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The connection between classical and supersymmetric turning points for multifold quasi-degenerate problems in one dimension

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Abstract

Matching between numbers of classical and supersymmetric turning points is the key point for the transition from the Wentzel–Kramers–Brillouin (WKB) to the supersymmetric WKB (SWKB) quantization condition. But mismatch between these numbers for quasi-degenerate problems challenges the traditional transition from WKB to SWKB methods. Here we resolve this problem for the n-fold quasi-degenerate case by suggesting a transition from the WKB quantization condition for the supersymmetric partner potential to the SWKB quantization condition. Our explicit example of threefold quasi-degeneracy nicely demonstrates the procedure proposed here.

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1. Introduction

A large variety of potentials are encountered in various branches of physics where exact analytic solutions of the Schrödinger equation are not possible; then one has to resort to approximation methods such as perturbation, variation or WKB methods. Among these, the WKB [1] method is the most useful since it can be applied to 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* [2] applied the concept of supersymmetric quantum mechanics (SSQM) [3] to the WKB method and proposed a modified semiclassical quantization condition known as the supersymmetric WKB (SWKB) condition which yields the exact eigenspectrum for all known shape-invariant potentials (SIPs) [4]. The accuracy of the lowest-order SWKB (LSWKB) quantization condition for non-SIPs is also remarkable [5, 6]. The LSWKB method has also been applied successfully to tunnelling

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problems [7]. The transition from the lowest-order WKB (LWKB) method to the LSWKB method is quite straightforward for single-well and single-barrier problems, where one can associate two SWKB turning points with two WKB turning points. But this transition following the simple association breaks down when there is quasi-degeneracy. Exact degeneracy does not appear in one dimension; however, quasi-degenerate states appear when two or more identical wells interact by tunnelling through intervening potential barriers. For quasi-degenerate states, the number of SWKB turning points exceeds the number of WKB turning points due to the superpotential having a number of oscillations. So a straightforward transition from the LWKB to the LSWKB condition is not possible. Mismatch between WKB and SWKB turning points challenges the straightforward transition and makes the problem more interesting. Recently we have studied the case of a double finite square well [8] and that of a double harmonic oscillator well [6]. Both of them exhibit twofold quasi-degeneracy; while the number of WKB turning points is four, the number of SWKB turning points is six. In [8], we proposed a reformulated SWKB quantization condition which successfully resolves the problem. But the situation becomes more complicated when multiple identical wells interact through intervening barriers exhibiting multifold quasi-degeneracy. A generalized procedure for transition from the WKB to the SWKB quantization condition—each having a different number of turning points—for an n-fold quasi-degenerate case has not been found so far. In [10], Milczarski and Giller have studied the exactness of conventional and supersymmetric JWKB formulae. But the most general questions of why the traditional WKB to SWKB transition procedure fails for multifold quasi-degeneracy and how to correlate SWKB turning points with WKB ones have not been answered clearly. In this paper we present a general survey using the wavefunction ansatz technique. We observe that the number of SWKB turning points *always* matches the number of classical turning points of the supersymmetric partner potential, $V_2(x)$. This leads to a general prescription for obtaining the SWKB quantization condition from the WKB quantization condition for $V_2(x)$ for quasi-degenerate cases. We also present an explicit example of a threefold quasi-degenerate problem to nicely demonstrate our prescription.

The paper is organized as follows. In section 2, we briefly review the LSWKB quantization condition for the single well and the single barrier. In section 3, we present the example of threefold quasi-degeneracy. In section 4 we generalize to the case of n-fold quasi-degeneracy. Lastly, in section 5, we draw our conclusions and also focus on some of the implications.

2. Transition from the LWKB to the LSWKB condition

In the lowest order, the WKB quantization for a particle of mass m moving in the one-dimensional potential $V(x)$ is [1]

$$\int_a^b \sqrt{2m(E_n^{WKB} - V(x))}\,\mathrm{d}x = (n + \tfrac{1}{2})\pi\hbar \qquad (n = 0, 1, 2, \ldots), \tag{1}$$

where a and b are the classical turning points defined by $E_n^{WKB} = V(a) = V(b)$.

