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Regularization of the WKB integrals

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Abstract. A simple general method of regularization of the higher-order Wentzel–Kramers–Brillouin (WKB) integrals for the bound state problem of the one-dimensional Schrödinger equation with a real-analytic potential is proposed. The method is based upon the explicit separation of the integrand singularities. As an example, a contribution of the higher-order WKB corrections to the energy eigenvalues for the quasi-exactly solvable potential, $V(x) = 10x^2+10x^4+x^6$, is considered.

1. Introduction

The Wentzel–Kramers–Brillouin (WKB) semiclassical approach [1–3] is one of the most useful methods for computing approximate energy eigenvalues of the one-dimensional Schrödinger equation. Recent success in extension of this technique to supersymmetric quantum mechanics [4–15] has, in its turn, revived interest in the original WKB quantization condition [16–21].

However, in general, the lowest-order WKB approximation yields moderately accurate eigenvalues. Hence, to improve the accuracy it is necessary to consider the higher-order corrections in $\hbar$.

The initial work in this direction was done by Dunham [22]. Although at first sight this problem seems relatively simple, it has proved to be hard due to nonintegrable singularities at the classical turning points. Several attempts have been made to avoid this difficulty and to transform the WKB integrals into integrable expressions. In particular, the higher-order corrections to the quantization conditions have been computed by rewriting the integrals in terms of derivatives, with respect to energy [23, 24] and in terms of complete elliptic integrals [25–28]; by means of replacement of the integrands by an approximate expression [29]; integrating in the complex x-plane [30, 31] and making use of quadrature routines [32].

In this paper we propose a new, computationally efficient technique for calculating the WKB integrals, based upon the regularization with explicit separation of the integrand singularities [33]. To the best of our knowledge such a straightforward approach to the regularization of the WKB quantization condition has not been so far considered in the literature.

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2. Higher-order WKB approximations

Let us briefly sketch the derivation of higher-order correction terms within the WKB framework. We shall confine our interest to the bound state problem for the one-dimensional Schrödinger equation

$$-\frac{\hbar^2}{2m}\Psi''(x)+[V(x)-E]\Psi(x)=0 \tag{1}$$

with two classical turning points given by $V(x_1)=V(x_2)=E$.

The WKB approximation consists in seeking a solution in the form

$$\Psi(x)=\exp\left(\frac{\mathrm{i}}{\hbar}\int^x S(x,E,\hbar)\,\mathrm{d}x\right). \tag{2}$$

Then the time independent Schrödinger equation (1) for $\Psi(x)$ goes over into the nonlinear Riccati equation for the function $S(x,E,\hbar)$,

$$\mathrm{i}\hbar S'-S^2+2m[E-V(x)]=0 \tag{3}$$

where the prime denotes differentiation with respect to x.

When the following asymptotic expansion in powers of the Planck constant:

$$S(x,E,\hbar)=\sum_{k=0}^{\infty}\left(\frac{\hbar}{\mathrm{i}}\right)^k S_k(x,E) \tag{4}$$

is substituted into the Riccati equation (3) and the coefficients of successive powers of $\hbar$ are equated to zero, one obtains the recurrent system

$$\begin{aligned} &S_0(x,E)=\sqrt{2m[E-V(x)]}\\ &S'_{n-1}(x,E)=-\sum_{k=0}^{n}S_{n-k}(x,E)S_k(x,E)\qquad n=1,2,\ldots. \end{aligned} \tag{5}$$

Further, we proceed following the analytic approach by Wentzel [1], Zwaan [34] and Dunham [22] (see also [35, 36]). In this approach, the eigenvalue selection is effectively achieved by enforcing not the square integrability of the eigenfunctions but their analyticity through considering the solution of equation (1) not only on the real axis but in the whole complex x-plane.

As is generally known, in the case of a discrete spectrum of the Schrödinger equation with a real-analytic potential, the eigenfunctions are the analytic functions with a finite number of simple real zeros. Therefore, we can apply the principle of argument, known from the analysis of complex variables to the logarithmic derivative, $\mathrm{i}S(x,E,\hbar)/\hbar$, of the wave function $\Psi(x)$.

