When is the lowest order WKB quantization exact?[1, 2]

R.K. Bhaduri, D.W.L. Sprung, and Akira Suzuki

Abstract: First, two conditions are specified for the lowest order Wentzel–Kramers–Brillouin quantization rule to yield exact results. These rules are related to the periodic orbit decomposition of the quantum density of states. This approach is then applied to supersymmetric quantum mechanics. It leads to a new derivation of the result that shape-invariant potentials give exact results when the classical action is calculated with the square of the super potential, but without the Maslov index or the Langer correction.

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Résumé : Nous précisons d'abord deux conditions pour que la quantification WKB à l'ordre le plus bas donne des résultats exacts. Ces règles sont reliées à la décomposition en orbite périodiques de la densité quantique d'états. Cette approche est alors appliquée à la mécanique quantique super-symétrique. Cela donne une nouvelle dérivation du résultat que les potentiels invariants de forme donnent des résultats exacts lorsque l'action classique est calculée avec le carré du super-potentiel, mais sans indice de Maslov ou correction de Langer.

[Traduit par la Rédaction]

1. Introduction

Much of this paper is based on some recent work [1] done in collaboration with some other colleagues. Before giving an account of this, we briefly recall the Wentzel–Kramers–Brillouin (WKB) approximation for the simplest cases.

Consider a potential V_1 in the coordinate x in one dimension. The results may be generalized to central potentials in higher dimensions for a specified partial wave. We define the classical action

$$S_1(E) = \oint p(x)\,\mathrm{d}x = 2\sqrt{2m}\int_{x_1}^{x_2} \sqrt{E - V_1(x)}\,\mathrm{d}x \tag{1}$$

In (1), the action integral is over a complete periodic orbit at energy E, where x_1 and x_2 are the classical turning points, and $V_1(x_1) = V_1(x_2) = E$ (see Fig. 1). The WKB quantization rule for the energy

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[1] This paper is one of thirty-two published from the Theory CANADA 1 conference.
[2] This paper is based on a talk with the same title that was given by one of us (R.K.B.) at the Theory CANADA meeting in Vancouver in early June, 2005.
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Fig. 1. An example of the potential $V_1(x)$ appearing in (1) with the classical turning points.

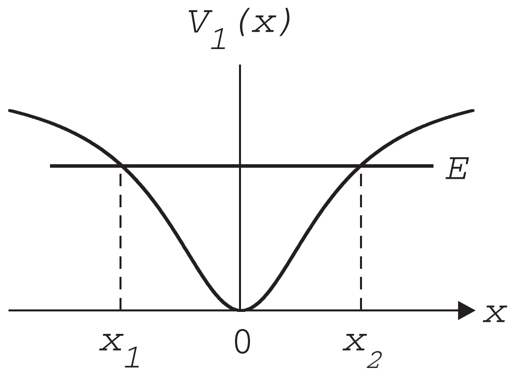
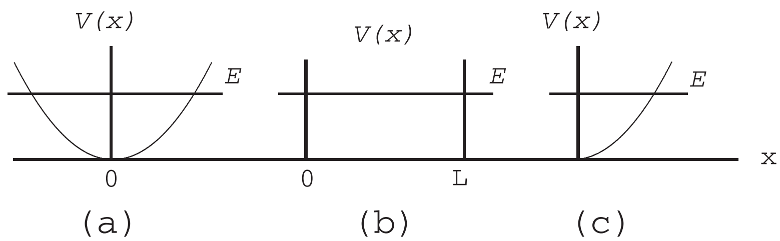


Fig. 2. Examples of one-dimensional potentials and corresponding Maslov indices. (*a*), depicts a harmonic well; (*b*), an infinite well, and (*c*) a three-dimensional central potential, respectively. The corresponding Maslov indices are for (*a*) $\eta = 1/2$, for (*b*) 1, and for (*c*) 3/4.



