Effective-range theory for quantum reflection amplitudes

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We formulate an effective-range theory for the near-threshold behavior of the amplitudes describing quantum reflection in attractive potential tails by adapting the effective-range theory of ordinary elastic scattering to the case of incoming boundary conditions at small distances. For homogeneous attractive potentials proportional to $-1/r^{\alpha}$ with $\alpha > 5$, the effective range turns out to be a real multiple (with known coefficient) of the complex scattering length which defines the leading, linear momentum dependence of phase and modulus of the quantum reflection amplitude. Analytical expressions are also given for the leading and next-to-leading terms in the near-threshold behavior of the quantum reflection amplitudes for homogeneous attractive potentials proportional to $-1/r^3$, $-1/r^4$, and $-1/r^5$.

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I. INTRODUCTION

The term "quantum reflection" describes classically forbidden reflection of a particle in a classically allowed region without classical turning points. It is generated in nonclassical regions of coordinate space, e.g., above potential barriers or purely attractive potential tails, as occur in the interaction of atoms and molecules with surfaces and with each other [1,2]. Quantum reflection has been observed in recent experiments involving ultracold atoms [3–9] and is always important at very low energies, because the quantum reflection probability tends to unity as the energy $E = \hbar^2 k^2/(2M)$ goes to zero.

For a particle of mass M approaching a long-ranged attractive potential $U(r)$ from large distances, the near-threshold behavior of the quantum reflection amplitude R up to and including terms linear in the asymptotic wave number $k = \sqrt{2ME}/\hbar$ is given by [1,10,11]

$$|R| \overset{k\to 0}{\sim} 1 - 2bk, \quad \arg R \overset{k\to 0}{\sim} \pi - 2\bar{a}k. \tag{1}$$

It is determined by two real parameters, the "threshold length" b [10], which is well defined as long as the potential falls off faster than $-1/r^2$ asymptotically [1], and the mean scattering length $\bar{a}$, which is well defined as long as U falls off faster than $-1/r^3$ [12].

Both b and $\bar{a}$ are "tail parameters," i.e., they depend only on the properties of the potential tail beyond a semiclassical region of comparatively "small" distances, where WKB wave functions with an unambiguously defined direction of motion are accurate solutions of the Schrödinger equation. These "small" distances are still beyond the close regime, corresponding typically to a few atomic units, where details of the structure of the interacting atoms, molecules, or surfaces become important. The interaction in the close regime is quite complicated and generally leads to inelastic reactions or absorption, so the yield of elastically reflected particles is essentially due to quantum reflection in the nonclassical region, which lies between the semiclassical region of "small" distances and the asymptotic regime ($r \to \infty$) of free-particle motion.

Quantum reflection is described by the same one-dimensional Schrödinger equation as ordinary, particle flux conserving elastic scattering [13], except that the solutions are defined via leftward-traveling (incoming) boundary conditions for the transmitted part of the wave at "small" distances, whereas the wave function for ordinary elastic scattering is generally taken as the regular wave function which vanishes at $r=0$. The observables of ordinary elastic scattering, such as the scattering phase shift, thus depend sensitively on the properties of the potential in the close regime, in particular on whether or not the whole potential supports a bound state close to threshold. The scattering length a_0, which describes the leading k dependence of the s-wave scattering phase shift $\delta_0(k)$ near threshold, becomes infinite when the potential supports an s-wave bound state at threshold. In contrast, the quantum reflection amplitude is insensitive to details of the interaction in the close region, where the incoming boundary conditions account for the loss of all particles which are transmitted through the quantum region of the potential tail.

In ordinary elastic scattering theory for potentials falling off faster than $1/r^5$ asymptotically, the next-to-leading term in the k dependence of the s-wave scattering phase shift is proportional to k^3, and it is determined by the effective range r_{eff} defined by [13]

$$\frac{k}{\tan \delta_0} \overset{k\to 0}{\sim} -\frac{1}{a_0} + \frac{1}{2} r_{\text{eff}} k^2. \tag{2}$$

This "effective-range expansion" has the misleading feature, that a vanishing value of r_{eff} does not coincide with the vanishing of the term proportional to k^3 in the low-energy behavior of the scattering phase shift. Inserting the right-hand side of Eq. (2) into a Taylor expansion of the $\tan \delta_0$ yields

$$\delta_0 \overset{k\to 0}{\sim} -a_0 k + \left(a_0^3 - \frac{3}{2} a_0^2 r_{\text{eff}}\right)\frac{k^3}{3}. \tag{3}$$

For example, a hard-core potential of radius L has scattering length $a_0 = L$ and effective range $r_{\text{eff}} = \frac{2}{3}L$ so that $\delta_0 = -kL$ to order k^3—and in fact to all higher orders as well. Equation (3) suggests an alternative notation for the low-energy behavior of the s-wave scattering phase shift

$$\delta_0 \overset{k\to 0}{\sim} -a_0 k + \frac{1}{3}(\lambda k)^3, \quad \text{with } \lambda = a_0\left(1 - \frac{3}{2}\frac{r_{\rm eff}}{a_0}\right)^{1/3}. \tag{4}$$

The effective-range expansion does not lead to a finite value of $r_{\rm eff}$ when the potential falls off as $1/r^5$ or slower asymptotically.

The aim of the present paper is to adapt the effective-range theory of ordinary elastic scattering to the case of quantum reflection and to derive appropriate parameters which describe the next-to-leading k dependence of quantum reflection amplitudes for attractive potential tails. Section II contains a general description of effective-range theory for quantum reflection amplitudes and Sec. III presents analytical results for homogeneous potential tails

$$U_\alpha(r) = -\frac{C_\alpha}{r^\alpha} = -\frac{\hbar^2}{2M}\frac{(\beta_\alpha)^{\alpha-2}}{r^\alpha}, \tag{5}$$

with $\alpha > 5$. Homogeneous potentials (5) with $\alpha \leqslant 5$ are treated in Sec. IV.

