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Numerical study of a phase-integral connection formula

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Abstract. In order to study the accuracy and properties of a certain type of arbitrary-order phase-integral approximations, especially as regards the connection formula for tracing a wavefunction from a classically forbidden region to a classically allowed region, the Schrödinger equation for the one-dimensional harmonic oscillator is solved by means of the first, third and fifth order of these approximations, and the resulting approximate wavefunctions, both when normalised and when fitted to the exact wavefunctions at $+\infty$, are compared with the corresponding exact wavefunctions. The numerical results show that, except for the lowest energy eigenstates, the higher-order phase-integral approximations in question are very accurate both in the classically allowed and in the classically forbidden regions.

The aim of the present investigation is also to illuminate and confirm numerically certain theoretical results of principal significance which are subject to confusion in the literature.

1. Introduction

While the accuracy of energy eigenvalues obtained by means of the half-integer Bohr–Sommerfeld quantisation condition, with or without higher-order corrections, has been examined, over the years, by many authors, studies of the accuracy of the wavefunctions themselves have not been made to the same extent. In a rather recent paper, however, Grunwald and Milano (1971) studied the accuracy of the first-order JWKB wavefunctions by evaluating the approximate expressions for the first ten eigenfunctions for the linear harmonic oscillator and comparing them with the exact wavefunctions. To the knowledge of the present authors no numerical study of the accuracy and range of validity of higher-order JWKB wavefunctions or similar higher-order approximate wavefunctions has been reported.

In the present paper we study the accuracy of the approximate wavefunctions obtained by means of a certain kind of phase-integral approximation, the first order of which is identical to the first-order JWKB approximation, while the higher orders are simpler than the corresponding JWKB approximations and also have other advantages, very important from a theoretical point of view (N Fröman 1966b, 1970; see also the review article by McHugh 1971). We have solved the Schrödinger equation for the one-dimensional harmonic oscillator by means of the first, third and fifth order of those approximations, when the quantum number n has the values 0, 1, 2, 3, 4, 5, 10, 15 and 20. The resulting approximate wavefunctions have then been compared with the corresponding exact wavefunctions. We use certain values of the wavefunctions to illuminate, in table 1, the high accuracy of the phase-integral wavefunctions, obtainable

when one is well away from the classical turning points. Of the complete numerical material we present in figure 2 the results for a few quantum numbers ($n = 0, 1, 5$ and 10) to illuminate graphically, how the phase-integral approximations fail in the neighbourhood of the classical turning points.

As will be explained in the last section, the numerical investigation in the present paper is of interest, not only for finding the accuracy obtainable, but also for illuminating numerically certain theoretical results of principal significance.

2. Exact solution

The Schrödinger equation for a one-dimensional harmonic oscillator, after introduction of dimensionless quantities, has the form

$$\frac{d^2\psi}{dz^2} + Q^2(z)\psi = 0 \tag{1}$$

where

$$Q^2(z) = \lambda - z^2. \tag{2}$$

The eigenvalues of λ are

$$\lambda = 2n + 1, \qquad n = 0, 1, 2, \ldots, \tag{3}$$

and the corresponding normalised exact solutions of (1) are (Schiff 1968, p 71 ff)

$$\psi_n(z) = (n!2^n\sqrt{\pi})^{-1/2} H_n(z) \exp(-z^2/2), \tag{4}$$

where $H_n(z)$ is the Hermite polynomial of order n.

3. Approximate solution

The approximate solutions of (1) which we shall study in the present paper are linear combinations of phase-integral approximations of the form

$$\psi = q^{-1/2}(z) \exp(\pm i w(z)), \tag{5}$$

where

$$w(z) = \int^z q(z)\, dz. \tag{6}$$

The functions $q(z)$ and $w(z)$, corresponding to the $(2N+1)$th-order phase-integral approximation, are given by

$$q(z) = \sum_{\nu=0}^{N} q^{(2\nu+1)}(z) \tag{7}$$

with

$$q^{(2\nu+1)}(z) = Q(z) Y_{2\nu}, \tag{8}$$

and

$$w(z) = \sum_{\nu=0}^{N} w^{(2\nu+1)}(z) \tag{9}$$

with

$$w^{(2\nu+1)}(z)=\int^{z} q^{(2\nu+1)}(z)\,\mathrm{d}z. \tag{10}$$

The first few functions $Y_{2\nu}$ are

$$Y_0=1, \tag{11a}$$

$$Y_2=\tfrac{1}{2}\epsilon_0, \tag{11b}$$

$$Y_4=-\frac{1}{8}\epsilon_0^2-\frac{1}{8}\frac{\mathrm{d}^2\epsilon_0}{\mathrm{d}\zeta^2} \tag{11c}$$

