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Accurate WKB wave functions for weakly attractive inverse-square potentials

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For a weakly attractive inverse-square potential, $V(x)=-g\hbar^2/(2mx^2)$ with $0<g\leqslant 1/4$, the standard WKB wave function shows unphysical divergence near the origin. Introducing an appropriate nonvanishing reference point and a related phase yields WKB wave functions whose deviation from the regular solution of the Schrödinger equation decreases asymptotically as $1/(kx)^3$. This is two orders better than the alternative technique involving the Langer modification of the potential. The performance of the correspondingly modified quantization conditions is demonstrated for the bound states of vanishing angular momentum in the two-dimensional circle billiard and in a two-dimensional Woods-Saxon well. [S1050-2947(99)05402-5]

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The accuracy of WKB wave functions has recently been shown to be improved considerably, if the connection formulas at classical turning points are generalized to allow for reflection phases deviating from the value $\pi/2$ appropriate in the short wave limit [1–6], and/or for amplitude factors deviating from the conventionally assumed value unity [7]. For a particle (mass m, energy E) in an inverse-square potential,

$$V(x)=\frac{\hbar^2}{2m}\frac{\gamma}{x^2},\quad x>0, \tag{1}$$

with $\gamma\geqslant 0$, the classical momentum $p(x)=\sqrt{2m[E-V(x)]}$ vanishes at the classical turning point x_1 given by $kx_1=\sqrt{\gamma}$ $(k=\sqrt{2mE}/\hbar)$, and the WKB wave function on the classically allowed side of the turning point is

$$\psi_{\mathrm{WKB}}(x)\propto\frac{1}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\int_{x_1}^{x}p(x')\,dx'-\frac{\phi}{2}\right). \tag{2}$$

The exact regular solution of the Schrödinger equation with the potential (1) is

$$\begin{aligned}\psi_{\mathrm{ex}}(x)&\propto\sqrt{kx}J_\nu(kx)\\&\sim\left(1-\frac{\gamma(\gamma-2)}{8(kx)^2}\right)\cos\left(kx-\nu\frac{\pi}{2}-\frac{\pi}{4}\right)\\&\quad-\frac{\gamma}{2kx}\sin\left(kx-\nu\frac{\pi}{2}-\frac{\pi}{4}\right)+O\left(\frac{1}{(kx)^3}\right),\end{aligned} \tag{3}$$

where J_ν is the Bessel function of order $\nu=\sqrt{\gamma+1/4}$. The difference between the appropriately normalized WKB wave function (2) and the exact wave function (3) vanishes as $1/(kx)^3$ asymptotically, if and only if the reflection phase ϕ in (2) is chosen as [1]

$$\phi=\frac{\pi}{2}+(\sqrt{\gamma+1/4}-\sqrt{\gamma})\pi. \tag{4}$$

This is two orders better than is achieved in the conventional approach [8–10], where the reflection phase is taken as $\pi/2$ and the WKB wave functions are calculated with the Langer-modified potential,

$$V_{\mathrm{L}}(x)=V(x)+\frac{\hbar^2}{8mx^2}=\frac{\hbar^2}{2m}\frac{\gamma+1/4}{x^2}. \tag{5}$$

Generalizations of the formula (4) have been successfully used to derive analytic expressions for the phase shifts in scattering by singular potentials [2] and to improve the accuracy obtained in WKB quantization in molecular potentials [4].

The condition $\gamma\geqslant 0$ restricts the applicability of Eq. (4) to repulsive (or vanishing) inverse-square potentials. Attractive inverse-square potentials can be generated, e.g., by the coupling of angular momentum and a monopole-dipole interaction, as for an electron or positron in the field of an excited hydrogen atom [11–13]. For $\gamma<-1/4$, the potential (1) supports an infinite number of bound states whose energies accumulate at $-\infty$ and at zero [14], and the Schrödinger equation only makes sense if the potential is modified at short distances. However, for weakly attractive potentials, $-1/4\leqslant\gamma<0$, the Schrödinger equation has no bound states, its regular positive energy solutions can still be written as (3), and the order $\nu=\sqrt{\gamma+1/4}$ remains real and non-negative in this range. The Langer modification (5) can be applied in this

case, but the more successful approach based on the reflection phase (4) cannot. In this Brief Report we close this gap by presenting a simple correction of WKB wave functions for weakly attractive inverse-square potentials, $-1/4 \leqslant \gamma < 0$. The correction leads to the same improved accuracy as the use of the appropriate reflection phase (4) does for repulsive inverse-square potentials.