II. EFFECTIVE-RANGE EXPANSION FOR QUANTUM REFLECTION

The Schrödinger equation for a particle of mass M moving with energy $E = \hbar^2 k^2/(2M)$ under the influence of the potential $U(r)$ is

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{2M}{\hbar^2}U(r)\right)u(r) = 0. \tag{6}$$

We assume that the potential vanishes asymptotically ($r\to\infty$), and that it is attractive and more singular than $-1/r^2$ for "small" values of r. The wave functions can then be described by WKB waves for small r, which allows an unambiguous identification of leftward (inward) and rightward (outward) traveling waves in this semiclassical region. The quantum reflection amplitude R for particles approaching from large distances is obtained by solving the Schrödinger equation (6) with the following boundary conditions:

$$u(r) \overset{r\to 0}{\sim} \frac{A}{\sqrt{p_k(r)}} \exp\left[-\frac{i}{\hbar}\int_{r_0}^{r} p_k(r')dr'\right],$$

$$u(r) \overset{r\to\infty}{\sim} B(e^{-ikr} + R(k)e^{+ikr}), \tag{7}$$

where $p_k(r) = \sqrt{2M[E - U(r)]}$ is the local classical momentum labeled by the asymptotic wave number $k = \sqrt{2ME}/\hbar$. The WKB wave in the upper line of Eq. (7) is defined with a fixed and finite point of reference r_0 and describes an inward traveling wave at small distances r.

In order to adapt the theory described, e.g., in Chap. 6 of Ref. [13] to the present situation, we choose the (arbitrary) parameter B in Eq. (7) to be $1/[1+R(k)]$ and obtain wave functions with the following behavior at large distances:

$$u(r) \overset{r\to\infty}{\sim} \left[e^{+ikr} - \frac{2i\sin(kr)}{1+R(k)}\right],$$

$$\frac{du}{dr} \overset{r\to\infty}{\sim} ik\left[e^{+ikr} - \frac{2\cos(kr)}{1+R(k)}\right]. \tag{8}$$

At small distances, the derivative of the inward traveling wave is

$$\frac{du}{dr} \overset{r\to 0}{\sim} -u(r)\left[\frac{p_k'(r)}{2p_k(r)} + \frac{i}{\hbar}p_k(r)\right]. \tag{9}$$

We call $u_1(r)$ the solution of the Schrödinger equation (6) for wave number k_1 and $u_2(r)$ the solution for wave number k_2. It then follows that $u_1(r)u_2''(r) - u_2(r)u_1''(r) = (k_1^2 - k_2^2)u_1(r)u_2(r)$ and

$$\int_{r_l}^{r_u}\left[u_1(r)\frac{d^2u_2}{dr^2} - u_2(r)\frac{d^2u_1}{dr^2}\right]dr = \left[u_1(r)\frac{du_2}{dr} - u_2(r)\frac{du_1}{dr}\right]_{r_l}^{r_u} = (k_1^2 - k_2^2)\int_{r_l}^{r_u} u_1(r)u_2(r)dr. \tag{10}$$

At the lower integration limit r_l we have

$$u_1(r_l)u_2'(r_l) - u_2(r_l)u_1'(r_l) = u_1(r_l)u_2(r_l)\left[\frac{p_{k_1}'(r_l)}{2p_{k_1}(r_l)} - \frac{p_{k_2}'(r_l)}{2p_{k_2}(r_l)} + \frac{i}{\hbar}[p_{k_1}(r_l) - p_{k_2}(r_l)]\right]. \tag{11}$$

For potentials behaving as Eq. (5) with $\alpha > 2$ for small r, we have $p_k(r_l) = (\hbar/\beta_\alpha)(\beta_\alpha/r_l)^{\alpha/2}\sqrt{1 + k^2 r_l^\alpha/(\beta_\alpha)^{\alpha-2}}$ and the expression (11) vanishes for $r_l \to 0$.

We use the letter v to denote solutions of the Schrödinger equation without the potential $U(r)$. Let $v_1(r)$ be the solution at wave number k_1 which has the same asymptotic ($r\to\infty$) behavior as $u_1(r)$; then $v_1(r)$ and $v_1'(r)$ are given by the right-hand sides of Eq. (8), with k_1 in place of k, not only asymptotically but for all values of r. Let v_2 be the solution of the free-wave equation at wave number k_2 which has the same asymptotic behavior as $u_2(r)$. Then

$$\int_{r_l}^{r_u}\left[v_1(r)\frac{d^2v_2}{dr^2} - v_2(r)\frac{d^2v_1}{dr^2}\right]dr = \left[v_1(r)\frac{dv_2}{dr} - v_2(r)\frac{dv_1}{dr}\right]_{r_l}^{r_u} = (k_1^2 - k_2^2)\int_{r_l}^{r_u} v_1(r)v_2(r)dr. \tag{12}$$

Subtracting Eq. (10) from Eq. (12) gives

$$\left[v_1(r)\frac{dv_2}{dr} - v_2(r)\frac{dv_1}{dr}\right]_{r_l}^{r_u} - \left[u_1(r)\frac{du_2}{dr} - u_2(r)\frac{du_1}{dr}\right]_{r_l}^{r_u} = (k_1^2 - k_2^2)\int_{r_l}^{r_u}[v_1(r)v_2(r) - u_1(r)u_2(r)]dr. \tag{13}$$

The contributions at the upper limit r_u on the left-hand side of Eq. (13) cancel as $r_u\to\infty$, because u_i and v_i ($i=1,2$) become equal asymptotically. At the lower limit r_l, the contributions of the $u's$ on the left-hand side vanish for $r_l\to 0$ as discussed above. The contribution of the $v's$ is

$$-v_1(r_l)\left.\frac{dv_2}{dr}\right|_{r_l}+v_2(r_l)\left.\frac{dv_1}{dr}\right|_{r_l} \overset{r_l\to 0}{\sim} i(k_1-k_2)+2i\left(\frac{k_2}{1+R(k_2)}-\frac{k_1}{1+R(k_1)}\right), \quad (14)$$

so, in the limits $r_l\to 0$, $r_u\to\infty$, Eq. (13) becomes

$$i(k_1-k_2)+2i\left(\frac{k_2}{1+R(k_2)}-\frac{k_1}{1+R(k_1)}\right) = (k_1^2-k_2^2)\int_0^\infty [v_1(r)v_2(r)-u_1(r)u_2(r)]dr. \quad (15)$$

Equation (15) is valid for any pair (k_1,k_2) of wave numbers. We can take the limit $k_2\to 0$ for which $1+R(k_2)\to 2(b+i\bar{a})k_2$ according to (1), so the quotient $2ik_2/[1+R(k_2)]$ approaches the constant value $1/(\bar{a}-ib)$. Dropping the index 1 on k_1, u_1 and v_1, Eq. (15) thus becomes

$$-\frac{2ik}{1+R(k)}+ik=-ik\frac{1-R(k)}{1+R(k)} = -\frac{1}{\bar{a}-ib}+k^2\int_0^\infty [v(r)v_0(r)-u(r)u_0(r)]dr, \quad (16)$$

where u_0 and v_0 now stand for the solutions of the Schrödinger equation, with and without potential respectively, at threshold, $k=0$.

