Tunneling near the base of a barrier

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Generalized WKB connection formulas are used to derive the transmission amplitude describing tunneling through a potential barrier via two isolated classical turning points. The resulting formulas correctly reproduce the behavior in the vicinity of the base of the barrier where the tunneling probability vanishes exactly, and where formulas available to date fail. [S1050-2947(98)06108-3]

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I. INTRODUCTION

The semiclassical formula for the probability T of tunneling through a potential barrier $V(x)$ at energy E is [1,2] $T=1/\Theta^2$, where Θ is the exponentiated action integral over the classically forbidden region $E<V(x)$,

$$\Theta(E)=\exp\left(\frac{1}{\hbar}\left|\int_{x_l}^{x_r}p(x)dx\right|\right). \tag{1}$$

The classically forbidden region is bounded by the left and right turning points x_l and x_r, and $p(x)=\sqrt{2m[E-V(x)]}$ is the local classical momentum, which is purely imaginary between x_l and x_r. Near the top of a barrier, Θ approaches unity and improved formulas are available, which account for the fact that the two classical turning points are not isolated in this case; an example is the formula $T=1/(\Theta^2+1)$ due to Kemble [3,4], which is exact for an inverted parabola potential. More realistic barriers approach a constant for $x\to\infty$ and for $x\to-\infty$, and $\Theta(E)$ tends to a finite value at the base of the barrier if the potential approaches its asymptotic value faster than $1/x^2$. The semiclassical formula and available variations thereof hence predict a finite tunneling probability at the base, in contrast to the exact quantum-mechanical result, which is zero. The failure of the conventional WKB formula and its various modifications to correctly describe tunneling near the base of a barrier has recently been emphasized by Chebotarev [4], and it can be attributed to the fact that the wavelengths are large and the conditions of the short-wave limit are not fulfilled.

Large wavelengths are important, e.g., in situations involving cold atoms, and numerically solving the Schrödinger equation in this regime is a nontrivial exercise. This is one reason why extending and generalizing WKB techniques so they remain applicable for long waves has recently become a topic of considerable interest [5–7].

The WKB approximation always breaks down at classical turning points, and the phases and amplitudes of WKB wave functions on either side of a turning point are related by connection formulas, which are conventionally derived under the conditions of the short-wave limit. When the conditions of the short-wave limit are not fulfilled, the WKB wave function on the classically allowed side of the turning point may still be a highly accurate approximation of the exact wave function, provided the appropriate connection formula is generalized to account for the correct "reflection phase" [8]. Detailed investigations of reflection phases away from the short-wave limit have recently led to the derivation of simple and accurate formulas for the scattering phase shifts of singular potentials [9] and of a modified quantization rule yielding highly accurate energies for very weakly bound states in molecular potentials [10].

For the description of tunneling, it is also important to discuss the relation of the amplitudes of the WKB waves on both sides of a turning point, and this shows that there can be an additional suppression of the wave function on the classically forbidden side when the conditions of the short-wave limit are not fulfilled, e.g., near the base of a barrier. In the present paper we use a generalization of the WKB connection formulas to derive expressions for the transition amplitude that include the effect of such additional suppression and behave correctly near the base of the barrier. The applicability of our formulas is demonstrated in a number of examples including barriers with tails decaying exponentially or as an inverse power of the coordinate.

II. GENERALIZATION OF THE WKB CONNECTION FORMULAS

The WKB method provides an accurate approximation to the quantum-mechanical wave function as long as the de Broglie wavelength, $\lambda(x)=2\pi\hbar/p(x)$, varies sufficiently slowly. This condition can be expressed quantitatively, e.g., in terms of the local classical momentum,

$$\hbar^2\left|\frac{p''}{2p^3}-\frac{3}{4}\frac{p'^2}{p^4}\right|\ll 1. \tag{2}$$

