Reflection above potential steps

R. Côté,[1] H. Friedrich,[1,2] and J. Trost[2]
[1]Harvard-Smithsonian Center for Astrophysics, ITAMP, 60 Garden Street, Cambridge, Massachusetts 02138
[2]Physik-Department, Technische Universität München, 85747 Garching, Germany
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Classically forbidden reflection by a potential step is analyzed by matching WKB waves to solutions of a Schrödinger equation involving the tail of the potential on the up side of the step. Analytic expressions for the leading deviation of the reflection probability from unity and the phase of the reflection amplitude at the top of the step are derived for potentials decaying as an inverse power of the coordinate $V(x)\propto -1/x^{\alpha}$, $\alpha>2$. [S1050-2947(97)05409-7]

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I. INTRODUCTION

The first-order WKB approximation is a powerful tool for accurately approximating solutions to the Schrödinger equation in the case of small and slowly varying wavelengths [1–3]. The probabilities for classically forbidden processes such as below-barrier tunneling or above-barrier reflection are then generally exponentially small and the standard procedures for treating such cases utilize the classical turning points in the complex plane [1–4]. Such procedures are difficult or impossible to implement if the turning-point structure is not known or not simple or if the potential is not analytic. An example for an alternative approach has been presented recently by Maitra and Heller, who used the WKB wave function without classically forbidden components as the input to a distorted-wave Born approximation and accurately reproduced the exact results for transmission well below a barrier and for reflection well above a barrier or step potential [5].

It remains a challenge to find a general procedure for describing classically forbidden transmission or reflection when the probabilities are large, which is typically the case for energies near the top of a barrier or step. Waves can become very long in such situations, which occur, e.g., in collisions of cold atoms, and the applicability of the WKB method in this regime recently has become a topic of some interest [6–8].

In this paper we study classically forbidden reflection by a potential step, in particular at energies close to the top of the step where the reflection probability approaches unity. The treatment is based on straightforward matching of a WKB wave function to an exact or good approximate solution of the Schrödinger equation at a real matching point, chosen such that the de Broglie wavelength varies sufficiently slowly in the entire domain extending from the matching point to the asymptotic region from which the incoming wave originates. The purpose of this paper is twofold. First we demonstrate that the probability for reflection by a sufficiently deep and smooth step is determined by the behavior of the tail of the potential on the up side of the step. Second we derive, for potentials decaying as $-1/x^{\alpha}$ with $\alpha>2$, analytic expressions for the leading deviation of the reflection probability from unity and for the phase of the reflection amplitude at the top of the step.

II. THE MATCHING PROCEDURE

In this section we explain our procedure, which is based on matching a superposition of incoming and reflected WKB waves to an exact or accurate approximate solution of the Schrödinger equation bridging the region where the WKB approximation is inaccurate. Consider a particle of mass m incident from $x\to-\infty$ with kinetic energy $\hbar^2k_1^2/2m$, which may be reflected by a potential $V(x)$ or transmitted to $x\to+\infty$ with kinetic energy $\hbar^2k_2^2/2m=E$; the potential is taken to vanish for $x\to+\infty$ and to assume a constant negative value $-V_0=-(k_1^2-k_2^2)\hbar^2/2m$ for $x\to-\infty$. The essential condition for applicability of the WKB method is that the de Broglie wavelength $\lambda=2\pi\hbar/p(x)$, with $p(x)=\sqrt{2m[E-V(x)]}$, varies sufficiently slowly,

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

If Eq. (1) is fulfilled in the entire region $x\leq x_m$, then the exact wave function should be well approximated by the WKB ansatz

$$\psi_{\mathrm{WKB}}=\frac{1}{\sqrt{p(x)}}\left[\exp\left(\frac{i}{\hbar}\int_{x_m}^{x}p(x')dx'\right)+R_{\mathrm{WKB}}\exp\left(-\frac{i}{\hbar}\int_{x_m}^{x}p(x')dx'\right)\right],\quad x\leq x_m. \tag{2}$$

Requiring the WKB wave function (2) to asymptotically ($x\to-\infty$) match the exact wave function, assumed proportional to $\exp(ik_1x)+R\exp(-ik_1x)$, leads to a relation between R_{WKB} and the conventionally defined reflection amplitude R,

$$R_{\mathrm{WKB}}=R\,\exp[i\eta(x_m)]. \tag{3}$$

The phase

$$\eta(x_m)=2\lim_{x\to-\infty}\left(\frac{1}{\hbar}\int_{x_m}^{x}p(x')dx'-k_1x\right) \tag{4}$$

accounts for the fact that the matching point x_m is not at $x=0$ and that the local momentum p may differ from its asymptotic value $\hbar k_1$ at finite values of x.