spectrum is given by

$$S_1(E) = (n + \eta)h, \qquad n = 0, 1, 2, 3 \ldots \tag{2}$$

where η is the Maslov index (independent of Planck's constant h), and is determined by matching the wave functions from both ends. The rule for determining the Maslov index η in the simple one-dimensional case is straightforward [2], and is illustrated in Figs. 2*a*–2*c*, for three different cases. We may express the rule by setting

$$\eta = C_1 + C_2 \tag{3}$$

where the constants C_i, $(i = 1, 2)$ are determined by the end points of the orbit in the potential. For a smooth wall at the intersection, $C_i = 1/4$, but for a sharp wall, $C_i = 1/2$. In Fig. 2*a*, for a harmonic well, the orbit encounters a smooth wall at both ends, so $C_1 = C_2 = 1/4$, and $\eta = 1/2$. In Fig. 2*b*, for an infinite well, $C_1 + C_2 = 1/2$, so $\eta = 1$. In the last case, shown in Fig. 2*c*, $\eta = 3/4$. For all three examples shown in Fig. 2, the WKB quantization rule, with the appropriate Maslov indices, gives the exact results. For completeness, we point out that in higher dimensions it is also necessary to implement the Langer correction [3] to the centrifugal barrier in each partial wave.

2. Exactness conditions for WKB

In general, the WKB series with higher order terms in $\hbar$ is an asymptotic one. In certain cases, however, the series may be absolutely convergent and may yield exact results. This happens when both conditions given below are satisfied

1. The Schrödinger eigenvalue equation with the potential is exactly solvable.

2. The energy spectrum E_n is given as an algebraic function of the quantum number n, i.e., $E_n = f_1(n)$, that may be solved analytically to obtain $n = F_1(E)$.

There are many potentials that satisfy the above conditions. These include the harmonic oscillator, square well, Coulomb, Morse, Rosen–Morse, Eckart, Pöschl–Teller, etc. that are listed in the text *Supersymmetry in quantum mechanics* by Cooper et al. [4]. Note that if only the first condition above is satisfied, but not the second one, the WKB results are not exact. An example is the two-dimensional disc billiard, where a particle is confined in a hard disc of radius R. The eigenvalues are given by the zeros of the cylindrical Bessel function $J_l(k_n R) = 0$, where the k_n's are the allowed wave numbers. This equation, however, cannot be inverted analytically, and the WKB quantization rule is, therefore, not exact.

3. Connection to periodic orbit theory

When the two conditions above are satisfied, there is a direct and exact way of decomposing the quantum density of states into a smooth and an oscillating part. This is a very special case of the more general periodic orbit theory (POT) [5] We recall that the energy spectrum is an algebraic function $f_1(n)$ of the quantum number n. At this stage, for reasons that will become clear later, let us shift the zero of energy at the ground state $n = 0$ of the spectrum, so that $f_1(0) = 0$. We may write

$$\delta\left(E - E_n^{(1)}\right) = \delta\left(E - f_1(n)\right) = \delta\left(n - F_1(E)\right) F_1'(E) \tag{4}$$

where the algebraic relation $E_n = f_1(n)$ has been inverted to define

$$n = F_1(E) \tag{5}$$

Note that we have used the algebraic expression between integer n's and E_n's to provide the relationship for continuous variables in (5). The continuous function $F_1(E)$ that we obtain in this way will be shown to satisfy the requirements of POT and classical mechanics (see (12)–(16)). In this sense, our choice of $F(E)$ using (5) is not only natural, but also necessary.

For the spectrum under consideration, $f_1(0) = 0$ implies the condition

$$F_1(0) = 0 \tag{6}$$

The quantum density of states $g_1(E)$ for the discrete spectrum of H_1 is defined as