The WKB wave functions $\propto p^{-1/2}\exp[\pm(i/\hbar)\int^x p(x')dx']$ are actually exact solutions of the Schrödinger equation when the left-hand side of the inequality (2) vanishes (e.g., [11]). The WKB approximation breaks down at a classical turning point x_0, because $p(x_0)=0$, and there is in general a region around the turning point, the "badlands," where the condition (2) is poorly fulfilled. The WKB approximation can soon become very accurate away from an isolated turning point, and the oscillating WKB wave functions on the classically allowed side are related to the decaying or growing WKB wave functions on the forbidden side via connection formulas, which in their most general form are

$$\frac{2}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\left|\int_{x_0}^{x}p(x')dx'\right|-\frac{\phi}{2}\right)$$
$$\leftrightarrow\frac{N}{\sqrt{|p(x)|}}\exp\left(-\frac{1}{\hbar}\left|\int_{x_0}^{x}p(x')dx'\right|\right),\qquad(3)$$

$$\frac{1}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\left|\int_{x_0}^{x}p(x')dx'\right|-\frac{\bar{\phi}}{2}\right)$$
$$\leftrightarrow\frac{\bar{N}}{\sqrt{|p(x)|}}\exp\left(\frac{1}{\hbar}\left|\int_{x_0}^{x}p(x')dx'\right|\right),\qquad(4)$$

with non-negative real amplitude factors $N,\bar{N}$, and real phases $\phi,\bar{\phi}$. If the potential can be linearized in a region around the classical turning point, which includes several wavelengths on the allowed side and a multiple of the penetration depth on the forbidden side, then the exact solutions of the Schrödinger equation are accurately approximated by Airy functions and matching leads to the standard result of conventional WKB theory [12]: $N=1$, $\phi=\pi/2$ in Eq. (3), and to $\bar{N}=1$, $\bar{\phi}=-\pi/2$ in Eq. (4). (Note that the latter formula is written with a sine instead of a cosine in [12].) The accuracy of the WKB wave functions away from the turning point does not, however, depend on fulfillment of the conditions of the short-wave limit. The WKB wave functions on either side of the turning point can be highly accurate, even for large wavelengths and penetration depths, provided the condition (2) is well fulfilled.

The phase ϕ and the amplitude factor N in Eq. (3) are uniquely determined by asymptotically matching the WKB wave function to an exact solution of the Schrödinger equation which decays to zero asymptotically on the classically forbidden side. Asymptotically here means far enough away from the turning point for the condition (2) to be well fulfilled, i.e., beyond the badlands. The phase $\bar{\phi}$ and the amplitude factor $\bar{N}$ in the second connection formula (4) are not well defined, because the wave function growing on the classically forbidden side of the turning point is not unique; any arbitrary admixture of the decaying wave does not change the asymptotic behavior of the wave function on the classically forbidden side. From the continuity equation we can, however, derive one condition relating $\bar{\phi}$ and $\bar{N}$ and the well-defined quantities ϕ and N.

Consider a linear superposition of the left-hand sides of Eqs. (3), (4), $\psi=A\times(3)+B\times(4)$, with arbitrary complex coefficients A and B. The corresponding current density $j=(\hbar/m)\mathrm{Im}(\psi^*\psi')$ on the classically allowed side of the turning point is

$$j_{\mathrm{allowed}}=\pm\frac{2}{m}\mathrm{Im}(A^*B)\sin\left(\frac{\phi-\bar{\phi}}{2}\right),\qquad(5)$$

where the plus (minus) sign refers to the case that the classically allowed side is to the left (right) of the turning point. On the other hand, the current density obtained with the same superposition of the right-hand sides of Eqs. (3) and (4) on the classically forbidden side of the turning point is

$$j_{\mathrm{forbidden}}=\pm\frac{2}{m}\mathrm{Im}(A^*B)N\bar{N}.\qquad(6)$$

Arbitrary superpositions of the WKB waves connected via Eqs. (3),(4) are thus consistent with the continuity equation if and only if