The reflection amplitude can be determined if we know, at the point x_m fulfilling Eq. (1), an exact or accurate approximate wave function $\psi(x)$ corresponding to a purely outgoing wave [proportional to exp (ik_2x)] for $x\to+\infty$. Matching the logarithmic derivative of the WKB wave function (2) to the logarithmic derivative $z=\psi'(x_m)/\psi(x_m)$ at x_m gives

$$R_{\mathrm{WKB}}=-\frac{z-\dfrac{i}{\hbar}p(x_m)+\dfrac{p'(x_m)}{2p(x_m)}}{z+\dfrac{i}{\hbar}p(x_m)+\dfrac{p'(x_m)}{2p(x_m)}}. \tag{5}$$

The conventional reflection amplitude R can be derived from R_{WKB} via the phase correction (3).

Fulfillment of the condition (1) at x_m means that the terms $p'/2p$ in the numerator and the denominator on the right-hand side of Eq. (5) are small compared to $p/\hbar$. Neglecting these terms leads to the simplified expression

$$R_{\mathrm{WKB}}=-\frac{z-\dfrac{i}{\hbar}p(x_m)}{z+\dfrac{i}{\hbar}p(x_m)}, \tag{6}$$

which actually corresponds to naïvely matching the wave function ψ to a superposition $\exp[ip(x_m)(x-x_m)/\hbar]+R_{\mathrm{WKB}}\exp[-ip(x_m)(x-x_m)/\hbar]$ of incoming and reflected plane waves with wave numbers given by the local classical momentum at the point x_m.

In the following section, we apply the straightforward matching procedure outlined above to a Woods-Saxon potential in order to illustrate that the reflection probability is solely determined by the tail of the potential on the up side of the step, when the step is deep enough. In Sec. IV we apply the same procedure to derive reflection amplitudes for potentials asymptotically proportional to $-1/x^{\alpha}$. For energies near the top of the step, we obtain, in Sec. V, analytic expressions for the leading deviation of the reflection probability from unity and for the phase of the reflection amplitude.

III. THE WOODS-SAXON STEP

Above-barrier reflection by a Woods-Saxon step

$$V_{\mathrm{WS}}(x)=\frac{V_0}{1+\ \exp(-x/a)}-V_0 \tag{7}$$

is described in detail in [1]. The reflection probability is

$$|R|^2=[\sinh\ \pi(k_1-k_2)a]^2/[\sinh\ \pi(k_1+k_2)a]^2. \tag{8}$$

For any given large or small value of k_2a, Eq. (8) reduces to

$$|R|^2\sim\ \exp(-4\pi k_2a) \tag{9}$$

in the limit of large k_1a, which corresponds to the limit of large values of the relative diffuseness a_r of the step $a_r\equiv a\sqrt{2mV_0}/\hbar=a\sqrt{k_1^2-k_2^2}$. The expression for the phase of R involves several complex Γ functions [1]; for large k_1a and energies near the top of the step, $k_2\to0$, it becomes

$$\arg(R)=-\frac{\pi}{2}+4k_1a\ln2,\ \ \text{for}\ \ k_1a\gg1\ \ ,\ \ k_2\to0. \tag{10}$$

This is the same phase as obtained for classically allowed reflection at energies approaching the top of the step from below. The term $+4k_1a\ln2$ in Eq. (10) is just twice the difference between the phases accumulated by the WKB wave between $-\infty$ and $+\infty$ and by a free wave with wave number k_1 between $-\infty$ and zero:

$$2\lim_{x_-\to-\infty}\left(\frac{1}{\hbar}\int_{x_-}^{\infty}p(x)dx+k_1x_-\right)=4k_1a\ln2; \tag{11}$$

the additional term $-\pi/2$ in Eq. (10) is the phase loss that the WKB wave undergoes, in the short-wave limit, when reflected at infinity [9].