with

$$\epsilon_0=Q^{-3/2}(z)\frac{\mathrm{d}^2}{\mathrm{d}z^2}Q^{-1/2}(z) \tag{12}$$

and

$$\zeta=\int^{z} Q(z)\,\mathrm{d}z. \tag{13}$$

The functions $Q^{1/2}(z)$ and $Q(z)$ have branch-points at the classical turning points, while the functions Y_{2n} are single-valued. In studying the wavefunction we choose to consider the upper edge of the real axis, and in figure 1(c) we show our choice of phase for $Q^{1/2}(x+\mathrm{i}0)$, real values of z being denoted by x. In the following, we shall for the sake of simplicity always write simply x instead of $x+\mathrm{i}0$.

According to (2), (8), (11a–c), (12) and (13), we obtain

$$q^{(1)}(z)=Q(z)=(\lambda-z^2)^{1/2}=-\mathrm{i}(z^2-\lambda)^{1/2}, \tag{14a}$$

$$q^{(3)}(z)=Q(z)\frac{3z^2+2\lambda}{8(\lambda-z^2)^3}, \tag{14b}$$

$$q^{(5)}(z)=-Q(z)\frac{297z^4+732\lambda z^2+76\lambda^2}{128(\lambda-z^2)^6}. \tag{14c}$$

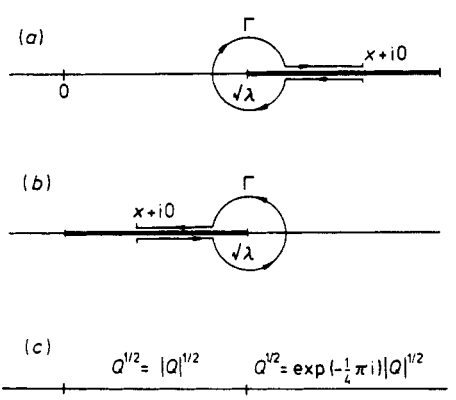

Figure 1. Contour of integration Γ (bold line indicates a cut), when x ($=x+\mathrm{i}0$) is located: (a) in the classically forbidden region; (b) in the classically allowed region; (c) the phase of $Q^{1/2}(x+\mathrm{i}0)$.

If in (14*a*, *b*, *c*) we replace z by x (which, as just mentioned, means $x+\mathrm{i}0$), we obtain with $Q(x)=(\lambda-x^2)^{1/2}$ the expressions for $q^{(1)}$, $q^{(3)}$ and $q^{(5)}$ in the classically allowed region ($|x|<\sqrt{\lambda}$), while with $Q(x)=-\mathrm{i}(x^2-\lambda)^{1/2}$ we obtain the functions in question in the classically forbidden region to the right of the well ($x>\sqrt{\lambda}$).

Since, in the present case, $Q^2(z)$ is an even function of z, the eigenfunctions are either symmetric or anti-symmetric functions of z, and it suffices to study the solutions on the positive part of the real axis. With a convenient choice of the constant lower limit in the integral (6) defining $w(z)$, we have (cf (10))

$$w^{(2\nu+1)}(x)=\tfrac{1}{2}\int_{\Gamma} q^{(2\nu+1)}(z)\,\mathrm{d}z, \tag{15}$$

where the contour of integration Γ is depicted in figures 1(*a*, *b*). Evaluating the integral in (15) for $2\nu+1$ equal to 1, 3 and 5, we obtain

$$w^{(1)}(x)=\begin{cases} \dfrac{x}{2}(\lambda-x^2)^{1/2}-\dfrac{\lambda}{2}\cos^{-1}\left(\dfrac{x}{\lambda^{1/2}}\right) & |x|<\sqrt{\lambda}, \qquad (16a)\\ -\mathrm{i}\left[\dfrac{x}{2}(x^2-\lambda)^{1/2}-\dfrac{\lambda}{2}\ln\left(\dfrac{x+(x^2-\lambda)^{1/2}}{\lambda^{1/2}}\right)\right] & x>\sqrt{\lambda}, \qquad (16a') \end{cases}$$

