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Reformulation of SWKB quantization condition for quasi-degeneracy in one dimension involving oscillating superpotential

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Abstract. Usual prescriptions for the supersymmetric Wentzel–Kramers–Brillouin (SWKB) formulation are applicable either in the case of broken or unbroken supersymmetry. However, they fail for one-dimensional potentials where there is a mixture of broken and unbroken supersymmetry, which corresponds to an oscillating superpotential. Such a situation arises when two or more identical wells interact by tunnelling through a potential barrier, exhibiting quasi-degeneracy. The simplest examples of twofold quasi-degeneracy are the double oscillator well and the double finite square well which are also very important from the point of view of application in real physics problems. The quasi-degenerate states are associated with six supersymmetric turning points in contrast with four classical turning points. This disagreement in the number of classical and supersymmetric turning points is responsible for the failure of the usual SWKB formulation and makes the case more interesting. Here we propose a modified version of the SWKB formulation using the partner potential to calculate the quasi-degenerate states. We apply our reformulated SWKB prescription to the double finite square well, which gives an excellent result.

The key ingredient of supersymmetric quantum mechanics (SSQM) is to build a partner potential $V_2(x)$, corresponding to a given $V_1(x)$, which has the same eigen spectrum as $V_1(x)$, except the absence of the ground state of $V_1(x)$. It gives a better understanding of the analytical solvability of some well known potentials [1,2]. Later, Comtet *et al* [3] applied this technique to the Wentzel–Kramers–Brillouin (WKB) approximation method and developed a supersymmetric WKB (SWKB) quantization condition, and also showed that the lowest-order SWKB quantization gives the exact spectrum for all shape-invariant potentials (SIPs) [4]. For such potentials, all higher-order contributions vanish identically [5]. Although the lowest-order SWKB is not exact for the excited states of non-SIPs [6], it is much better than the standard WKB approximation. Recently the concept of supersymmetry has been applied in coupled systems [7].

In all these works, the SWKB formalism was applied either to the case of a broken or an unbroken supersymmetry. In the case of an unbroken supersymmetry the SWKB turning points (x_1, x_2) are determined by $-W(x_1) = W(x_2) = \sqrt{E}$, i.e., the superpotential has opposite signs at the two turning points. However, in the case of a broken supersymmetry, the superpotential has the same sign at the two turning points and is determined by $W(x_1) = W(x_2) = \pm\sqrt{E}$. In this paper, we address the question of the formulation of an SWKB quantization condition in the case where there is a mixture of broken and unbroken supersymmetry. This mixing appears for a quasi-degenerate spectrum, for which two or more identical wells interact by

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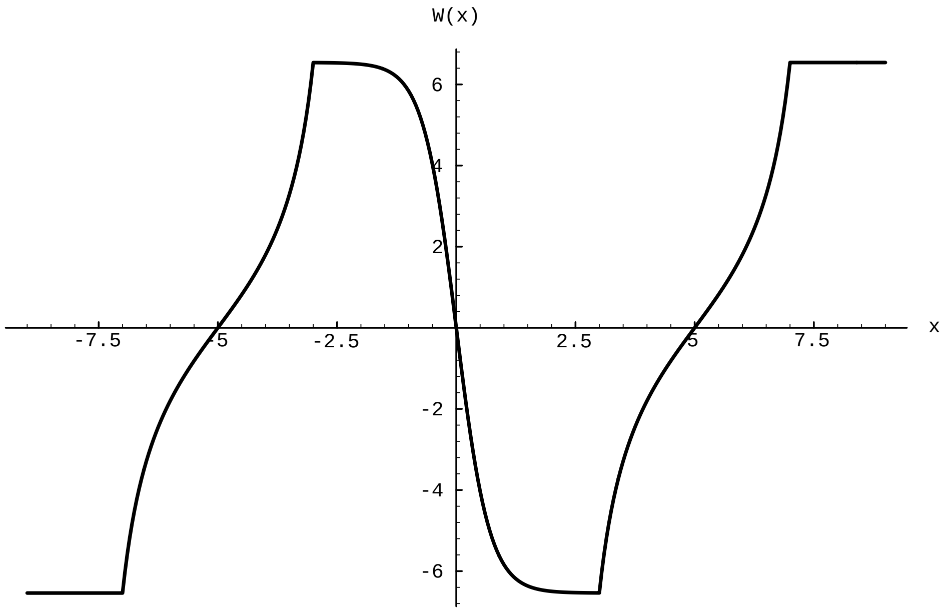

