Nonintegral Maslov indices

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The phase loss of a wave reflected by a smooth potential generally varies continuously from π in the long-wave limit to $\pi/2$ in the limit of short waves. Incorporating the corresponding nonintegral multiples of $\pi/2$ as nonintegral Maslov indices in the formulation of the WKB approximation leads to a substantial improvement of accuracy when the conditions for applicability of the WKB method are violated only near the classical turning points. We demonstrate the efficacy of using nonintegral Maslov indices for a Woods-Saxon potential and a repulsive $1/x^2$ potential. The nonintegral Maslov index for a given $1/x^2$ potential yields far more accurate wave functions than the conventional Langer modification of the potential in conjunction with phase loss $\pi/2$. The energy spectrum of the radial harmonic oscillator (including the centrifugal potential), which is reproduced exactly by the standard WKB method with the Langer modification, is also reproduced exactly without the Langer modification when the nonintegral Maslov index is used. We suggest a method for approximately calculating the nonintegral Maslov index near the long-wave limit from the decaying WKB wave function in the classically forbidden region. [S1050-2947(96)06108-2]

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I. INTRODUCTION

In the WKB approximation, the quantum-mechanical wave function for a particle of mass m moving with total energy E in a potential $V(x)$ is approximated by [1–3]

$$\psi(x)=\frac{1}{\sqrt{p(x)}}\exp\left[\pm\frac{i}{\hbar}\int_{x_0}^{x}p(x')dx'\right],\tag{1}$$

where $p(x)$ is the local momentum

$$p(x)=\sqrt{2m[E-V(x)]}.\tag{2}$$

The wave function (1) is, in general, a good approximate solution of the quantum-mechanical Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi\tag{3}$$

as long as the (local) de Broglie wavelength $\lambda(x)=2\pi\hbar/|p(x)|$ varies sufficiently slowly

$$\frac{1}{2\pi}\left|\frac{d\lambda}{dx}\right|=\hbar\left|\frac{m}{p^3}\frac{dV}{dx}\right|\ll 1.\tag{4}$$

The condition (4) is always violated at a classical turning point x_0 because $p(x_0)=0$. If the potential can be approximated linearly around the turning point, the exponentially decreasing real wave function on the classically forbidden side of the turning point should be associated with the oscillating wave functions on the classically allowed side of the turning point via the famous connection formula [1,2]

$$\frac{1}{\sqrt{|p(x)|}}\exp\left[-\frac{1}{\hbar}\left|\int_{x_0}^{x}|p(x')|dx'\right|\right]\to\frac{2}{\sqrt{p(x)}}\cos\left[\frac{1}{\hbar}\left|\int_{x_0}^{x}p(x')dx'\right|-\frac{\phi}{2}\right].\tag{5}$$

The phase $\phi/2$ appearing in the argument of the cosine on the right-hand side of (5) corresponds to a reflection coefficient with phase ϕ in front of the wave reflected at the turning point, relative to the incoming wave traveling towards the turning point. This *phase loss* ϕ at reflection is equal to $\pi/2$ in the semiclassical limit of short wave [1,2]. For a particle oscillating in the classically allowed region between two turning points x_1 and x_2, the WKB quantization condition is obtained by requiring the total phase during one period of oscillation to be an integral multiple of 2π,

$$\frac{1}{\hbar}\oint p(x)dx-\phi_1-\phi_2=\frac{2}{\hbar}\int_{x_1}^{x_2}p(x)dx-\phi_1-\phi_2=2\pi n,\tag{6}$$

where ϕ_1 is the phase loss due to reflection at the turning point x_1 and ϕ_2 is the phase loss due to reflection at x_2. Taking ϕ_1 and ϕ_2 to be equal to $\pi/2$ leads to the conventional form of the WKB quantization condition, viz.,

$$\int_{x_1}^{x_2}p(x)dx=\left(n+\frac{\mu}{4}\right)\pi\hbar,\tag{7}$$

where $\mu=2$ is the total Maslov index corresponding to the two reflections during one period of oscillation.

For reflection by an infinite steep wall the phase loss is π rather than $\pi/2$ and the WKB quantization rule (7) reproduces the correct spectrum of quantum-mechanical eigenvalues for a particle oscillating freely between two such walls if we insert 4 rather than 2 for the total Maslov index μ. In this case any wavelength is large at the turning points, where the potential changes abruptly, but the condition (4) is fullfilled in between the turning points. In the more general case the wavelength may be too large for the semiclassical limit to be invoked near the classical turning points, but the WKB approximation may still be useful away from the turning points if the potential is sufficiently smooth.

We demonstrate in the following that this is actually the case in various physically important and realistic situations. The key to obtaining a good approximation of the quantum-mechanical wave functions in the classically allowed region and of energy eigenvalues in the framework of the WKB method lies in correctly accounting for the phase loss of the wave function due to reflection at the classical turning points. In between the limits of long and short waves this amounts to allowing nonintegral Maslov indices, because the phase losses are in general nonintegral multiples of $\pi/2$.

Modified WKB quantization conditions have been investigated from a different perspective by Robbins, Creagh, and Littlejohn, who studied contributions due to tunneling orbits for the Hecht Hamiltonian describing molecular rotations [4]. In a recent paper, Popov, Karnakov, and Mur discuss in some detail how the ratio of the amplitudes appearing on both sides of the connection formula (5) should be modified, when the conditions of the short-wave limit are not fulfilled, but the phase loss is taken as $\pi/2$ [5]. In this paper we focus on how to modify the phase loss, which plays a crucial role in improving the WKB approximation in the classically allowed region.

In Sec. II we discuss the reflection of a particle by a smooth potential step and use the analytically known phase loss to obtain energies and wave functions for bound eigenstates in a Woods-Saxon potential. Section III is devoted to repulsive $1/x^2$ potentials and critically analyzes the role of the Langer modification. In Sec. IV we discuss quadratic potentials and in Sec. V we present a method, with which the phase loss might be calculated approximately from the WKB wave functions when it is not known analytically.

