, we draw our conclusions.

2. SWKB quantization condition

In the lowest order, the WKB quantization condition [8] for a one-dimensional potential $V(x)$ is:

$$\int_{x_1}^{x_2} \sqrt{2m(E_n^{WKB} - V(x))}\,\mathrm{d}x = (n + \frac{1}{2})\pi\hbar \qquad (n = 0, 1, 2, ...), \tag{1}$$

where x_1 and x_2 are the classical turning points defined by:

$$E_n^{WKB} = V(x_1) = V(x_2). \tag{2}$$

In the supersymmetric quantum mechanics (SSQM) approach [6], all energy scales are shifted by the ground-state energy (E_0), so that in the new energy scale, the ground state has zero energy. The potential becomes:

$$V_1(x) = V(x) - E_0 \tag{3}$$

and the Schrödinger equation for the ground state becomes:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_0(x)}{\mathrm{d}x^2} + V_1(x)\psi_0(x) = 0. \tag{4}$$

A superpotential is defined in terms of the ground-state wave function $\psi_0(x)$ as

$$W(x) = -\frac{\hbar}{\sqrt{2m}}\frac{\psi_0'(x)}{\psi_0(x)} \tag{5}$$

so that

$$V_1(x) = W^2(x) - \frac{\hbar}{\sqrt{2m}}W'(x). \tag{6}$$

Substituting Eqs. (3) and (6) into Eq. (1), one has

$$\int\limits_{x_1}^{x_2}\sqrt{2m[E_n^{(1)SWKB} - W^2(x) + \frac{\hbar}{\sqrt{2m}}W'(x)]}\,\mathrm{d}x = (n+\frac{1}{2})\pi\hbar \tag{7}$$

where $E_n^{(1)SWKB} = E_n^{SWKB} - E_0$ is the SWKB energy (in shifted scale) of the n^{th} state corresponding to the potential $V_1(x)$. Expanding the left side of Eq. (7) in powers of $\hbar$, one can see [2–5] that the SWKB quantization condition for $V_1(x)$ becomes:

$$\int\limits_{c}^{d}\sqrt{2m[E_n^{(1)SWKB} - W^2(x)]}dx = n\pi\hbar \qquad (n = 0, 1, 2, ...) \tag{8}$$

where the turning points c, d are defined through:

$$\sqrt{E_n^{(1)SWKB}} = -W(c) = W(d). \tag{9}$$

It has been shown [2-5] that the SWKB gives the exact energies for all states and all SIP obtained by translations of parameters.

In SSQM, one also defines a potential V_2(x), which is a partner to V_1(x) as

$$V_2(x) = W^2(x) + \frac{\hbar}{\sqrt{2m}}W'(x)\cdot \tag{10}$$

Then it can be shown [6] that both $V_1(x)$ and $V_2(x)$ have identical energy spectrum, except that the ground state of $V_1(x)$ is missing in the energy spectrum of $V_2(x)$. The same result can also be obtained in SWKB, if we substitute $V_2(x)$ from Eq. (10) in Eq. (1), which results in the SWKB quantization for $V_2(x)$ as:

$$\int_c^d \sqrt{2m[E_n^{(2)SWKB} - W^2(x)]}dx = (n+1)\pi\hbar \qquad (n = 0, 1, 2, ...) \tag{11}$$

showing that the level degeneracy of the exact eigenvalue spectra of $V_1(x)$ and $V_2(x)$ are preserved.