We shall now use the procedure outlined in Sec. II to demonstrate that the probability for reflection by the (sufficiently deep) step is determined by the tail of the potential alone. The Woods-Saxon potential (7) approaches an exponential decay

$$V_{\mathrm{WS},as}(x)=-V_0\exp(-x/a) \tag{12}$$

for large x/a. At zero energy, the variation of the de Broglie wavelength in this potential is given by

$$\frac{1}{2\pi}\left|\frac{d\lambda}{dx}\right|=\frac{\exp(x/2a)}{2a_r}. \tag{13}$$

For $E>0$ the variation of the de Broglie wavelength is a monotonically decreasing function of energy. For a sufficiently large relative diffuseness a_r the right-hand side of Eq. (13) can be much smaller than unity, even for values of the coordinate that are so much larger than a, that the asymptotic form (12) is a good approximation of the potential. In such a situation, we may use the exact solution of the Schrödinger equation with the potential (12), namely [10],

$$\psi(x)=J_\nu(y), \tag{14}$$

to match the WKB wave function Eq. (2). In (14) $J_\nu(y)$ is the Bessel function of order $\nu=-2ik_2a$ and its argument is $y=2a_r\exp(-x/2a)$, which is equal to the inverse of the right-hand side of Eq. (13).

At a fixed value of k_2, the asymptotic situation $x\to+\infty$ corresponds to small values of the argument y, for which the Bessel function (14) approaches $\exp(+ik_2x)$, corresponding to a rightward-traveling transmitted wave. On the other hand, a small value of Eq. (13) means a large value of y, so at an appropriate matching point x_m with the corresponding large y_m we may use the large argument expansion of the Bessel function,

$$\psi(x_m)\approx\sqrt{\frac{2}{\pi y_m}}\cos(y_m+i\pi k_2a-\pi/4), \tag{15}$$

whereby the logarithmic derivative z at x_m becomes

$$z=\frac{1}{2a}[y_m \tan(y_m+i\pi k_2 a-\pi/4)+O(1)]. \quad (16)$$

Inserting this value of z into the matching equation (6) and using $y_m \gg 2k_2 a$ leads to

$$R_{\rm WKB}= \exp(-2\pi k_2 a)\exp(2iy_m-i\pi/2). \quad (17)$$

The reflection probability $|R_{\rm WKB}|^2=|R|^2= \exp(-4\pi k_2 a)$ is precisely the expression (9), valid for large relative diffuseness. The phase of $R_{\rm WKB}$ contains the term $-\pi/2$ as in Eq. (10) and the contribution $2y_m$; at the top of the step, $k_2\to 0$, $2y_m$ is twice the action integral $(1/\hbar)\int_{x_m}^{\infty}p(x)dx$. With Eq. (11) we see that the expression (17) yields the correct phase (10) for the conventionally defined reflection amplitude R via Eqs. (3) and (4) at the top of the step.

The derivation above shows that the probability for reflection by a sufficiently deep Woods-Saxon step is determined by the asymptotic tail of the potential alone; the shape of the step itself and its depth are irrelevant for the derivation. The shape and the precise value of the depth do, however, enter crucially into the WKB wave function (2), which now offers an accurate approximation to the exact wave function in the entire range $x \leqslant x_m$. These features of reflection are characteristic of any sufficiently smooth step potential for which the variation of the de Broglie wavelength is small everywhere except in the tail region of the potential. The example of potentials decaying as an inverse power of the coordinate is treated in the next section.

IV. POTENTIAL ASYMPTOTICALLY PROPORTIONAL TO $-1/x^{\alpha}$

Consider a step potential $V(x)$ that behaves asymptotically, $x\to+\infty$, as

$$V_\alpha(x)=-\frac{\hbar^2}{2m}\frac{\beta^{\alpha-2}}{x^\alpha}. \quad (18)$$

The variation (1) of the de Broglie wavelength at energy zero is

$$\frac{1}{2\pi}\left|\frac{d\lambda}{dx}\right|=\frac{\alpha}{2}\left(\frac{x}{\beta}\right)^{\alpha/2-1}. \quad (19)$$

The properties of the Schrödinger equation with the homogeneous potential (18) depend only on the dimensionless ''reduced wave number'' $k_2\beta$. For energies near zero the wavelengths become arbitrarily large asymptotically, but Eq. (19) shows that the WKB condition (1) is fulfilled if

$$\left(\frac{x}{\beta}\right)^{(\alpha-2)/2}\ll\frac{2}{\alpha}, \quad (20)$$

which can be achieved for sufficiently small values of x/β, as long as $\alpha>2$.