Straightforward application of the WKB method for a weakly attractive inverse-square potential (without Langer modification) is impossible near the origin $x \to 0$, because $p(x) \sim 1/x$ and the integral $\int_0^x p(x')\,dx'$ diverges. This problem does not occur when using the Langer modified potential (5), and, except for $\nu = 0$, the WKB wave function then actually has the right behavior $\propto x^{\nu+1/2}$ near the origin. This fact is not very significant, however, because the Langer modified potential has a wrong classical turning point x_{L} at $kx_{\mathrm{L}} = \sqrt{\gamma + 1/4}$, and the WKB wave function becomes singular at x_{L}.

The WKB wave function (2) can be formulated consistently for a weakly attractive potential (without Langer modification), if we choose the point of reference x_1 to be not the origin but a (small) positive number. The leading asymptotic behavior of the WKB wave function (2) then is

$$\psi_{\mathrm{WKB}}(x) \sim \left(1 - \frac{g(g+2)}{8(kx)^2}\right)\cos\left(kx - c_1 - \frac{\phi_1}{2}\right) + \frac{g}{2kx}\sin\left(kx - c_1 - \frac{\phi_1}{2}\right) + O\left(\frac{1}{(kx)^3}\right), \quad (6)$$

where we have written g for the positive number $-\gamma$ and labeled the phase ϕ with the subscript ''1'' to indicate that its choice will depend on the choice of x_1. The constant c_1 in (6) comes from the lower limit of integration and is given by

$$c_1 = \sqrt{g}\left[\sqrt{1 + \frac{1}{a}} - \ln\left(\sqrt{1+a} + \sqrt{a}\right)\right], \qquad a = \frac{g}{(kx_1)^2} = \frac{|\gamma|}{(kx_1)^2}. \quad (7)$$

The asymptotic behavior of the WKB wave function (6) agrees with that of the exact wave function (3) up to and including terms of order $1/(kx)^2$, if the constant phase $c_1 + \phi_1/2$ in (6) is identical to the corresponding phase $\nu(\pi/2) + \pi/4$ appearing in the exact wave function (3). The correct phase ϕ_1 to be inserted in the WKB wave function (6) is thus, for a given choice of the reference point x_1,

$$\phi_1 = \frac{\pi}{2} + \pi\sqrt{\frac{1}{4} - g} + 2\sqrt{g}\left[\ln\left(\sqrt{1+a} + \sqrt{a}\right) - \sqrt{1 + \frac{1}{a}}\right]. \quad (8)$$

The difference between the appropriately normalized WKB wave function (2) and the exact wave function (3) vanishes as $1/(kx)^3$ asymptotically, as long as reference point x_1 and phase ϕ_1 fulfill the relation (8). This is two orders better than the WKB wave function constructed via the Langer-modified potential (5), where only the leading asymptotic terms agree and the error is proportonal to $1/(kx)$.

Our recipe for improving the WKB wave function in the presence of a weakly attractive inverse-square potential contains the reference point x_1 as a free parameter. The WKB wave function beyond x_1 does not depend on the choice of x_1 as long as Eq. (8) is fulfilled. In a potential consisting of a sum of a weakly attractive inverse-square potential and a further potential behaving smoothly near the origin, the choice of x_1 will not significantly affect the WKB wave function, as long as it is chosen in a region where the full potential in the Schrödinger equation is essentially given by the inverse-square potential. If we choose x_1 to correspond to a given finite value of the parameter a (7), then the phase (8) does not depend on energy. In the limit of vanishing strength of the inverse-square potential, $\gamma \to 0$, the reference point x_1 tends to zero for finite a and the reflection phase (8) becomes π, as for the s-wave radial Schrödinger equation in three dimensions.

In order to demonstrate the usefulness of the current prescription, we study the energies of the bound states of the radial Schrödinger equation of the two-dimensional circle billiard and a two-dimensional Woods-Saxon well for vanishing angular momentum. For two-dimensional (plane) systems the radial Schrödinger equation contains a centrifugal potential [15],

$$V^{(m_{\mathrm{ang\,mom}})}(x) = \frac{\hbar^2}{2m}\,\frac{m_{\mathrm{ang\,mom}}^2 - 1/4}{x^2}, \quad (9)$$

where $m_{\mathrm{ang\,mom}} = 0, \pm 1, \pm 2 \ldots$ is the quantum number of the angular momentum component perpendicular to the plane. For vanishing angular momentum, the potential (9) has the form (1) with $\gamma = -1/4$, which corresponds to the maximum strength in our range of weakly attractive potentials. Berry and Ozorio de Almeida [15] pointed out the problems associated with the WKB treatment of the two-dimensional radial Schrödinger equation for vanishing angular momentum, and they studied an alternative approach based on the method of comparison equations. In an application to bound states in a logarithmic potential, they managed to reduce the error in the WKB approach based on the Langer modification by a factor of 12 to 30. Our present treatment is as simple as the conventional WKB treatment, and the quantization condition is [1]

$$\int_{x_1}^{x_2} p(x)\,dx = \left(n + \frac{\mu}{4}\right)\pi\hbar, \quad (10)$$

where

$$\mu = \frac{\phi_1 + \phi_2}{\pi/2} \quad (11)$$

is the, not necessarily integral, Maslov index accounting for the phase loss ϕ_2 of the WKB wave function at the outer turning point x_2 and the phase ϕ_1 from the inner point of reference x_1.