Figure 1. Plot of oscillating superpotential $W(x)$ for the double finite square well with $a = 6$ fm and $b = 4$ fm.

tunnelling through one or more inter-well barriers. As we will see later, this corresponds to an oscillating superpotential causing a mixture of unbroken and broken supersymmetry for the SWKB turning points. An important example is the double oscillator (which has extensive applications in many branches of physics, e.g. vibration of the ammonia molecule) or double finite square well (which can be extended to multiple finite square wells for producing band structure in solid state physics), where twofold degeneracy appears due to an interaction between two identical wells separated by a central barrier.

In the cases of SIPs and also for non-SIPs, having only two classical turning points (a_1, a_2), given by $V(a_1) = V(a_2) = E$, quasi-degeneracy does not appear and $W(x)$ is a monotonically varying odd function of x. In such cases, there are only two SWKB turning points (x_1, x_2), given by $-W(x_1) = W(x_2) = \sqrt{E}$, and supersymmetry is unbroken. Then the transition from the WKB quantization condition to the SWKB quantization condition is straightforward and one replaces $\int_{a_1}^{a_2} \sqrt{\frac{2m}{\hbar^2}(E - V(x))}\, \mathrm{d}x$ of the WKB method by $\int_{x_1}^{x_2} \sqrt{\frac{2m}{\hbar^2}(E - W^2(x))}\, \mathrm{d}x + \frac{\pi}{2}$ for the SWKB approximation [4,9]. It is interesting to note that for all these cases the number of supersymmetric turning points is the same as the number of classical turning points. However, in the case of the double oscillator [8] or double finite square well, the potential $V(x)$ has four classical turning points. The superpotential $W(x)$ is not a monotonically varying function, but shows a typical one-cycle oscillation and has six supersymmetric turning points for the low-lying quasi-degenerate pairs of states (see figure 1, which is a plot of $W(x)$ for the double finite square well). Oscillation of the superpotential is a necessary consequence of the quasi-degeneracy. For a two-fold quasi-degeneracy in one dimension, the ground state wave function $(\psi_0(x))$ must have two peaks (but no nodes) corresponding to large and equal position probability densities in two locations, and hence three extrema in $\psi_0(x)$. Then the superpotential, $W(x) = -\frac{\hbar}{\sqrt{2m}} \frac{\psi_0'(x)}{\psi_0(x)}$, will have three zeros, exhibiting one complete oscillation. In this case, the number of SWKB turning points (given, in general, by $W^2(x_i) = E$ for the ith

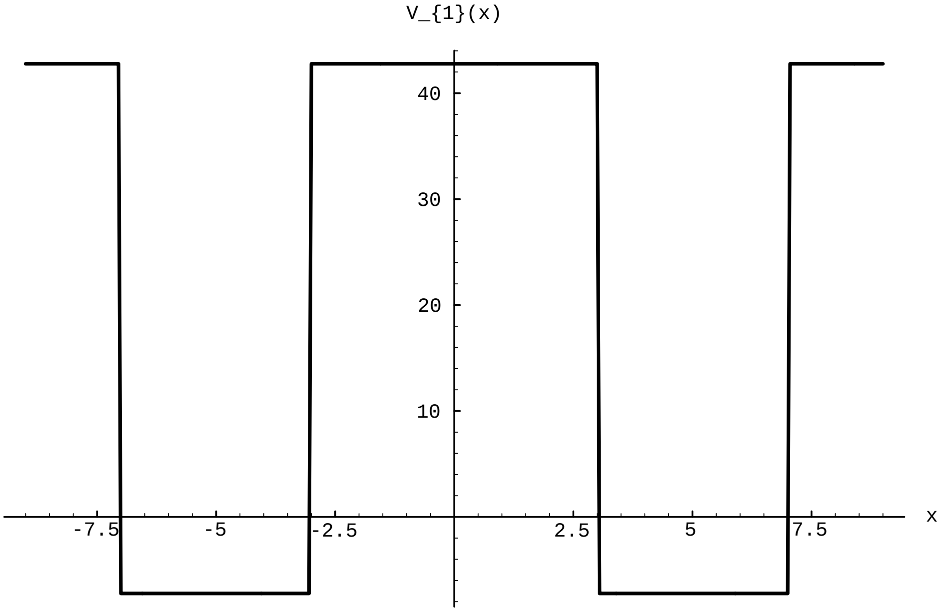

Figure 2. Plot of the calculated partner potential $V_1(x)$ (reproducing $V(x)$ in a shifted energy scale), showing four classical turning points.