Except for a minus sign, the reflection amplitude R corresponds to the S matrix of s-wave scattering, which is usually written in terms of the s-wave scattering phase shift δ_0 as $e^{2i\delta_0}$, $R\equiv -e^{2i\delta_0}$. In terms of δ_0, Eq. (16) has the form of the ordinary effective-range expansion (2). In the present case, the modulus $|R|$ of the reflection amplitude can be less than unity, so the corresponding "scattering phase shift" is in general complex,

$$\delta_0\equiv\delta_r+i\delta_i, \quad R=-e^{-2\delta_i}e^{2i\delta_r}. \quad (17)$$

Also, the scattering length a_0 of ordinary scattering theory is now replaced by a complex scattering length $\bar{a}-ib$, where $\bar{a}$ and b are the tail parameters of the potential as defined in Eq. (1). Adopting the nomenclature of the effective-range expansion in ordinary scattering theory we write the near-threshold expansion of Eq. (16) as

$$-ik\frac{1-R(k)}{1+R(k)}=\frac{k}{\tan(\delta_r+i\delta_i)}\overset{k\to 0}{\sim}-\frac{1}{\bar{a}-ib}+\frac{1}{2}\mathcal{R}_{\rm eff}k^2, \quad (18)$$

and the complex effective range $\mathcal{R}_{\rm eff}$ is defined via the value of the integral on the right-hand side of Eq. (16) at threshold

$$\mathcal{R}_{\rm eff}=2\int_0^\infty [v_0(r)^2-u_0(r)^2]dr. \quad (19)$$

The functions v_0 and u_0 are defined via the asymptotic boundary conditions (8) in the limit $k\to 0$

$$v_0(r)=1-\frac{r}{\bar{a}-ib}, \quad u_0(r)\overset{r\to\infty}{\sim}1-\frac{r}{\bar{a}-ib}, \quad (20)$$

and the only difference to effective-range theory for ordinary elastic scattering is the appearance of the complex scattering length $\bar{a}-ib$ instead of the real s-wave scattering length a_0.

For convenience we introduce

$$\mathcal{A}\overset{\rm def}{=}\bar{a}-ib \quad (21)$$

as the complex scattering length whose imaginary and real parts determine the leading near-threshold k dependence of modulus and phase of the quantum reflection amplitude (17) according to Eq. (1). The leading near-threshold behavior of the complex phase shift can then be written as

$$\delta_r+i\delta_i\overset{k\to 0}{\sim}-k\mathcal{A}+\frac{1}{3}(k\Lambda)^3, \quad \Lambda=\left(1-\frac{3}{2}\frac{\mathcal{R}_{\rm eff}}{\mathcal{A}}\right)^{1/3}\mathcal{A}, \quad (22)$$

in analogy to Eq. (4). This is the desired expression for the leading and next-to-leading behavior of modulus and phase of the quantum reflection amplitude (17).

The function $u_0(r)$ is the zero energy solution of the Schrödinger equation (6) defined by its asymptotic behavior (20). If the potential behaves as Eq. (5) asymptotically, then the asymptotic behavior of u_0 is given [1,11] via Bessel functions $J_{\pm\nu}(z)$, whose order and argument are defined by

$$\nu=\frac{1}{\alpha-2}, \quad z=2\nu\left(\frac{\beta_\alpha}{r}\right)^{1/(2\nu)}. \quad (23)$$

Explicitly we have [11]

$$u_0(r)\overset{r\to\infty}{\sim}\frac{\Gamma(1+\nu)}{\nu^\nu}\sqrt{\frac{r}{\beta_\alpha}}J_\nu(z)-\frac{\beta_\alpha}{\bar{a}-ib}\Gamma(1-\nu)\nu^\nu\sqrt{\frac{r}{\beta_\alpha}}J_{-\nu}(z). \quad (24)$$

Inserting the asymptotic $(r\to\infty, z\to 0)$ behavior of the Bessel functions [14] yields

$$u_0(r)\overset{r\to\infty}{\sim}1-\frac{(z/2)^2}{1+\nu}+O(z^4)-\frac{r}{\bar{a}-ib}\left(1-\frac{(z/2)^2}{1-\nu}+O(z^4)\right) = 1-\frac{r}{\bar{a}-ib}+O(r^{3-\alpha}). \quad (25)$$

The leading asymptotic terms of $v_0(r)^2-u_0(r)^2$ are proportional to $r^{4-\alpha}$, so the integral in the definition (19) of the effective range converges to a well-defined value when $\alpha>5$.

Remember that the quantum reflection amplitude depends not only on the leading asymptotic behavior of the potential, but on the potential tail in the whole nonclassical region beyond semiclassical regime at "small" distances. Deviations from the homogeneous form (5) are important, if they are not negligible beyond the semiclassical region.

