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Phase Loss in WKB Waves Due to Reflection by a Potential

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We study the WKB method away from the short-wave limit. Incorporating the correct phase loss due to reflection at a classical turning point, in place of the usual choice $\pi/2$, can greatly improve the accuracy of the WKB wave function in the classically allowed region. For a repulsive $1/x^2$ potential this leads to far more accurate WKB wave functions that the usual Langer modification of the potential. [S0031-9007(96)00463-2]

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The WKB wave function for a particle of mass m moving with total energy E in a potential $V(x)$ is [1,2]

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

where $p(x)$ is the local momentum, $p(x) = \sqrt{2m[E - V(x)]}$. It is, in general, a good approximate solution of the Schrödinger equation,

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} V(x)\psi = E\psi\,, \quad (2)$$

as long as the (local) de Broglie wavelength $\lambda(x) = 2\pi\hbar/p(x)$ varies sufficiently slowly. This condition is always violated at a classical turning point x_0, because $\lambda(x_0) = \infty$. The monotonically 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 via the famous connection formula [1,2]

$$\frac{1}{\sqrt{|p(x)|}} \exp\left[-\frac{1}{\hbar} \left| \int_{x_0}^{x} |p(x')|\, dx' \right| \right] \longrightarrow \frac{2}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar} \left| \int_{x_0}^{x} p(x')\, dx' \right| - \frac{\phi}{2} \right]. \quad (3)$$

The phase $\phi/2$ in (3) corresponds to a reflection coefficient $\exp(-i\phi)$ in front of the wave reflected at the turning point, relative to the incoming wave traveling towards the turning point. The *phase loss* ϕ due to reflection at an isolated classical turning point is equal to $\pi/2$ in the semiclassical limit of short waves [1,2]. In the long-wave limit, e.g., for a free particle reflected by an infinite steep wall, the reflection coefficient is -1 and the phase loss is π rather than $\pi/2$. In between the limits of long and short waves, the phase loss is, in general, a nonintegral multiple of $\pi/2$. We demonstrate in the following that the WKB approximation can be highly accurate away from the short-wave limit, provided that the phase losses due to reflection at the classical turning points are accounted for correctly. Popov *et al.* [3] have recently discussed in some detail how the ratio of the *amplitudes* appearing on both sides of the connection formula (3) should be modified when the conditions of the short-wave limit are not fulfilled, but the phase loss is taken as $\pi/2$. This Letter focuses on how to modify the phase loss, which plays a crucial role in improving the WKB approximation in the classically allowed region.

First consider the potential

$$V_\gamma(x) = \frac{c}{x^2} = \frac{\hbar^2}{2m} \frac{\gamma}{x^2}\,. \quad (4)$$

How close the wave functions are to the semiclassical limit depends not on energy, but only on the dimensionless parameter $\gamma = 2mc/\hbar^2$, which is $l(l+1)$ for the 3D centrifugal potential, but can, in general, be any non-negative real number. The solution of the Schrödinger equation which is regular at the origin is $\psi(x) \propto \sqrt{kx}\, J_\nu(kx), k = \sqrt{2mE}/\hbar$, where J_ν is the

Bessel function of order $\nu = \sqrt{\gamma + 1/4}$. Asymptotically

$$\psi(x) \propto \left(1 - \frac{\gamma(\gamma-2)}{8(kx)^2}\right)\cos\left[kx - \left(\nu + \frac{1}{2}\right)\frac{\pi}{2}\right] - \frac{\gamma}{2kx}\sin\left[kx - \left(\nu + \frac{1}{2}\right)\frac{\pi}{2}\right] + O((kx)^{-3}). \tag{5}$$