SWKB turning point) is six. The number of classical turning points, on the other hand, will be four. The numbers of supersymmetric and classical turning points only match when there is no quasi-degeneracy; for this case $\psi_0(x)$ has only one maximum and $W(x)$ is a monotonically varying odd function having only one zero.

Thus, a mismatch in the number of classical and SWKB turning points is an inherent property of the quasi-degeneracy in one dimension and the associated oscillation in $W(x)$. In such a situation, we can formulate a WKB quantization condition for four classical turning points by the usual prescription found in text books of quantum mechanics [10], but cannot correlate six supersymmetric turning points with four classical turning points. Hence the usual SWKB procedure fails. We seek an alternative formulation.

As an example, we choose a double finite square well

$$V(x) = \left\{ \begin{array}{lllll} -V_0 & \text{for} & -(\frac{a}{2}+b) \leqslant x \leqslant -\frac{a}{2} & \text{and} & \frac{a}{2} \leqslant x \leqslant (\frac{a}{2}+b) \\ 0 & \text{otherwise} & & & \end{array} \right\} \tag{1}$$

Here b is the width of each square well of depth V_0, which are separated by a distance a. The choice of this potential over the double oscillator well has the advantage that $W(x)$ is given by an analytic expression for the former only. On the other hand, both have the same qualitative features, namely, quasi-degeneracy and an oscillatory superpotential. Both are non-SIPs. In figure 1 we plot the superpotential $W(x)$ for the double finite square well. The calculated partner potentials $V_1(x)$ and $V_2(x)$ (in the energy scale, shifted by the ground state energy of $V(x)$) are shown in figure 2 and 3, respectively. Note that $V_2(x)$ also has finite discontinuities of magnitude V_0 at $x = \pm\frac{a}{2}$ and $x = \pm(\frac{a}{2}+b)$. Both $V_1(x)$ and $V_2(x)$ have been calculated using the superpotential $W(x)$ given by equation (16) (see later). The potential $V_1(x)$ presents four classical turning points (a_1, a_2, a_3, a_4) and the WKB quantization condition for the case

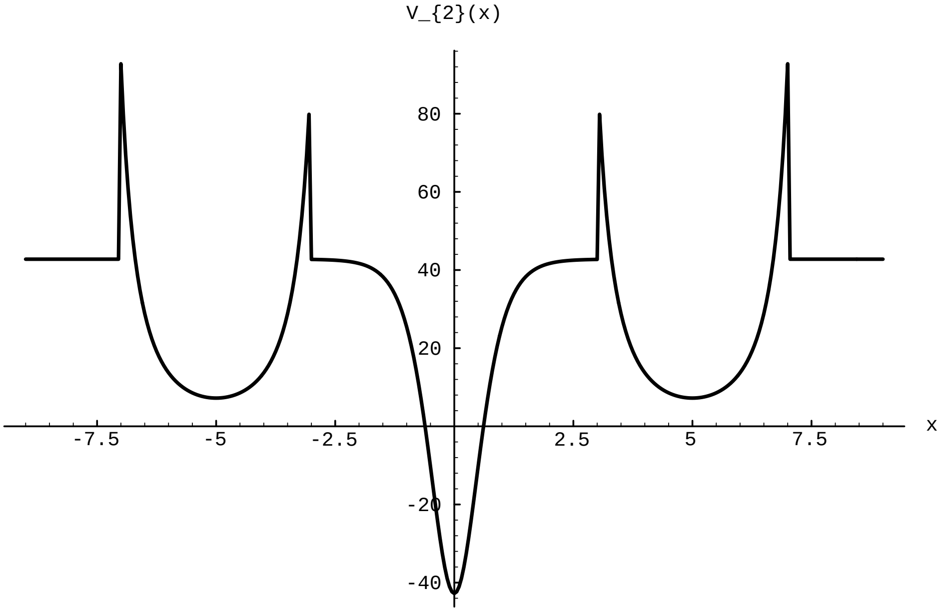

Figure 3. Plot of the calculated partner potential $V_2(x)$ showing six classical turning points.