$$g_1(E) = \sum_{n=0}^{\infty} d(n)\delta\left(E - E_n^{(1)}\right) \tag{7}$$

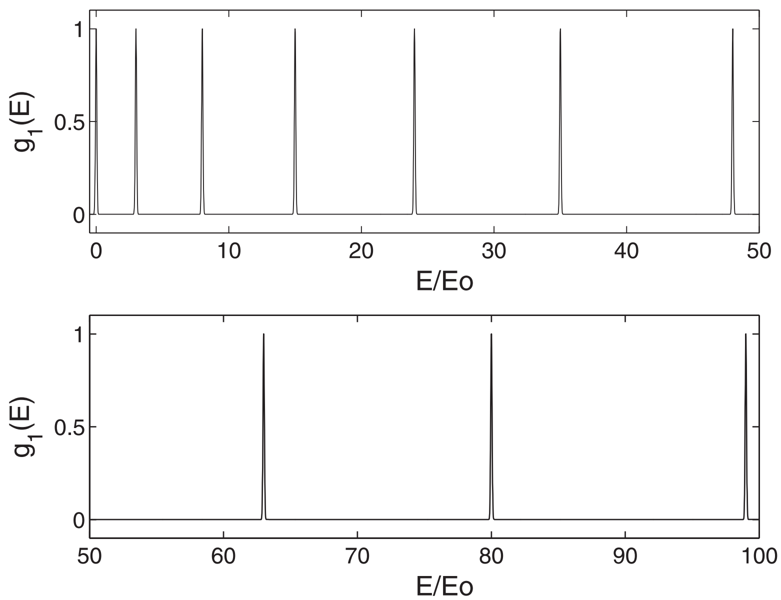
where $d(n)$ is the degeneracy of states at $E = E_n$. Writing $d(n) = d(F_1(E)) = D(E)$, and using (4), we obtain

$$g_1(E) = D(E)F_1'(E) \sum_{n=0}^{\infty} \delta\left(n - F_1(E)\right) \tag{8}$$

($D(E) = 1$ for one-dimensional potentials). We now use the identity

$$\sum_{n=0}^{\infty} \delta(n - x) = \sum_{k=-\infty}^{\infty} \exp\left(2i\pi kx\right), \quad x \geq 0 \tag{9}$$

Fig. 3. Numerical evaluation of the trace formula (10) for an infinite square-well potential. The spectrum is given by $f(n) = n(n+2)E_0$ with $n = 0, 1, 2, \ldots$and $E_0 = \hbar^2\pi^2/(2mL^2)$. We get $F_1(E) = (1+E/E_0)^{1/2} - 1$. In this figure, E is plotted in units of E_0. To ensure uniform line shapes, correct degeneracies, and strict numerical convergence, we have employed the usual prescription used in numerical semiclassics (see, for example, Sect. 5.5 of ref. 6), which is to convolve the trace formula with a Gaussian of width σ. For this particular calculation, we have truncated the sum at $k_{\max} = 10^4$, while prescribing $\sigma = 0.05$.



to obtain the desired expression [6, 7]

$$g_1(E) = D(E)F_1'(E)\left[1 + 2\sum_{k=1}^{\infty}\cos\left[2\pi k F_1(E)\right]\right] \tag{10}$$

For a given $F_1(E)$, this is an *exact* expression for the quantum density of states $g_1(E)$ (see the example of a square-well potential in Fig. 3). It is in the form of a trace formula in POT [6] when $F_1(E)$ (to within a dimensionless additive constant η) is identified with the action $S_1(E)$ of the primitive classical periodic orbit of the potential $V_1(x)$

$$\frac{S_1(E)}{h} = F_1(E) + \eta \tag{11}$$

$$S_1(E) = 2\sqrt{2m}\int_{x_1}^{x_2}\sqrt{E - V_1}\,\mathrm{d}x \tag{12}$$

In the above, x_1 and x_2 are the classical turning points at which $E = V_1(x)$. The (h-independent) constant η may be determined by using (11), and applying the condition given by (6) for $E = 0$. We then obtain

$$\eta = \frac{S_1(0)}{h} \tag{13}$$

We may prove (11) by noting that the (smooth) Thomas–Fermi density of states, given by the first term on the right-hand side of (10), is the Laplace inverse of the classical canonical partition function [8] of the Hamiltonian $H_1^{\rm cl}(x, p) = p^2/2m + V_1(x)$

$$F_1'(E) = \mathcal{L}_E^{-1}\, Z_1^{\rm cl}(\beta) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} Z_1^{\rm cl}(\beta)\,{\rm e}^{\beta E}\,{\rm d}\beta \tag{14}$$