A simple example for the effective-range expansion (18) and (22) is provided by the finite sharp-step potential, which vanishes beyond $r=L$ and has the constant value $U_{\rm step}=-\hbar^2K_0^2/(2M)$ for $0<r<L$. Here the nonclassical re-

gion is restricted to a single point, namely, $r=L$, and the quantum reflection amplitude is given by

$$R_{\rm step} = -\frac{1-k/\sqrt{K_0^2+k^2}}{1+k/\sqrt{K_0^2+k^2}}e^{-2ikL},$$

$$\delta_r + i\delta_i = -kL - \frac{i}{2}\ln\left[\frac{1-k/\sqrt{K_0^2+k^2}}{1+k/\sqrt{K_0^2+k^2}}\right] \overset{k\to 0}{\sim} -k\left(L-\frac{i}{K_0}\right) - \frac{i}{6}\left(\frac{k}{K_0}\right)^3. \quad (26)$$

This corresponds to the complex scattering length $\mathcal{A}=L-i/K_0$ and the effective range

$$\mathcal{R}_{\rm eff} = \frac{2}{3}\mathcal{A} + \frac{i}{3K_0^3\mathcal{A}^2} \Rightarrow \Lambda = \frac{i}{2^{1/3}K_0}. \quad (27)$$

III. HOMOGENEOUS POTENTIALS

For the calculation of quantum reflection amplitudes, a potential with the asymptotic behavior (5) can be assumed to be of this homogeneous form, if deviations from Eq. (5) are restricted to the semiclassical regime at "small" distances. In this case, the zero-energy solution $u_0(r)$ of the Schrödinger equation can be taken as given by Eq. (24) in the whole range of r values and not only asymptotically, and the definition of the effective range via Eq. (19) gives a well defined result as long as $\alpha > 5$. For homogeneous potentials (5), the properties of the Schrödinger equation (6) depend not on energy $E=\hbar^2k^2/(2M)$ and potential strength independently, but only on the dimensionless parameter $k\beta_\alpha$. This also holds for all lengths when expressed in units of β_α.

The mean scattering length $\bar{a}_\alpha$ and the threshold length b_α are well known [11] for homogeneous potential tails (5),

$$\frac{\bar{a}_\alpha}{\beta_\alpha} = \nu^{2\nu}\frac{\Gamma(1-\nu)}{\Gamma(1+\nu)}\cos(\pi\nu), \quad \frac{b_\alpha}{\beta_\alpha} = \nu^{2\nu}\frac{\Gamma(1-\nu)}{\Gamma(1+\nu)}\sin(\pi\nu) \quad (28)$$

[remember, $\nu=1/(\alpha-2)$], so the complex scattering length $\mathcal{A}_\alpha$ is given by

$$\mathcal{A}_\alpha = \bar{a}_\alpha - ib_\alpha = \beta_\alpha\nu^{2\nu}\frac{\Gamma(1-\nu)}{\Gamma(1+\nu)}e^{-i\pi\nu}. \quad (29)$$

The effective-range expansion for ordinary elastic scattering by potentials with inverse-power tails (5) was studied by Flambaum *et al.* in Ref. [15]. They calculate the effective range by evaluating an integral as in Eq. (19) with wave functions v_0 and u_0 defined as in Eqs. (20) and (24), and the only difference is the use of the real scattering length a_0 instead of the complex scattering length $\bar{a}-ib \equiv \mathcal{A}_\alpha$. The relevant equation (24) of Ref. [15] can be directly transferred to the present case of quantum reflection by writing $\mathcal{A}_\alpha$ in place of the real scattering length of ordinary elastic scattering

$$\frac{\mathcal{R}_{\rm eff}}{\beta_\alpha} = f_\alpha - g_\alpha\frac{\beta_\alpha}{\mathcal{A}_\alpha} + h_\alpha\left(\frac{\beta_\alpha}{\mathcal{A}_\alpha}\right)^2. \quad (30)$$

We have referred all lengths to the strength parameter β_α of the potential (5) so that the coefficients in Eq. (30) become dimensionless,

$$f_\alpha = \frac{2}{3}\frac{\pi\nu^{2\nu}}{\sin(\pi\nu)}\frac{\Gamma(\nu)\Gamma(4\nu)}{\Gamma(2\nu)^2\Gamma(3\nu)},$$

$$g_\alpha = \frac{4}{3}\frac{\pi\nu^{4\nu}}{\sin(\pi\nu)}\frac{\Gamma(1-2\nu)\Gamma(4\nu)}{\nu\Gamma(\nu)\Gamma(2\nu)\Gamma(3\nu)},$$

$$h_\alpha = \frac{2}{3}\frac{\pi\nu^{6\nu}}{\sin(\pi\nu)}\frac{\Gamma(1-3\nu)\Gamma(1-\nu)\Gamma(4\nu)}{\nu^2\Gamma(\nu)^2\Gamma(2\nu)^2}. \quad (31)$$

Inserting Eq. (29) into Eq. (30) and exploiting some properties [14] of the gamma function, in particular the identity $\Gamma(1+x)\Gamma(1-x)=\pi x/\sin(\pi x)$, leads to the following explicit expression for the complex effective range of the quantum reflection amplitude for a homogeneous potential tail (5):

$$\mathcal{R}_{\rm eff} = \frac{2}{3}\mathcal{A}_\alpha\frac{\Gamma(1-2\nu)^2\Gamma(1-3\nu)\Gamma(1+\nu)}{\Gamma(1-4\nu)\Gamma(1-\nu)^2}. \quad (32)$$

An alternative method of obtaining the same result is to study ordinary elastic scattering by the repulsive homogeneous potential

$$U_\alpha^{\rm (rep)}(r) = -U_\alpha(r) = \frac{\hbar^2}{2M}\frac{(\beta_\alpha)^{\alpha-2}}{r^\alpha}. \quad (33)$$

Del Giudice and Galzenati [16] studied the near-threshold behavior of the s-wave scattering phase shift $\delta_0^{\rm (rep)}$ in the potential (33), and this involved studying the asymptotic $(r\to\infty)$ behavior of the regular solutions $\psi_{\rm reg}(r)$, which are correctly given by the WKB expression near the origin as long as $\alpha > 2$ [11],

$$\psi_{\rm reg}(r) \overset{r\to 0}{\propto} \frac{1}{\sqrt{p_k^{\rm (rep)}(r)}}\exp\left[-\frac{1}{\hbar}\int_r^{r_0} p_k^{\rm (rep)}(r')dr'\right]. \quad (34)$$