In SSQM, one replaces the potential $V(x)$ by the Riccati equation [3]

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

where $W(x)$ is called the superpotential and is defined in terms of the ground-state wavefunction $\psi_0(x)$: as

$$W(x) = -\frac{\hbar}{\sqrt{2m}} \frac{\psi_0'}{\psi_0}. \tag{3}$$

In equation (2), $V_1(x)$ is the original potential $V(x)$, but on a shifted energy scale such that its ground-state energy is zero. That is,

$$V_1(x) = V(x) - E_0 \tag{4}$$

where E_0 is the ground-state energy of $V(x)$. In terms of the superpotential (substituting the Riccati equation in (1)), the lowest-order SWKB quantization condition becomes [2]

$$\int_{x_1}^{x_2} \sqrt{2m(E_n^{(1)} - W^2(x))}\,\mathrm{d}x = n\pi\hbar \qquad (n = 0, 1, 2, \ldots) \tag{5}$$

where $E_n^{(1)}$ is the energy in the shifted energy scale and x_1 and x_2 are the SWKB turning points corresponding to the WKB turning points a and b, and are defined through

$$E_n^{(1)} = W^2(x_1) = W^2(x_2). \tag{6}$$

Of the two solutions, $W(x_1) = -W(x_2) = \sqrt{E_n^{(1)}}$ corresponds to unbroken supersymmetry [2, 3]. For broken supersymmetry the SWKB turning points are defined through $W(x_1) = W(x_2) = \sqrt{E_n^{(1)}}$ and the lowest-order SWKB quantization condition becomes [3]

$$\int_a^b \sqrt{\frac{2m}{\hbar^2}(V(x) - E_n^{WKB})}\,\mathrm{d}x \Rightarrow \int_{x_1}^{x_2} \sqrt{\frac{2m}{\hbar^2}(W^2(x) - E_n^{SWKB})}\,\mathrm{d}x. \tag{7}$$

In SSQM, one can construct a partner potential V_2 in terms of W:

$$V_2 = W^2 + \frac{\hbar}{\sqrt{2m}}W'. \tag{8}$$

The SSQM algebra shows that the two partners, V_1 and V_2, will have the same eigenspectrum except that the ground state of V_1 is missing in the spectrum of V_2 ($E_{n+1}^{(1)} = E_n^{(2)}$, $n = 0, 1, 2, \ldots$). The leading-order SWKB quantization condition for V_2 becomes [3]

$$\int_{x_1}^{x_2} \sqrt{2m(E_n^{(2)} - W^2(x))}\,\mathrm{d}x = (n+1)\pi\hbar \qquad (n = 0, 1, 2, \ldots). \tag{9}$$

Comparing equation (9) with (5), one notices that they are consistent with the level degeneracy ($E_{n+1}^{(1)} = E_n^{(2)}$, $n = 0, 1, 2, \ldots$). The lowest-order SWKB quantization condition has been successfully applied to various bound-state problems, such as the harmonic oscillator, Coulomb and Morse problems [3, 4], and also to one-dimensional barriers [9]. One can easily see that, in each of these cases, the superpotential has a monotonic nature, exhibiting either broken or unbroken supersymmetry, and the number of supersymmetric turning points always matches the number of classical turning points. But this nature changes drastically when $V(x)$ has two or more interacting wells. The superpotential becomes oscillating, losing its monotonic nature, and exhibits mixing of broken and unbroken supersymmetry. In [6, 8], we have studied two important examples exhibiting twofold quasi-degeneracy. One is the double harmonic oscillator [6] and the other one is the double finite square well [8]. In both cases, the superpotential exhibits one complete oscillation, having six SWKB turning points in contrast with the four WKB turning points of V_1. This immediately indicates the failure of the traditional transition scheme. In [8] we present an elegant alternative way to bypass the problem. Application of this reformulated SWKB quantization to the double finite square well nicely reproduces the twofold quasi-degenerate states [8]. In the following sections we study the threefold quasi-degenerate problem by using the wavefunction ansatz technique and generalize the connection between classical and supersymmetric turning points for n-fold quasi-degeneracy.