II. REFLECTION BY A POTENTIAL STEP

Consider a smooth potential step of the form

$$V_a(x)=\frac{V_0}{1+\exp(-x/a)}. \tag{8}$$

The exact solution of the Schrödinger equation (3) for this potential is given in paragraph 25 of [2] for energies $E>V_0$ and can easily be extended to energies in the range $0<E<V_0$. The solution that decays exponentially in the classically forbidden region is asymptotically proportional to $e^{ikx}+re^{-ikx}$ in the classically allowed region $x\to-\infty$ and $r=\exp(-i\delta)$ is the reflection coefficient with the phase

$$\delta=2\arg\frac{\Gamma(-2ika)}{\Gamma(\kappa a-ika)\Gamma(1+\kappa a-ika)}. \tag{9}$$

The constants k and κ in (9) are the asymptotic wave numbers in the classically allowed and classically forbidden regions, respectively,

$$k=\frac{1}{\hbar}\sqrt{2mE}=k_{V_0}\sqrt{\frac{E}{V_0}},$$

$$\kappa=\frac{1}{\hbar}\sqrt{2m(V_0-E)}$$

$$=k_{V_0}\sqrt{1-\frac{E}{V_0}}. \tag{10}$$

At the top of the potential step ($E=V_0$) the asymptotic wave number in the allowed region is

$$k_{V_0}=\frac{1}{\hbar}\sqrt{2mV_0} \tag{11}$$

and the inverse of k_{V_0} defines a scale for lengths.

The exact wave function is asymptotically proportional to $\cos(kx+\delta/2)$. Comparing this to the asymptotic form of the WKB wave function (5) for $x\to-\infty$ yields

$$\phi=\delta+2ka\left[2\ln 2-\ln\left(1+\frac{\kappa^2}{k^2}\right)-2\frac{\kappa}{k}\arctan\frac{k}{\kappa}\right]. \tag{12}$$

The phase δ in (12) is just the phase (9) of the reflection coefficient r above, where the point of reference is $x=0$. The second term on the right-hand side of (12) accounts for the fact that we are taking the point of reference to be the classical turning point x_0 and that the WKB wave function is not exactly a plane wave away from the turning point.

For small values of the diffuseness parameter a, the Gamma functions in (9) can be approximated with the help of the identity $\Gamma(z)=\Gamma(1+z)/z$ and the approximation $\Gamma(1+z)\approx 1-Cz+O(z^2)$ (C is Euler's constant) to yield $\delta=2\arctan(\kappa/k)+O(a^2)$. In the limit $a\to 0$ we obtain the phase loss due to reflection by a sharp step, $\phi=2\arctan(\kappa/k)$ [6].

For a very diffuse step, assuming $ka\gg 1$, $\kappa a\gg 1$, and using Stirling's formula to approximate the Gamma functions yields a phase loss $\phi\to\pi/2$. Note, however, that no matter how large we choose the diffuseness parameter a, ka is always small sufficiently close to the long-wave limit $E=0$ and hence ϕ always approaches π in this limit.

The right-hand side of (12) depends on ka and κa and for a given value of the dimensionless *relative diffuseness* $\alpha=k_{V_0}a$ the phase loss ϕ is a function of E/V_0 alone. Examples are illustrated for various values of the relative diffuseness α in Fig. 1. For any value of α, the phase ϕ is π at the bottom of the step and decreases monotonically, passing the value $\pi/2$ at an energy that is close to half the height of the step in the case of small α and decreases with increasing α. The limiting value at the top of the step is zero for $\alpha=0$ and approaches $\pi/2$ for large α.

Consider s waves in a Woods-Saxon potential

$$V_{\mathrm{WS}}(x)=V_a(x-R)-V_0=-\frac{V_0}{1+\exp\left(\dfrac{x-R}{a}\right)},\quad x>0, \tag{13}$$

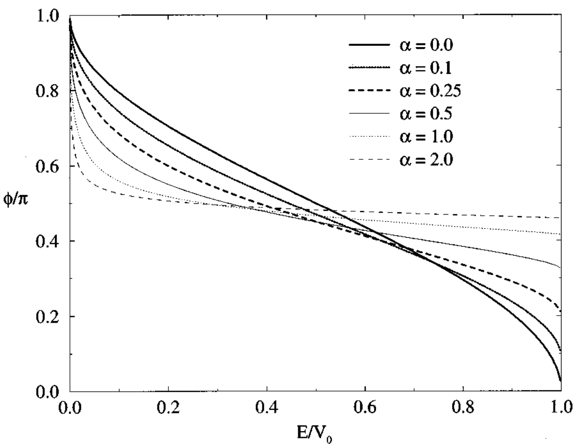

FIG. 1. Phase loss ϕ due to reflection by the potential step (8) as given by (12) for various values of the relative diffuseness α.

which is widely used for modeling self-consistent fields in atomic nuclei and, more recently, atomic clusters [7]. At the origin, $x=0$, the quantum-mechanical wave function vanishes and the phase loss due to reflection is π. The phase loss ϕ due to reflection at the outer turning point $x_0=R+a\ln(V_0/|E|-1)$ $[V_{\rm WS}(0)<E<0]$ is given by (12) and the asymptotic wave numbers κ and k are as in (10), except that the energy E is now replaced by $V_0+E=V_0-|E|$. The WKB quantization condition in this case is

$$\int_0^{x_0}\sqrt{2m[E-V_{\rm WS}(x)]}dx=\left(n+\frac{\mu}{4}\right)\pi\hbar \quad \text{with} \quad \mu=2+\frac{\phi}{\pi/2}. \tag{14}$$

Due to the dependence of ϕ on energy, the right-hand side of (14) is an energy-dependent function and the positions of the energy levels are obtained by numerically locating the intersections of both sides of (14).

We have calculated the energy eigenvalues in the Woods-Saxon potential whose depth V_0 is chosen such that $k_{V_0}=1$ and the diffuseness and range parameter are $a=0.5$ and $R=30$, respectively (Table I). The energies E/V_0 obtained with the conventional ''simple'' WKB quantization condition, which corresponds to a Maslov index $\mu=3$ in this case, deviate from the exact quantum-mechanical values by typically 0.004 near the bottom of the potential well and by up to 0.01 near the top of the potential well. [Results of comparable accuracy are obtained in the standard WKB method by including a centrifugal potential as prescribed by the Langer modification (see Sec. III).] In contrast, the energy values derived with the nonintegral Maslov index according to (14) reproduce the exact quantum-mechanical result within our numerical accuracy, i.e., better than 5×10^{-9}, except for the weakly bound ninth state near the top of the well, where the error is roughly 6×10^{-7}. Note that the simple first-order WKB approximation is highly accurate, even close to the long-wave limit, provided the appropriate nonintegral Maslov index is used.