$$N\bar{N}=\sin\left(\frac{\phi-\bar{\phi}}{2}\right).\qquad(7)$$

The uncertainty in $\bar{\phi}$, $\bar{N}$ can be overcome, e.g., by requiring the oscillating waves on the allowed sides of Eqs. (3),(4) to be asymptotically phase shifted by a quarter of a wave, $\bar{\phi}=\phi-\pi$, as is the convention in defining the irregular solution of the radial Schrödinger equation in scattering theory. This would imply $\bar{N}=1/N$ according to Eq. (7). Other choices can, however, be justified, and, for the purposes of the present investigation, no harm is done in leaving the barred quantities arbitrary, except that $\phi-\bar{\phi}$ must not be an integral multiple of 2π, because the left-hand sides of Eqs. (3),(4) would be linearly dependent in this case.

III. DERIVATION OF THE TRANSMISSION AMPLITUDE

We now study tunneling through a potential barrier $V(x)$ with two classical turning points, x_l on the left and x_r on the right. $V(x)$ is assumed to approach constant (not necessarily equal) values for $x\to+\infty$ and $x\to-\infty$. The wave function far left of x_l is described as a superposition of incoming and reflected WKB waves,

$$\psi^l(x)=\frac{1}{\sqrt{p(x)}}\exp\left(\frac{i}{\hbar}\int_{x_l}^{x}p(x')dx'\right)$$
$$+r_{\mathrm{WKB}}\frac{1}{\sqrt{p(x)}}\exp\left(-\frac{i}{\hbar}\int_{x_l}^{x}p(x')dx'\right),\qquad(8)$$

and the wave function far right of x_r is a transmitted WKB wave,

$$\psi^r(x)=t_{\mathrm{WKB}}\frac{1}{\sqrt{p(x)}}\exp\left(\frac{i}{\hbar}\int_{x_r}^{x}p(x')dx'\right).\qquad(9)$$

The WKB reflection amplitude r_{WKB} and transmission amplitude t_{WKB} can be related to the conventionally defined reflection and transmission amplitudes by identifying the wave functions (8),(9) with the exact solution of the Schrödinger equation in the asymptotic region. The modulus of the WKB reflection amplitude is of course equal to the modulus of the conventionally defined reflection amplitude, and the modulus of the WKB transmission amplitude is related to the modulus of the conventionally defined transmission amplitude t by $|t_{\mathrm{WKB}}|=\sqrt{k_r/k_l}|t|$, where k_l is the asymptotic wave number to the left and k_r is the asymptotic wave number to the right of the barrier. The factor $\sqrt{k_r/k_l}$ is needed, because the conventional transmission coefficient t is defined as a ratio of amplitudes of dimensionless plane waves, whereas the reference waves for ψ^l (8) and ψ^r (9) contain the amplitude $1/\sqrt{p}$. Furthermore, there is a phase correction to account for the fact that the WKB waves are defined with respect to the classical turning points as reference rather than, e.g., the origin $x=0$, and that the local momentum $p(x)$ may differ from its asymptotic value for finite x [7]. The WKB transmission amplitude $t_{\rm WKB}$ in Eq. (9) is thus related to the conventionally defined transmission amplitude t via

$$\sqrt{\frac{k_r}{k_l}}\,t=t_{\rm WKB}\exp\left[\lim_{x\to\infty}\left(\frac{i}{\hbar}\int_{-x}^{x_l}p(x')dx'-ik_lx+\frac{i}{\hbar}\int_{x_r}^{x}p(x')dx'-ik_rx\right)\right]. \tag{10}$$

In order to derive an explicit expression for the transmission amplitude we write the wave function in between the two turning points as a superposition of decaying and growing WKB waves,

$$\psi^m(x)=\frac{A}{\sqrt{|p(x)|}}e^{-(1/\hbar)\int_{x_l}^{x}|p(x')|dx'}+\frac{B}{\sqrt{|p(x)|}}e^{+(1/\hbar)\int_{x_l}^{x}|p(x')|dx'}. \tag{11}$$