Here $p_k^{\rm (rep)}(r)=|\hbar\sqrt{k^2-(\beta_\alpha)^{\alpha-2}/r^\alpha}|$ is the absolute value of the local classical momentum in the classically forbidden region near $r=0$. Matching the regular solution (34) to the asymptotic form

$$\psi_{\rm reg}(r) \overset{r\to\infty}{\sim} \sin(kr) + \tan\delta_0^{\rm (rep)}\cos(kr) \propto e^{-ikr} - e^{2i\delta_0^{\rm (rep)}}e^{+ikr} \quad (35)$$

leads to the following near-threshold behavior of $\tan\delta_0^{\rm (rep)}$:

$$\tan\delta_0^{\rm (rep)} \overset{k\to 0}{\sim} \frac{\Gamma(-\nu)}{\Gamma(\nu)}\nu^{2\nu}k\beta_\alpha + \frac{\Gamma(-\nu)\Gamma(-2\nu)^2\Gamma(-3\nu)}{\Gamma(\nu)^2\Gamma(-4\nu)}\nu^{1+6\nu}(k\beta_\alpha)^3. \quad (36)$$

For $\alpha > 5$, Eq. (36) represents a standard effective-range expansion

TABLE I. Mean scattering length $\bar{a}_\alpha$ and threshold length b_α defining the real and imaginary parts of the scattering length $\mathcal{A}_\alpha=\bar{a}_\alpha-ib_\alpha$ for quantum reflection by homogeneous potential tails (5). Also shown is the ratio of the effective range $\mathcal{R}_{\rm eff}$ to $\mathcal{A}_\alpha$ and the quotient $\Lambda_\alpha/\mathcal{A}_\alpha$, where Λ_α is the parameter determining the next-to-leading momentum dependence in the near-threshold behavior of the complex phase shift according to Eq. (22). The constant c_∞ in the last row and column is as given by Eq. (48)

α	6	7	8	9	10	$\alpha\to\infty$
$\bar{a}/\beta_\alpha$	0.4779888	0.5388722	0.5798855	0.6108042	0.6356215	1
b/β_α	0.4779888	0.3915136	0.3347971	0.2941478	0.2632830	$\pi/(\alpha-2)$
$\mathcal{R}_{\rm eff}/\mathcal{A}_\alpha$	0	0.4839001	0.5888796	0.6259995	0.6426344	$\frac{2}{3}$
$\Lambda_\alpha/\mathcal{A}_\alpha$	1	0.6496249	0.4886519	0.3936512	0.3303405	$c_\infty/(\alpha-2)$

$$\frac{k}{\tan\delta_0^{\rm (rep)}} \overset{k\to0}{\sim} -\frac{1}{a_\alpha^{\rm (rep)}}+\frac{1}{2}R_{\rm eff}k^2, \tag{37}$$

where

$$a_\alpha^{\rm (rep)}=\nu^{2\nu}\frac{\Gamma(1-\nu)}{\Gamma(1+\nu)}\beta_\alpha \tag{38}$$

is the scattering length, and the effective range $R_{\rm eff}$ is given by

$$R_{\rm eff}=2a_\alpha^{\rm (rep)}\frac{\Gamma(-2\nu)^2\Gamma(-3\nu)\nu^2\Gamma(1+\nu)}{\Gamma(-4\nu)\Gamma(1-\nu)^2}. \tag{39}$$

The repulsive homogeneous potential (33) becomes the attractive homogeneous potential (5) if we replace [17] $(\beta_\alpha)^{\alpha-2}$ by $-(\beta_\alpha)^{\alpha-2}$,

$$(\beta_\alpha)^{\alpha-2}\to-(\beta_\alpha)^{\alpha-2}=e^{-i\pi}(\beta_\alpha)^{\alpha-2},\quad \beta_\alpha\to\beta_\alpha e^{-i\pi\nu}. \tag{40}$$

The regular wave function $\psi_{\rm reg}$ then becomes a complex wave function $\psi_{\rm in}$, whose behavior near the origin corresponds to an inward traveling WKB wave

$$\psi_{\rm reg}(r)\to\psi_{\rm in}(r)\overset{r\to0}{\propto}\frac{1}{\sqrt{p_k(r)}}\exp\left[\frac{i}{\hbar}\int_r^{r_0}p_k(r')dr'\right], \tag{41}$$

where $p_k(r)=\hbar\sqrt{k^2+(\beta_\alpha)^{\alpha-2}/r^\alpha}$ is the local classical momentum in the attractive homogeneous potential (5). Equation (41) is just the small-r behavior of the wave function used to define the quantum reflection amplitude according to Eq. (7), so the correct quantum reflection amplitude is obtained via Eq. (17) if we replace the s-wave scattering phase shift $\delta_0^{\rm (rep)}$ by the complex phase shift obtained for the attractive homogeneous potential via the replacement $\beta_\alpha\to\beta_\alpha e^{-i\pi\nu}$. According to Eq. (36), the near-threshold behavior of the tangent of this complex phase shift is

$$\tan(\delta_r+i\delta_i)\overset{k\to0}{\sim}\frac{\Gamma(-\nu)}{\Gamma(\nu)}\nu^{2\nu}k\beta_\alpha e^{-i\pi\nu} + \frac{\Gamma(-\nu)\Gamma(-2\nu)^2\Gamma(-3\nu)}{\Gamma(\nu)^2\Gamma(-4\nu)}\nu^{1+6\nu}(k\beta_\alpha e^{-i\pi\nu})^3. \tag{42}$$

While Eqs. (37) and (39) follow from Eq. (36) for the repulsive homogeneous potential, the corresponding equations following from Eq. (42) in the attractive case are obtained by simply writing $\beta_\alpha e^{-i\pi\nu}$ instead of β_α,

$$\frac{k}{\tan(\delta_r+i\delta_i)}\overset{k\to0}{\sim}-\frac{1}{a_\alpha^{\rm (rep)}e^{-i\pi\nu}}+\frac{1}{2}\mathcal{R}_{\rm eff}k^2, \tag{43}$$

$$\mathcal{R}_{\rm eff}=2a_\alpha^{\rm (rep)}e^{-i\pi\nu}\frac{\Gamma(-2\nu)^2\Gamma(-3\nu)\nu^2\Gamma(1+\nu)}{\Gamma(-4\nu)\Gamma(1-\nu)^2}. \tag{44}$$

From Eqs. (29) and (38) it follows that

$$a_\alpha^{\rm (rep)}e^{-i\pi\nu}=\mathcal{A}_\alpha=\bar{a}_\alpha-ib_\alpha, \tag{45}$$

and some elementary transcriptions of the gamma functions show that Eq. (44) is indeed the same equation as Eq. (32).