3. *Calculations for the finite square well*

We consider a symmetric one dimensional finite square well potential given by:

$$V(x) = \left\{ \begin{array}{cc} -V_0 & \text{for } -a \leq x \leq a \\ 0 & |x| > a \end{array} \right\}. \tag{12}$$

Analytic solution of the Schrödinger equation for this potential can be found in any standard textbook on quantum mechanics [9]. Since the potential is symmetric about the origin, solutions have definite parity. Matching the oscillatory solution within the well with the solution decaying exponentially outwards, one gets transcendental equations for the energy eigenvalues:

$$\eta \tan \eta = \xi \qquad \text{(for even parity)}, \tag{13}$$

$$\eta \cot \eta = -\xi \qquad \text{(for odd parity)}, \tag{14}$$

and

$$\xi^2 + \eta^2 = \frac{2m}{\hbar^2} V_0 a^2, \tag{15}$$

where

$$\eta = \alpha a, \qquad \alpha = \sqrt{\frac{-2mE}{\hbar^2}}, \tag{16}$$

and

$$\xi = \beta a, \qquad \beta = \sqrt{\frac{2m}{\hbar^2}(V_0 + E)}, \tag{17}$$

with $E < 0$ for a bound state. As $V_0 a^2$ increases, the number of bound states also increases. For a given value of $V_0 a^2$, the set of equations (13) – (16) is solved numerically to obtain the energy eigenvalue E.

For even-parity states, the wave function is given by:

$$u(x) = \left\{ \begin{array}{ll} A\cos\beta x & |x| < a \\ B\mathrm{e}^{-\alpha|x|} & |x| > a \end{array} \right\} \tag{18}$$

and for odd-parity states by:

$$u(x) = \left\{ \begin{array}{ll} A\sin\beta x & |x| < a \\ B\mathrm{e}^{-\alpha|x|} & |x| > a. \end{array} \right\} \tag{19}$$

The constants A and B are determined by matching at $x = a$ and by overall normalization. The WKB quantization condition is given by Eq. (1) with the classical turning points $x_1 = -a$ and $x_2 = a$ and $V(x) = -V_0$. The result is:

$$E_n^{WKB} = \frac{(n+\frac{1}{2})^2\pi^2\hbar^2}{8ma^2} - V_0 \qquad (n = 0, 1, 2, ...). \tag{20}$$

The quantum number n takes integral values 0,1,2,...... upto a maximum value, such that $E_n^{WKB} < 0$.

For the SWKB treatment, we assume that the ground state energy is $E_0 = -B_0 \;\; (B_0 > 0)$. The ground state wave function is:

$$u_0(x) = \left\{ \begin{array}{ll} A\cos\beta_0 x & |x| < a \\ B\mathrm{e}^{-\alpha_0|x|} & |x| > a \end{array} \right\} \tag{21}$$

with

$$\alpha_0 = \sqrt{\frac{2mB_0}{\hbar^2}}, \qquad \beta_0 = \sqrt{\frac{2m}{\hbar^2}(V_0 - B_0)}. \tag{22}$$

Then, by Eq. (5), the superpotential is given by:

$$W(x) = \left\{ \begin{array}{cc} \frac{\hbar}{\sqrt{2m}}\beta_0 tan\beta_0 x & |x| < a \\ \frac{\hbar}{\sqrt{2m}}\alpha_0 & x > a \\ -\frac{\hbar}{\sqrt{2m}}\alpha_0 & x < -a \end{array} \right\}. \tag{23}$$

Since $W(x)$ is positive for $x \to +\infty$ and negative for $x \to -\infty$, supersymmetry is not broken [6].

We can verify that $V_1(x)$ given by Eq. (6), with the superpotential given by Eq. (23), is the correct potential given by Eqs. (3) and (12). With the superpotential given by Eq. (23), the turning points are c and d, ($c = -d$), where

$$W(d) = \frac{\hbar}{\sqrt{2m}}\beta_0 \tan\beta_0 d = \sqrt{E_n^{(1)SWKB}}. \tag{24}$$

Hence,

$$d = \frac{1}{\beta_0} \tan^{-1} \left\{ \frac{1}{\beta_0} \sqrt{\frac{2mE_n^{(1)SWKB}}{\hbar^2}} \right\}. \tag{25}$$