For larger values of the diffuseness a the phase loss ϕ is closer to $\pi/2$. The standard WKB becomes a better approximation in this case, but use of the phase ϕ of (12) generally improves the result further. For smaller values of the diffuseness a the standard WKB approximation becomes progressively worse, whereas the quantization condition (14) with the phase (12) becomes better and yields the exact eigenvalues in the limit of a sharp step $a=0$.

III. REFLECTION BY A REPULSIVE $1/x^2$ POTENTIAL

Consider the potential

$$V_\gamma(x)=\frac{c}{x^2}=\frac{\hbar^2}{2m}\frac{\gamma}{x^2}. \tag{15}$$

How close the solutions of the Schrödinger equation with this potential are to the long-wave or the short-wave limit depends not on energy but only on the dimensionless parameter

$$\gamma=\frac{2mc}{\hbar^2}\geqslant 0, \tag{16}$$

TABLE I. Energies of the bound states in the Woods-Saxon potential (13) with the parameters $k_{V_0}=1$, $a=0.5$, and $R=30$. The exact quantum-mechanical results are compared with the present results obtained via (14) using the nonintegral Maslov index corresponding to the phase loss (12) at the outer turning point and with the simple WKB ansatz based on the phase loss $\pi/2$ at the outer turning point. The last column contains the WKB results obtained with a centrifugal potential corresponding to the Langer modification $l(l+1)\rightarrow(l+1/2)^2$ for $l=0$ and a phase loss $\pi/2$ at the inner turning point as well as the outer turning point.

n	$E_n^{\rm exact}/V_0$	$E_n^{\rm present}/V_0$	$E_n^{\rm simple}/V_0$	$E_n^{\rm Langer}/V_0$
0	−0.98931658	−0.98931658	−0.99252241	−0.99284005
1	−0.95733492	−0.95733492	−0.96165414	−0.96194975
2	−0.90425814	−0.90425814	−0.90830332	−0.90858855
3	−0.83041962	−0.83041962	−0.83332836	−0.83360627
4	−0.73628786	−0.73628786	−0.73744628	−0.73771764
5	−0.62249893	−0.62249893	−0.62140847	−0.62167285
6	−0.48995387	−0.48995387	−0.48615942	−0.48641611
7	−0.34009410	−0.34009410	−0.33314992	−0.33339578
8	−0.17588806	−0.17588806	−0.16540815	−0.16563339
9	−0.01083777	−0.01083835	−0.00095238	−0.00091497

which is equal to $l(l+1)$ for the three-dimensional centrifugal potential corresponding to the orbital angular momentum quantum number l. (In general, γ can be any non-negative real number.)

The Schrödinger equation with the potential (15) can be solved analytically [8] and the solution regular at the origin is

$$\psi(x)\propto\sqrt{kx}J_\nu(kx),\quad k=\frac{\sqrt{2mE}}{\hbar},\tag{17}$$

where J_ν is the Bessel function of order

$$\nu=\sqrt{\gamma+\frac{1}{4}}.\tag{18}$$

Asymptotically,

$$\psi(x)\propto\left(1-\frac{\gamma(\gamma-2)}{8(kx)^2}\right)\cos\left[kx-\left(\nu+\frac{1}{2}\right)\frac{\pi}{2}\right]-\frac{\gamma}{2kx}\sin\left[kx-\left(\nu+\frac{1}{2}\right)\frac{\pi}{2}\right]+O((kx)^{-3}).\tag{19}$$

The classical turning point is at $x_0=\sqrt{\gamma}/k$ and the integral $\int_{x_0}^{x}\sqrt{2m[E-V_\gamma(x')]}dx'$ occurring in the WKB wave function can be calculated analytically. The asymptotic behavior of the WKB wave function in the classically allowed region is

$$\psi_{\text{WKB}}(x)\propto\left(1-\frac{\gamma(\gamma-2)}{8(kx)^2}\right)\cos\left[kx-\sqrt{\gamma}\frac{\pi}{2}-\frac{\phi}{2}\right]-\frac{\gamma}{2kx}\sin\left[kx-\sqrt{\gamma}\frac{\pi}{2}-\frac{\phi}{2}\right]+O((kx)^{-3}).\tag{20}$$

In the standard WKB method the phase ϕ in (20) is taken to be $\pi/2$ and the asymptotic phases in the exact wave function (19) and in the WKB wave function (20) are reconciled by subjecting the potential (15) for the WKB calculation to the *Langer modification* [1–3,9],

$$\gamma\to\gamma'=\gamma+\frac{1}{4},\tag{21}$$

which amounts to replacing $l(l+1)$ by $(l+1/2)^2$ when $\gamma=l(l+1)$. This gives the right argument of sine and cosine in (20), but the coefficients proportional to $1/(kx)$ and $1/(kx)^2$ are changed, so only the leading term of (20) agrees with the exact expression (19).

However, a comparison of Eqs. (19) and (20) shows that we also obtain the correct asymptotic phase in the WKB wave function if we leave the potential intact and interpret

$$\phi=\left(\nu+\frac{1}{2}-\sqrt{\gamma}\right)\pi=\frac{\pi}{2}+\left(\sqrt{\gamma+\frac{1}{4}}-\sqrt{\gamma}\right)\pi\tag{22}$$

as the phase loss due to reflection at the classical turning point. The phase (22) is independent of energy; it approaches $\pi/2$ in the semiclassical limit $\gamma\to\infty$ and it approaches π in the anticlassical (long-wave) limit $\gamma\to 0$. Explicit numbers are given in Table II for a few values of γ corresponding to orbital angular momentum $l=0,\ldots,10$ in the three-dimensional centrifugal potential, $\gamma=l(l+1)$.