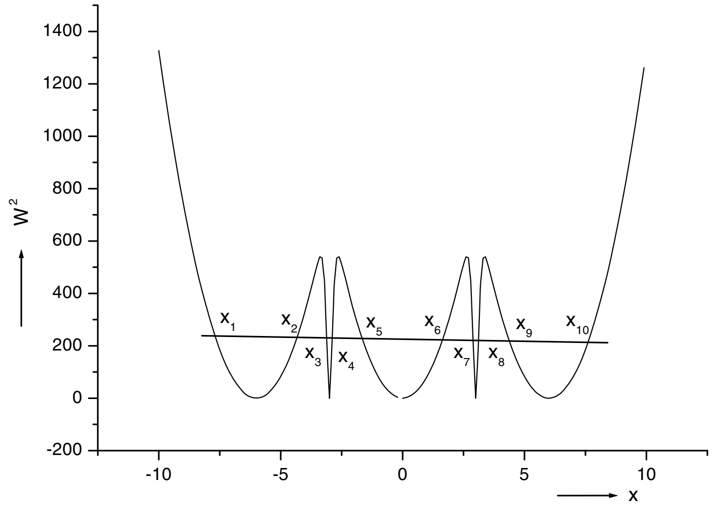

Figure 1. A plot of W^2 for three wells ($x_0 = 6$) showing ten SWKB turning points.

3. Threefold quasi-degeneracy

Here we use the wavefunction ansatz technique (i.e., start with a chosen ground-state wavefunction) to analytically build up the triple wells. We start with ψ_0 as the sum of three Gaussians representing three wells centred at $x = 0$, x_0 and $-x_0$:

$$\psi_0(x) = \mathrm{e}^{-(x-x_0)^2} + \mathrm{e}^{-x^2} + \mathrm{e}^{-(x+x_0)^2}. \tag{10}$$

We calculate W^2, V_1 and V_2 by using equations (3), (2) and (8), respectively and plot them in figures 1–3, respectively. It is easy to see that ten turning points of the superpotential do not match with six WKB turning points of the original potential V_1. So one cannot correlate them, because classically accessible regions become supersymmetrically inaccessible and vice versa. To solve this riddle we need the help of SSQM. The partner potential V_2 is isospectral with V_1. Figure 3 shows that the numbers of classical turning points for $V_2(x)$ and supersymmetric turning points of $W(x)$ match. So instead of V_1, we can use its partner V_2 and can make the transition from the WKB to SWKB condition in a straightforward way. All the energy levels of V_1 are obtained from the sypersymmetric level degeneracy:

$$E_{n+1}^{(1)} = E_n^{(2)} \qquad (n = 0, 1, 2, \ldots). \tag{11}$$

We first formulate the WKB quantization condition for ten turning points by the standard WKB procedure [1] and use the WKB to SWKB transitions to accessible and inaccessible regions separately. The accessible regions $a_i < x < a_{i+1}$ (with $i = 1, 3, 5, 7, 9$) correspond to unbroken supersymmetry where $-W(x_i) = W(x_{i+1}) = \sqrt{E^{SWKB}}$ and we have

$$\int_{a_i}^{a_{i+1}} \sqrt{\frac{2m}{\hbar^2}(E_n^{(2)} - V_2(x))}\,\mathrm{d}x = \int_{x_i}^{x_{i+1}} \sqrt{\frac{2m}{\hbar^2}(E_n^{(2)} - W^2(x))}\,\mathrm{d}x - \frac{\pi}{2} \qquad (i = 1, 3, 5, 7, 9). \tag{12}$$