is [11]

$$\left(\sin\int_{a_1}^{a_2} k(x)\,\mathrm{d}x\right)\left(\exp - \int_{a_2}^{a_3} K(x)\,\mathrm{d}x\right)\left(\sin\int_{a_3}^{a_4} k(x)\,\mathrm{d}x\right)$$
$$-4\left(\cos\int_{a_1}^{a_2} k(x)\,\mathrm{d}x\right)\left(\exp\int_{a_2}^{a_3} K(x)\,\mathrm{d}x\right)\left(\cos\int_{a_3}^{a_4} k(x)\,\mathrm{d}x\right) = 0 \qquad (2)$$

where

$$k(x) = \sqrt{\frac{2m}{\hbar^2}(E - V_1(x))} \qquad (E > V_1(x)) \qquad (3)$$

and

$$K(x) = \sqrt{\frac{2m}{\hbar^2}(V_1(x) - E)} \qquad (E < V_1(x)). \qquad (4)$$

Since along x there are some regions which are accessible ($E > V(x)$) using the WKB formulation but inaccessible ($E < W^2(x)$) using the SWKB formulation (figure 4) and vice versa, we cannot follow the process of transition from WKB to SWKB, and also cannot correlate between the four classical and six supersymmetric turning points.

How can we solve the riddle and formulate the SWKB prescription when $W(x)$ has an oscillation? Again, we use SSQM to find the solution. SSQM asserts that knowing the superpotential $W(x)$ in terms of the ground state wave function $\psi_0(x)$, one can form two partner potentials:

$$V_1(x) = W^2(x) - \frac{\hbar}{\sqrt{2m}} W'(x) \qquad (5)$$

and

$$V_2(x) = W^2(x) + \frac{\hbar}{\sqrt{2m}} W'(x). \qquad (6)$$

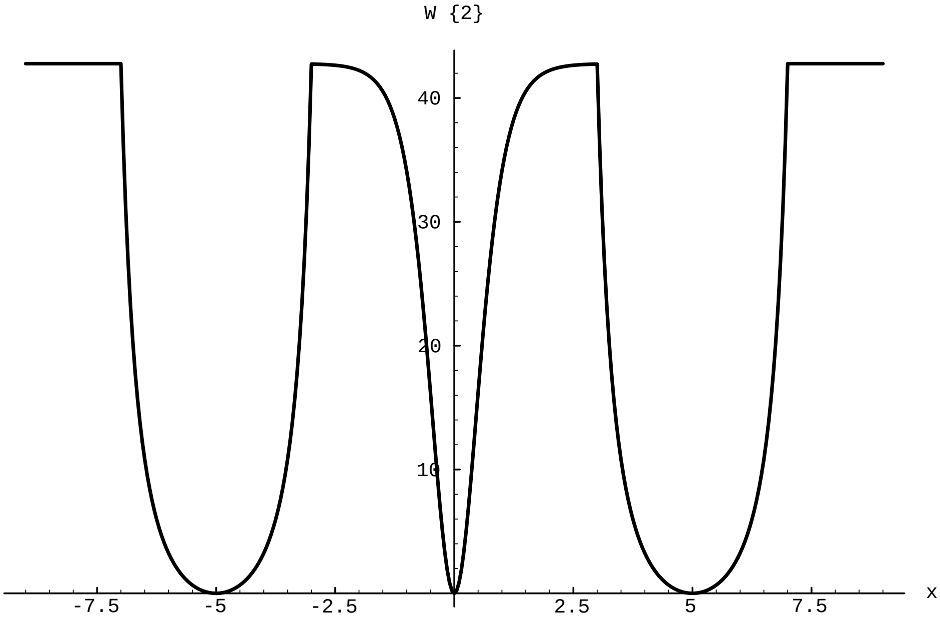

Figure 4. Plot of $W^2(x)$ showing that all quasi-degenerate states have six SWKB turning points.

Then $V_1(x)$ and $V_2(x)$ have the same eigenspectra except that the ground state of $V_1(x)$ is absent in the spectrum of $V_2(x)$. Here $V_1(x)$ is our starting potential (in the shifted energy scale), having four classical turning points. A plot of $V_2(x)$ against x (figure 3) shows that it has six classical turning points. Since the number of classical turning points for $V_2(x)$ and supersymmetric turning points of $W(x)$ match, we can make a transition from the WKB procedure for $V_2(x)$ to the SWKB quantization condition by the standard procedure and will be able to calculate all the energy levels of $V_1(x)$ by the supersymmetric level degeneracy relation

$$E_{n+1}^{(1)} = E_n^{(2)} \qquad (n = 0, 1, 2, \ldots) \tag{7}$$

where $E_n^{(i)}$ is the energy of the nth state of $V_i(x)$ $(i = 1, 2)$, in an energy scale which is shifted by the ground state energy of $V(x)$, such that $E_0^{(1)} = 0$. We will see later that the ground state energy of $V_1(x)$ is correctly reproduced by the reformulated SWKB procedure.