Interestingly, $\mathcal{R}_{\rm eff}$ is a real multiple of the complex scattering length $\mathcal{A}_\alpha$. This cannot be a general property of quantum reflection amplitudes, however, because it does not hold for the sharp step potential, see Eq. (27). The ratio $\mathcal{R}_{\rm eff}/\mathcal{A}_\alpha$ tends to the value $2/3$ as $\alpha\to\infty$ ($\nu\to0$), so the correction of order $O(k^3)$ in Eq. (22) or, equivalently, in the expression

$$R(k)=-e^{-2b_\alpha k}e^{-2i\bar{a}_\alpha k}\{1+O[(k\beta_\alpha)^3]\}, \tag{46}$$

becomes smaller and smaller for increasing powers α. The increasing accuracy of the exponential representation (46) with increasing α has been noticed in previous studies of quantum reflection probabilities [18].

For the homogeneous potentials (5), the parameter Λ_α, which defines the strength of the next-to-leading term in the k dependence of the complex phase shift as in Eq. (22) is also a real multiple of the complex scattering length $\mathcal{A}_\alpha$,

$$\frac{\Lambda_\alpha}{\mathcal{A}_\alpha}=\left[1-\frac{\Gamma(1-2\nu)^2\Gamma(1-3\nu)\Gamma(1+\nu)}{\Gamma(1-4\nu)\Gamma(1-\nu)^2}\right]^{1/3}. \tag{47}$$

Numerical values of the mean scattering length $\bar{a}_\alpha$, the threshold length b_α, the ratio $\mathcal{R}_{\rm eff}/\mathcal{A}_\alpha$ and the ratio $\Lambda_\alpha/\mathcal{A}_\alpha$ are listed in Table I. The constant c_∞ in the last row and column follows from the low-ν expansion of the gamma functions in Eq. (47), where the leading nonvanishing contribution to the expression in the square bracket turns out to be $(c_\infty\nu)^3$ with

$$c_\infty=[8\gamma^3-12\gamma\Gamma''(1)-4\Gamma'''(1)]^{1/3}=2.12653077\cdots. \tag{48}$$

IV. POTENTIALS FALLING OFF AS $-1/r^3$, $-1/r^4$, AND $-1/r^5$

As mentioned after Eq. (25) in Sec. II, the integral on the right-hand side of Eq. (19) diverges when the potential falls off as $1/r^5$ or slower asymptotically and the wave function v_0 is exactly given by Eq. (20). For homogeneous repulsive potentials (33) with α=3, 4, and 5, Del Giudice and Galzenati [16] gave the following expressions for the near-threshold behavior of the s-wave scattering phase shift $\delta_0^{(\mathrm{rep})}$:

$$\tan\delta_0^{(\mathrm{rep})} \overset{k\to 0}{\sim} k\beta_3\ln(k\beta_3) + \left(\ln 2 + 3\gamma - \frac{3}{2}\right)k\beta_3 + O((k\beta_3)^2), \quad \alpha=3, \tag{49}$$

$$\tan\delta_0^{(\mathrm{rep})} \overset{k\to 0}{\sim} -k\beta_4 + \frac{\pi}{3}(k\beta_4)^2 + \frac{4}{3}(k\beta_4)^3\ln(k\beta_4) + \left(\frac{8}{3}(\gamma+\ln 2) - \frac{28}{9}\right)(k\beta_4)^3 + O((k\beta_4)^4), \quad \alpha=4, \tag{50}$$

$$\tan\delta_0^{(\mathrm{rep})} \overset{k\to 0}{\sim} -\left(\frac{1}{3}\right)^{2/3}\frac{\Gamma\left(\frac{2}{3}\right)}{\Gamma\left(\frac{4}{3}\right)}k\beta_5 - \frac{1}{3}(k\beta_5)^3\ln(k\beta_5) + \left(\frac{13}{36} + \frac{\ln 3}{18} - \frac{\ln 2}{3} - \frac{5}{9}\gamma - \frac{\pi}{6\sqrt{3}}\right)(k\beta_5)^3 + O((k\beta_5)^4), \quad \alpha=5. \tag{51}$$

Here $\gamma=-\Gamma'(1)=0.57721566\cdots$ is Euler's constant. We can transfer the results of Ref. [16] to the case of quantum reflection by attractive potentials in the same way as already discussed in Sec. III, i.e., we replace the parameter β_α describing the strength of the repulsive potential by $\beta_\alpha e^{-i\pi\nu}$, with $\nu=1/(\alpha-2)$.

A. α=3

For α=3 we have ν=1, so Eq. (49) becomes

$$\tan(\delta_r + i\delta_i) \approx \delta_r + i\delta_i \overset{k\to 0}{\sim} -k\beta_3\ln(k\beta_3) - \left(\ln 2 + 3\gamma - \frac{3}{2} - i\pi\right)k\beta_3 + O((k\beta_3)^2). \tag{52}$$

The term $-k\beta_3\ln(k\beta_3)$ remains the leading contribution, even if the potential contains shorter ranged deviations from proportionality to $-1/r^3$, see, e.g., Ref. [19], but the coefficient in front of $k\beta_3$ in the next term only has the given form if the potential can be regarded as homogeneous in the nonclassical region important for quantum reflection. Note that the leading contribution to the imaginary part δ_i of the phase shift is $\pi k\beta_3$ in Eq. (52), in accordance with the fact that the threshold length b_3 is equal to $\pi\beta_3$ for the homogeneous attractive $-1/r^3$ potential [1]. The threshold length b, which is minus the imaginary part of the scattering length, is well defined for potentials falling off as $1/r^3$ asymptotically, even though a real part of the complex scattering length cannot be defined [11].