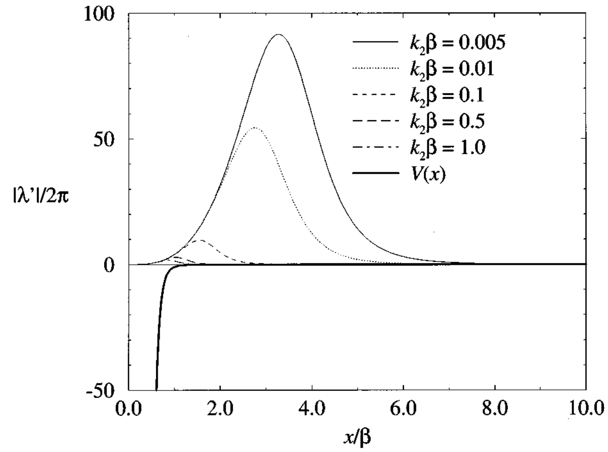

FIG. 1. Variation $(1/2\pi)|d\lambda/dx|$ of the de Broglie wavelength for the attractive inverse power-law potential (18) for $\alpha=8$ and various values of the reduced momentum $k_2\beta$.

For finite values of $k_2\beta$ the quantity $d\lambda/dx$ has a maximum at $(\beta/x)^\alpha=2(\alpha+1)(k_2\beta)^2/(\alpha-2)$ and decreases monotonically towards lower and higher values of x/β. Its maximum value becomes equal to $3^{-3/2}\alpha/k_2\beta$ for large α and is arbitrarily large for sufficiently small $k_2\beta$. The dependence of $(1/2\pi)d\lambda/dx$ on $x/\beta=k_2x/k_2\beta$ is illustrated in Fig. 1 for the case $\alpha=8$ and various values of the reduced wave number $k_2\beta$. The localized peak grows and moves towards larger values of x/β as $k_2\beta$ approaches zero. Note that $(1/2\pi)d\lambda/dx$ at any given point x is a monotonically decreasing function of energy as long as $E>V(x)$.

The behavior of $(1/2\pi)d\lambda/dx$ is qualitatively similar to that shown in Fig. 1 for any negative potential vanishing faster than $1/x^2$ asymptotically. At small but finite energies the condition (1) is fulfilled in the limits $x\to\infty$ and, for the inverse power-law potentials (18) with $\alpha>2$, also for $x\to 0$, but there are ''badlands'' in between, where the WKB approximation breaks down.

The efficacy of the matching equations (5) and (6) for obtaining the reflection probability is illustrated in Fig. 2 for the power $\alpha=8$ and the reduced momentum $k_2\beta=0.1$. Figure 2(a) shows two linearly independent solutions of the Schrödinger equation, $\psi_c(x)$ and $\psi_s(x)$, which evolve into $\cos k_2x$ and $\sin k_2x$, respectively, in the asymptotic region $x\to+\infty$. The wave function $\psi(x)=\psi_c(x)+i\psi_s(x)$ corresponds to a rightward-traveling outgoing wave asymptotically. The acceleration of the particle as x approaches zero is indicated by decreasing wavelengths and amplitudes of the oscillations. Figure 2(c) shows the reflection probabilities as derived by matching incoming and reflected WKB waves to $\psi(x)$ via Eqs. (5) and (6) as functions of the matching point x_m. After violent variations as x_m passes through the badlands [Fig. 2(b)], $|R_{\rm WKB}|^2$ settles down and oscillates with rapidly diminishing amplitude to a well-defined limiting value as x_m approaches zero. Note that the full WKB matching condition (5) (dotted line) leads to more rapid convergence than the truncated condition (6) (solid line). If $|R_{\rm WKB}|^2$ as calculated from the tail part of the potential has converged to a given number at a point x_m, then this number defines the reflection probability for any step potential obtained by continuing the potential sufficiently smoothly into the region $x<x_m$.