The classical turning point for the potential (4) is $x_0 = \sqrt{\gamma}/k$, and the integral $\int_{x_0}^{x} p(x')\,dx'$ can be calculated analytically. The asymptotic behavior of the WKB wave function (3) is

$$\psi_{\mathrm{WKB}} \propto \left(1 - \frac{\gamma(\gamma-2)}{8(kx)^2}\right)\cos\left[kx - \sqrt{\gamma}\,\frac{\pi}{2} - \frac{\phi}{2}\right] - \frac{\gamma}{2kx}\sin\left[kx - \sqrt{\gamma}\,\frac{\pi}{2} - \frac{\phi}{2}\right] + O((kx)^{-3}). \tag{6}$$

In the standard WKB method the phase ϕ in (6) is taken to be $\pi/2$, and the asymptotic phases in the leading term of the exact wave function (5) and in the WKB wave function (6) are reconciled by subjecting the potential (4) for the WKB calculation to the *Langer modification* [1,2,4,5],

$$\gamma \longrightarrow \gamma' = \gamma + \tfrac{1}{4}, \tag{7}$$

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 (6), but the coefficients proportional to $1/kx$ and $1/(kx)^2$ are changed, so only the leading term of (6) agrees with the exact expression (5).

However, we also obtain the correct arguments of sine and cosine in the asymptotic expansion (6) of the WKB wave function, if we leave the potential intact and interpret

$$\phi = \left(\nu + \frac{1}{2} - \sqrt{\gamma}\right)\pi = \frac{\pi}{2} + \left(\sqrt{\gamma + \frac{1}{4}} - \sqrt{\gamma}\right)\pi \tag{8}$$

as the phase loss due to reflection at the classical turning point. The asymptotic expansion of the WKB wave function is then identical to the exact wave function (5) up to and including terms of order $1/(kx)^2$, and the deviation is of the order $1/(kx)^3$. The WKB wave function based on the true potential and the phase loss (8) approaches the exact wave function more rapidly by 2 orders in $1/kx$ and is a far better approximation at finite distances. This is illustrated in Fig. 1. The phase (8) 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 $\gamma \to 0$.

Now consider a smooth potential step

$$V_a(x) = \frac{V_0}{1 + \exp(-x/a)}, \quad V_0 > 0. \tag{9}$$

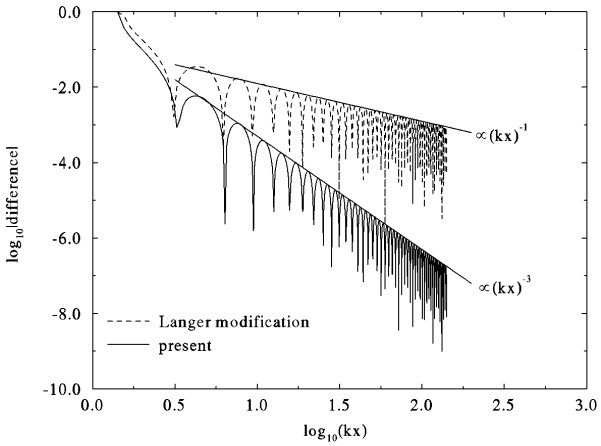

FIG. 1. Accuracy of WKB wave functions in the classically allowed region for the potential (4) with $\gamma = 2$ ($l = 1$). The absolute values of the difference between the WKB wave function and the exact wave function as a function of kx are shown in a doubly logarithmic plot. The dashed curve shows 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 (8) and the true potential without Langer modification. The straight lines indicate proportionality to $1/kx$ and $1/(kx)^3$, respectively.

Asymptotically comparing the WKB wave function (3) in the classically allowed region, $x \to -\infty$, with the exact solution [2] of the Schrödinger equation (2) in the energy range $0 < E < V_0$ leads to the following phase loss ϕ in the WKB wave function [6]:

$$\phi = \delta + 2ka\left[2\ln 2 - \ln\left(1 + \frac{\kappa^2}{k^2}\right) - 2\,\frac{\kappa}{k}\arctan\frac{k}{\kappa}\right], \tag{10}$$

with

$$\delta = 2\arg\frac{\Gamma(-2ika)}{\Gamma(\kappa a - ika)\Gamma(1 + \kappa a - ika)}. \tag{11}$$