Since the wavefunction of the nth excited state has precisely n zeros we have

$$\oint_\gamma S(x,E,\hbar)\,\mathrm{d}x=2\pi\hbar n \tag{6}$$

where the integral is taken in a counter-clockwise sense along some contour γ enclosing the classical turning points and no other singularities of $S(x,E,\hbar)$.

Taking into account that within the WKB approach the passage to the classical limit is implemented using the rule

$$\hbar\to 0\qquad n\to\infty\qquad\text{and}\qquad \hbar n=\text{const} \tag{7}$$

the quantization condition (6) combined with the expansion (4)

$$\sum_{k=0}^{\infty}\left(\frac{\hbar}{\mathrm{i}}\right)^{2k}\oint_\gamma S_{2k}(x,E)\,\mathrm{d}x=2\pi\hbar\left(n+\frac{1}{2}\right) \tag{8}$$

where integration of the quantity $S_1(x, E)$ is performed explicitly, giving the addition of $\pi\hbar$ on the right-hand side of this equality, and all other odd terms $S_3(x, E)$, $S_5(x, E)$ etc, being total derivatives, vanish when integrating around a closed loop [37].

Upon rewriting in explicit form, this equation up to the order of $\hbar^8$ reads

$$\oint_\gamma \left\{ \sqrt{E-V} + \frac{\hbar^2}{96m} V''(E-V)^{-3/2} - \frac{\hbar^4}{6144m^2}[7(V'')^2 - 5V'V^{(3)}](E-V)^{-7/2} + \frac{\hbar^6}{196\,608m^3}[93(V'')^3 - 224V'V''V^{(3)} + 35(V')^2V^{(4)}](E-V)^{-11/2} - \frac{\hbar^6}{4096m^3}(V^{(3)})^2(E-V)^{-9/2} + \mathrm{O}(\hbar^8) \right\} \mathrm{d}x = \frac{2\pi\hbar}{\sqrt{2m}}\left(n+\frac{1}{2}\right) \tag{9}$$

where even terms $S_{2k}(x, E)$ are simplified by repeated integration by parts [38].

It is customary to represent this quantization condition as an integral over the real variable. From equation (5) it is seen that the above-mentioned classical turning points x_1 and x_2 prove to be the square root branch points for the functions $S_{2k}(x, E)$. Hence the single valuedness of the integrand requires that the cut joins these points.

As a next step, we have to choose the branch of the square root and to draw the contour of integration, γ, to the cut. However, it becomes evident that the integrand has nonintegrable singularities at the turning points and its regularization is needed.

Usually one follows the method of Krieger *et al* [23, 24] and expresses this quantization condition in the tantamount form [9]

$$\int_{x_1}^{x_2} \sqrt{E-V}\,\mathrm{d}x - \frac{\hbar^2}{48m}\frac{\mathrm{d}}{\mathrm{d}E}\int_{x_1}^{x_2} V''(E-V)^{-1/2}\,\mathrm{d}x + \frac{\hbar^4}{11\,520m^2}\frac{\mathrm{d}^3}{\mathrm{d}E^3}\int_{x_1}^{x_2}[7V''^2 - 5V'V^{(3)}](E-V)^{-1/2}\,\mathrm{d}x - \frac{\hbar^6}{5806\,080m^3}\left\{216\frac{\mathrm{d}^4}{\mathrm{d}E^4}\int_{x_1}^{x_2}(V^{(3)})^2(E-V)^{-1/2}\,\mathrm{d}x + \frac{\mathrm{d}^5}{\mathrm{d}E^5}\int_{x_1}^{x_2}[93(V'')^3 - 224V'V''V^{(3)} + 35(V')^2V^{(4)}](E-V)^{-1/2}\,\mathrm{d}x\right\} + \mathrm{O}(\hbar^8) = \frac{2\pi\hbar}{\sqrt{2m}}\left(n+\frac{1}{2}\right) \tag{10}$$

where singularities already become integrable.

Then the integrals derived are evaluated numerically for different values of E near each other and the derivatives are obtained by taking differences. However, having used the numerical evaluation of derivatives, it is difficult to control errors and, hence, to estimate the accuracy of results [33].

Now we describe a different way of a regularization of the higher-order WKB corrections that results in easily integrable expressions without derivatives with respect to the energy.