TABLE II. Phase loss (22) due to reflection by the three-dimensional centrifugal potential.

l	ϕ/π
0	1.0
1	0.58578644
2	0.55051026
3	0.53589838
4	0.52786405
5	0.52277442
6	0.51925930
7	0.51668523
8	0.51471863
9	0.51316702
10	0.51191152

WKB wave functions based on the Langer modification (21) and a phase loss $\pi/2$ or on the true potential and the phase loss (22) both have the correct asymptotic behavior to leading order, but the latter wave function is a far better approximation of the true solution of the Schrödinger equation at finite distances because it approaches the exact wave function more rapidly by two orders in $1/kx$. This is illustrated in Fig. 2 and, more dramatically in Fig. 3, where we plot the differences of the respective WKB wave function and the exact solution as functions of kx in a doubly logarithmic plot. All wave functions are normalized to unit amplitude asymptotically.

Summarizing the situation, we can say that a phase loss $\pi/2$ at reflection is too small and the Langer modification of the potential, which reduces the kinetic energy and hence increases the wavelengths of the WKB wave function, enables the wave to catch up to the correct phase asymptoti-

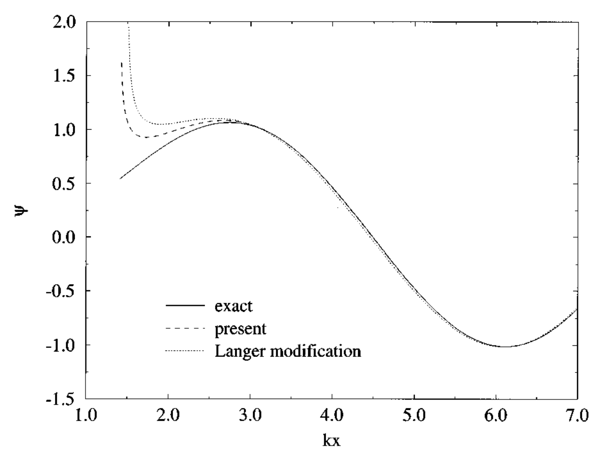

FIG. 2. Wave functions in the classically allowed region for the potential (15) with $\gamma=2$ (corresponding to $l=1$ in the three-dimensional centrifugal potential). The standard WKB wave function based on a phase loss $\pi/2$ due to reflection and the Langer-modified potential and the present wave function based on the phase loss (22) ($\phi\approx 0.5858\pi$ for $\gamma=2$) and the true potential without Langer modification are compared with the exact solution of the Schrödinger equation (17).

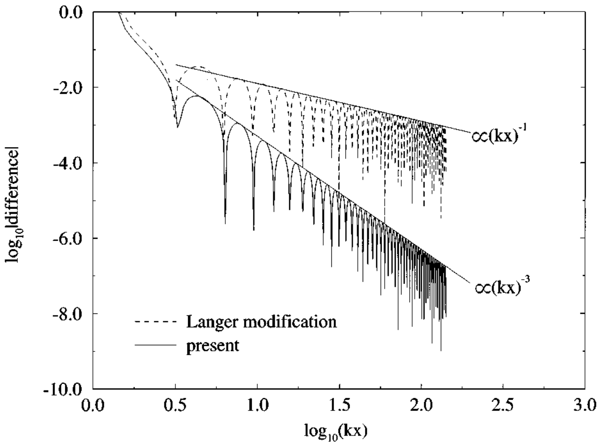

FIG. 3. Absolute value of the difference between the WKB wave functions of Fig. 2 and the exact quantum-mechanical wave function as function of kx in a doubly logarithmic plot. The dashed curve shows the result for the standard WKB wave function based on a phase loss $\pi/2$ due to reflection and the Langer-modified potential, the solid curve shows the result for the wave function obtained with the phase loss (22) and the true potential without Langer modification. The straight lines indicate proportionality to $1/(kx)$ and $1/(kx)^3$, respectively.

cally. With the correct phase loss at reflection (22), the WKB wave function based on the true potential (15) approaches the exact quantum-mechanical wave function more rapidly by two orders in $1/kx$.

The results obtained for the Woods-Saxon potential in Sec. II and for the centrifugal potential (15) can be combined to investigate the radial Woods-Saxon potential

$$V_{\mathrm{WS}}^{(l)}(x)=\frac{\hbar^2}{2m}\frac{l(l+1)}{x^2}-\frac{V_0}{1+\exp\left(\frac{x-R}{a}\right)},\quad x>0. \quad (23)$$

We have calculated the exact eigenvalues of the quantum-mechanical bound states and compared them with the results obtained via the WKB quantization condition

$$\int_{x_1}^{x_2}\sqrt{2m[E-V_{\mathrm{WS}}^{(l)}(x)]}dx=\left(n+\frac{\mu}{4}\right)\pi\hbar$$

$$\text{with}\quad \mu=\frac{\phi_1+\phi_2}{\pi/2}. \quad (24)$$

The inner and outer turning points, x_1 and x_2, respectively, are close to but not exactly equal to the turning points for the centrifugal potential or the Woods-Saxon potential alone. The phase losses ϕ_1 and ϕ_2 are both taken to be $\pi/2$ in the "simple" application of the WKB method. This is also the case in the "Langer" version, but the centrifugal potential is subjected to the Langer modification (21). The "present" WKB method we are proposing uses the energy-independent expression (22) for the phase loss ϕ_1 due to reflection at the inner turning point, the expression (12) for the phase loss ϕ_2 due to reflection at the outer turning point, and is based on the true centrifugal potential: there is no Langer modification.

The resulting eigenvalues are given in Table III for angular momentum $l=1$ and in Table IV for angular momentum $l=2$. The parameters of the Woods-Saxon potential are $k_{V_0}=1$, $R=30$, and $a=0.5$ in both cases. For $l=1$ the error in the conventional WKB calculation based on the Langer modification and a phase loss $\pi/2$ at both turning points is of the order of 0.002 to 0.012, except for the fourth excited state, where it is only 0.0004. Note that the simple WKB ansatz without the Langer modification yields qualitatively similar results. The results obtained with nonintegral Maslov index based on the phase losses (12) and (22), without the Langer modification, show a maximum error of 0.0002, which is two orders of magnitude better than the standard WKB results. The same holds for $l=2$ (Table IV), where a maximum error of 0.0005 with the nonintegral Maslov index is to be compared with errors up to 0.01 in the standard WKB method.