B. α=4

For α=4 we have ν=1/2, so β_4 is replaced by $-i\beta_4$ in Eq. (50),

$$\tan(\delta_r + i\delta_i) \overset{k\to 0}{\sim} ik\beta_4 - \frac{\pi}{3}(k\beta_4)^2 + \frac{4}{3}i(k\beta_4)^3\ln(k\beta_4) + \frac{2\pi}{3}(k\beta_4)^3 + \left(\frac{8}{3}(\gamma+\ln 2) - \frac{28}{9}\right)i(k\beta_4)^3 \tag{53}$$

or, equivalently,

$$\delta_r + i\delta_i \overset{k\to 0}{\sim} ik\beta_4 - \frac{\pi}{3}(k\beta_4)^2 + \frac{4}{3}i(k\beta_4)^3\ln(k\beta_4) + \frac{2\pi}{3}(k\beta_4)^3 + \left(\frac{8}{3}(\gamma+\ln 2) - \frac{25}{9}\right)i(k\beta_4)^3. \tag{54}$$

In a classic article in 1961 [20], O'Malley, Spruch and Rosenberg studied potentials with attractive tails asymptotically proportional to $1/r^4$. They modified the standard effective-range theory by replacing the free-wave solution v_0 by an appropriate solution of a Schrödinger equation which includes the homogeneous potential

$$U_4(r) = -\frac{C_4}{r^4} = -\frac{\hbar^2}{2M}\frac{\beta_4^2}{r^4}. \tag{55}$$

This leads to the "modified effective-range expansion"

$$\frac{k}{\tan\delta_0} \overset{k\to 0}{\sim} -\frac{1}{a_0} + \frac{\pi\beta_4^2}{3a_0^2}k + \frac{4\beta_4^2}{3a_0}k^2\ln\left(\frac{k\beta_4}{4}\right) + \left[\frac{1}{2}\tilde{r}_{\mathrm{eff}} + \frac{\pi\beta_4}{3} + \frac{20\beta_4^2}{9a_0} - \frac{8\beta_4^2}{3a_0}\psi\left(\frac{3}{2}\right) - \frac{\pi\beta_4^3}{3a_0^2} - \frac{\pi^2\beta_4^4}{9a_0^3}\right]k^2, \tag{56}$$

where ψ is the digamma function $\psi(\frac{3}{2})=0.036489974\cdots$. The contribution $\frac{1}{2}\tilde{r}_{\mathrm{eff}}k^2$ on the right-hand side of Eq. (56) contains a modified effective range $\tilde{r}_{\mathrm{eff}}$, which is defined as in Eq. (19), but with v_0 standing for a zero-energy solution of the Schrödinger equation including the potential (55).

Adapting the procedure of Ref. [20] to quantum reflection by the homogeneous potential tail (55) means that the wave functions u_0 and v_0 in Eq. (19) are identical, and the contribution containing $\tilde{r}_{\mathrm{eff}}$ vanishes. All other terms on the right-hand side of Eq. (56) are derived from near-threshold solutions of the Schrödinger equation with the potential (55), which can be expressed analytically in terms of Mathieu functions [14,20]. The correct expression for the case of quantum reflection is obtained by replacing the ordinary scattering length a_0 by the complex scattering length, which is $\mathcal{A}_4=-i\beta_4$ for α=4. Remembering that $\psi(\frac{3}{2})=2-\gamma-2\ln 2$, it is easy to show that Eq. (56) is equivalent to Eqs. (53) and (54) when δ_0 and a_0 are replaced by $\delta_r+i\delta_i$ and $-i\beta_4$, respectively, and $\tilde{r}_{\mathrm{eff}}$ is set equal to zero.

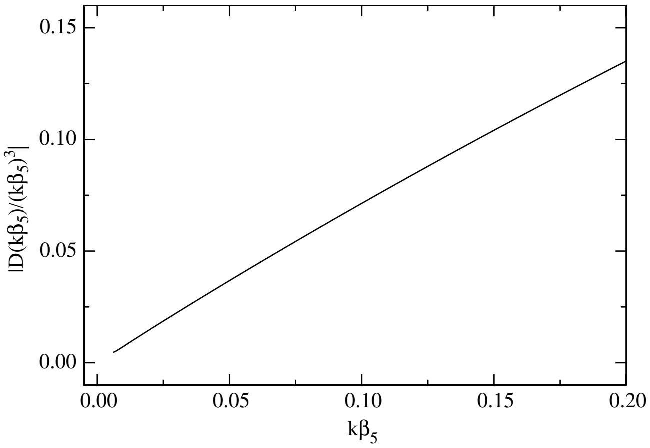

FIG. 1. Absolute value of the difference $\mathcal{D}(k\beta_5)$ of left- and right-hand sides of Eq. (57) divided by $(k\beta_5)^3$ as function of $k\beta_5$.

C. $\alpha=5$

For $\alpha=5$ we have $\nu=1/3$, so β_5 is replaced by $\beta_5 e^{-i\pi/3}$ in Eq. (51),

$$\tan(\delta_r+i\delta_i) \overset{k\to 0}{\sim} -\left(\frac{1}{3}\right)^{2/3}\frac{\Gamma\left(\frac{2}{3}\right)}{\Gamma\left(\frac{4}{3}\right)}k\beta_5\left(\cos\frac{\pi}{3}-i\sin\frac{\pi}{3}\right) + \frac{1}{3}(k\beta_5)^3\ln(k\beta_5) - \left(\frac{13}{36}+\frac{\ln 3}{18}-\frac{\ln 2}{3}-\frac{5}{9}\gamma - \frac{\pi}{6\sqrt{3}}+i\frac{\pi}{9}\right)(k\beta_5)^3 \quad (57)$$

or, equivalently,

$$\delta_r+i\delta_i \overset{k\to 0}{\sim} -\left(\frac{1}{3}\right)^{2/3}\frac{\Gamma\left(\frac{2}{3}\right)}{\Gamma\left(\frac{4}{3}\right)}k\beta_5\left(\cos\frac{\pi}{3}-i\sin\frac{\pi}{3}\right) + \frac{1}{3}(k\beta_5)^3\ln(k\beta_5) - \left[\frac{13}{36}+\frac{\ln 3}{18}-\frac{\ln 2}{3}-\frac{5}{9}\gamma - \frac{\pi}{6\sqrt{3}}+\frac{1}{27}\left(\frac{\Gamma\left(\frac{2}{3}\right)}{\Gamma\left(\frac{4}{3}\right)}\right)^3+i\frac{\pi}{9}\right](k\beta_5)^3. \quad (58)$$