$$w^{(3)}(x)=\begin{cases} -\dfrac{x^3-6\lambda x}{24\lambda(\lambda-x^2)^{3/2}} & |x|<\sqrt{\lambda}, \qquad (16b)\\ +\mathrm{i}\dfrac{x^3-6\lambda x}{24\lambda(x^2-\lambda)^{3/2}} & x>\sqrt{\lambda}, \qquad (16b') \end{cases}$$

$$w^{(5)}(x)=\begin{cases} -\dfrac{56x^9-252\lambda x^7+441\lambda^2x^5+1860\lambda^3x^3+3420\lambda^4x}{5760\lambda^3(\lambda-x^2)^{9/2}} & |x|<\sqrt{\lambda}, \qquad (16c)\\ -\mathrm{i}\dfrac{56x^9-252\lambda x^7+441\lambda^2x^5+1860\lambda^3x^3+3420\lambda^4x}{5760\lambda^3(x^2-\lambda)^{9/2}} & x>\sqrt{\lambda}. \qquad (16c') \end{cases}$$

Since we are concerned with a bound-state problem, only the solution which tends to zero as $x\to\infty$ is acceptable. Apart from a constant normalisation factor, we can obtain approximate expressions for the wavefunction on the real axis, except in the neighbourhood of the classical turning points $x=\pm\sqrt{\lambda}$, by tracing the bound-state phase-integral wavefunction from the classically forbidden region to the classically allowed region with the aid of the pertinent connection formula, derived with reference to any conveniently chosen order of the phase-integral approximations (N Fröman 1970, equation (21)). The normalisation factor, which has been given in a simple form for arbitrary-order phase-integral approximations (Yngve 1971, 1972, P O Fröman 1974), is in the present case equal to $(2\pi)^{-1/2}$, independently of the order of the phase-integral approximation (Yngve 1971). The approximate, normalised wavefunction obtained is

$$\psi_n(x)=\begin{cases} (2\pi)^{-1/2}2|q^{-1/2}(x)|\cos(|w(x)|-\pi/4) & |x|<\sqrt{\lambda}, \qquad (17a)\\ (2\pi)^{-1/2}|q^{-1/2}(x)|\exp(-|w(x)|) & x>\sqrt{\lambda}, \qquad (17b) \end{cases}$$

with $q(x)$ and $w(x)$ given by (7) and (9) with (14*a*–*c*) and (16*a*–*c*′), respectively.

4. Discussion

The accuracy of the normalised eigenfunctions obtained in the first-, third- and fifth-order phase-integral approximations, respectively, is obtained by comparison with the exact, normalised wavefunctions (2). Graphical representations of the approximate and the exact wavefunctions are, for some quantum numbers, given in figure 2. As is well known, the approximations break down in the neighbourhood of the classical turning points. In the first-order approximation we have $q(z) = Q(z)$, and hence $q(z)$ is zero at the classical turning points. For the higher-order approximations $q(z)$ is singular at such a point and has, in its neighbourhood, a certain number of zeros ($3N$ for the approximation of order $2N+1$), which, with increasing N, spread out over a larger