We assume that the turning points x_l and x_r are isolated, meaning that the badlands associated with the two turning points should not overlap, i.e., there is a region between x_l and x_r where the condition (2) is well fulfilled. The ansatz (11) is then an accurate approximation of the true wave function in this range of values of x. To the right of the barrier, the wave function ψ^r (9) can be written as

$$\psi^r=\frac{C}{\sqrt{p}}\cos\left(\frac{1}{\hbar}\int_{x_r}^{x}p\ dx'-\frac{\phi_r}{2}\right)+\frac{\bar{C}}{\sqrt{p}}\cos\left(\frac{1}{\hbar}\int_{x_r}^{x}p\ dx'-\frac{\bar{\phi}_r}{2}\right), \tag{12}$$

with

$$C=\frac{2t_{\rm WKB}e^{-i\phi_r/2}}{e^{-i\phi_r}-e^{-i\bar{\phi}_r}},\quad \bar{C}=-\frac{2t_{\rm WKB}e^{-i\bar{\phi}_r/2}}{e^{-i\phi_r}-e^{-i\bar{\phi}_r}}. \tag{13}$$

The subscript r on the phases marks reference to the right-hand turning point. The two cosine terms in Eq. (12) are matched according the connection formulas (3),(4) to the growing and decaying terms $\exp[\pm(1/\hbar)\int_x^{x_r}|p|dx']$ to the left of x_r, which can be written as $\Theta^{\pm1}\exp[\mp(1/\hbar)\int_{x_l}^{x}|p|dx']$, with Θ defined as in Eq. (1), and represent decaying and growing terms on the classically forbidden side of the left-hand turning point x_l. The coefficients A and B which determine the wave function ψ^m [Eq. (11)] in the classically forbidden region are thus

$$A=\bar{N}_r\Theta\bar{C},\quad B=\frac{N_r}{2\Theta}C, \tag{14}$$

and the subscript r again marks reference to the right-hand turning point. The decaying and growing terms to the right of x_l, proportional to A and B respectively, are then matched to the appropriate cosine terms to the left of x_l according to Eqs. (3),(4), and decomposition of the cosines into exponentials enables comparison with ψ_l [Eq. (8)]. The coefficient of the incoming WKB wave is

$$\frac{A}{N_l}e^{i\phi_l/2}+\frac{B}{2\bar{N}_l}e^{i\bar{\phi}_l/2}, \tag{15}$$

where the subscript l marks reference to the left-hand turning point. Equating the expression (15) with unity and exploiting the relations (13), (14), and (7) yields the general expression for the transmission amplitude $t_{\rm WKB}$,

$$t_{\rm WKB}=iN_lN_r\left(\Theta\ e^{i(\phi_l+\phi_r)/2}-\frac{N_lN_r}{\bar{N}_l\bar{N}_r}\frac{1}{4\Theta}e^{i(\bar{\phi}_l+\bar{\phi}_r)/2}\right)^{-1}. \tag{16}$$

With the assumptions of conventional WKB theory at both turning points, $N_{l,r}=\bar{N}_{l,r}=1$, $\phi_{l,r}=-\bar{\phi}_{l,r}=\pi/2$, Eq. (16) reduces to $t_{\rm WKB}=[\Theta+1/(4\Theta)]^{-1}$, a result given in the textbook by Merzbacher [12]. We emphasize that the present formula (16) is much more general. It does not depend on fulfillment of the conditions of the short-wave limit and it remains valid for arbitrarily long waves, as occur, e.g., near the base of a barrier.

In Eq. (16) the term in the bracket containing the poorly defined barred parameters is smaller than the dominant term to the extent that Θ is a large (but still finite) number. Thus, for a sufficiently dense barrier, we can ignore the subdominant contribution and obtain a formula for the transition amplitude, in which all ingredients are well defined,

$$t_{\rm WKB}\approx i\ N_l\ N_r\ e^{-i(\phi_l+\phi_r)/2}/\Theta. \tag{17}$$

For a symmetric barrier the conditions at the left and right turning points are the same at a given energy, so we can drop the subscripts and Eq. (16) becomes

$$t_{\rm WKB}=iN^2\left(\Theta\ e^{i\phi}-\frac{N^2}{\bar{N}^2}\frac{1}{4\Theta}e^{i\bar{\phi}}\right)^{-1}. \tag{18}$$