For the homogeneous potential (5) with $\alpha=5$, analytical solutions of the Schrödinger equation are not available at finite energies $E=\hbar^2k^2/(2M)>0$, and we are not aware of a modified effective-range expansion analogous to Eq. (56) for this case. A numerical verification of the near-threshold expansion (57) can be achieved by studying the difference $\mathcal{D}(k\beta_5)$ of the left-hand side $\mathrm{LH}(k\beta_5)$, obtained by numerically solving the Schrödinger equation, and the right-hand side $\mathrm{RH}(k\beta_5)$, as given analytically. Figure 1 shows the absolute value $|\mathcal{D}(k\beta_5)/(k\beta_5)^3|$ of the difference

$$\mathcal{D}(k\beta_5)=\mathrm{LH}(k\beta_5)-\mathrm{RH}(k\beta_5) \quad (59)$$

divided by $(k\beta_5)^3$ as function of $k\beta_5$ for values of $k\beta_5$ down to 0.01 and below. The fact that $|\mathcal{D}(k\beta_5)/(k\beta_5)^3|$ clearly tends to zero as $k\beta_5\to 0$ confirms that Eq. (57) is correct up to and including terms of order $(k\beta_5)^3$. We have also subjected the analytical formulas (42), (52), and (53) to analogous numerical tests.

V. SUMMARY AND DISCUSSION

A straightforward adaptation of effective-range theory of ordinary elastic scattering to the case of quantum reflection by an attractive potential tail leads to a simple formula (18) or (22) for the leading and next-to-leading terms in the near-threshold behavior of the complex phase shift, whose real and imaginary parts describe the phase and the modulus of the quantum reflection amplitude according to Eq. (17). For potentials falling off faster than $-1/r^3$ asymptotically, the leading near-threshold behavior of the complex phase shift is $\delta_r+i\delta_i \overset{k\to 0}{\sim} -\mathcal{A}k$, where $\mathcal{A}=\bar{a}-ib$ is a complex scattering length whose real and imaginary part are the mean scattering length $\bar{a}$ and minus the threshold length b of the potential tail. For potentials falling off faster than $-1/r^5$, the next-to-leading term is proportional to k^3—see Eq. (22), and it is determined by a complex effective range (19). This complex effective range is completely defined via zero-energy solutions of the Schrödinger equation, which are taken to obey incoming boundary conditions in the semiclassical region on the near side of the nonclassical region where quantum reflection is generated. Analytical solutions of the Schrödinger equation are known at energy zero for all potentials which can be regarded as homogeneous (5) in the nonclassical region, and for a number of nonhomogeneous potential tails as well [11,21,22]. Even if the zero-energy solutions are not known analytically, the complex scattering length and effective range can be calculated by solving the Schrödinger equation numerically at threshold, and this gives the parameters for the near-threshold behavior of the complex phase shift up to and including $O(k^3)$ as long the potential falls off faster than $-1/r^5$.

For (attractive) homogeneous potential tails, i.e. those with neglible deviations from the homogeneous form (5) in the nonclassical region, both complex scattering length $\mathcal{A}_\alpha$ and effective range $\mathcal{R}_{\mathrm{eff}}$ are proportional to the parameter β_α describing the strength of the potential, with known constants of proportionality depending only on α, see Eqs. (29) and (32). The ratio $\mathcal{R}_{\mathrm{eff}}/\mathcal{A}_\alpha$ is real and tends to $2/3$ for large α, meaning that the corrections of order $(k\beta_\alpha)^3$ to the complex phase shift become smaller and smaller with increasing power α.

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[1] R. Côté, H. Friedrich, and J. Trost, Phys. Rev. A **56**, 1781 (1997).

[2] H. Friedrich, G. Jacoby, and C. G. Meister, Phys. Rev. A **65**, 032902 (2002).

[3] F. Shimizu, Phys. Rev. Lett. **86**, 987 (2001).

[4] F. Shimizu and J. I. Fujita, Phys. Rev. Lett. **88**, 123201 (2002).

[5] T. A. Pasquini, Y. Shin, C. Sanner, M. Saba, A. Schirotzek, D. E. Pritchard, and W. Ketterle, Phys. Rev. Lett. **93**, 223201 (2004).

[6] H. Oberst, D. Kouznetsov, K. Shimizu, J. I. Fujita, and F. Shimizu, Phys. Rev. Lett. **94**, 013203 (2005).

[7] H. Oberst, Y. Tashiro, K. Shimizu, and F. Shimizu, Phys. Rev. A **71**, 052901 (2005).

[8] D. Kouznetsov, H. Oberst, A. Neumann, Y. Kuznetsova, K. Shimizu, J.-F. Bisson, K. Ueda, and S. R. J. Brueck, J. Phys. B **39**, 1605 (2006).

[9] T. A. Pasquini, M. Saba, G. Jo, Y. Shin, W. Ketterle, D. E. Pritchard, T. A. Savas, and N. Mulders, Phys. Rev. Lett. **97**, 093201 (2006).

[10] H. Friedrich and A. Jurisch, Phys. Rev. Lett. **92**, 103202 (2004); **335**, 43 (2005); A. Jurisch and H. Friedrich, Phys. Rev. A **70**, 032711 (2004).

[11] H. Friedrich and J. Trost, Phys. Rep. **397**, 359 (2004).

[12] G. F. Gribakin and V. V. Flambaum, Phys. Rev. A **48**, 546 (1993).

[13] P. G. Burke, *Potential Scattering in Atomic Physics* (Plenum Press, New York, 1977).

[14] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover Publications, New York, 1972).

[15] V. V. Flambaum, G. F. Gribakin, and C. Harabati, Phys. Rev. A **59**, 1998 (1999).

[16] E. Del Giudice and E. Galzenati, Nuovo Cimento **38**, 443 (1965).

[17] At this point, writing $e^{+i\pi}$ for -1 seems equally possible; the present choice guarantees the right value of the mean scattering length for the attractive potential.

[18] M. J. Moritz, Ph.D. thesis, Technical University Munich, 2001.

[19] P. S. Ganas, Physica (Amsterdam) **68**, 164 (1973).

[20] T. F. O'Malley, L. Spruch, and L. Rosenberg, J. Math. Phys. **2**, 491 (1961).

[21] C. Eltschka, M. J. Moritz, and H. Friedrich, J. Phys. B **33**, 4033 (2000).

[22] G. Jacoby and H. Friedrich, J. Phys. B **35**, 4839 (2002).