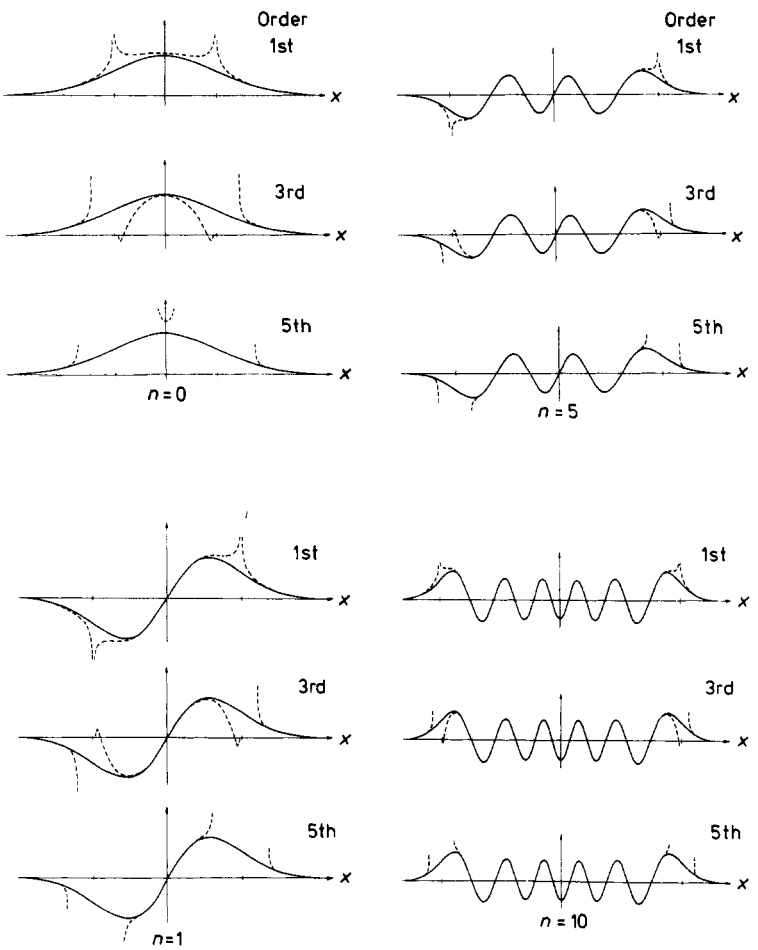

Figure 2. Full curves represent exact, normalised wavefunctions. Broken curves represent approximate wavefunctions obtained by using phase-integral approximations of the first, third and fifth orders. Except for regions in the neighbourhood of the classical turning points, located at $x = \pm(2n+1)^{1/2}$, and except for the lowest states, the difference between the approximate and the exact results is too small to be distinguished in this figure. We note that, roughly speaking, the approximate solution becomes useful already at the first extremum of the wavefunction in the classically allowed region.

and larger region around the zero of $Q^2(z)$ in question. As a consequence, in this region the approximations fail, the function $q(z)$, when $N>0$, changes violently, and the picture of Stokes' and anti-Stokes' lines becomes, correspondingly, very complicated (N Fröman 1970, figures 1(*a*, *b*)). The fact that, for a fixed quantum number n, the region around a classical turning point in which the approximations fail becomes wider with increasing order of the approximations used, is seen from the curves in figure 2. On the other hand, when x lies outside the region, in which the zeros of $q(z)$ are located, and moves away from the classical turning point, the approximate solution rapidly becomes very accurate. When x lies well away from the classical turning points, the approximate solution improves with increasing order of the phase-integral approximation used until an optimal order is reached. For instance, it is seen from table 1 (and also from figure 2) that for $n = 0$ and $n = 1$ and for the values of x at the origin and at the first extremum of the wavefunction, respectively, the third order provides the optimum.

Table 1. Absolute value of the relative error of the phase-integral wavefunction at the extremum lying at the origin, when n is even, and nearest to the origin, when n is odd: (*a*) when $(\psi_n)_{\text{approx}}$ is normalised, i.e. calculated according to (17*a*); (*b*) when $(\psi_n)_{\text{approx}}$ is fitted to $(\psi_n)_{\text{exact}}$ at infinity.

