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Higher-order JWKB approximations for radial problems: I. Modification of the effective potential

M Seetharaman and S S Vasan

Department of Theoretical Physics, University of Madras, Guindy Campus, Madras-600025, India

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Abstract. In the context of higher-order JWKB approximations for radial problems, the need for modifying the strength of the centrifugal barrier is considered. For spherically symmetric potentials $V(r)$ satisfying the condition $r^2V(r)\to 0$ as $r\to 0$, it is shown how to determine the modification required in an arbitrary order n that will ensure that the nth-order JWKB wavefunction has the correct behaviour ($\sim r^{l+1}$) near the origin. The second-order modification of Beckel and Nakhleh is a special case of the proposed nth-order modification, as are those of Fröman and Fröman. It is demonstrated that, with the correct modification, the JWKB series truncated at any order n leads to the exact energy spectrum for both the harmonic oscillator and the Coulomb potentials.

1. Introduction

A natural way of applying the JWKB approximation to three-dimensional problems with spherical symmetry is to apply the one-dimensional JWKB formalism to the radial Schrödinger equation, treating the sum of the true potential and the centrifugal barrier term as the effective potential V_e. Such a straightforward application entails certain difficulties which are not encountered in true one-dimensional problems (see Berry and Mount 1972 for details). For instance, the JWKB radial wavefunction has a behaviour near the origin $r=0$ which is different from that of the exact wavefunction. This defect can be remedied if one treats the strength of the centrifugal term not as a fixed quantity $l(l+1)$ but as an adjustable parameter L^2 whose value is to be chosen suitably. In the lowest order of approximation, L^2 should be taken as $(l+\frac{1}{2})^2$, which then ensures that the corresponding JWKB wavefunction goes like r^{l+1} near $r=0$. This replacement $l(l+1)\to(l+\frac{1}{2})^2$ is known as the Langer–Kemble modification (Langer 1937, Kemble 1937).

When one goes beyond the lowest order and includes higher-order corrections in a one-dimensional treatment with the potential $V_e(r)$, the difficulty at the origin surfaces again. The Langer–Kemble replacement which sufficed in the lowest order needs further modification. In fact, in different orders of approximation the parameter L^2 has to be chosen differently. In the second order, L^2 has to be chosen to be the root of the equation $x+1/64x=l(l+1)$. This was shown by Beckel and Nakhleh (1963) from an analysis of the differential equation obeyed by the second-order JWKB wavefunction. Later Fröman and Fröman (1974) included up to eighth-order terms in a different (phase integral) analysis of the problem, and showed that L^2 must be taken

to be the root (that lies closest to $l(l+1)$) of the equations

$$x^4 - l(l+1)x^3 - 2^{-9}x + 2^{-14} = 0,$$
$$x^6 - l(l+1)x^5 - 5\times 2^{-14}x^2 - 2^{-16}x + 2^{-20} = 0,$$
$$x^8 - l(l+1)x^7 - 7\times 2^{-17}x^3 - 5\times 2^{-24}x + 25\times 2^{-30} = 0,$$

in the fourth, sixth and eighth orders of approximation respectively. The modifications necessary in still higher orders have not been reported in the literature.

The main objective of this work is to show how the effective potential V_e has to be modified in the nth-order JWKB approximation in order that the wavefunction vanishes as r^{l+1} at the origin. With the modified effective potential, the one-dimensional formalism for higher-order corrections can be applied to radial problems *in toto*. By a simple analysis based on Dunham's formulation of the higher-order JWKB approximations in one dimension (Dunham 1932), we determine the behaviour of ψ_{JWKB} near the origin in any order of approximation. Requiring this to be r^{l+1}, we get an equation that determines the parameter L^2. A gratifying consequence of this equation is that, when all orders are summed, L^2 is identically equal to $l(l+1)$. As a further check, we apply our result to the eigenvalue problems of the isotropic oscillator $V(r) = \frac{1}{2}r^2$ and the Coulomb potential $V(r) = -1/r$. We show that, in both cases, the exact spectrum results, not only when all orders are summed, but also in any finite order of approximation. This interesting fact explains why even the lowest-order approximation is exact for these potentials.