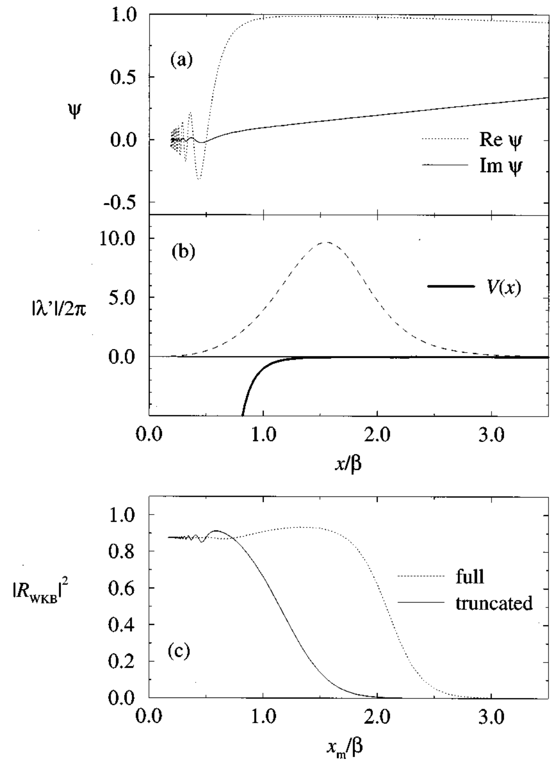

FIG. 2. (a) Real and imaginary parts of the solution of the Schrödinger equation with the potential (18), which asymptotically ($x \to +\infty$) corresponds to a rightward-traveling outgoing wave $\exp(ik_2x)$. Here $\alpha=8$ and the reduced momentum is $k_2\beta=0.1$. The potential and the variation of the de Broglie wavelength for this case are shown in (b). (c) Reflection probability $|R_{\rm WKB}|^2$ derived by matching incoming and reflected WKB wave functions to the exact solution ψ [(a)] according to the full matching condition (5) (dotted line) and to the truncated matching condition (6) (solid line) as functions of the matching point x_m. As x_m approaches zero, the reflection probability converges to a well-defined value, which is 0.8747 . . . in this case.

In order to demonstrate this in a concrete example, we have calculated the reflection probabilities in the potential

$$V(x) = -\frac{V_0}{1+\{\ln[1+\exp(x/a)]\}^{\alpha}}. \tag{21}$$

For $x\to+\infty$ this potential has the form (18) with

$$\beta^{\alpha-2} = \frac{2m}{\hbar^2} V_0 a^{\alpha}; \tag{22}$$

for $x\to-\infty$ we have

$$V(x) \sim -V_0\left[1-\exp\left(-\frac{\alpha|x|}{a}\right)\right], \tag{23}$$

i.e., $V(x)$ approaches $-V_0$ exponentially on the down side of the step.

We fixed the scale for the reduced momentum by choosing $\beta=1$ and calculated the reflection probability by numerically integrating the Schrödinger equation with the potential (21) for various values of the parameter a, which defines the range over which $V(x)$ differs from its asymptotic forms and is related to the depth of the potential via Eq. (22). The results are shown in Fig. 3 for $\alpha=8$ and in Fig. 4 for $\alpha=3$. As a is decreased, the reflection probabilities converge rapidly, not necessarily monotonically, to the limiting case $a=0$, where the potential becomes infinitely deep, and the homogeneous tail (18) solely determines the reflection prob-

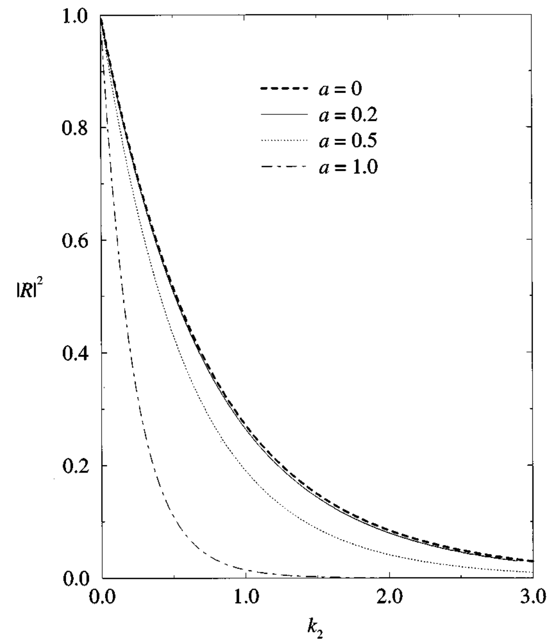

FIG. 3. Probability for reflection by the potential step (21) as a function of the asymptotic ($x\to+\infty$) momentum k_2 ($\beta=1$) for $\alpha=8$ and various values of the parameter a.