The inaccessible regions $a_i < x < a_{i+1}$ (with $i = 2, 4, 6, 8$) correspond to broken supersymmetry where $W(x_i) = W(x_{i+1}) = \pm\sqrt{E^{SWKB}}$ and we have [3]

$$\int_{a_i}^{a_{i+1}} \sqrt{\frac{2m}{\hbar^2}(V_2(x) - E_n^{(2)})}\,\mathrm{d}x = \int_{x_i}^{x_{i+1}} \sqrt{\frac{2m}{\hbar^2}(W^2(x) - E_n^{(2)})}\,\mathrm{d}x \qquad (i = 2, 4, 6, 8). \tag{13}$$

Using the above transition procedure we get the SWKB quantization condition for the ten turning points $(x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10})$ as

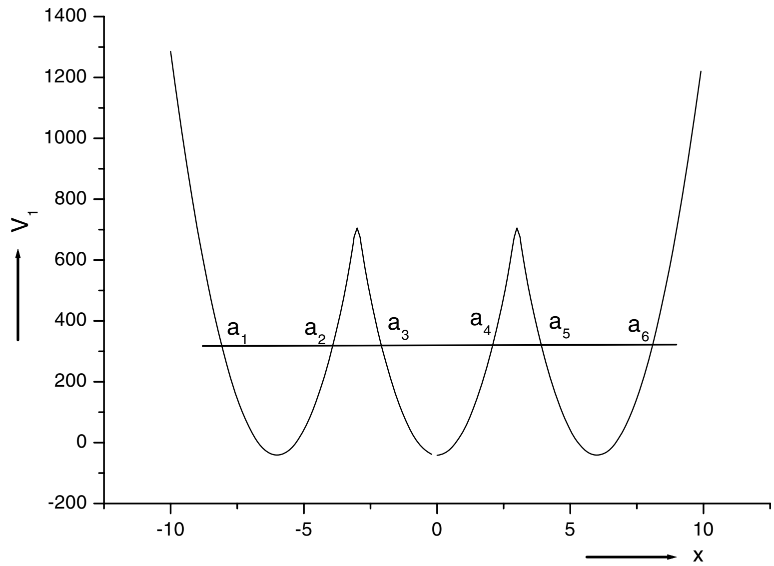

Figure 2. A plot of V_1 for three wells ($x_0 = 6$) showing six WKB turning points.