For the two-dimensional circle billiard, the outer turning point is at its radius R and the wave function is required to

TABLE I. Wave numbers k_n of the eigenstates of the two-dimensional circle billiard of radius $R=1$ for vanishing angular momentum. The ''conventional'' values are obtained via the quantization condition (12) based on the Langer modification of the potential; the ''present'' values are obtained via WKB quantization in the (attractive) centrifugal potential according to Eq. (14); the ''exact'' values are the exact quantum-mechanical eigenvalues corresponding to the zeros of the Bessel function $J_0(kR)$.

n	Conventional	Present	Exact
0	2.356194490	2.407922305	2.404825558
1	5.497787144	5.520414929	5.520078110
2	8.639379797	8.653820273	8.653727913
3	11.78097245	11.79157166	11.79153444
4	14.92256510	14.93093620	14.93091771
5	18.06415776	18.07107445	18.07106397
6	21.20575041	21.21164313	21.21163663
7	24.34734307	24.35247584	24.35247153
8	27.48893572	27.49348213	27.49347913

have a node at R, so $\phi_2=\pi$. The Langer-modified potential vanishes in this case, so the conventional WKB quantization condition is simply

$$kR=\left(n+\frac{3}{4}\right)\pi. \tag{12}$$

With our present recipe, the action integral on the left-hand side of Eq. (10) is evaluated with the true potential, $V(x)=-\hbar^2/(8mx^2)$ and a nonvanishing inner point of reference x_1, and the quantization condition (10) and (11) contains the nontrivial phase ϕ_1. The quantization condition now reads,

$$\begin{aligned}\frac{1}{\hbar}\int_{x_1}^{R}p(x)\,dx&\\ &\equiv\frac{1}{2}\left[\sqrt{1+(2kR)^2}-\ln\left(\frac{1}{2kR}+\sqrt{1+\frac{1}{(2kR)^2}}\right)\right]-c_1\\ &=\left(n+\frac{\mu}{4}\right)\pi,\quad \mu=\frac{\phi_1+\pi}{\pi/2}.\end{aligned} \tag{13}$$

With c_1 given by (7) and ϕ_1 by (8) we now ($g=-1/4$) have $\phi_1=(\pi/2)-2c_1$, so the quantization condition (13) reduces to

$$\frac{1}{2}\left[\sqrt{1+(2kR)^2}-\ln\left(\frac{1}{2kR}+\sqrt{1+\frac{1}{(2kR)^2}}\right)\right]=\left(n+\frac{3}{4}\right)\pi. \tag{14}$$

The resulting wave numbers k_n of the radial eigenfunctions are listed in Table I for $R=1$ and quantum numbers up to $n=8$. Comparison with the exact quantum-mechanical results, which are simply the zeros of the Bessel function $J_0(kR)$, shows that the present quantization rule (14) leads to far more accurate values than the conventional quantization rule (12); the error is reduced by a factor which is about 16 for $n=0$, about 70 for $n=1$, and more than 10^3 for $n\geqslant 7$.

TABLE II. Energies E_n/V_0 of the eigenstates of the two-dimensional Woods-Saxon well for vanishing angular momentum. The parameters were chosen as $k_0=1, b=0.5, R=30$. The ''present'' values are obtained via WKB quantization in the potential (15) according to Eq. (10); x_1 is given by Eq. (18), $\phi_1=\pi/2, x_2$ is the outer turning point in the potential, and ϕ_2 is given by Eq. (16). The ''conventional'' values are obtained via the WKB quantization in the Langer-modified potential in which the inverse-square contribution vanishes, $x_1=0$, and $\phi_2=\pi/2$. The ''exact'' values are the exact quantum-mechanical eigenvalues in the potential (15).

n	Conventional	Present	Exact
0	−0.9965786	−0.9937022	−0.993739
1	−0.9715200	−0.9670365	−0.967054
2	−0.9236975	−0.9192126	−0.919224
3	−0.8540595	−0.8505310	−0.850539
4	−0.7633378	−0.7614254	−0.761432
5	−0.6522609	−0.6524848	−0.652490
6	−0.5217072	−0.5245293	−0.524534
7	−0.3729500	−0.3788203	−0.378825
8	−0.2084060	−0.2177515	−0.217756
9	−0.0365539	−0.0490030	−0.049006