IV. QUADRATIC POTENTIAL

For a parabolic potential

$$V_\omega(x)=\frac{m}{2}\omega^2x^2\quad \text{for}\ x\geqslant 0,\quad V_\omega(x)=0\quad \text{for}\ x<0, \quad (25)$$

TABLE III. Energies of the bound states in the radial Woods-Saxon potential (23) with potential parameters $k_{V_0}=1$, $a=0.5$, and $R=30$ with angular momentum quantum number $l=1$. The exact quantum-mechanical results are compared with the present results obtained via (24) with the phase loss ϕ_1 given by (22) and ϕ_2 given by (12), with the simple WKB result in which both phase losses are taken as $\pi/2$, and with the standard WKB result obtained with the Langer-modified potential and phase loss $\pi/2$ at both turning points.

n	E_n^{exact}/V_0	$E_n^{\mathrm{present}}/V_0$	$E_n^{\mathrm{simple}}/V_0$	$E_n^{\mathrm{Langer}}/V_0$
0	−0.97815416	−0.97834291	−0.98383228	−0.98284962
1	−0.93556613	−0.93566866	−0.94235308	−0.94037733
2	−0.87203511	−0.87210568	−0.87893902	−0.87602379
3	−0.78795362	−0.78800723	−0.79425753	−0.79043683
4	−0.68386491	−0.68390852	−0.68900609	−0.68431253
5	−0.56051533	−0.56055291	−0.56399138	−0.55846381
6	−0.41901295	−0.41904703	−0.42031999	−0.41401662
7	−0.26131274	−0.26134508	−0.25989745	−0.25293155
8	−0.09248716	−0.09251698	−0.08776052	−0.08054343

TABLE IV. Same as Table III but with angular momentum quantum number $l=2$.

n	E_n^{exact}/V_0	E_n^{present}/V_0	E_n^{simple}/V_0	E_n^{Langer}/V_0
0	−0.96407673	−0.96457292	−0.97046925	−0.96973473
1	−0.91078135	−0.91105425	−0.91698240	−0.91566039
2	−0.83681851	−0.83700949	−0.84225964	−0.84038718
3	−0.74257027	−0.74271811	−0.74669583	−0.74429501
4	−0.62864921	−0.62877193	−0.63097475	−0.62806680
5	−0.49593660	−0.49604452	−0.49599832	−0.49261024
6	−0.34583435	−0.34593422	−0.34314953	−0.33932501
7	−0.18117566	−0.18127168	−0.17523388	−0.17107759
8	−0.01365981	−0.01366466	−0.00518905	−0.00183653

the Schrödinger equation (3) can be solved analytically in terms of the parabolic cylinder functions and the solution decaying in the classically forbidden region $x\to\infty$ is $U(-E/(\hbar\omega),y)$, where $y=x\sqrt{2m\omega/\hbar}$ [8]. Matching the logarithmic derivative of this solution to a superposition of incoming and reflected waves $\exp(ikx)+r\exp(-ikx)$ at $x=0$ leads to a reflection coefficient $r=(1-\mathrm{i}\beta)/(1+\mathrm{i}\beta)$, with

$$\beta=\sqrt{\frac{2\hbar\omega}{E}}\frac{\Gamma(\frac{3}{4}-E/(2\hbar\omega))}{\Gamma(\frac{1}{4}-E/(2\hbar\omega))}. \tag{26}$$

Comparing the WKB wave function (5) in the ''asymptotic'' region $x<0$ with the exact solution shows that the phase loss ϕ due to reflection at the classical turning point $x_0=\sqrt{2E/m}/\omega$ amounts to

$$\begin{aligned}\phi&=-\arg(r)+\frac{E}{\hbar\omega}\pi\\&=2\arctan\left(\sqrt{\frac{2\hbar\omega}{E}}\frac{\Gamma(\frac{3}{4}-E/(2\hbar\omega))}{\Gamma(\frac{1}{4}-E/(2\hbar\omega))}\right)+\frac{E}{\hbar\omega}\pi.\end{aligned} \tag{27}$$

The phase loss (27) is shown in Fig. 4. For half integral values of the ratio $E/\hbar\omega$ we have $\phi=\pi/2$, which is not surprising considering that standard WKB quantization gives the exact results for the quantum-mechanical energy eigenvalues of the harmonic oscillator, $E_n=(n+1/2)\hbar\omega$. The formula (27) goes further and it also shows how the phase approaches the long-wave limit π for $E\to 0$, viz.,

$$\phi=\pi-\sqrt{2}\,\frac{\Gamma(1/4)}{\Gamma(3/4)}\sqrt{\frac{E}{\hbar\omega}}+\frac{E}{\hbar\omega}\pi+O(E^{3/2})\quad\text{for } E\to 0. \tag{28}$$

If, for example, we study the bound states in a symmetric potential well consisting of two half parabolas (25) separated by a finite stretch where the potential vanishes, then there will be bound states at energies different from $(n+1/2)\hbar\omega$ and in particular one or more below $\hbar\omega/2$. Applying the WKB quantization condition with a Maslov index $\mu=2\phi/(\pi/2)$ gives, by construction, the exact eigenvalues for this potential if we insert the phase loss (27). Again we observe that the first-order WKB approximation can give highly accurate (in this case exact) results, even close to the long-wave limit, provided that the appropriate nonintegral Maslov index is used.