Substituting in Eq. (8), the SWKB quantization condition becomes:

$$\int_0^d \sqrt{\tan^2 \beta_0 d - \tan^2 \beta_0 x}\, \mathrm{d}x = \frac{n\pi\hbar}{2\sqrt{2m(V_0 - B_0)}} \qquad (n = 0, 1, 2, ...). \tag{26}$$

With the substitution $\tan \beta_0 x = y \tan \beta_0 d$, the condition (26) can be put in the form:

$$\int_0^1 \frac{\sqrt{1 - y^2}}{y^2 + \left\{ \frac{V_0 - B_0}{E_n^{(1)SWKB}} \right\}} \mathrm{d}y = \frac{n\pi}{2} \qquad (n = 0, 1, 2, ...). \tag{27}$$

For the ground state ($n = 0$), the integral on the left side must vanish. The only way this can happen is by putting $E_0^{(1)SWKB} = 0$ in the shifted energy scale. Thus, the SWKB quantization condition gives the correct result for the ground state. For $n > 0$, $E_n^{(1)SWKB} > 0$. Now, since the turning point d should be less than or equal to a, Eq. (24) shows that:

$$E_n^{(1)SWKB} \leq (V_0 - B_0) \tan^2 \beta_0 a. \tag{28}$$

Thus the SWKB energies are obtained by Eq. (27) for $n = 0, 1, 2, ...$ upto the maximum value of n for which condition (28) is satisfied.

4. *Numerical results*

The exact energies are obtained by solving numerically Eqs. (13), (15), (16) and (17) for even-parity states and Eqs. (14), (15), (16) and (17) for odd-parity states. Eliminating one of the variables, the equations are written with E as the unknown variable. A preliminary search for E is obtained by the bisection method [10]. An improvement of this value is done by the Newton-Rhapson method [10]. The results are obtained with a precision of one part in 10^8. All the solutions in the range $0 > E > -V_0$ are obtained.

The WKB results are simply calculated from Eq. (20) for all values of n satisfying $0 > E_n^{WKB} > -V_0$.

Finally, for the SWKB result, Eq. (27) is solved by first evaluating the integral on the left side with a trial value of $E_n^{(1)SWKB}$. The integral is evaluated by dividing the integration interval [0, 1] into a number of equispaced subintervals and using a 32 point Gaussian quadrature [10,11] for each of the subintervals. The number of subintervals needed is found from the condition that the evaluated integral has a precision of one part in 10^{10}. Finally, Eq. (27) is solved initially by the bisection method to get a fairly accurate value of

$E_n^{(1)SWKB}$, followed by the Newton-Rhapson method for an accurate determination with a precision of one part in 10^8.

TABLE 1. Comparison of exact, WKB and SWKB energies (in MeV*) for* $V_0 = 50$ MeV.

a(fm)	n	exact energy	WKB energy	SWKB energy
3	0	-46.165022	-48.578847	-46.165022
	1	-34.903114	-37.209625	-34.660119
	2	-17.261409	-14.471180	-15.485253
4	0	-47.633023	-49.200602	-47.633023
	1	-40.600594	-42.805414	-40.532111
	2	-29.156011	-30.015039	-28.697241
	3	-14.006306	-10.829476	-12.128416
5	0	-48.395881	-49.488385	-48.395881
	1	-43.608629	-45.395465	-43.583538
	2	-35.724757	-37.209625	-35.562954
	3	-24.941503	-24.930865	-24.334132
	4	-11.765276	-8.559185	-9.897072
6	0	-48.841863	-49.644712	-48.841863
	1	-45.378370	-46.802406	-45.367462
	2	-39.645688	-41.117795	-39.576786
	3	-31.718607	-32.590878	-31.469836
	4	-21.749954	-21.221656	-21.046612
	5	-10.123111	-7.010128	-8.307115

For a representative calculation, the mass parameter has been taken as the nuclear mass and two values of the depth parameter (V_0), namely 50 MeV and 60 MeV have been chosen. For each of these values of V_0, four values of the width parameter (a), viz; $a = 3, 4, 5$ and 6 fm, have been taken. The number of bound states increases as $V_0 a^2$ increases. The values of V_0 and a are so chosen that a fairly large number of bound states exists, facilitating a critical comparison of the exact, WKB and SWKB energies. The results are presented in Table 1 and Table 2. The first column lists the value of a, next column gives the excitation quantum number (n). The third, fourth and fifth columns present the exact, WKB and SWKB energies, respectively.