In the expression for the associated tunneling probability, the phases can be eliminated via Eq. (7) giving

$$T=|t_{\rm WKB}|^2=\left[\left(\frac{\Theta}{N^2}-\frac{1}{4\Theta\bar{N}^2}\right)^2+1\right]^{-1}. \tag{19}$$

Keeping only the dominant term gives

$$T\approx\frac{N^4}{\Theta^2}=N^4\exp\left(-\frac{2}{\hbar}\left|\int_{x_l}^{x_r}p(x)dx\right|\right). \tag{20}$$

IV. APPLICATIONS

A simple illustrative example is the rectangular barrier of height V_0 and length L. Energies below the barrier top are characterized by the wave number $k=\sqrt{2mE}/\hbar$ of the oscillating waves in the classically allowed region and the inverse penetration depth $q=\sqrt{2m(V_0-E)}/\hbar$ of the exponentially rising or falling wave functions in the forbidden region. The left and right turning points are separated by the distance L

and are, for any large or small finite value of L, truly isolated, because the WKB approximation for the wave function is exact in the whole region $x_r < x < x_l$ (and of course also for $x < x_l$ and $x > x_r$). The amplitude factor N and reflection phase ϕ are obtained by comparing the WKB waves on either side of a turning point with the exact wave function for the sharp potential step of height V_0, which is treated in elementary quantum-mechanics classes; the result is

$$N = 2\sqrt{\frac{kq}{k^2+q^2}}, \quad \phi = 2 \arctan\left(\frac{q}{k}\right). \tag{21}$$

Note that N approaches zero as $\sqrt{k} \propto E^{1/4}$ at the base of the barrier. This is a consequence of matching at the turning point; here the value of the oscillating wave is essentially given by $k^{-1/2} \cos(\phi/2)$, and the value of the decaying wave is essentially the amplitude factor N, because the factor $1/\sqrt{|p|}$ approaches a constant on the forbidden side as $k \to 0$. The reflection phase ϕ approaches the value π characteristic of the long-wave limit [8], and $\cos(\phi/2)$ goes to zero as the wave number k. Thus N must go to zero as $\sqrt{k}$ for $k \to 0$. This mechanism of additional supression of the wave function in the classically forbidden region is most clearly illustrated for the sharp step, but it also occurs for other potential shapes when $k \to 0$ corresponds to the long-wave limit; this is the case for potentials falling off faster than $1/x^2$ [9].

For the rectangular barrier we can also determine $\bar{N}$ and $\bar{\phi}$, because p' vanishes in the classically forbidden region, so the exponentially growing solution can be defined unambiguously. The results are $\bar{N} = N/2$, $\bar{\phi} = -\phi$. With Eq. (21) and $\Theta = e^{qL}$, Eq. (18) thus becomes

$$t_{\mathrm{WKB}} = \frac{4ikq}{e^{qL}(k+iq)^2 - e^{-qL}(k-iq)^2}, \tag{22}$$

which agrees with the exact quantum-mechanical result [12] when the phase correction (10) is taken into account. Near the base of the barrier, $k \to 0$, $q \to q_0 = \sqrt{2mV_0}/\hbar$, the leading term is $t_{\mathrm{WKB}} \sim -2i\, k/[q_0 \sinh(q_0 L)]$ and the tunneling probability to leading order is $T \sim 4k^2/[q_0 \sinh(q_0 L)]^2$. Neglecting the subdominant term in the denominator on the right-hand side of Eq. (22) corresponds to replacing $\sinh(q_0 L)$ by $[\exp(q_0 L)]/2$ in these two expressions.