2. Dunham's JWKB formalism and its radial generalisation

We briefly summarise here the results of Dunham's analysis for one-dimensional potentials, and indicate how they can be adapted for radial problems. In his analysis Dunham takes the solution of the one-dimensional Schrödinger equation

$$\psi'' + (2m/\hbar^2)(E - V(x))\psi = 0 \tag{2.1}$$

in the form

$$\psi = \exp\left((\mathrm{i}/\hbar)\int y\,\mathrm{d}x\right). \tag{2.2}$$

The function y then satisfies the Riccati equation

$$-\mathrm{i}\hbar y' = 2m(E - V) - y^2. \tag{2.3}$$

Expanding y as a power series in $\hbar$ (the JWKB series)

$$y = \sum_{n=0}^{\infty} (-\mathrm{i}\hbar)^n y_n \tag{2.4}$$

and substituting in (2.3), one obtains

$$y_0^2 = 2m(E - V), \tag{2.5}$$

$$2y_0 y_n + y'_{n-1} + \sum_{m=1}^{n-1} y_m y_{n-m} = 0, \qquad n \geqslant 1. \tag{2.6}$$

These relations determine all the y_n's recursively†. With the y_n's thus determined, (2.2) provides an asymptotic series for the wavefunction which is valid away from the turning points.

For potentials $V(x)$ that have only two classical turning points with a single minimum lying in between, Dunham has obtained a quantisation formula for the energy eigenvalues in terms of the y_n's, which reads

$$\oint \sum (-i\hbar)^n y_n \, dx = 2\pi N\hbar. \tag{2.7}$$

Here the closed contour encloses a branch cut along the real axis between the two turning points which are branch points of y_0 and hence of y. The branch of y_0 chosen is that which is negative real on the upper lip of the cut, and the contour is traversed in the counterclockwise sense. N is a non-negative integer.

To apply the above analysis to the radial equation, let us first assume that the true potential $V(r)$ is such that $r^2V(r) \to 0$ as $r \to 0$, and that the sum of $V(r)$ and the centrifugal term has a single minimum and gives rise to two classical turning points corresponding to bound states. Typical potentials satisfying these conditions are $V(r) = -1/r$, $r^n (n = 1, 2, 3, \ldots)$. Under these assumptions the radial problem is quite analogous to the one-dimensional one, except for the fact that the radial wavefunction is required to vanish as r^{l+1} as $r \to 0$. For bound states, it also vanishes as $r \to \infty$. As noted in § 1, the JWKB radial wavefunction can be made to obey the boundary condition at the origin by treating the strength of the centrifugal term as an adjustable parameter L^2 and choosing its value suitably. As will be shown below, the value of L^2 depends on the order of approximation. Taking the effective potential therefore as

$$V_e = V(r) + \hbar^2 L^2 / 2mr^2, \tag{2.8}$$

the one-dimensional formalism outlined above can be applied *in toto*, after replacing $V(x)$ by $V_e(r)$. Thus the radial wavefunction is given by

$$u = \exp\left((i/\hbar) \int \sum (-i\hbar)^n y_n \, dr \right) \tag{2.9}$$

where

$$y_0^2 = 2m(E - V_e),$$

the other y_n's being determined by (2.6). The energy quantisation condition is still given by (2.7).

3. Determination of L^2

As L^2 is to be determined by the boundary condition at the origin, we need to know first of all how the JWKB wavefunction behaves near $r = 0$. For this purpose, we note that as long as $r^2V(r) \to 0$ as $r \to 0$, the leading r-dependence in V_e is governed by the centrifugal barrier term. Thus we find that

$$y_0 \to -iL/r, \qquad r \to 0 \tag{3.1}$$

† Some numerical studies on the structure of the JWKB series and the properties of the y_n's have been carried out by Bender *et al* (1977).

(we take $\hbar = 1$ and $m = 1$ for convenience). Substituting this in the recurrence relation (2.6), the behaviour of other y_n's near $r = 0$ can also be successively determined:

$$y_1 \to +1/2r, \qquad y_2 \to -1/8\mathrm{i}Lr, \ldots .$$

It is easy now to verify that, as $r \to 0$, the ansatz

$$y_n \to (-)^n (\mathrm{i}/L)^{n-1} C_n / r \tag{3.2}$$

solves the recurrence relation (2.6), provided the coefficients C_n obey the relation

$$-2C_{n+1} = C_n + \sum_{m=1}^{n} C_m C_{n+1-m}, \qquad n \geqslant 1.$$

The solution to this relation is given by

$$\begin{aligned} &C_0 = 1, \qquad C_1 = -\tfrac{1}{2}, \\ &C_{2n} = 2^{-2n}\binom{\frac{1}{2}}{n}, \qquad n = 1, 2, 3, \ldots, \\ &C_{2n+3} = 0, \qquad n = 0, 1, 2, \ldots . \end{aligned} \tag{3.3}$$