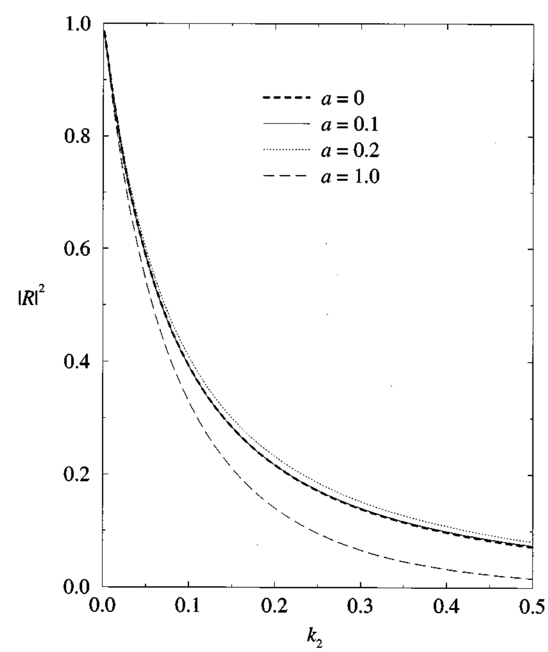

FIG. 4. Probability for reflection by the potential step (21) as a function of the asymptotic ($x\to+\infty$) momentum k_2 ($\beta=1$) for $\alpha=3$ and various values of the parameter a.

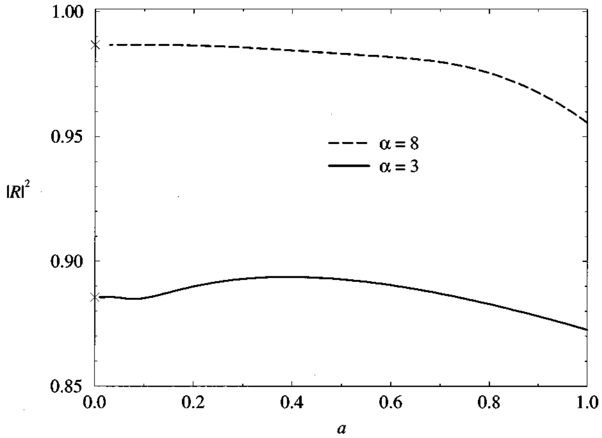

FIG. 5. Convergence of the probability for reflection by the potential (21) with a decreasing value of the parameter a (increasing depth of the potential). The results are for $\beta=1$ and the reduced momentum $k_2\beta=0.01$. The crosses on the ordinate mark the respective limiting values for $a\rightarrow 0$.

ability. The convergence of the reflection probability as $a\rightarrow 0$ is demonstrated in detail in Fig. 5 for $k_2=0.01$. The crosses on the ordinate indicate the limiting values calculated with the limiting form (18) of the potential (21) via Eq. (5) as described above.

V. ANALYTIC RESULTS

There are no known analytic solutions for step potentials with the asymptotic behavior (18), but the Schrödinger equation with this potential alone can be solved in terms of Bessel functions at $E=0$ [10], and this is sufficient to deduce the leading behavior of the reflection amplitude at the top of the step. Two linearly independent solutions are

$$\psi_1(x)=\sqrt{x}\,J_\nu(y),\quad \psi_2(x)=\sqrt{x}\,J_{-\nu}(y), \tag{24}$$

with

$$\nu=\frac{1}{\alpha-2},\quad y=\frac{2}{\alpha-2}\left(\frac{\beta}{x}\right)^{\alpha/2-1}. \tag{25}$$

Asymptotically, $x\rightarrow+\infty$, the solutions (24) behave as

$$\psi_1(x)\sim c_1+O(x^{2-\alpha})\quad,\quad \psi_2(x)\sim c_2x+O(x^{3-\alpha}), \tag{26}$$

with

$$c_1=\left(\frac{1}{\alpha-2}\right)^{1/(\alpha-2)}\frac{\sqrt{\beta}}{\Gamma\left(1+\frac{1}{\alpha-2}\right)},$$

$$c_2=\frac{1}{\sqrt{\beta}}\frac{(\alpha-2)^{1/(\alpha-2)}}{\Gamma\left(1-\frac{1}{\alpha-2}\right)}. \tag{27}$$