3. Regularization of the WKB integrals

As has been already noted, the integrands of the higher-order terms in equation (9) have nonintegrable singularities. We intend to circumvent this difficulty by means of a regularization based upon the explicit separation of singularities [33].

With this end in view let us investigate the behaviour of the singular integrands. In the vicinity of the turning point x_1, their general form may be written as $f(x)/(x-x_1)^{m-1/2}$.

Because a function $f(x)$ is regular, it is expanded in a Taylor series, yielding

$$\frac{f(x)}{(x-x_1)^{m-1/2}} = \sqrt{x-x_1}\left\{F(x) + \sum_{k=1}^{m} \frac{c_k}{(x-x_1)^k}\right\} \tag{11}$$

where a function $F(x)$ is regular too.

The behaviour of integrands at the second turning point x_2 is obviously analogous.

From equation (11) we observe that the non-integrability at the turning points arises from the pole terms of the right-hand side. For removing these singularities let us consider the preselected appropriate functions

$$\begin{aligned} P_k(x) &= (x-x_1)^{-k}\sqrt{(x-x_1)(x_2-x)} \\ Q_k(x) &= (x-x_2)^{-k}\sqrt{(x-x_1)(x_2-x)} \end{aligned} \tag{12}$$

whose behaviour in the complex x-plane is qualitatively similar to the behaviour of integrands. The useful feature of these functions is their integrability along the contour γ encircling the branch cut. Choosing the branch of the square root with the negative values on the upper side of the cut, as well as in equation (10), and evaluating the residue at infinity, we find

$$\begin{aligned} \oint P_1(x)\,\mathrm{d}x &= -\oint Q_1(x)\,\mathrm{d}x = \pi(x_2-x_1) \\ \oint P_2(x)\,\mathrm{d}x &= \oint Q_2(x)\,\mathrm{d}x = -2\pi \end{aligned} \tag{13}$$

other integrals being zero.

Clearly, if we add the linear combination

$$\sum_{k\geqslant 1}[p_k(\hbar)P_k(x) + q_k(\hbar)Q_k(x)] \tag{14}$$

to the integrand, providing its equality to zero at the turning points, the singularities under consideration may have to be removed.

Note that parameters $p_k(\hbar)$ and $q_k(\hbar)$, which we must find by demanding equality of the integrand to zero at the points x_1 and x_2, are really polynomials in $\hbar^2$ whose order is determined by the order of approximation.

Thus a general formula for the renormalized quantization condition of the WKB approach is readily obtainable as follows:

$$\begin{aligned} \int_{x_1}^{x_2} \Bigg\{ &\sqrt{E-V} + \frac{\hbar^2}{96m}V''(E-V)^{-3/2} - \frac{\hbar^4}{6144m^2}[7(V'')^2 - 5V'V^{(3)}](E-V)^{-7/2} \\ &+ \frac{\hbar^6}{196\,608m^3}[93(V'')^3 - 224V'V''V^{(3)} + 35(V')^2V^{(4)}](E-V)^{-11/2} \\ &- \frac{\hbar^6}{4096m^3}(V^{(3)})^2(E-V)^{-9/2} \\ &+ \sum_{k\geqslant 1}[p_k(\hbar)P_k(x) + q_k(\hbar)Q_k(x)] + \mathrm{O}(\hbar^8)\Bigg\}\,\mathrm{d}x \\ &= \frac{\pi\hbar}{\sqrt{2m}}\left(n+\frac{1}{2}\right) - \pi(q_2+p_2) - \frac{\pi}{2}(x_2-x_1)(q_1-p_1) \end{aligned} \tag{15}$$

where integrals may be computed routinely.