An interesting application of the concept of nonintegral Maslov indices is the radial harmonic oscillator

$$V_\omega^{(\gamma)}(x)=\frac{\hbar^2}{2m}\frac{\gamma}{x^2}+\frac{m}{2}\omega^2x^2,\qquad \gamma=l(l+1), \tag{29}$$

for which the standard WKB method in conjunction with the Langer-modified centrifugal potential is known to reproduce the energy eigenvalues exactly [3]. The integral $\int_{x_1}^{x_2}p(x)dx$ between the classical turning points x_1 and x_2 can be calculated analytically,

$$\int_{x_1}^{x_2}\sqrt{2m[E-V_\omega^{(\gamma)}(x)]}dx=\left(\frac{E}{2\hbar\omega}-\frac{1}{2}\sqrt{\gamma}\right)\pi\hbar. \tag{30}$$

In the standard WKB method the centrifugal potential is subjected to the Langer modification (21), whereby $\sqrt{\gamma}$ becomes $l+1/2$, and the right-hand side of Eq. (30) is equated to $(n+\mu/4)\pi\hbar$ with a Maslov index $\mu=2$. This immediately gives the correct quantum-mechanical energy eigenvalues

$$E=\left(2n+l+\frac{3}{2}\right)\hbar\omega. \tag{31}$$

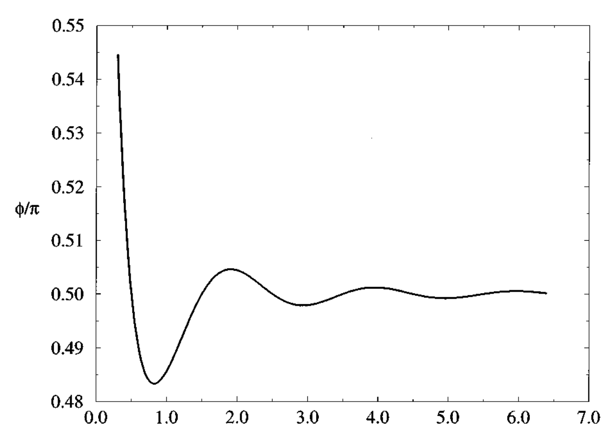

FIG. 4. Phase loss (27) due to reflection by the quadratic potential (25) as function of $\varepsilon=E/(\hbar\omega)$.

In the alternative procedure we are proposing, the centrifugal potential remains intact — there is no Langer modification — so the integral (30) contains the correct expression for $\sqrt{\gamma}$, viz., $\sqrt{l(l+1)}$. The right-hand side of (30) is equated to $(n+\mu/4)\pi\hbar$, but we now assume that the phase loss due to reflection at the centrifugal barrrier is given by (22) rather than $\pi/2$. The phase loss due to reflection at the outer turning point may be assumed to be $\pi/2$ because this is the correct value for a harmonic potential at the energies where we expect the eigenvalues to be [cf. Eq. (27) and Fig. 4]. Thus the Maslov index μ is

$$\mu = 1 + 2\left(l + \frac{1}{2} - \sqrt{l(l+1)} \right) + 1 \tag{32}$$

and the energies are again given by (31).

V. CALCULATING ϕ

In the examples discussed so far, we could make use of analytic expressions for the phase loss ϕ based on exact solutions of the Schrödinger equation containing all or a part of the potential being studied. It would of course be desirable to have a model-independent prescription for calculating the phase loss due to reflection at a classical turning point and the related nonintegral Maslov index in the general case without reference to exact wave functions. In order to achieve this, we must use in some way the information on how the wave function decays in the classically forbidden region because this determines its logarithmic derivative at the turning point, where it is matched to the wave function in the classically allowed region.

The WKB wave function is (weakly) singular at the classical turning point, so its logarithmic derivative cannot be used directly. One way of using the WKB wave function to construct an approximate wave function regular at the classical turning point is to insert it in the right-hand side of the Lippmann-Schwinger equation

$$\psi(x) = \psi_0(x) + \int_{-\infty}^{\infty} G(x,x')\mathcal{V}(x')\psi(x')dx', \tag{33}$$

where $G(x,x')$ is a Green's function for the "homogeneous" part of the Schrödinger equation, for which ψ_0 is a solution, and $\mathcal{V}$ stands for the "inhomogeneous" potential not accounted for in G.

Near the classsical turning point x_0 we have $E \approx V(x)$, so we may assume the term $[V(x)-E]\psi(x) = [V(x)-V(x_0)]\psi(x)$ in the Schrödinger equation (3) to be the small inhomogeneity and apply the Lippmann-Schwinger equation based on the Green's function

$$G(x,x') = \frac{2m}{\hbar^2}(x'-x)\Theta(x'-x),$$

$$\frac{\hbar^2}{2m}\frac{d^2}{dx^2}G(x,x') = \delta(x-x'). \tag{34}$$

We assume the classically forbidden region to be $x > x_0$. The wave function at x_0 is now

$$\psi(x_0) = \frac{2m}{\hbar^2}\int_{x_0}^{\infty}(x-x_0)[V(x)-V(x_0)]\psi(x)dx \tag{35}$$

and its derivative is

$$\psi'(x_0) = -\frac{2m}{\hbar^2}\int_{x_0}^{\infty}[V(x)-V(x_0)]\psi(x)dx. \tag{36}$$

The correct boundary conditions $\psi(x)\to 0$ for $x\to\infty$ are obtained by choosing the solution of the homogeneous equation to vanish.

If the potential were to vanish identically on the classically allowed side of the turning point, then the correct wave function would be proportional to $\cos(k|x-x_0|-\phi/2)$, $k=\sqrt{2mE}/\hbar$, on the allowed side, and the matching condition would be

$$\phi = -2\arctan\left(\frac{1}{k}\frac{\psi'(x_0)}{\psi(x_0)}\right). \tag{37}$$

Inserting the decaying WKB wave function as given on the left-hand side of (5) into Eqs. (35) and (36) and matching the logarithmic derivative according to (37) defines one way of obtaining an approximate value for the phase loss ϕ on the basis of the WKB wave functions alone. The matching condition (37) neglects the difference between the exact wave function and the free wave on the classically allowed side of the turning point. For a potential barrier that vanishes for $x \leqslant 0$ and rises monotonically for $x>0$, this means approximating the wave function between $x=0$ and the classical turning point $x=x_0$. In terms of wavelengths, the distance over which the wave function is approximated is measured by the dimensionless parameter kx_0, which goes to zero in the long-wave limit, because both $k\to 0$ and $x_0\to 0$.