For small wave numbers k_2, the wave function

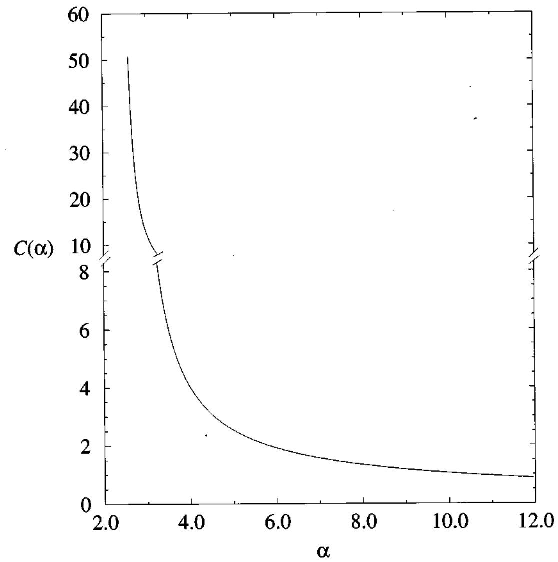

FIG. 6. Coefficient $C(\alpha)$ of the leading deviation of the reflection probability from unity for reflection by a sufficiently deep and smooth potential step decaying asymptotically as $-1/x^\alpha$; cf. Eq. (36).

$$\psi(x)=\frac{1}{c_1}\,\psi_1(x)+\frac{ik_2}{c_2}\,\psi_2(x) \tag{28}$$

is a solution of the Schrödinger equation in the region $x>0$ up to $O(k_2^2)$ and its asymptotic ($x\rightarrow+\infty$) behavior

$$\psi(x)\sim 1+ik_2x \tag{29}$$

corresponds to a rightward-traveling outgoing wave. For small values of x/β the argument y of the Bessel functions in Eq. (24) is large, giving [10]

$$\psi(x)\propto\sqrt{\frac{x}{y}}\left[\cos\left(y-\frac{\pi}{4}-\frac{\nu\pi}{2}\right)+ik_2B\,\cos\left(y-\frac{\pi}{4}+\frac{\nu\pi}{2}\right)\right], \tag{30}$$

with

$$B=\frac{c_1}{c_2}=\left(\frac{1}{\alpha-2}\right)^{2/(\alpha-2)}\frac{\pi\beta}{\Gamma\left(\frac{1}{\alpha-2}\right)\Gamma\left(1+\frac{1}{\alpha-2}\right)\sin\left(\frac{\pi}{\alpha-2}\right)}. \tag{31}$$

At an appropriate matching point x_m fulfilling Eq. (20) the logarithmic derivative of the wave function (30) is

$$z=\frac{\alpha-2}{2x_m}\left[y_m\frac{\sin\left(y_m-\frac{\pi}{4}-\frac{\nu\pi}{2}\right)+ik_2B\sin\left(y_m-\frac{\pi}{4}+\frac{\nu\pi}{2}\right)}{\cos\left(y_m-\frac{\pi}{4}-\frac{\nu\pi}{2}\right)+ik_2B\cos\left(y_m-\frac{\pi}{4}+\frac{\nu\pi}{2}\right)}+\frac{\alpha}{2(\alpha-2)}\right]. \tag{32}$$

The constant term in the square brackets can be neglected since the value of y_m, which is related to x_m by Eq. (25), is large. Inserting z into the matching condition (6) yields the expressions for modulus and phase of the reflection amplitude $R_{\rm WKB}$,

$$|R_{\rm WKB}|^2=1-4k_2B\sin\left(\frac{\pi}{\alpha-2}\right), \tag{33}$$

$$\arg R_{\rm WKB}=\frac{4}{\alpha-2}\left(\frac{\beta}{x_{\rm m}}\right)^{(\alpha/2)-1}-\left(\frac{\pi}{2}+\frac{\pi}{\alpha-2}\right). \tag{34}$$

Note that the factor $\sin[\pi/(\alpha-2)]$ in Eq. (33) cancels the corresponding factor in the denominator of the expression (31) for B, so that Eq. (33) is continuous in α and has no singularity at the values $\alpha=2+1/n$, $n=1,2,3,\ldots$, where the sine vanishes. Corrections to the formulas (33) and (34) are of the order $(k_2\beta)^2$ for $\alpha\geqslant3$ and of order $(k_2\beta)^{\alpha-1}$ for $\alpha\leqslant3$. This can be seen by estimating the corrections to the approximation (29) for finite momenta [11]. The matching-point-dependent contribution to the phase (34) again has the form $(2/\hbar)\int_{x_m}^{\infty}p(x)\,dx$, so the phase of the conventionally defined reflection amplitude consists of the standard contribution as on the left-hand side of Eq. (11) minus a term that may be interpreted as the phase loss in the WKB wave function due to the reflection at infinity [9].