Therefore, the behaviour of y near $r = 0$ is fully determined:

$$y = \sum_{n=0} (-\mathrm{i})^n y_n \to \frac{-\mathrm{i}}{r}\left[L + \tfrac{1}{2} + \sum_{n=1}^{\infty} \left(\frac{1}{L}\right)^{2n-1} C_{2n} \right].$$

Substituting for C_{2n} and formally summing the series, we get

$$y \to (-\mathrm{i}/r)[\tfrac{1}{2} + L(1 + 1/4L^2)^{1/2}]. \tag{3.4}$$

Putting this in (2.9), we see that near $r = 0$ the JWKB wavefunction has the form

$$u \to r^{1/2} + L(1 + 1/4L^2)^{1/2}. \tag{3.5}$$

This shows that the true wavefunction and its JWKB approximant will have the same r-dependence near $r = 0$, if L is chosen to satisfy

$$\tfrac{1}{2} + L(1 + 1/4L^2)^{1/2} = l + 1,$$

i.e.

$$L(1 + 1/4L^2)^{1/2} = l + \tfrac{1}{2}. \tag{3.6}$$

We now briefly consider the implications of this equation. The solution is easily seen to be $L^2 = l(l+1)$. We thus have the gratifying result that the correct strength of the centrifugal barrier in the Schrödinger equation is reproduced, when the *entire* JWKB series is summed. On the other hand, it is also clear from the foregoing analysis that, if the series is truncated at a finite n, L^2 will not be equal to $l(l+1)$. Nonetheless, the JWKB wavefunction in any finite order can still be made to have the correct behaviour near $r = 0$ by choosing L^2 properly. This necessarily implies that L^2 is different in different orders. Formally expanding the square root in (3.6), we get the series

$$L + \tfrac{1}{2} + 1/8L - 1/128L^3 + \ldots = (l+1). \tag{3.7}$$

If we keep only the first two terms, we get the Langer–Kemble modification $L^2 = (l + \frac{1}{2})^2$, known to be correct in the lowest (zeroth plus first) order. Approximating the LHS of (3.7) as $L + \frac{1}{2} + 1/8L$ we obtain the second-order result of Backel and Nakhleh quoted in § 1: $L^2 + 1/64L^2 = l(l+1)$. The results of Fröman and Fröman for higher orders

quoted in § 1 also follow from (3.7) when appropriate truncations of the series expansion are made. It may be noted that if the JWKB series is truncated at the third order ($n=3$), the value of L^2 to be used will be the same as that for the second order. This is because $C_3=0$ in (3.2). For similar reasons, the value of L^2 appropriate to the $(2n+1)$th order, for $n>1$, will be the same as that for the $2n$th order. The value of L^2 for the $2n$th order (with $n\geq 1$) will be determined by (3.7) in which the first $(n+2)$ terms on the LHS alone are retained. Explicity, it is given by

$$L+\tfrac{1}{2}+L\sum_{r=1}^{n}\left(\frac{1}{4L^2}\right)^r\binom{\frac{1}{2}}{r}=l+1, \qquad n\geq 1.$$

4. Application to the harmonic oscillator and the Coulomb potentials

We apply the results of the foregoing analysis to the harmonic oscillator and the Coulomb problems and show that when the value of L^2 appropriate to any given order is used, the exact eigenvalues of these potentials are reproduced in that order. This provides a check on our formalism.