The method based on (37), with the WKB wave functions in the integrands in the expressions (35) for $\psi(x_0)$ and (36) for $\psi'(x_0)$, gives the correct phase loss π in the long-wave limit and should be useful for small values of the dimensionless parameter kx_0. In order to obtain a quantitative estimate of how accurate it may be, we now study the special example of power-law potentials

$$V_\beta(x) = \begin{cases} V_0 x^\beta & \text{for } x \geqslant 0 \\ 0 & \text{for } x<0, \end{cases} \tag{38}$$

where $V_0>0$ and $\beta>0$. With the length b defined by $b=[\hbar^2/(2mV_0)]^{1/(\beta+2)}$, the classical turning point is $x_0=(E/V_0)^{1/\beta}=b(kb)^{2/\beta}$ and the dimensionless parameter kx_0 is related to kb by $kx_0=(kb)^{1+2/\beta}$. The exact phase loss due to reflection is defined as the phase loss ϕ with which the WKB wave function (5) is proportional to the exact solution of the Schrödinger equation in the asymptotic region $x<0$; the corresponding nonintegral Maslov index is, of course, $\phi/(\pi/2)$. In terms of the exact solution $\psi_{\rm ex}$ of the Schrödinger equation, which decays in the classically forbidden region $x>x_0$, the exact phase loss ϕ is

$$\phi_{\rm ex} = -2\arctan\left(\frac{1}{k}\frac{\psi'_{\rm ex}(0)}{\psi_{\rm ex}(0)}\right) + \frac{2}{\hbar}\int_0^{x_0}p(x)dx. \tag{39}$$

The second term on the right-hand side of (39) accounts for the phase accumulated in the WKB wave function between the classical turning point x_0 and the point $x=0$, where the WKB wave function is matched to the exact wave function. It can be evaluated analytically and is proportional to $kx_0=(kb)^{1+2/\beta}$.

In the long-wave limit the leading deviation of the phase loss from π is twice the inverse of the argument of the arctangent in (39), which can be calculated analytically at zero energy from the modified Bessel function representing the exact wave function (at zero energy). The leading terms for the phase loss in the long-wave limit are thus

$$\phi_{\rm ex}=\pi-\frac{2}{(\beta+2)^{\beta/(\beta+2)}}\frac{\Gamma\left(\frac{1}{\beta+2}\right)}{\Gamma\left(\frac{\beta+1}{\beta+2}\right)}kb+\frac{2}{\beta}\frac{\Gamma\left(\frac{1}{\beta}\right)\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{1}{\beta}+\frac{3}{2}\right)}(kb)^{1+2/\beta}+O((kb)^3); \qquad (40)$$

this is a generalization of (28) where $\beta=2$. If we calculate the phase loss approximately via the wave function (35) with the decaying WKB wave function in the integrand, then the corresponding expansion for ϕ near the long-wavelength limit is

$$\phi=\pi-2\left(\frac{\beta+2}{2}\right)^{2/(\beta+2)}\frac{\Gamma\left(\frac{3\beta+8}{2\beta+4}\right)}{\Gamma\left(\frac{3\beta+4}{2\beta+4}\right)}kb+\frac{2}{\beta}\frac{\Gamma\left(\frac{1}{\beta}\right)\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{1}{\beta}+\frac{3}{2}\right)}(kb)^{1+2/\beta}+O((kb)^3), \qquad (41)$$

Up to order $(kb)^3$ the approximate expression (41) differs from the exact expression (40) only in the coefficient of kb. The relative error in this coefficient approaches zero both for $\beta\to 0$ and for $\beta\to\infty$; its largest value is near 3% for $\beta\approx 1$ and it amounts to 2.4% for $\beta=4$.

The behavior of the approximate phase loss derived via (37) from the wave function (35) with the decaying WKB wave function in the integrand is illustrated for $\beta=4$ in Fig. 5, together with the exact phase loss derived from the numerically calculated exact solution of the Schrödinger equation. The abscissa is labeled by the energy in units of $E_0=\hbar^2/mb^2$, i.e. $\varepsilon=E/E_0=(kb)^2/2$. The approximate phase loss is quite close to the exact value near the long-wave limit and it remains within a few percent up to $\varepsilon\approx 2$, beyond which approximating ϕ by its semiclassical limit $\pi/2$ yields comparable or better accuracy. Similar results are observed for other powers β [10]: the relative error of the approximate phase loss is at most a few percent up to energies where the exact phase has approached the short-wavelength limit $\pi/2$ to within a few percent. At higher energies, the approximate phase loss becomes increasingly inaccurate, in particular it does not converge to the correct short-wave limit $\pi/2$. The usefulness of the procedure based on Eqs. (35)–(37) and the decaying WKB wave function lies in the fact that it is accurate to within a few percent near the long-wave limit, where the standard WKB breaks down.

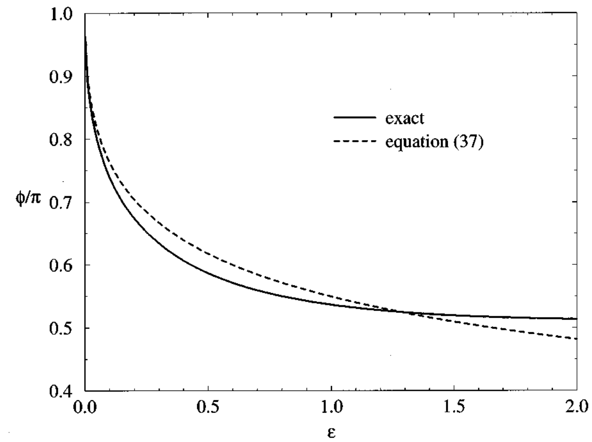

FIG. 5. Phase loss due to reflection by the quartic potential $V(x)=[\hbar^2/(2mb^2)](x/b)^4$ as function of $\varepsilon=E/[\hbar^2/(mb^2)]=(kb)^2/2$. The exact result derived from the numerical solution of the Schrödinger equation is compared with the approximate phase loss derived via Eq. (37) using the decaying WKB wave function in the classically forbidden region in the integrands of (35) and (36).