The individual steps in the derivation above are essentially the same as those used for deriving scattering lengths as in Sec. 4.3. of [2] and in [8,12], where real superpositions of the solutions (24) are used. Their coefficients are determined by matching to WKB approximations of the regular solutions for s-wave scattering. In the present approach we use a *fixed* superposition (28) to determine $R_{\rm WKB}$ by matching it to Eq. (2) at x_m.

From the above derivation it follows that for a sufficiently deep and smooth step potential behaving asymptotically as Eq. (18), the reflection probability $|R|^2$ near the top of the step is given to leading order by

$$|R|^2=1-C(\alpha)k_2\beta \tag{35}$$

and the coefficient of the term linear in the reduced momentum is

$$C(\alpha)=\left(\frac{1}{\alpha-2}\right)^{2/(\alpha-2)}\frac{4\pi}{\Gamma\left(\frac{1}{\alpha-2}\right)\Gamma\left(1+\frac{1}{\alpha-2}\right)}. \tag{36}$$

This result holds for any real value of the power α as long as $\alpha>2$. The behavior of $C(\alpha)$ is illustrated in Fig. 6.

The phase of the conventionally defined reflection amplitude R at the top of the step can be derived from Eq. (34) via Eqs. (3) and (4),

$$\arg R=2\lim_{x\to-\infty}\left(\frac{1}{\hbar}\int_x^{\infty}p(x')\,dx'+k_1x\right)-\phi, \tag{37}$$

with

$$\phi=\frac{\pi}{2}+\frac{\pi}{\alpha-2}. \tag{38}$$

The first term on the right-hand side of Eq. (37) is just twice the difference between the phase accumulated by the WKB wave function between $-\infty$ and $+\infty$ and the phase accumulated by the free wave with wave number k_1 between $-\infty$ and $x=0$. This term depends of course on the precise shape of the whole potential and not only on the decaying tail. The second term on the right-hand side of Eq. (37) describes the phase loss ϕ in the WKB wave due to the reflection at $+\infty$, being the classical turning point at the top of the step. For large powers α this phase loss (38) approaches $\pi/2$ as for the Woods-Saxon step with large relative diffuseness [9]. For inverse power-law potentials with $\alpha>2$, vanishing reduced momentum corresponds to the anticlassical limit of the Schrödinger equation, and WKB waves reflected by repulsive inverse power-law potentials acquire a phase loss π in this limit [13]. For the attractive inverse power-law potentials studied in this section, the phase loss for vanishing reduced momentum depends on the power α; it increases monotonically from the value $\pi/2$ for $\alpha\to\infty$, passes π at $\alpha=4$, and grows beyond bound as α approaches the value 2, where the present theory breaks down.

VI. CONCLUSION

We have studied classically forbidden reflection by a potential step that is sufficiently deep and smooth, so that the variation of the de Broglie wavelength is small except in the tail region of the potential. The probability for reflection is then determined by the decaying tail of the potential on the up side and is independent of the precise shape and depth of the potential step.

For potentials decaying asymptotically ($x\to+\infty$) as an inverse power of the coordinate $V(x)\sim-\beta^{\alpha-2}/x^{\alpha}$, $\alpha>2$, we have derived analytic expressions for the leading deviation of the reflection probability from unity and for the phase of the reflection amplitude at the top of the step. The decrease of the reflection probability from unity is linear in the reduced momentum $k_2\beta$, and the coefficient (36) of this linear dependence increases monotonically from zero to infinity as α varies from ∞ to 2, according to Eq. (36) (Fig. 6). The phase (37) of the reflection amplitude contains a general contribution describing the accumulated phase difference of the incoming and reflected WKB waves in comparison with free waves and an additional contribution describing the phase loss ϕ of the WKB wave due to reflection. At the top of the step, the phase loss ϕ increases monotonically from the value $\pi/2$ in the limit of large powers α to $+\infty$ as α approaches 2; see Eq. (38). The result (35) with Eq. (36) and the result (37) with Eq. (38) are valid for any sufficiently deep and smooth step potential decaying asymptotically as Eq. (18) with any real power $\alpha > 2$.

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