The WKB quantization condition for six turning points (a_1, a_2, a_3, a_4, a_5, a_6) can be obtained by the standard WKB procedure connecting across the six turning points and has the following form:

$$\begin{aligned}
\tfrac{1}{2}&\left(\sin\int_{a_1}^{a_2} k(x)\,\mathrm{d}x\right)\left(\exp-\int_{a_2}^{a_3} K(x)\,\mathrm{d}x\right)\left(\cos\int_{a_3}^{a_4} k(x)\,\mathrm{d}x\right)\\
&\times\left(\exp-\int_{a_4}^{a_5} K(x)\,\mathrm{d}x\right)\left(\sin\int_{a_5}^{a_6} k(x)\,\mathrm{d}x\right)\\
&+2\left(\sin\int_{a_1}^{a_2} k(x)\,\mathrm{d}x\right)\left(\exp-\int_{a_2}^{a_3} K(x)\,\mathrm{d}x\right)\left(\sin\int_{a_3}^{a_4} k(x)\,\mathrm{d}x\right)\\
&\times\left(\exp\int_{a_4}^{a_5} K(x)\,\mathrm{d}x\right)\left(\cos\int_{a_5}^{a_6} k(x)\,\mathrm{d}x\right)
\end{aligned}$$

$$
\begin{aligned}
&+2\left(\cos\int_{a_1}^{a_2} k(x)\,\mathrm{d}x\right)\left(\exp\int_{a_2}^{a_3} K(x)\,\mathrm{d}x\right)\left(\sin\int_{a_3}^{a_4} k(x)\,\mathrm{d}x\right)\\
&\times\left(\exp-\int_{a_4}^{a_5} K(x)\,\mathrm{d}x\right)\left(\sin\int_{a_5}^{a_6} k(x)\,\mathrm{d}x\right)\\
&-8\left(\cos\int_{a_1}^{a_2} k(x)\,\mathrm{d}x\right)\left(\exp\int_{a_2}^{a_3} K(x)\,\mathrm{d}x\right)\left(\cos\int_{a_3}^{a_4} k(x)\,\mathrm{d}x\right)\\
&\times\left(\exp\int_{a_4}^{a_5} K(x)\,\mathrm{d}x\right)\left(\cos\int_{a_5}^{a_6} k(x)\,\mathrm{d}x\right)=0
\end{aligned}
\tag{8}
$$

where $k(x)$ and $K(x)$ have the same meaning as before (cf equations (3) and (4)). From equation (8) one notices that the WKB quantization condition involves both classically accessible and inaccessible regions. For the accessible regions $a_i < x < a_{i+1}$ (with $i = 1, 3, 5$), the SWKB turning points are given by $-W(x_i) = W(x_{i+1}) = \sqrt{E^{\mathrm{SWKB}}}$ (unbroken supersymmetry), where E^{SWKB} is the SWKB energy. Then we have [12]

$$
\begin{aligned}
\int_{a_i}^{a_{i+1}} \sqrt{\frac{2m}{\hbar^2}(E_n^{(2)} - V_2(x))}\,\mathrm{d}x &= \int_{a_i}^{a_{i+1}} \sqrt{\frac{2m}{\hbar^2}\left(E_n^{(2)} - W^2(x) - \frac{\hbar}{\sqrt{2m}}W'\right)}\,\mathrm{d}x\\
&= \int_{x_i}^{x_{i+1}} \sqrt{\frac{2m}{\hbar^2}(E_n^2 - W^2(x))}\,\mathrm{d}x - \frac{\pi}{2} \qquad (i = 1, 3, 5)
\end{aligned}
\tag{9}
$$