Quantum number	$\lvert(\psi_n)_{\text{approx}}-(\psi_n)_{\text{exact}}\rvert/\lvert(\psi_n)_{\text{exact}}\rvert$					
	First order		Third order		Fifth order	
n	(*a*) Normalised	(*b*) Fitted at $+\infty$	(*a*) Normalised	(*b*) Fitted at $+\infty$	(*a*) Normalised	(*b*) Fitted at $+\infty$
0	$6{\cdot}3\times10^{-2}$	$6{\cdot}3\times10^{-2}$	$4{\cdot}9\times10^{-2}$	$5{\cdot}5\times10^{-2}$	$3{\cdot}1\times10^{-1}$	$3{\cdot}2\times10^{-1}$
1	$3{\cdot}9\times10^{-2}$	$5{\cdot}4\times10^{-2}$	$3{\cdot}4\times10^{-2}$	$3{\cdot}5\times10^{-2}$	$2{\cdot}0\times10^{-1}$	$2{\cdot}0\times10^{-1}$
2	$4{\cdot}7\times10^{-3}$	$1{\cdot}3\times10^{-2}$	$3{\cdot}8\times10^{-4}$	$4{\cdot}4\times10^{-4}$	$1{\cdot}0\times10^{-4}$	$1{\cdot}0\times10^{-4}$
3	$3{\cdot}0\times10^{-3}$	$9{\cdot}0\times10^{-3}$	$2{\cdot}0\times10^{-4}$	$2{\cdot}3\times10^{-4}$	$5{\cdot}2\times10^{-5}$	$5{\cdot}4\times10^{-5}$
4	$1{\cdot}5\times10^{-3}$	$6{\cdot}1\times10^{-3}$	$4{\cdot}1\times10^{-5}$	$5{\cdot}4\times10^{-5}$	$3{\cdot}9\times10^{-6}$	$4{\cdot}5\times10^{-6}$
5	$1{\cdot}4\times10^{-4}$	$5{\cdot}2\times10^{-3}$	$3{\cdot}2\times10^{-5}$	$3{\cdot}4\times10^{-5}$	$2{\cdot}7\times10^{-6}$	$3{\cdot}3\times10^{-6}$
10	$3{\cdot}0\times10^{-4}$	$2{\cdot}3\times10^{-3}$	$1{\cdot}5\times10^{-6}$	$1{\cdot}3\times10^{-6}$	$4{\cdot}0\times10^{-8}$	$2{\cdot}4\times10^{-7}$
15	$1{\cdot}8\times10^{-4}$	$1{\cdot}5\times10^{-3}$	$5{\cdot}3\times10^{-7}$	$5{\cdot}3\times10^{-7}$	$9{\cdot}8\times10^{-8}$	$9{\cdot}8\times10^{-8}$
20	$7{\cdot}3\times10^{-5}$	$1{\cdot}1\times10^{-3}$	$9{\cdot}2\times10^{-8}$	$9{\cdot}2\times10^{-8}$	$1{\cdot}3\times10^{-8}$	$1{\cdot}2\times10^{-8}$

The optimal order, yielding the highest accuracy obtainable, is higher the larger the quantum number n is and the farther from the classical turning points x lies. In this connection we also draw attention to the striking manner in which the errors in the wavefunctions creep further and further outwards from the turning points, as the order of approximation increases (cf figure 2). This observation extends our understanding of the asymptotic nature of the approximation used. With increasing order of approximation the accuracy first increases but then in general starts decreasing, when the errors, spreading out from the sources of the eventual divergence, i.e. the turning points, approach and reach the point where the wavefunction is to be calculated.

The fact that the phase-integral approximations cannot be used in a certain region around a classical turning point may at first seem to be a serious drawback, which should limit considerably the usefulness of these approximations. In particular, one might be tempted to think that the usefulness of higher-order approximations would be highly restricted because of this fact. The improvement of the accuracy gained far away from

the turning point, with increasing order of approximation, might seem to be of limited value in view of the fact that, at the same time, the region where the solution fails in the neighbourhood of the turning point becomes broader. Fortunately, it turns out that there are only few physical problems for the solution of which it is necessary to know the wavefunction in the neighbourhood of classical turning points. Such knowledge is, of course, needed when there is a boundary condition imposed on the wavefunction in the neighbourhood of a classical turning point. It is, however, in general not needed for the calculation of important physical quantities such as energy eigenvalues, phase shifts and transmission coefficients, as is well known from the application of the usual JWKB approximation. Recently, accurate phase-integral formulae, not involving wavefunctions, have been obtained also for quantal expectation values (N Fröman 1974) and matrix elements (N Fröman and P O Fröman 1977) in a single-well potential.

Except for the lowest quantum states, the right-hand side of (17*a*) approximates the exact, normalised wavefunction in the classically allowed region extremely accurately, when one is well away from the classical turning points, and especially when higher-order approximations are used. To illustrate this statement concretely we give in the columns labelled (*a*) in table 1 the absolute value of the relative error at the extremum at the origin, when n is even, and at the extremum nearest to the origin, when n is odd. For large quantum numbers n, the relative error is seen to be several orders of magnitude less in the third-order than in the first-order approximation and about one order of magnitude less in the fifth-order than in the third-order approximation. For all values of n investigated, the sign of the error is such that the extrema are alternately too big and too small, when calculated in the first-, third-, and fifth-order approximations, respectively. Studying the accuracy at other maxima or minima of the wavefunction in the classically allowed region, we find similar features. We also find that, for a fixed order of the phase-integral approximations studied, the relative error may be negative in certain intervals of the classically allowed region and positive in others.