Another soluble example is the $\cosh^{-2}$ potential,

$$V(x) = V_0 \cosh^{-2}(x/a), \quad V_0 > 0, \tag{23}$$

for which the exact transmission probability is [1]

$$T = \frac{\sinh^2(\pi\, k\, a)}{\sinh^2(\pi\, k\, a) + \cosh^2[\pi\sqrt{(2mV_0 a^2/\hbar^2) - \frac{1}{4}}]}, \tag{24}$$

when the argument of the square root is non-negative. For $k \to 0$ the leading contribution is

$$T \sim \pi^2\, k^2\, a^2 \cosh^{-2}[\pi\sqrt{(2mV_0 a^2/\hbar^2) - \tfrac{1}{4}}]. \tag{25}$$

Near the base of the barrier, the classical turning points lie in the exponential tail of the potential, e.g., for $x_l < 0$,

$$V(x) \approx U(x) = 4V_0 e^{2x/a}, \tag{26}$$

and we can derive an approximate expression for the amplitude factor N if we replace $V(x)$ by the exponential potential $U(x)$ when determining the parameters of the generalized connection formula (3). For the exponential potential $U(x)$ the exact wave function decaying to zero on the classically forbidden side is a modified Bessel function [13], $\psi(x) = K_{ika}(2\sqrt{2mV_0}a\; e^{x/a}/\hbar)$, and the reflection phase and amplitude factor can be derived analytically in this case. The reflection phase is [14]

$$\phi = \pi - 2 \arg \Gamma(1+ika) + 2ka[\ln(ka) - 1] \tag{27}$$

and the amplitude factor is

$$N = e^{-\pi ka/2}\sqrt{2 \sinh(\pi ka)} \sim \begin{cases} \sqrt{2\pi ka}, & k \to 0 \\ 1, & k \to \infty. \end{cases} \tag{28}$$

These expressions are accurate, as long as the full potential is well approximated by the exponential tail (26) in a region around the turning point large enough to contain the badlands. Again we observe, that N approaches zero as $\sqrt{k}$ at the base. With Eq. (28) the formula (20) gives

$$T \approx 4\, e^{-2\pi ka} \sinh^2(\pi ka)/\Theta^2 \tag{29}$$

for a barrier with exponential tails (26). The tunneling probability (29) approaches the conventional semiclassical result $1/\Theta^2$ when $ka \gg 1$ and tends to zero as $k^2 \propto E$ at the base of the barrier. For the potential (23), we have

$$\Theta = \exp\left[\pi\, ka\left(\frac{\sqrt{2mV_0}}{\hbar k} - 1\right)\right] \overset{k\to 0}{\sim} \exp\left(\pi\, a\frac{\sqrt{2mV_0}}{\hbar}\right),$$

and the leading contribution to the tunneling probability (29) at the base of the barrier is

$$T \sim 4\pi^2 k^2 a^2 \exp(-2\pi\sqrt{2mV_0 a^2/\hbar^2}). \tag{30}$$

This coincides with the low-energy expansion (25) of the exact expression, when $2mV_0 a^2/\hbar^2$ is large enough, so that the 1/4 in the square root can be neglected and the cosh replaced by half the exponential of the argument.

Now consider barriers decaying asymptotically as an inverse power of the coordinate, e.g., for $x \to \infty$,

$$V(x) \approx U_\alpha(x) = \frac{\hbar^2}{2m}\frac{c^{\alpha-2}}{x^\alpha}, \quad c > 0, \quad \alpha > 2. \tag{31}$$

At sufficiently low energy, the right-hand turning point is essentially the turning point x_0 of the homogeneous potential U_α, which is given by $x_0/c = (kc)^{-2/\alpha}$. The low-energy behavior of the amplitude factor and reflection phase for the homogeneous potential can be derived in the spirit of an effective range expansion [14,15] from the zero-energy regular solution χ_{reg} of the Schrödinger equation with U_α, which is essentially a modified Bessel function [13],

$$\chi_{\rm reg}(x)=c_1\sqrt{x}K_{1/(\alpha-2)}\left[\frac{2}{\alpha-2}\left(\frac{c}{x}\right)^{(\alpha-2)/2}\right]$$
$$\stackrel{x\to 0}{\sim} c_1\frac{\sqrt{(\alpha-2)\pi}}{2}\sqrt{x}\left(\frac{x}{c}\right)^{(\alpha/4)-(1/2)}$$
$$\times\exp\left[-\frac{2}{\alpha-2}\left(\frac{c}{x}\right)^{(\alpha-2)/2}\right]. \tag{32}$$