The effective potential for the harmonic oscillator is

$$V_e=\tfrac{1}{2}r^2+L^2/2r^2.$$

The energy is to be computed from the condition

$$2\pi n_r=\oint\sum(-\mathrm{i})^n y_n\,\mathrm{d}r=\sum(-\mathrm{i})^n I_n \tag{4.1}$$

with

$$y_0=-(2E-r^2-L^2/r^2)^{1/2},$$

the other y_n's being determined from (2.6). For this potential, it is easy to verify by induction that the following form for y_n solves (2.6):

$$y_n=P^{1-3n}\sum_{k=0}^{2n}A_{n,k}\,r^{2k-1} \tag{4.2}$$

where $P=-(-r^4+2Er^2-L^2)^{1/2}$ and $A_{n,k}$ are constants. Consider the integral

$$I_n=\oint y_n\,\mathrm{d}r.$$

The integration contour encloses the branch cut from r_1 to r_2, where r_1 and r_2 are the positive roots of $P=0$. The other singularities of y_n in the complex r-plane are a simple pole at $r=0$ and two branch points at $-r_1$ and $-r_2$. Therefore there is a symmetrical left-hand cut from $-r_2$ to $-r_1$. The integral around the right-hand cut is equal to that around the left-hand cut. Therefore, by Cauchy's theorem,

$$2I_n=-(2\pi\mathrm{i}\times\text{residue of } y_n \text{ at } r=0)+\oint_{C_R}y_n\,\mathrm{d}r$$

where C_R is a circle of radius R. Now, as $R\to\infty$, the integral over C_R tends to zero for all $n>1$, because $y_n\to 0$ as $|r|\to\infty$, as is clear from (4.2). The residue at the origin is simply the coefficient of $1/r$ in y_n and is read from (3.2). Therefore

$$2I_n=-2\pi\mathrm{i}(-1)^n(\mathrm{i}/L)^{n-1}C_n.$$

Using the value of C_n from (3.3), it follows then that for $n>0$

$$I_{2n+1}=0, \qquad I_{2n}=(-1)^{n+1}\pi L\left(\frac{1}{4L^2}\right)^n\binom{\frac{1}{2}}{n}.$$

We are left with the integrals I_0 and I_1, and these are easily evaluated to be $\pi(E-L)$ and $-\pi i$ respectively. Collecting all the terms, we have

$$\begin{aligned}2\pi n_r &= \pi(E-L)-\pi-\pi L\sum_{n=1}\binom{\frac{1}{2}}{n}\left(\frac{1}{4L^2}\right)^n \\ &= \pi[E-1-L(1+1/4L^2)^{1/2}],\end{aligned}$$

and therefore

$$E=2n_r+1+L(1+1/4L^2)^{1/2}.$$

Hence, it follows from (3.6) that when the correct L^2 in any order is used, the exact spectrum results.

For the Coulomb problem also a similar analysis can be carried out. For $n\geqslant 1$, the integral of y_n is the same as that in the harmonic oscillator case. Only the integral I_0 has a different value, leading to the Coulomb spectrum.

5. Discussion

We have demonstrated that the one-dimensional JWKB formalism can be applied *in toto* to radial problems for computing higher-order corrections, provided the strength of the centrifugal term is treated as a parameter L^2. The value of L^2 in any order of approximation is then fully determined by the boundary condition on the wavefunction at the origin. In the test cases of the harmonic oscillator and the hydrogen atom, our procedure leads to the known energy spectra in every order of approximation. That the JWKB series can be summed is a special feature of these potentials. For a general potential $V(r)$, the singularity structure of y_n in the complex r-plane is quite complicated. For instance in the quartic oscillator case, $V(r)=r^4$, in addition to right-hand and left-hand cuts along the real axis and a pole at $r=0$, y_n will have additional cuts along the imaginary axis. In a subsequent paper we shall show how, for the quartic oscillator case, one can calculate higher-order JWKB integrals I_n for $n\leqslant 4$ and obtain an expression for the energy eigenvalues.

We conclude with a comment on the applicability of our analysis to S-waves. When $l=0$, the centrifugal term is absent in the radial Schrödinger equation, and there will be only one turning point, for potentials of the type discussed. This means that our analysis cannot be applied directly to S-waves. If one tries to apply the above analysis to S-waves by adding a fictitious term L^2/r^2 to $V(r)$, and thereby generating a second turning point, there may arise difficulties. The observation of Beckel and Nakhleh that in second-order JWKB the parameter L^2 becomes imaginary for S-waves is an illustration. Similar difficulties may be present in higher orders. It is interesting to observe that if all orders of JWKB are taken into account, the value of L^2 to be chosen for the S-wave is the correct value zero. The corresponding S-wave energies will also be then reproduced correctly, as illustrated in the harmonic oscillator and the hydrogen atom problems. For obtaining the energy eigenvalues specifically for S-waves, the works of Fröman (1978) and Pasupathy and Singh (1981) may be consulted.

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