From the tables, it is seen that in general the SWKB energies are more precise than the WKB energies. However, the WKB results for the low-lying states are below the exact energies, while those for the high-lying states near the top of the well are above the exact energies. As a consequence, the WKB results for some intermediate values of n are quite accurate. Examples of this are provided by $n = 3$ state with V_0=50, a=5 or n=4 state with V_0=50, a=6 and n=4, 5 states with V_0=60, a=6. The SWKB results are always larger than the corresponding exact values, the error increasing as the excitation increases. Once again the error for the states lying near the top of the well is large, while that for the low-lying states is quite small. As discussed earlier, the SWKB result for the ground state turns out to be exact. The observation that the error in both WKB and SWKB energies for the states lying near the top of the well is large is a standard feature for the WKB method. This is because such states have a small negative energy (in the original scale) and so α is small (see Eq. (16)). Hence the wave function spills considerably outside the well, [Eq. (18)], which is contrary to the semiclassical picture.

TABLE 2. Comparison of exact, WKB and SWKB energies (in MeV*) for* $V_0 = 60$ MeV.

a(fm)	n	exact energy	WKB energy	SWKB energy
3	0	-56.040323	-58.578847	-56.040323
	1	-44.357233	-47.209625	-44.161324
	2	-25.746563	-24.471181	-24.362965
4	0	-57.573619	-59.200602	-57.573619
	1	-50.349141	-52.805414	-50.294495
	2	-38.522252	-40.015039	-38.162603
	3	-22.587963	-20.829477	-21.177948
5	0	-58.363064	-59.488385	-58.363064
	1	-53.472149	-55.395465	-53.452270
	2	-45.394360	-47.209625	-45.267601
	3	-36.274649	-34.930865	-33.809060
	4	-20.438938	-18.559185	-19.076647
6	0	-58.821855	-59.644712	-58.821855
	1	-55.296025	-56.802406	-55.287430
	2	-49.450588	-51.117795	-49.396712
	3	-41.341562	-42.590878	-41.149704
	4	-31.075454	-31.221656	-30.546406
	5	-18.879021	-17.010128	-17.586782

5. Summary and conclusions

The SWKB is known to produce exact results for potentials which are shape-invariant through the translation of one or more parameters. We have applied both the SWKB and the WKB approximations to a simple one-dimensional finite square well potential for which analytic treatment is possible and an analytic expression for the superpotential is obtained. But this potential is not shape invariant. Consequently, SWKB is not expected to produce exact energies, which agree with our calculation. However, the errors of the energies are quite small, particularly for the low-lying states. In almost all cases, the SWKB approximation turns out to be better than the WKB results.

Thus, the SWKB is a better approximation than the WKB even for potentials that are not shape-invariant but have a discrete, well separated energy spectrum and the superpotential is obtained analytically.

Acknowledgements

The author wishes to acknowledge financial assistance from the University Grants Commission (UGC) for a senior research fellowship (SRF).

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USPOREDBA SKWB I WKB APROKSIMACIJA ZA KONAČNU PRAVOKUTNU JAMU

Razmatraju se Wentzel-Kramers-Brillouin (WKB) i suprasimetrična WKB (SWKB) aproksimacija za pravokutnu jamu konačne dubine, te uspoređuju s rezultatima točnih računa. Iako promatrani potencijal nije invarijantan po obliku, moguće je analitičko rješenje za suprapotencijal te se nalazi da su rješenja SWKB točnija nego rješenja WKB.