Since

$$\begin{aligned} Z_1^{\rm cl}(\beta) &= \frac{1}{h}\int \exp\left[-\beta\, H_1^{\rm cl}(x, p)\right]\,{\rm d}x\,{\rm d}p \\ &= \frac{1}{2\pi\hbar}\sqrt{\frac{2m\pi}{\beta}}\int_{-\infty}^{\infty}\exp\left[-\beta V_1(x)\right]\,{\rm d}x \end{aligned} \tag{15}$$

it follows from (14) that

$$F_1'(E) = \frac{\sqrt{2m}}{2\pi\hbar}\int_{x_1}^{x_2}\frac{{\rm d}x}{\sqrt{[E - V_1(x)]}} \tag{16}$$

From this, (11) follows on integration over energy. Note that $F_1'(E)/h$ is the period of the classical periodic orbit and is unique, whereas $F_1(E)$ involves a constant of integration, η. Using (5) together with (11) and (12), we obtain the important result that the lowest order WKB quantization rule is *exact* for V_1

$$S_1(E) = \oint p(x)\,{\rm d}x = (n + \eta)h \tag{17}$$

where $p(x) = \sqrt{2m[E - V_1(x)]}$. We also see that the constant η is the so-called Maslov index, which may vary from one potential to another.

4. Supersymmetric WKB

The Maslov index η may be eliminated by performing WKB in the framework of supersymmetric (SUSY) quantum mechanics (QM), which is dubbed SWKB [4, 9]. We first set the notation by reviewing the relevant equations of SUSY QM. Consider a potential $V(x; a_1)$ of a single variable x, and a set of parameters denoted by a_1. One defines a "super potential"

$$W(x; a_1) = -\frac{\hbar}{\sqrt{2m}}\frac{\phi_0'(x)}{\phi_0(x)} \tag{18}$$

where $\phi_0(x)$ is the ground-state solution of the Schrödinger equation at energy E_0 for the potential $V_1(x, a_1)$, and the prime denotes a spatial derivative. Let us define

$$V_1(x; a_1) = V(x; a_1) - E_0 \tag{19}$$

so that the ground-state energy of the Hamiltonian

$$H_1 = -\frac{\hbar^2}{2m}\frac{{\rm d}^2}{{\rm d}x^2} + V_1(x; a_1)$$

lies at zero energy, i.e., $E_0^{(1)} = 0$. Then it is easy to show that

$$V_1(x; a_1) = W^2(x; a_1) - \frac{\hbar}{\sqrt{2m}}W'(x; a_1)$$

The SUSY partner Hamiltonian H_2 has the potential $V_2(x; a_1)$, and has an energy spectrum identical to that of H_1, except for the absence of the zero-energy state. The ground state of H_2, denoted by $E_0^{(2)}$ coincides with the first excited state $E_1^{(1)}$ of H_1, and so on. The partner potential $V_2(x; a_1)$ is

$$V_2(x; a_1) = W^2(x; a_1) + \frac{\hbar}{\sqrt{2m}} W'(x; a_1)$$

Shape invariance in the partner potentials is defined by the relation

$$V_2(x; a_1) = V_1\,(x; a_2) + R\,(a_1) \tag{20}$$

where the new parameters a_2 are some function of a_1, and the remainder $R(a_1)$ is independent of the variable x. We restrict our consideration of shape invariance to those cases where a_2 and a_1 are related by translation, $a_2 = a_1 + \alpha$. A shape-invariant potential in this class is exactly solvable and its energy spectrum is expressible as an algebraic function of the quantum number.

We now show that the Maslov index η may be eliminated from the quantization rule [1] by employing the superpotential formalism, and the result of Barclay and Maxwell [10]. They made the important observation that the shape-invariant class of potentials under consideration obey one or other of the following equations:

Class I

$$\frac{\hbar}{\sqrt{2m}} \frac{\mathrm{d}W}{\mathrm{d}x} = A + BW^2(x) + CW(x) \tag{21}$$

Class II

$$\frac{\hbar}{\sqrt{2m}} \frac{\mathrm{d}W}{\mathrm{d}x} = A + BW^2(x) + CW(x)\sqrt{A + BW^2} \tag{22}$$

where A, B, and C are constants. Using these equations, we now show that $S_1(E)$, as defined by (12), obeys the relation (x_{1s}, x_{2s} are the turning points in SWKB)

$$S_1(E) = 2\sqrt{2m} \int_{x_{1s}}^{x_{2s}} \sqrt{E - W^2}\, \mathrm{d}x + h\eta \tag{23}$$