The constants k and κ in (10) are the asymptotic wave numbers in the classically allowed and forbidden regions, respectively,

$$k = k_{V_0}\sqrt{E/V_0}, \quad \kappa = k_{V_0}\sqrt{1 - E/V_0}; \tag{12}$$

$k_{V_0} = \sqrt{2mV_0}/\hbar$ is the asymptotic wave number in the allowed region at the top of the barrier, and $1/k_{V_0}$ defines a scale for lengths. The phase (10) is illustrated in Fig. 2 for various values of the *relative diffuseness* $\alpha = k_{V_0}a$. In the limit of small α we obtain the phase loss due to reflection by a sharp step, $\phi = 2\arctan(\kappa/k)$. For a very diffuse step, assuming $ka \gg 1$, $\kappa a \gg 1$ yields a phase loss $\phi \to \pi/2$. Note, however, that for any value of a, ka is always small sufficiently close to the long-wave limit $E = 0$, and ϕ always approaches π in this limit.

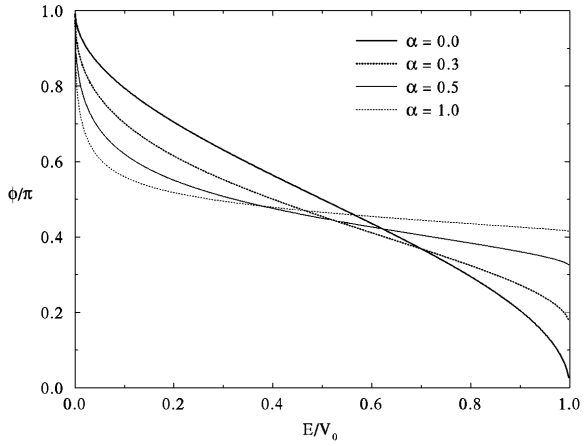

FIG. 2. Phase loss ϕ due to reflection by the potential step (9) as given by (10) for various values of the relative diffuseness $\alpha = k_{V_0} a$.

For a particle oscillating between two turning points x_1 and x_2, the WKB quantization condition is obtained by requring the total phase during one period of oscillation to be an integral multiple of 2π: $(1/\hbar) \oint p(x)\, dx - \phi_1 - \phi_2 = 2\pi n$, where ϕ_1 is the phase loss due to reflection at the turning point x_1 and ϕ_2 is the phase loss at x_2. This leads to the well known formulation of the quantization condition,

$$\int_{x_1}^{x_2} p(x)\, dx = \left(n + \frac{\mu}{4}\right)\pi\hbar, \quad \mu = \frac{\phi_1 + \phi_2}{\pi/2}. \tag{13}$$

The *Maslov index* μ stands for the total phase loss during one period in units of $\pi/2$. Allowing the phase losses to be nonintegral multiples of $\pi/2$ corresponds to allowing nonintegral Maslov indices in the quantization condition (13).

The phase losses due to reflection by a centrifugal potential (8) and by the smooth potential step (10) may be used to apply the concept of nonintegral Maslov indices to the quantization of the radial Woods-Saxon potential, which is, e.g., used in the description of atomic clusters [7],

$$V_{\mathrm{WS}}^{(l)}(x) = \frac{\hbar^2}{2m}\frac{l(l+1)}{x^2} - \frac{V_0}{1 + \exp[(x - R)/a]}, \quad x > 0. \tag{14}$$

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 step alone. In the present application of the quantization condition (13) we take the phase loss ϕ_1 at the inner turning point to be the energy-independent value (8), and the phase loss ϕ_2 is taken as the energy-dependent value (10)—note that k and κ are given by (12) with E replaced by $V_0 + E = V_0 - |E|$. Since the right-hand side of the quantization condition (13) now depends on energy, the positions of the eigenvalues are determined as the intersections of both sides of the equation. Energy eigenvalues obtained in this way are given in Table I and compared with conventional WKB results and exact energies. In this example the present results show a maximum error of 0.0002, which is 2 orders of magnitude better than the standard WKB results.