The vicinity of the long-wave limit is relevant, e.g., for low-lying bound states in the potential

$$V_R(x)=\begin{cases} V_0(x-R)^\beta & \text{for } x\geqslant R \\ 0 & \text{for } -R<x<R \\ V_0|x+R|^\beta & \text{for } x\leqslant -R \end{cases} \qquad (42)$$

describing a particle moving freely over a distance $2R$ bounded on each side by the power-law potential. We have calculated the energies of the lowest few eigenstates in the potential defined by $\beta=4$ and $R/b=5$ and the results are shown in Table V. The exact eigenvalues are compared with the present results derived via the quantization condition (7), but with the nonintegral Maslov index corresponding to the approximate phase loss ϕ, as shown in Fig. 5, at each turning point; we also show the results obtained with standard WKB quantization, i.e., with $\phi=\pi/2$, and with the opposite limit $\phi=\pi$. The eigenvalues obtained with the present quantization condition based on the (approximate) nonintegral Maslov index are quite accurate for the lowest few states and they remain more accurate than the standard WKB results, as long as the approximate phase loss is closer to the exact phase loss than is the standard choice $\pi/2$. The error relative to the separation of successive levels is uniformly less than 3% in the energy range studied. Note that choosing the phase loss to be π at each turning point gives very poor results even for the ground-state energy. The reason for this is that the leading deviation of the phase loss from its long-wave limit π is proportional to the square root of the energy [cf. Fig. 5 and Eqs. (40) and (41)] so that small increments in energy lead to large shifts in phase loss. [See also Figs. 1 and 4 as well as Eqs. (12) and (28).] For reflection by a steep wall, which is an essential feature of various two-dimensional billard systems so extensively studied

TABLE V. Eigenvalues $\varepsilon_n = E_n/[\hbar^2/(mb^2)]$ of the lowest eight bound states in the potential (42) for $\beta = 4$ and $R/b = 5$. The exact eigenvalues are compared with the present results obtained via first-order WKB quantization (7) with a nonintegral Maslov index corresponding to the approximate phase loss ϕ as shown in Fig. 5 at each turning point. Also shown are the standard WKB results based on phase loss $\pi/2$ as well as the results obtained with $\phi = \pi$, which would be appropriate for steep wall potentials at the classical turning points.

n	Exact	Present	$\phi = \pi/2$	$\phi = \pi$
0	0.0292434	0.0300133	0.0108349	0.0412557
1	0.1167859	0.1197302	0.0895180	0.1544972
2	0.2620643	0.2677489	0.2353420	0.3313643
3	0.4641405	0.4713903	0.4419855	0.5667067
4	0.7217078	0.7286595	0.7050893	0.8567424
5	1.0331110	1.0369163	1.0213137	1.1984827
6	1.3963910	1.3943704	1.3879559	1.5894626
7	1.8093647	1.7992174	1.8027518	2.0275898

nowadays [11], we may expect that even a slight smoothing of the wall will necessitate substantial modification of the Maslov indices in the quantization formulas.

When β is an even integer and the length R is taken to vanish, the potential (42) is an analytic function; for $\beta = 4$ we have the quartic oscillator. The semiclassical quantization of the quartic oscillator was studied by Bender *et al.* [12] using the WKB series derived from Dunham's formulation of the quantization condition [13]. This theory yields an asymptotic series for the eigenvalues and gives extremely accurate results for highly excited states. For the ground state of the quartic oscillator the series does not converge well and provides a rather poor approximation. The exact ground-state energy is $\varepsilon = 0.530\,181\,05\ldots$ and standard WKB quantization, which corresponds to the leading term of the Dunham series, predicts $\varepsilon = 0.43$, which is off by 18%. In the next order, standard WKB gives $\varepsilon = 0.49$, which is about 8% off, and the error grows again in higher orders [12]. The first-order WKB quantization condition (7) with the nonintegral Maslov index corresponding to the approximate phase losses ϕ as shown in Fig. 5 gives the ground-state energy of the quartic oscillator at $\varepsilon = 0.560\,615$, which is within 6% of the exact result. This error is smaller than the error obtained in standard WKB quantization in any order.

VI. CONCLUSION

The WKB ansatz may be an accurate approximation of the quantum-mechanical Schrödinger equation away from the semiclassical limit of short waves if the potential is sufficiently smooth so that the condition of applicability (4) is violated only near the classical turning points. The key to obtaining accurate wave functions in the classically allowed region is the correct choice of the phase loss ϕ due to reflection at the classical turning points. Away from the limit of short waves, this phase loss is in general not equal to $\pi/2$ and it approaches the value π continuously in the limit of long waves. The fact that the phase losses due to reflection are in general nonintegral multiples of $\pi/2$ between the limits of long and short waves can be expressed by nonintegral Maslov indices in the WKB ansatz.

We have demonstrated the efficacy of the concept of nonintegral Maslov indices in a number of physically relevant cases. For the bound states in a Woods-Saxon potential (with or without centrifugal potential) the use of the nonintegral Maslov indices improves the accuracy of the WKB results by orders of magnitude. The energy eigenvalues of the radial harmonic oscillator, which are given exactly in the standard WKB theory, are also reproduced exactly in the present ansatz based on nonintegral Maslov indices.

An especially important case is the repulsive γ/x^2 potential, which is treated in the standard WKB method by assuming a phase loss $\pi/2$ at reflection and subjecting the potential to the Langer modification $\gamma \to \gamma' = \gamma + 1/4$. The WKB wave function constructed in this way approaches the exact solution of the Schrödinger equation asymptotically, but the difference between WKB wave function and exact wave function decreases only as $1/kx$. If we incorporate the correct energy-independent phase loss (22) in the WKB ansatz (which is no more difficult than assuming a phase loss $\pi/2$), then there is no need for the Langer modification of the potential and the difference between the WKB wave function and exact wave function decreases as $1/(kx)^3$, i.e., the WKB wave function approaches the exact solution of the Schrödinger equation more rapidly by two orders in $1/kx$.

We have presented a method by which the phase loss can be derived approximately from the decaying WKB wave functions in the classically forbidden region. For power-law potentials this method yields approximate phase losses that are within a few percent of the exact phase losses for energies ranging from the long-waves limit up to values where the exact phase loss is already within a few percent of the short-wave limit $\pi/2$. With the approximate phase loss derived in this way, first-order WKB quantization reproduces the ground-state energy of the quartic oscillator more accurately than standard WKB quantization in any order.

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