$$
\begin{aligned}
&-32\sin(I_1)\exp(J_2)\sin(I_3)\exp(J_4)\sin(I_5)\exp(J_6)\sin(I_7)\exp(J_8)\sin(I_9)\\
&+8\sin(I_1)\exp(J_2)\sin(I_3)\exp(J_4)\sin(I_5)\exp(J_6)\cos(I_7)\exp(-J_8)\cos(I_9)\\
&+8\sin(I_1)\exp(J_2)\sin(I_3)\exp(J_4)\cos(I_5)\exp(-J_6)\cos(I_7)\exp(J_8)\sin(I_9)\\
&+2\sin(I_1)\exp(J_2)\sin(I_3)\exp(J_4)\cos(I_5)\exp(-J_6)\sin(I_7)\exp(-J_8)\cos(I_9)\\
&+8\sin(I_1)\exp(J_2)\cos(I_3)\exp(-J_4)\cos(I_5)\exp(J_6)\sin(I_7)\exp(J_8)\sin(I_9)\\
&-2\sin(I_1)\exp(J_2)\cos(I_3)\exp(-J_4)\cos(I_5)\exp(J_6)\cos(I_7)\exp(-J_8)\cos(I_9)\\
&+2\sin(I_1)\exp(J_2)\cos(I_3)\exp(-J_4)\sin(I_5)\exp(-J_6)\cos(I_7)\exp(J_8)\sin(I_9)\\
&+\tfrac{1}{2}\sin(I_1)\exp(J_2)\cos(I_3)\exp(-J_4)\sin(I_5)\exp(-J_6)\sin(I_7)\exp(-J_8)\cos(I_9)\\
&+8\cos(I_1)\exp(-J_2)\cos(I_3)\exp(J_4)\sin(I_5)\exp(J_6)\sin(I_7)\exp(J_8)\sin(I_9)\\
&-2\cos(I_1)\exp(-J_2)\cos(I_3)\exp(J_4)\sin(I_5)\exp(J_6)\cos(I_7)\exp(-J_8)\cos(I_9)\\
&-2\cos(I_1)\exp(-J_2)\cos(I_3)\exp(J_4)\cos(I_5)\exp(-J_6)\cos(I_7)\exp(J_8)\sin(I_9)\\
&-\tfrac{1}{2}\cos(I_1)\exp(-J_2)\cos(I_3)\exp(J_4)\cos(I_5)\exp(-J_6)\sin(I_7)\exp(-J_8)\cos(I_9)\\
&+\tfrac{1}{2}\cos(I_1)\exp(-J_2)\sin(I_3)\exp(-J_4)\sin(I_5)\exp(-J_6)\cos(I_7)\exp(J_8)\sin(I_9)\\
&+\tfrac{1}{8}\cos(I_1)\exp(-J_2)\sin(I_3)\exp(-J_4)\sin(I_5)\exp(-J_6)\sin(I_7)\exp(-J_8)\cos(I_9)\\
&+2\cos(I_1)\exp(-J_2)\sin(I_3)\exp(-J_4)\cos(I_5)\exp(J_6)\sin(I_7)\exp(J_8)\sin(I_9)\\
&-\tfrac{1}{2}\cos(I_1)\exp(-J_2)\sin(I_3)\exp(-J_4)\cos(I_5)\exp(J_6)\cos(I_7)\exp(-J_8)\cos(I_9)=0
\end{aligned}
\tag{14}
$$

where

$$
\begin{aligned}
I_i &= \int_{x_i}^{x_{i+1}} \sqrt{\frac{2m}{\hbar^2}(E^{SWKB}-W^2)} \qquad (i = 1, 3, 5, 7, 9)\\
J_i &= \int_{x_i}^{x_{i+1}} \sqrt{\frac{2m}{\hbar^2}(W^2-E^{SWKB})} \qquad (i = 2, 4, 6, 8).
\end{aligned}
\tag{15}
$$

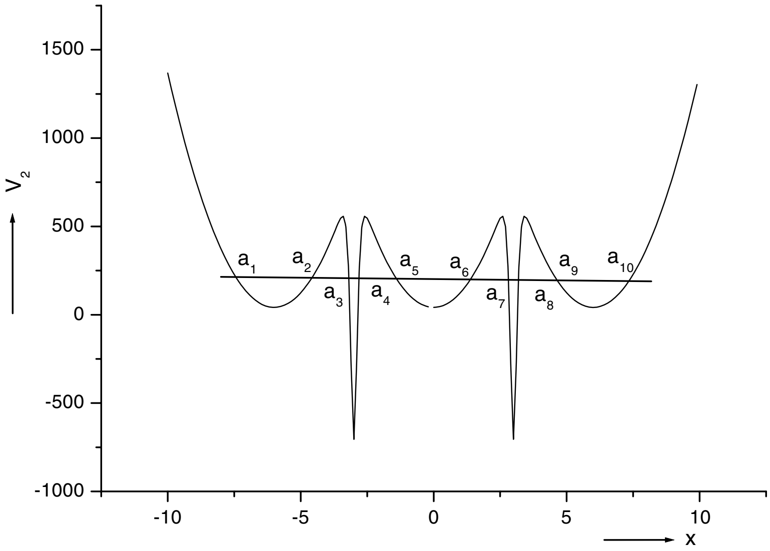

Figure 3. A plot of V_2 for three wells ($x_0 = 6$) showing ten WKB turning points.