Next we consider the radial harmonic oscillator,

$$V_\omega^{(\gamma)}(x) = \frac{\hbar^2}{2m}\frac{\gamma}{x^2} + \frac{m}{2}\omega^2 x^2, \quad \gamma = l(l+1), \tag{15}$$

for which the standard WKB method in conjunction with the Langer-modified centrifugal potential is known to reproduce the energy eigenvalues exactly [5]. The integral $\int_{x_1}^{x_2} p(x)\, dx$ between the classical turning points x_1 and x_2 can be calculated analytically,

$$\int_{x_1}^{x_2} \sqrt{2m[E - V_\omega^{(\gamma)}(x)]}\, dx = \left(\frac{E}{2\hbar\omega} - \frac{1}{2}\sqrt{\gamma}\right)\pi\hbar. \tag{16}$$

TABLE I. Energies of the bound states in the radial Woods-Saxon potential (14) with potential parameters $k_{V_0} = 1$, $a = 0.5$, $R = 30$, and $l = 1$. The *exact* quantum mechanical results are compared with the *present* results obtained via (13) with the phase loss ϕ_1 given by (8) and ϕ_2 given by (10), the *simple* WKB results in which both phase losses are taken as $\pi/2$, and the standard WKB results 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	−0.978 154 16	−0.978 342 91	−0.983 832 28	−0.982 849 62
1	−0.935 566 13	−0.935 668 66	−0.942 353 08	−0.940 377 33
2	−0.872 035 11	−0.872 105 68	−0.878 939 02	−0.876 023 79
3	−0.787 953 62	−0.788 007 23	−0.794 257 53	−0.790 436 83
4	−0.683 864 91	−0.683 908 52	−0.689 006 09	−0.684 312 53
5	−0.560 515 33	−0.560 552 91	−0.563 991 38	−0.558 463 81
6	−0.419 012 95	−0.419 047 03	−0.420 319 99	−0.414 016 62
7	−0.261 312 74	−0.261 345 08	−0.259 897 45	−0.252 931 55
8	−0.092 487 16	−0.092 516 98	−0.087 760 52	−0.080 543 43

In the standard WKB method the centrifugal potential is subjected to the Langer modification (7), whereby $\sqrt{\gamma}$ becomes $l + 1/2$, and the right-hand side of Eq. (16) is equated to $(n + \mu/4)\pi\hbar$ with a Maslov index $\mu = 2$. This immediately gives the correct quantum mechanical energy eigenvalues,

$$E = (2n + l + \tfrac{3}{2})\hbar\omega\,. \tag{17}$$

In the procedure we are proposing, the centrifugal potential remains intact—there is no Langer modification—so the integral (16) contains the correct expression for $\sqrt{\gamma}$, viz. $\sqrt{l(l+1)}$. The right-hand side of (16) is equated to $(n + \mu/4)\pi\hbar$, but we now take the phase loss due to reflection at the centrifugal barrier to be (8) rather than $\pi/2$; at the outer turning point we use the phase loss due to reflection by a quadratic potential, which can be derived via parabolic cylinder functions and is equal to $\pi/2$ at the energies where we expect the eigenvalues to be [6]. Thus the total Maslov index is $\mu = 1 + 2[l + 1/2 - \sqrt{l(l+1)}] + 1$, and the energies are again given by (17).