To this end, note that the action S_1 can be expressed as an inverse Laplace transform

$$S_1(E) = \sqrt{2m\pi}\,\mathcal{L}_E^{-1} \int_{-\infty}^{\infty} \frac{\exp\left(-\beta\left[W^2 - \hbar W'/\sqrt{2m}\right]\right)}{\beta^{3/2}}\, \mathrm{d}x \tag{24}$$

At this point, for simplicity of notation, let us temporarily put $\hbar/\sqrt{2m} = \gamma$. Expanding the exponential in powers of W', we have

$$\begin{aligned} S_1(E) &= \sqrt{2m\pi}\,\mathcal{L}_E^{-1} \int_{-\infty}^{\infty} \frac{\mathrm{e}^{-\beta W^2}}{\beta^{3/2}} \left(1 + \sum_{k=0}^{\infty} \frac{\left(\gamma\beta W'\right)^{k+1}}{(k+1)!}\right) \mathrm{d}x \\ &= 2\sqrt{2m} \int_{x_{1s}}^{x_{2s}} \sqrt{E - W^2}\, \mathrm{d}x + \sum_{k=0}^{\infty} \frac{\hbar}{(k+1)!} \frac{\partial^k}{\partial E^k} \int_{-\sqrt{E}}^{\sqrt{E}} \frac{(\gamma W')^k}{\sqrt{E - W^2}}\, \mathrm{d}W \end{aligned} \tag{25}$$

Note that now the limits in x are replaced by the condition $W^2(x) = E$. The integral for $k = 0$ may be done immediately, yielding π. To evaluate the integrals for integer $k \geq 1$, we assume that $\gamma\, W'$ obeys Barclay's equation (21) (Class I) or (22) (Class II).

For Class I, we require integrals of the type

$$I_k = \int_{-\sqrt{E}}^{\sqrt{E}} \frac{\left(A + BW^2 + CW\right)^k}{\sqrt{E - W^2}}\, \mathrm{d}W \tag{26}$$

On expanding the numerator, terms with odd powers of W vanish on integration. One now sees that only the piece of I_k involving the highest power of W^2 survives the differentiation in (25). Consider the integral with W^{2k}. With the substitution $W = \sqrt{E}\sin\theta$

$$\int_{-\sqrt{E}}^{\sqrt{E}} \frac{W^{2k}}{\sqrt{E - W^2}}\, \mathrm{d}W = E^k \int_{-\pi/2}^{\pi/2} \sin^{2k}\theta\, \mathrm{d}\theta = E^k \frac{(2k-1)!!}{(2k)!!}\pi \tag{27}$$

Accordingly, (25) reduces to

$$S_1(E) = 2\sqrt{2m} \int_{x_{1s}}^{x_{2s}} \sqrt{E - W^2}\, \mathrm{d}x + \hbar\pi \left[1 + \sum_{k=1}^{\infty} \frac{B^k\,(2k-1)!!}{(k+1)\,(2k)!!}\right] \tag{28}$$

By construction, $W^2(x)$ has coincident turning points at $E = 0$, so the first term on the right-hand side above vanishes at this energy. Comparing with (13), we deduce that

$$\eta = \frac{1}{2}\left[1 + \sum_{k=1}^{\infty} \frac{B^k\,(2k-1)!!}{(k+1)\,(2k)!!}\right] = \frac{1}{B}\left[1 - \sqrt{1-B}\right] \tag{29}$$

Note, from (21), that B is independent of Planck's constant h. Comparing now with (11), we deduce our main result

$$2\pi\hbar F_1(E) = \sqrt{2m} \oint \sqrt{E - W^2}\, \mathrm{d}x \tag{30}$$

Using (5), we get as the *exact* result the SWKB expression

$$\oint \sqrt{2m(E - W^2)}\, \mathrm{d}x = 2\pi\hbar n, \quad n = 0, 1, 2, 3, \ldots \tag{31}$$

that yields the quantum spectrum of $V_1(x)$.