We solve the SWKB quantization condition (equation (14)) using W given by equation (3) together with equation (10). The numerical results for a few low-lying triplet states are presented in table 1 for $x_0 = 6$ fm and $\hbar^2/2m = 20.735$ MeV fm^2. The parameters are so chosen as to make the degeneracy effect pronounced. For comparison, we present exact numerical results as well as the WKB results in the same table. The WKB results are obtained from the WKB quantization condition with six WKB turning points (TPs) given by

$$\begin{aligned}
\frac{1}{2}&\left(\sin\int_{a_1}^{a_2} k(x)\,\mathrm{d}x\right)\left(\exp-\int_{a_2}^{a_3} K(x)\,\mathrm{d}x\right)\left(\cos\int_{a_3}^{a_4} k(x)\,\mathrm{d}x\right)\\
&\times\left(\exp-\int_{a_4}^{a_5} K(x)\,\mathrm{d}x\right)\left(\sin\int_{a_5}^{a_6} k(x)\,\mathrm{d}x\right)\\
&+2\left(\sin\int_{a_1}^{a_2} k(x)\,\mathrm{d}x\right)\left(\exp-\int_{a_2}^{a_3} K(x)\,\mathrm{d}x\right)\left(\sin\int_{a_3}^{a_4} k(x)\,\mathrm{d}x\right)\\
&\times\left(\exp\int_{a_4}^{a_5} K(x)\,\mathrm{d}x\right)\left(\cos\int_{a_5}^{a_6} k(x)\,\mathrm{d}x\right)\\
&+2\left(\cos\int_{a_1}^{a_2} k(x)\,\mathrm{d}x\right)\left(\exp\int_{a_2}^{a_3} K(x)\,\mathrm{d}x\right)\left(\sin\int_{a_3}^{a_4} k(x)\,\mathrm{d}x\right)\\
&\times\left(\exp-\int_{a_4}^{a_5} K(x)\,\mathrm{d}x\right)\left(\sin\int_{a_5}^{a_6} k(x)\,\mathrm{d}x\right)\\
&-8\left(\cos\int_{a_1}^{a_2} k(x)\,\mathrm{d}x\right)\left(\exp\int_{a_2}^{a_3} K(x)\,\mathrm{d}x\right)\left(\cos\int_{a_3}^{a_4} k(x)\,\mathrm{d}x\right)\\
&\times\left(\exp\int_{a_4}^{a_5} K(x)\,\mathrm{d}x\right)\left(\cos\int_{a_5}^{a_6} k(x)\,\mathrm{d}x\right)=0
\end{aligned}\tag{16}$$

Table 1. Comparison of exact, WKB and SWKB energies (MeV) for the triple wells.

n	Exact energy	WKB energy	SWKB energy
1	82.939 948	82.938 083	82.938 868
2	82.940 058	82.938 098	82.938 970
3	82.940 231	82.939 342	82.940 131
4	165.878 803	165.875 497	165.877 652
5	165.880 676	165.876 835	165.880 204
6	165.883 236	165.880 228	165.887 138
7	248.805 144	248.796 097	248.810 339
8	248.824 559	248.815 690	248.837 458
9	248.848 569	248.838 303	248.888 389

where

$$\begin{aligned} k(x) &= \sqrt{\frac{2m}{\hbar^2}(E - V_1(x))} \qquad && (E > V_1(x)) \\ K(x) &= \sqrt{\frac{2m}{\hbar^2}(V_1(x) - E)} \qquad && (E < V_1(x)). \end{aligned} \tag{17}$$

All the energy values in table 1 are given on the shifted scale. The results of the WKB calculations starting from $V_2(x)$ agree closely with those obtained from $V_1(x)$ (as expected) and are not presented in table 1. It is very interesting to observe that SWKB energies (obtained from the quantization condition with ten TPs) agree excellently (especially for low-lying states where the effect of degeneracy is most prominent) with the exact ones obtained by solving the Schrödinger equation numerically. It is seen that the SWKB approximation is better than the WKB approximation in most cases, especially for low-lying triplet states, which are most difficult to calculate. In a few cases (the states numbered 6, 8 and 9), the WKB appears to be slightly better than the SWKB. This appears to be due to a relatively large numerical error in the exact calculation.