As a less trivial example we now study a two-dimensional Woods-Saxon well for angular momentum zero. The total potential in the radial Schrödinger equation is

$$V_{\mathrm{WS}}^{(0)}(x)=-\frac{\hbar^2}{8mx^2}-\frac{V_0}{1+\exp[(x-R)/b]}\ ,\quad x>0. \tag{15}$$

The phase loss for reflection by a pure Woods-Saxon potential is known analytically and is given (for $-V_0<E<0$) by [1]

$$\begin{aligned}\phi=2\arg\frac{\Gamma(-2ikb)}{\Gamma(\kappa b-ikb)\Gamma(1+\kappa b-ikb)}&\\ +2kb\left[2\ln 2-\ln\left(1+\frac{\kappa^2}{k^2}\right)-2\frac{\kappa}{k}\arctan\frac{k}{\kappa}\right].&\end{aligned} \tag{16}$$

Here k corresponds to the asymptotic ($x\to-\infty$) wave number on the classically allowed side of the pure Woods-Saxon potential (without centrifugal term) and κ is the asymptotic ($x\to+\infty$) value of the decay parameter on the classically forbidden side,

$$k=k_0\sqrt{1-\frac{|E|}{V_0}},\quad \kappa=k_0\sqrt{\frac{|E|}{V_0}},\quad k_0=\frac{\sqrt{2mV_0}}{\hbar}. \tag{17}$$

The energy eigenvalues are obtained via the quantization condition (10). As a natural choice for the inner reference point x_1, we take that for which the expression in the lower line of Eq. (8) vanishes. This is achieved for $a=2.276\,717\,531\,22\ldots$ implying

$$kx_1=0.662\,743\,419\,35\ldots\times\sqrt{|\gamma|}=0.331\,371\,709\,675\ldots. \tag{18}$$

The corresponding phase (8) is then simply

$$\phi_1 = \frac{\pi}{2} + \pi\sqrt{\frac{1}{4} - |\gamma|}. \tag{19}$$

In the present example, $\gamma = -1/4$, this corresponds to $\phi_1 = \pi/2$ as in the conventional WKB treatment, but in the conventional treatment the WKB wave function is calculated via the Langer-modified potential [in which the inverse-square contribution now vanishes, Eq. (5)], and the reference point is $x_1 = 0$. In our treatment, the potential is left intact and the reference point x_1 is given by Eq. (18). The upper limit x_2 of the action integral in Eq. (10) is the outer turning point in the potential (15), and ϕ_2 is taken to be the phase loss (16) of the pure Woods-Saxon potential.

Table II shows the energy eigenvalues obtained in this way for the following values of the potential parameters: $k_0 = 1, b = 0.5, R = 30$. The results are compared with the exact eigenvalues and with the results of the conventional WKB treatment, based on $x_1 = 0, \phi_2 = \pi/2$ and the Langer-modified potential, in which the inverse-square contribution vanishes. The error in the present results is smaller than the error in the conventional treatment by a factor which varies from 100 for the ground state to 4000 for the least bound state, $n = 9$. The present results are essentially independent of the choice of the inner reference point x_1, as long as it does not substantially exceed the value given by Eq. (18). It is worth mentioning, that the excellent results displayed in Table II depend on the correct choice both of the reflection phase at the outer turning point and of the inner reference point and phase. Correcting for the reflection phase at the outer turning point alone already reduces the error in the energies E_n/V_0 to values between 2×10^{-4} and 3×10^{-4}; introducing the nonvanishing inner point of reference with the associated phase further reduces the error to the values between 3×10^{-5} and 3×10^{-6} in Table II.

Summary. Weakly attractive inverse square potentials can be accurately treated within the WKB approximation by introducing a nonvanishing point of reference x_1 near the origin in conjunction with a phase depending on x_1 via Eq. (8). The accuracy achieved in this way is comparable to that obtained in repulsive inverse-square potentials via the correct reflection phase (4), and it is better than conventional treatments by two orders in $1/(kx)$. For the bound states of vanishing angular momentum in the two-dimensional circle billiard and in a two-dimensional Woods-Saxon well, we have demonstrated that the accuracy obtained in conventional WKB quantization can be improved by orders of magnitude when the quantization rule is modified by incorporating an appropriate point of reference and the correct phases.

Note added in proof: Eigenvalues of the two-dimensional circle billiard have recently been calculated by harmonic inversion of the expansion of the periodic orbit signal [16]. The present results in Table I, obtained via improved WKB quantization (14), are systemically closer to the exacta eigenvalues than the eigenvalues obtained (for vanishing angular momentum) in Ref. [16].

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