For inaccessible regions $a_i < x < a_{i+1}$ (with $i = 2, 4$), supersymmetry is broken and $W(x_i) = W(x_{i+1}) = \pm\sqrt{E^{\mathrm{SWKB}}}$, and we have [12]

$$
\int_{a_i}^{a_{i+1}} \sqrt{\frac{2m}{\hbar^2}(V_2(x) - E_n^{(2)})}\,\mathrm{d}x = \int_{x_i}^{x_{i+1}} \sqrt{\frac{2m}{\hbar^2}(W^2(x) - E_n^{(2)})}\,\mathrm{d}x \qquad (i = 2, 4)
\tag{10}
$$

The contribution of $W'(x)$ in the above equation vanishes identically [12]. Substituting these equations into the WKB quantization condition (equation (8)), the SWKB quantization condition for potentials showing six SWKB turning points ($x_1, x_2, x_3, x_4, x_5, x_6$) becomes

$$
\begin{aligned}
&\tfrac{1}{2}\left(\cos\int_{x_1}^{x_2} \gamma\,\mathrm{d}x\right)\left(\exp-\int_{x_2}^{x_3} \delta\,\mathrm{d}x\right)\left(\sin\int_{x_3}^{x_4} \gamma\,\mathrm{d}x\right)\\
&\quad\times\left(\exp-\int_{x_4}^{x_5} \delta\,\mathrm{d}x\right)\left(\cos\int_{x_5}^{x_6} \gamma\,\mathrm{d}x\right)\\
&\quad+2\left(\cos\int_{x_1}^{x_2} \gamma\,\mathrm{d}x\right)\left(\exp-\int_{x_2}^{x_3} \delta\,\mathrm{d}x\right)\left(\cos\int_{x_3}^{x_4} \gamma\,\mathrm{d}x\right)\\
&\quad\times\left(\exp\int_{x_4}^{x_5} \delta\,\mathrm{d}x\right)\left(\sin\int_{x_5}^{x_6} \gamma\,\mathrm{d}x\right)\\
&\quad+2\left(\sin\int_{x_1}^{x_2} \gamma\,\mathrm{d}x\right)\left(\exp\int_{x_2}^{x_3} \delta\,\mathrm{d}x\right)\left(\cos\int_{x_3}^{x_4} \gamma\,\mathrm{d}x\right)\\
&\quad\times\left(\exp-\int_{x_4}^{x_5} \delta\,\mathrm{d}x\right)\left(\cos\int_{x_5}^{x_6} \gamma\,\mathrm{d}x\right)\\
&\quad-8\left(\sin\int_{x_1}^{x_2} \gamma\,\mathrm{d}x\right)\left(\exp\int_{x_2}^{x_3} \delta\,\mathrm{d}x\right)\left(\sin\int_{x_3}^{x_4} \gamma\,\mathrm{d}x\right)\\
&\quad\times\left(\exp\int_{x_4}^{x_5} \delta\,\mathrm{d}x\right)\left(\sin\int_{x_5}^{x_6} \gamma\,\mathrm{d}x\right)=0
\end{aligned}
\tag{11}
$$

where

$$
\gamma = \sqrt{\frac{2m}{\hbar^2}(E^{\mathrm{SWKB}} - W^2)} \qquad \delta = \sqrt{\frac{2m}{\hbar^2}(W^2 - E^{\mathrm{SWKB}})}
\tag{12}
$$

Note that $\int_{x_i}^{x_{i+1}} \alpha\, \mathrm{d}x = 0$, for $i = 1, 3, 5$, satisfy equation (11) identically—this is possible when x_i and x_{i+1} ($i = 1, 3, 5$) coalesce, corresponding to $E_0^{\mathrm{SWKB}} = 0$, where E_n^{SWKB} is the SWKB energy for the nth state of $V_1(x)$ (see figure 4). Thus the ground state of $V_1(x)$ is again reproduced exactly, even for the oscillatory superpotential. The double finite square well is an exceptional case, where all the bound states are quasi-degenerate and have six turning points, whereas for the double oscillator only the low-lying states are quasi-degenerate.