A similar derivation may be carried out for Class II superpotentials obeying (22). The starting point, as before, is (25), and the integral to be considered is now of the form

$$J_k = \int_{-\sqrt{E}}^{\sqrt{E}} \frac{\left(A + BW^2\right)^k \left(1 + CW/\sqrt{A + BW^2}\right)^k}{\sqrt{E - W^2}}\, \mathrm{d}W \tag{32}$$

The second bracketed term in the numerator on the right-hand side may be expanded binomially, and the odd-powered terms in W vanish on integration. We then have

$$J_k = \sum_{n=0}^{n_{\max}} \frac{k!}{(k-2n)!\,(2n)!} \int_{-\sqrt{E}}^{\sqrt{E}} \frac{\left(A + BW^2\right)^{k-n} (CW)^{2n}}{\sqrt{E - W^2}}\, \mathrm{d}W \tag{33}$$

where $n_{\max} = k/2$ for k even, and $(k-1)/2$ for k odd. The highest power of W in the numerator is again W^{2k} and again only terms with this highest power (with coefficient $B^{k-n}C^{2n}$) will survive when J_k is differentiated k times. Accordingly, (25) reduces to

$$S_1(E) = 2\sqrt{2m} \int_{x_{1s}}^{x_{2s}} \sqrt{E - W^2}\, \mathrm{d}x + \hbar\pi \left[1 + \sum_{k=1}^{\infty} \frac{(2k-1)!!}{(k+1)\,(2k)!!} \sum_{n=0}^{n_{\max}} \frac{k!\,B^{k-n}C^{2n}}{(k-2n)!\,(2n)!}\right] \tag{34}$$

The main results given earlier by (30) and (31) remain valid.

The summation in (34) can be done similarly to that in (29). The inner summation provides the mean of $\left(B \pm C\sqrt{B}\right)^k$. Then we find

$$\eta = \frac{1}{2z_+}\left[1 - \sqrt{1 - z_+}\right] + \frac{1}{2z_-}\left[1 - \sqrt{1 - z_-}\right] \tag{35}$$

where

$$z_\pm = B \pm C\sqrt{B} \tag{36}$$

The results (29) and (36) are a simple demonstration of the relation between WKB and SWKB, which Barclay [11] approached in a different manner.

It may now be instructive to illustrate our results with a few examples:

1. Infinite square well. In this example, $W(x) = -[\hbar\pi/(\sqrt{2m}L)][\cot(\pi x/L)]$. It belongs to Class I with $A = \hbar^2\pi^2/(2mL^2) = E_0$, $B = 1$, and $C = 0$. The quantum spectrum of V_1 is given by $f(n) = n(n+2)E_0$, with $n = 0, 1, 2, \ldots$. Then $F_1(E) = (1 + E/E_0)^{1/2} - 1$. A careful numerical evaluation of the trace formula (10) with this $F_1(E)$ reproduces the quantum spectrum (see Fig. 3). It is also easy to check (30) by evaluating the action integral of $W^2(x)$ analytically, and (23) using (29) ($\eta = 1$).

2. The three-dimensional harmonic oscillator in the lth partial wave. In this example, $W(r) = \sqrt{2m}\omega r/2 - [\hbar/(\sqrt{2m})][(l+1)/r]$. It belongs to Class II with $A = \hbar\omega$, $B = 1/(2l+2)$, and $C = -\sqrt{B}$. The quantum spectrum, measured from the lowest state in a fixed partial wave is $f(n) = 2n\hbar\omega$, so $F(E) = E/(2\hbar\omega)$. Again, (30) may be checked explicitly.

To verify (23), we find from (36) that

$$\eta = \frac{1}{2} + \frac{1}{2}\left[\ell + \frac{1}{2} - \sqrt{\ell(\ell+1)}\right] \tag{37}$$

in this example. The first 1/2 represents the usual half-integer quantization in lowest order WKB, while the terms in square brackets arise from the sum of order $\hbar^2$ and higher corrections. As discussed in detail by Seetharaman [12] and Barclay [11] they can be removed by adopting the Langer prescription. We have also checked other examples analytically.

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