At small energies the potential $U_\alpha(x)$ [Eq. (31)] rapidly dominates over the energy term in the Schrödinger equation as x moves away from the turning point into the classically forbidden region. On the allowed side of the turning point we approximate the wave function by a free wave,

$$\psi_{\rm reg}(x)=c_2\cos\left[kx-kx_0g(\alpha)-\frac{\phi}{2}\right]. \tag{33}$$

The constant $g(\alpha)$ is chosen as

$$g(\alpha)=\frac{\sqrt{\pi}}{2}\frac{\Gamma\left(1-\frac{1}{\alpha}\right)}{\Gamma\left(\frac{3}{2}-\frac{1}{\alpha}\right)}, \tag{34}$$

so that $(1/\hbar)\int_{x_0}^{x}p(x')dx'\sim kx-kx_0g(\alpha)$ for $x\to\infty$, and Eq. (33) is consistent with the definition of the reflection phase in Eq. (3).

To lowest order in k the zero-energy solution (32) on the classically forbidden side of the turning point x_0 and the free wave (33) on the classically allowed side approximate the exact solution not only asymptotically, but also close to x_0. Matching these wave functions and their derivatives at x_0 thus provides an accurate approximation of the exact wave function, to which the WKB wave function can be matched asymptotically, $x\to 0$ and $x\to\infty$, in order to determine the leading-order behavior of the amplitude factor N and the reflection phase ϕ. The result for the reflection phase is

$$\phi\sim\pi-2g(\alpha)(ck)^{1-(2/\alpha)}+2f(\alpha)ck, \tag{35}$$

with the constant $f(\alpha)$ given by

$$f(\alpha)=(\alpha-2)^{-[2/(\alpha-2)]}\frac{\Gamma\left(1-\frac{1}{\alpha-2}\right)}{\Gamma\left(1+\frac{1}{\alpha-2}\right)}. \tag{36}$$

The leading contribution to the amplitude factor N is

$$N\sim\frac{2\sqrt{\pi\ kc}}{\Gamma\left(1+\frac{1}{\alpha-2}\right)(\alpha-2)^{[\alpha/2(\alpha-2)]}}. \tag{37}$$

Again $N\propto E^{1/4}$ near $E=0$. Inserting Eq. (37) into the formula (20) gives

$$T\approx\frac{16\pi^2k^2c^2}{\left[\Gamma\left(1+\frac{1}{\alpha-2}\right)(\alpha-2)^{[\alpha/2(\alpha-2)]}\right]^4\Theta^2}$$

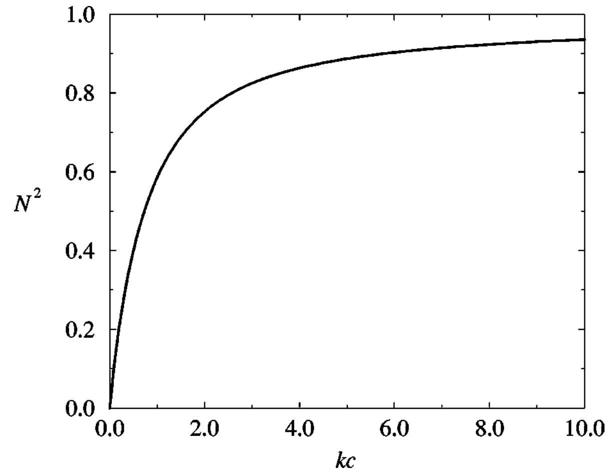

FIG. 1. Square of the amplitude factor N derived by matching the WKB wave functions (3) to numerically calculated exact wave functions on either side of the turning point for the power-law potential U_α (31) with $\alpha=8$.

for the tunneling probability T at low energies.