4. Multifold quasi-degeneracy

Using the wavefunction ansatz technique (choose the ground-state wavefunction as the sum of Gaussian terms), one can easily build up multiple wells analytically. From this, further calculations of the superpotential and the partner potentials are quite straightforward. One can easily verify how the number of WKB turning points (in V_1 and V_2) and the number of SWKB turning points (in W^2) increase as the degree of quasi-degeneracy increases. The connection between the numbers of classical and supersymmetric turning points is presented in table 2, from which it is easy to generalize the cases of n-fold quasi-degeneracy problems. One can easily see that, in each case, the number of classical turning points for V_2 and (not for V_1) matches with the number of SWKB turning points. Although V_1 and V_2 are two partners and according to SSQM must have same eigenspectrum, to proceed further with SSQM one has to start with V_2 and not with V_1. The generalization shows that for n-fold quasi-degeneracy, the number of turning points in V_1 is $2n$ and the number of turning points in W^2 is $(4n-2)$ (since one extra well introduces one additional complete oscillation in $W(x)$), which matches the number of turning points in V_2. Thus one has to use the WKB quantization condition for $V_2(x)$ (and *not* $V_1(x)$) to derive the SWKB quantization condition using $W(x)$, whenever quasi-degeneracy appears. Note also that, for an n-fold quasi-degeneracy, each one of $V_1(x)$, $V_2(x)$ and $W^2(x)$ has an $(n-2)$-fold periodic symmetry and a twofold symmetry at the two edges. These symmetries can be utilized in simplifying the SWKB quantization condition, resulting in a much simpler numerical calculation.

Table 2. The connection between classical and supersymmetric turning points.

Degeneracy	No of classical turning points in V_1	No of classical turning points in V_2	No of supersymmetric turning points in W^2	Comment
2-fold	4	6	6	Same No of
3-fold	6	10	10	turning
4-fold	8	14	14	points in
5-fold	10	18	18	V_2 and W^2
—	—	—	—	
n-fold	$2n$	$4n-2$	$4n-2$	

5. Summary and conclusions

The transition from the WKB to the SWKB quantization condition is straightforward for single wells or single barriers for which there are two turning points for both the WKB and SWKB procedures. This case corresponds to no quasi-degeneracy. Quasi-degeneracy in one dimension appears when two or more identical wells interact through intervening finite barriers. For n such identical wells, there will be n-fold quasi-degeneracy and $2n$ classical turning points. In such a case, the superpotential has $(n-1)$ complete oscillations and there are $(4n-2)$ SWKB turning points. The difference in the numbers of WKB and SWKB turning points for $n > 1$ makes a straightforward transition from the WKB to the SWKB quantization condition impossible. The difficulty is removed if, instead of the original potential, one uses its supersymmetric partner (V_2), which has the same number ($=4n-2$) of classical turning points as there are SWKB turning points. Use of twofold symmetry at the two edges and $(n-2)$-fold symmetry of the internal wells further simplifies the LSWKB quantization conditions. Earlier works established that the reformulated SWKB procedure accurately reproduces the quasi-degenerate states of double wells [8]. In the present paper we extend our work to n-fold quasi-degeneracy and explicitly calculate the threefold quasi-degenerate states of a triple well. It unambiguously establishes our argument that for n-fold quasi-degeneracy (with $n > 1$) one always has to use the partner potential V_2 instead of original potential V_1 in the SWKB transition. SWKB calculation using V_2 together with its periodic symmetries may be more interesting for physical systems exhibiting periodic identical potential wells, resulting in band structure.

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