It is, of course, desirable to have a model-independent prescription for calculating the phase loss without reference to exact wave functions. For 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. One way of constructing an approximate wave function regular at the classical turning point is to insert the WKB wave function in the right-hand side of the Lippmann-Schwinger equation,

$$\psi(x_0) = \frac{2m}{\hbar^2}\int_{x_0}^{\infty}(x - x_0)[V(x) - V(x_0)]\psi(x)\,dx\,, \tag{18}$$

where the classically forbidden region is $x > x_0$. The derivative of (18) is

$$\psi'(x_0) = -\frac{2m}{\hbar^2}\int_{x_0}^{\infty}[V(x) - V(x_0)]\psi(x)\,dx\,. \tag{19}$$

If the potential were to vanish identically on the classically allowed side of the turning point, then the matching condition would be

$$\phi = -2\arctan\left(\frac{1}{k}\,\frac{\psi'(x_0)}{\psi(x_0)}\right). \tag{20}$$

Inserting the decaying WKB wave function as given on the left-hand side of (3) into Eqs. (18) and (19) and matching the logarithmic derivative according to (20) defines one way of obtaining an approximate value for the phase loss ϕ on the basis of the WKB wave functions alone. This gives the correct value π for $k \to 0$ and should be useful for long waves.

We applied this procedure numerically to a few potentials, $V_n(x) = |x|^n/2$ ($\hbar = m = 1$). The phase loss is shown in Fig. 3 together with the "exact" phase, which was derived by comparing WKB and exact wave functions at $x = 0$. The ground state energy is given via (13) [$\phi_1 = \phi_2 = \phi$] by the intersection of the action integral $\hbar^{-1}\int_{x_1}^{x_2} p(x)\,dx$ with ϕ/π. The energies obtained using the approximate phases are listed in Table II together with the exact energies and the results obtained in standard WKB quantization with $\phi = \pi/2$. The present approximate procedure gives ground state energies uniformly within about 6% of the exact values, whereas the standard WKB result is 18% off for $n = 4$ and becomes rapidly worse as n increases. Note, however, that better results have been obtained in the traditional WKB for $n = 4$ by including complex-coordinate turning points [8].

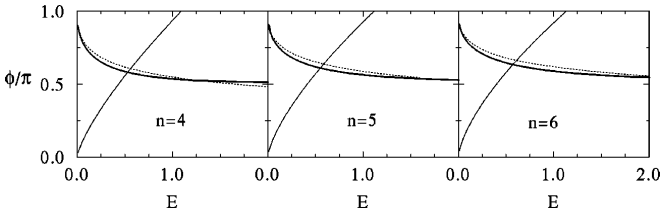

FIG. 3. Phase loss due to reflection by the potentials $V_n(x) = |x|^n/2$. The exact results (thick solid lines) are compared with the approximate phase losses (dashed lines) derived via equation (20) using the WKB wave functions in the classically forbidden region in the integrands of (18) and (19). The action integral $\hbar^{-1}\int_{x_1}^{x_2} p(x)\,dx$ is shown as a thin solid line in each panel, and its intersection with ϕ/π defines the ground state energy for the respective potential.

The examples above show that the WKB ansatz may be an accurate approximation of the quantum mechanical wave function away from the semiclassical limit of short waves, if the potential is sufficiently smooth so that the condition of applicability is violated only near the classical turning points. The key to obtaining accurate wave functions in the classically allowed region is correctly accounting for the phase loss due to reflection at the classical turning points. For a repulsive $1/x^2$ potential as occurs in the radial Schrödinger equation, the correct phase loss is an energy-independent constant, and it can be incorporated into the WKB ansatz as easily as the standard choice $\pi/2$. Compared with the standard WKB wave functions based on a phase loss $\pi/2$ and a Langer modification of the

TABLE II. Ground state energies in the potentials $V_n(x) = |x|^n/2$ ($\hbar = m = 1$). The exact results are compared with the results obtained in first order WKB quantization using the present method based on the (approximate) phase losses in Fig. 3 and using the standard procedure based on a phase loss $\pi/2$ at each reflection.

n	4	5	6
Exact	0.530 181	0.551 149	0.572 401
Present	0.560 664	0.586 680	0.610 391
Standard	0.433 573	0.414 535	0.400 415

potential, the present WKB wave functions based on the correct phase loss and the true centrifugal potential approach the exact wave function more rapidly by 2 orders in $1/kx$.

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