The behavior of N and ϕ at finite energies can be obtained by numerically solving the Schrödinger equation with the potential U_α and asymptotically comparing the WKB wave functions (3) with the exact wave function. The resulting amplitude factor N is illustrated in Fig. 1 for $\alpha=8$. The amplitude factor obtained in this way is accurate for all barriers for which the potential can be approximated by the power-law tail (31) in a region around the classical turning point which is large enough to contain the badlands.

As an example we have calculated the transmission probabilities for the potential,

$$V(x)=\frac{V_0}{1+(x/a)^8}. \tag{38}$$

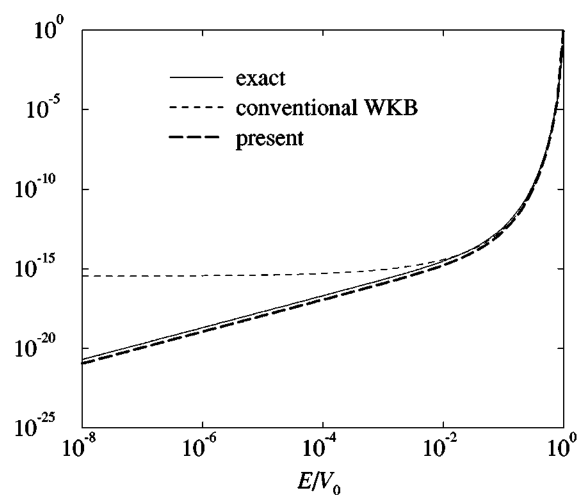

FIG. 2. Numerically calculated exact transmission probabilities (solid line) for the potential Eq. (38) with $\alpha=8$ and $\sqrt{mV_0/\hbar^2}a=5$, together with the result of Eq. (20) containing the amplitude factor derived from the power-law tail of the potential (thick dashed line). The thin dashed line shows the conventional semiclassical result $1/\Theta^2$.

The asymptotic tail of this potential corresponds to Eq. (31) with $\alpha=8$ and $c^6=(2mV_0/\hbar^2)a^8$. In Fig. 2 the exact transmission probability (full line) is plotted for $\sqrt{mV_0/\hbar^2}a=5$. The thin dashed line shows the conventional WKB result $T=\Theta^{-2}$, which deviates from the exact result and approaches a finite constant at low energies. The result of formula (20) with the approximate amplitude factor N of Fig. 1 is shown as a thick dashed line. It reproduces the low-energy behavior correctly and merges into the conventional semiclassical result as N approaches unity.

V. CONCLUSION

We have used the generalized connection formulas (3),(4) to derive amplitudes for tunneling through a potential barrier with two classical turning points. The expression (16) was derived using only the assumption, that the two turning points be isolated, i.e., that the WKB approximation be accurate somewhere in between. Neglecting the subdominant term in Eq. (16) leads to the expression (17) for the transmission amplitude, which contains only well-defined quantities.

If the potential on the classically allowed side of a turning point approaches its asymptotic (constant) value faster than $1/x^2$, then the amplitude factor N approaches zero as $\sqrt{k}$. This additional suppression of the wave function on the classically forbidden side of the turning point is characteristic of the long-wave limit, where the reflection phase approaches π. For a barrier potential approaching the same constant ($E=0$, say) faster than $1/x^2$ on both sides, the transmission probability vanishes as the energy E near the base of the barrier. If the barrier approaches a constant ($E=0$, say) on one side of the barrier, and a different, lower constant on the other side, then the transmission probability vanishes only as $\sqrt{E}$ near the base. Previous semiclassical formulas have been unable to reproduce this vanishing behavior of the tunneling probability at the base of a barrier.

For potential tails decaying exponentially the reflection phase and amplitude factor are given analytically in Eqs. (27) and (28), respectively. For potentials decaying as $1/|x|^\alpha$, $\alpha>2$, the formulas (35) and (37) give the leading behavior of phase and amplitude near the base of the barrier.

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