In order to study the error due to the connection procedure itself, without the smearing out of the error resulting from the normalisation, we fitted the exponentially decreasing phase-integral function to the pertinent exact wavefunction such that they agreed exactly for $x = +\infty$. This means that for each value of λ we had to multiply the right-hand sides of (17*a*) and (17*b*) by a certain constant (depending on λ). In the columns labelled (*b*) in table 1 we give the relative error of the approximate wavefunction obtained in this way, calculated at the same point as the relative error of the normalised wavefunction displayed in the columns labelled (*a*). We note that, in the first-order approximation, the wavefunction obtained by fitting at $+\infty$ improves only slowly when the quantum number n increases. Thus, in other words, in the first-order approximation the connection formula does not yield very accurate wavefunctions even for large quantum numbers. By the normalisation we achieve, for large quantum numbers, a considerable improvement of the first-order wavefunction, as can be seen from table 1. In the third-order as well as in the fifth-order approximation, the errors in column (*a*) and column (*b*) in table 1 do not differ significantly and are very small, except for the lowest states. Thus, we realise the great improvement in the accuracy of the connection formula which can be achieved when one uses higher-order approximations.

Beside the aim of studying quantitatively the accuracy of the wavefunctions obtained by means of the arbitrary-order phase-integral approximations under consideration, our purpose is also to confirm numerically certain results, which have been questioned (Dingle 1965, 1973, Berry and Mount 1972).

Let us first say a few general words about the theory, on which the formulae investigated in the present paper, are based. The derivation of the connection formula for arbitrary-order phase-integral approximations (N Fröman 1970) used in the present investigation was made by means of an extension of the method, developed by N Fröman and P O Fröman (1965), for handling the connection problems of the first-order JWKB approximation. This extension (N Fröman 1966b) could, after certain precautions, be made quite straightforwardly, and several results could be directly generalised to higher orders. Although the derivation of the arbitrary-order connection formula yielding (17*a*), when (17*b*) is given, is rigorous, we found it worthwhile, for illustrative and didactic purposes, to make the numerical investigation presented above, because already the well known first-order connection formulae have given rise to a great deal of discussion over the years, and continue to do so. The very accurate values of the higher-order phase-integral wavefunctions discussed in the present investigation confirm numerically in a direct way that the connection formula in question has the correct form and thus, in turn, that the just mentioned extension of the method for handling connection problems to arbitrary-order phase-integral approximations works efficiently.

Finally let us make some comments on the fact that the Stokes' constants are independent of the order of approximation. For the type of phase-integral approximations used in the present paper, the theory, developed by N Fröman and P O Fröman (1965) and extended to higher-order approximations by N Fröman (1966b), yields the same Stokes' constants independently of the order of approximation. Implicitly, this result is confirmed by the fact that the phase-integral formulae *not involving wavefunctions*, obtained according to this theory, have been found to yield physical quantities very accurately. See, for instance, some papers concerning the double oscillator (N Fröman 1966a, N Fröman and Myhrman 1970, N Fröman *et al* 1972) and a paper on the calculation of transmission and reflection coefficients (Karlsson 1975). The high accuracy achieved *for wavefunctions* reported in the present paper confirms directly that the connection formula corresponding to (17*a*, *b*), involving Stokes' constants independent of the order of approximation, has the correct form. If Stokes' constants depended on the order of approximation used, this would imply that, with (17*b*) given, the right-hand side of (17*a*) should be multiplied by a certain constant, and the phase of the cosine should be changed by a constant, both of these constants being dependent on the order of approximation, in order that we should obtain accurate values of the wavefunction in the classically allowed region. Thus, the great numerical accuracy achieved confirms the fact that the Stokes' constants are independent of the order of approximation used. The conclusion that the Stokes' constants are independent of the order of approximation, confirmed for the arbitrary-order phase-integral approximations used in the present paper, must be true also for the arbitrary-order JWKB approximations which, although they are of a more complicated analytic form, have an accuracy comparable to that of the phase-integrable approximations used in the present paper.

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