Exact solutions of the double finite square well can be obtained by standard quantum mechanics. The energy eigenvalues are obtained from the transcendental equations

$$\sqrt{\frac{B}{V_0 - B}} \tanh\left(\frac{a}{2}\sqrt{\frac{2mB}{\hbar^2}}\right) = \tan\left\{b\sqrt{\frac{2m}{\hbar^2}(V_0 - B)} - \tan^{-1}\left(\sqrt{\frac{B}{V_0 - B}}\right)\right\} \qquad \text{(for even parity)} \tag{13}$$

and

$$\sqrt{\frac{B}{V_0 - B}} \coth\left(\frac{a}{2}\sqrt{\frac{2mB}{\hbar^2}}\right) = \tan\left\{b\sqrt{\frac{2m}{\hbar^2}(V_0 - B)} - \tan^{-1}\left(\sqrt{\frac{B}{V_0 - B}}\right)\right\} \qquad \text{(for odd parity)} \tag{14}$$

where

$$\alpha = \sqrt{\frac{2mB}{\hbar^2}} \qquad \beta = \sqrt{\frac{2m}{\hbar^2}(V_0 - B)} \tag{15}$$

and $B = -E$ is the binding energy. The superpotential is obtained from the ground state wave function (even parity) and is given by

$$W(x) = \left\{\begin{array}{cc} -\frac{\hbar}{\sqrt{2m}}\alpha_0 \tanh(\alpha_0 x) & 0 \leqslant x \leqslant \frac{a}{2} \\ -\frac{\hbar}{\sqrt{2m}}\beta_0 \tan\{\beta_0(d - x) - \tan^{-1}(\frac{\alpha_0}{\beta_0})\} & \frac{a}{2} \leqslant x \leqslant d \\ \frac{\hbar}{\sqrt{2m}}\alpha_0 & d \leqslant x \end{array}\right\} \tag{16}$$

where $d = \frac{a}{2} + b$ and

$$\alpha_0 = \sqrt{\frac{2mB_0}{\hbar^2}} \qquad \beta_0 = \sqrt{\frac{2m}{\hbar^2}(V_0 - B_0)} \tag{17}$$

where B_0 denotes the ground state binding energy, which is the lowest solution for B of equations (13) and (15). We solve the SWKB quantization condition given by equations (11) and (12) for energy (E_{SWKB}, n), where $W(x)$ is given by equation (16).

We compare the SWKB energy with the exact energy solution of equations (15) and either (13) or (14). For a further comparison with the WKB approximation, we use the WKB quantization condition for $V(x)$, which has only four classical turning points and hence solve equation (2) with equations (3) and (4) numerically. For the numerical solution, we use a preliminary bisection method followed by a Newton–Raphson method [13], to reach a precision of up to 9 significant digits—the units are chosen suitably according to convenience. In table 1, we present the exact, WKB and SWKB results for three representative values of a (the width of the barrier between the wells) $= 5, 6, 7$ (fm) and for a fixed value of b (the width of each well) $= 4$ (fm). The depth of the potential (V_0) is chosen as 50 Mev for each case and the unit is chosen $\frac{\hbar^2}{2m} = 20$ Mev fm^2. All the energy values in table 1 are given in the original (unshifted) scale. As a increases, the degeneracy effect becomes more pronounced

Table 1. Comparision of exact, WKB and SWKB energies (MeV) for the double finite square well ($V_0 = 50$ Mev, $b = 4$ fm).

a	n	Exact energy	WKB energy	SWKB energy
5	0	−42.774 9435	−46.803 5145	−42.774 9435
	1	−42.770 0854	−46.801 2895	−42.590 7551
	2	−22.498 0129	−21.260 2471	−21.805 7056
	3	−22.409 6970	−21.182 6106	−21.641 7171
6	1	−42.773 0918	−46.802 6504	−42.773 0918
	2	−42.771 9365	−46.802 1551	−42.609 7884
	3	−22.469 6684	−21.235 7057	−21.727 8001
	4	−22.438 4736	−21.207 4769	−21.668 0305
7	0	−42.772 6515	−46.802 4574	−42.772 6515
	1	−42.772 3767	−46.802 3473	−42.628 7700
	2	−22.459 6124	−21.226 7489	−21.698 7191
	3	−22.448 5934	−21.216 4847	−21.677 0231

(especially for the lowest-lying states), since the two wells are then separated by a larger distance and the interference effect is weak. Since the double finite square well is a non-SIP, we cannot expect that the SWKB quantization condition given by equations (11) and (12) will produce exact results as in the case of SIPs with monotonically varying $W(x)$. In the SWKB quantization condition, equation (11), we have kept only the term of order $\hbar$, which is again an approximation. Unlike the case of SIPs, the contribution of terms of higher order in $\hbar$ will not vanish identically. Here only the ground state is exactly reproduced. From table 1, we see that the first-order SWKB results are much better than the first-order WKB results and the quasi-degeneracy is fairly well reproduced.

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