4. Example of application

As a check, we apply our technique to the linear harmonic oscillator and show straightforwardly that higher-order corrections are equal to zero, that is to be expected because the first-order integral already gives the exact eigenvalues. In this case $V(x) = x^2$ and equation (15) becomes

$$\int_{x_1}^{x_2} \left\{ \sqrt{E - x^2} + \frac{\hbar^2}{48m}(E - x^2)^{-3/2} - \frac{7\hbar^4}{1536m^2}(E - x^2)^{-7/2} + \frac{31\hbar^6}{8192m^3}(E - x^2)^{-11/2} + \sum_{k=1}^{6}[p_k P_k(x) + q_k Q_k(x)] + \mathrm{O}(\hbar^8) \right\} \mathrm{d}x = \frac{\pi\hbar}{\sqrt{2m}}\left(n + \frac{1}{2}\right) - \pi(q_2 + p_2) - \frac{\pi}{2}(x_2 - x_1)(q_1 - p_1). \tag{16}$$

Upon equating the integrand to zero at the turning points $x_1 = -\sqrt{E}$ and $x_2 = \sqrt{E}$, we obtain

$$\begin{aligned}
q_1 &= -p_1 = \frac{\hbar^2}{192E^{3/2}m} - \frac{35\hbar^4}{49\,152E^{7/2}m^2} + \frac{1953\hbar^6}{4194\,304E^{11/2}m^3} \\
q_2 &= p_2 = -\frac{\hbar^2}{192Em} + \frac{35\hbar^4}{49\,152E^3m^2} - \frac{1953\hbar^6}{4194\,304E^5m^3} \\
q_3 &= -p_3 = -\frac{7\hbar^4}{12\,288E^{5/2}m^2} + \frac{217\hbar^6}{524\,288E^{9/2}m^3} \\
q_4 &= p_4 = \frac{7\hbar^4}{24\,576E^2m^2} - \frac{651\hbar^6}{2097\,152E^4m^3} \\
q_5 &= -p_5 = \frac{93\hbar^6}{524\,288E^{7/2}m^3} \\
q_6 &= p_6 = -\frac{31\hbar^6}{524\,288E^3m^3}
\end{aligned}$$

that results in identical zeros both for the higher-order part of the integrand and the renormalization contribution to the right-hand side of equation (16).

In addition, we have computed with our technique the higher-order WKB corrections to the energy eigenvalues for the potential $V(x) = x^2 + \lambda x^4$ and have obtained the same numerical results as given by Kesarwani and Varshni [26].

As an example of application, we consider now the contribution of the higher-order WKB corrections to the energy eigenvalues of the Schrödinger equation with the quasi-exactly solvable potential, $V(x) = 10x^2 + 10x^4 + x^6$, for which the energy levels are determined by the equality [39–41]

$$E^4 - 140E^3 + 6110E^2 - 88\,540E + 252\,105 = 0 \qquad n = 0, 2, 4. \tag{17}$$

Table 1 illustrates how the inclusion of the higher-order corrections in the quantization condition (15) improves the accuracy of the WKB eigenvalues. From the table it is seen that, according to the rule of passage to the classical limit (7), ground states are not accurately calculated by the WKB method, even if the higher-order corrections are taken into account. The error, which was equal to 0.5% after including the first correction, decreases only to 0.1% when third- and fourth-order integrals are considered. However, the error rapidly decreases for increasing main quantum number, and already for the second excited state becomes less than 10^{-7}%.

Table 1. The energy eigenvalues for the potential, $V(x) = 10x^2 + 10x^4 + x^6$, computed with the regularized WKB quantization condition (15), included corrections of the order up to $\hbar^{2k}$. Here n is the quantum number and E_{exact} is given by (17).

k	$n = 0$	$n = 2$	$n = 4$
0	3.483 289 04	21.631 370 779	44.239 398 6553
1	3.706 117 47	21.745 513 565	44.325 317 4643
2	3.717 768 96	21.745 741 462	44.325 354 1810
3	3.718 643 63	21.745 705 806	44.325 350 2556
4	3.715 138 65	21.745 700 678	44.325 350 1080
5	3.702 718 85	21.745 700 559	44.325 350 1124
6	3.659 044 83	21.745 700 933	44.325 350 1144
E_{exact}	3.725 616 03	21.745 704 430	44.325 350 1153

5. Conclusion

We have proposed a general method for calculating the higher-order WKB integrals with real-analytic potentials. The method is based upon the explicit separation of the integrand singularities which occur in the WKB quantization condition. Then transformed integrals may be computed routinely for obtaining the energy eigenvalues to a high degree of accuracy. This is demonstrated by calculating the eigenvalues for the quasi-exactly solvable potential, $V(x) = 10x^2 + 10x^4 + x^6$.

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