Improved effective-range expansions for small and large values of scattering length

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The textbook effective-range expansion of scattering theory is useful in the analysis of low-energy scattering phenomenology when the scattering length $|a|$ is much larger than the range $R$ of the scattering potential: $|a| \gg R$. Nevertheless, the same has been used for systems where the scattering length is much smaller than the range of the potential, which could be the case in many scattering problems. We suggest and numerically study improved two-parameter effective-range expansions for the cases $|a| > R$ and $|a| < R$. The improved effective-range expansion for $|a| > R$ reduces to the textbook expansion for $|a|/R \gg 1$.

I. INTRODUCTION

The textbook effective-range expansion of scattering theory with short-range potential in three spatial dimensions is the following Taylor series of the function $k \cot \delta$ analytic in $k^2$ [1–4]:

$$k \cot \delta = -\frac{1}{a} + \frac{1}{2} r_0 k^2 + O(k^4) + ..., \quad (1)$$

where $k^2$ is the energy in units of $h^2/2m$, $m$ is the reduced mass, $a$ is the scattering length, $r_0$ is the effective range of interaction, and $\delta$ is the $S$-wave phase shift satisfying the low energy limit $k^2 \rightarrow 0 \delta = -ka$. At small energies when the higher order terms in (1) can be neglected, the $k \cot \delta$--$k^2$ plot is a straight line for large values of scattering length $|a|$, which can be used to predict the phase shift $\delta$ at different energies. The effective range expansion (1) was indeed used in the study and analysis of low-energy scattering problems in nuclear [5] and atomic [6] physics. In the general case, $r_0$ is just a coefficient of the Taylor series expansion of $k \cot \delta$. However, for a short-range potential, e.g., a square-well, a Gaussian well, a Yukawa well, or an exponential well, etc., it has been shown [5, 6] that for large values of scattering length $|a|$, the parameter $r_0$ relates approximately to the range of the potential. For $|a|/R \gg 1$, this relation becomes exact for a square-well potential with range $R$. Similar effective range expansions have been suggested for potential scattering in one [5] and two spatial dimensions [7].

The applicability of the effective-range expansion is limited to the cases where the scattering can be described by a short-range potential, which may not be the case for scattering by many composite systems. In addition one should have the condition $|a|/R \gg 1$ [1], otherwise the effective range $r_0$ could be very different from the actual range $R$ of the potential.

Originally, the effective-range expansion (1) was applied [6, 7] to the triplet $S (^3S_1)$ and singlet $S (^1S_0)$ channels of neutron-proton scattering at low energies, where the scattering lengths were $a \approx 5$ fm and $\approx -17$ fm, respectively, with $|a|$ much larger than the range of the interaction potential ($R \sim 1$ fm, $|a|/R \gg 1$) [6, 7]. For small values of scattering length $|a| \rightarrow 0$ the function $k \cot \delta$ of (1) develops a pole in $k^2$ near $k^2 = 0$ as found in the scattering of neutron-deuteron and pion-pion [11] systems and for $a = 0$ this pole appears at $k^2 = 0$. Then the first term on the right-hand-side (rhs) of (1) diverges and for $k \cot \delta$ to be finite at low energies, the coefficients of the subsequent terms in this equation has to diverge, e.g., $r_0 \rightarrow \infty$. Consequently, the $k \cot \delta$--$k^2$ plot ceases to be a straight line at small energies and the effective-range function $k \cot \delta$ is not a convenient function for expansion in $k^2$ as $a \rightarrow 0$. Indeed, the effective range expansion (1) breaks down in this limit. The deficiency of the function (1) for small $a$ ($k|a|, |a|/R \ll 1$) was discussed [1] and noted [13, 14] before. For small phase shifts $\delta \approx \tan \delta - \tan^2 \delta/3$, which leads to an alternate parametrization of phase shift for $a \rightarrow 0$ [13]:

$$\frac{-\delta}{k} = a - \left[ \frac{a^3}{3} - \frac{a^2 r_0}{2} \right] k^2 + ... \quad (2)$$

However, no proper effective-range expansion was given in [13] for $|a|/R \ll 1$. It has been pointed out [14] that in studies of scattering from cold atoms often the scattering length could be tuned to zero near a Feshbach resonance [15] and in such a case the necessity of an appropriate effective range expansion in this limit cannot be over-emphasized. In this study, we provide two such two-parameter (scattering length and range) effective-range expansions valid in the limit $|a| < R$, viz. (22) and (23), suitable for low-energy scattering phenomenology. Equation (22) should be considered to be complimentary to (1) and without (22) the effective range theory, a fundamental topic in an introductory course on quantum scattering theory, cannot be considered complete. Expansion (23) reduces to (22) in the limit $|a| \ll R$. In addition, we provide an improved two-parameter (scattering length and range) effective-range expansion for large values of scattering length: $|a| > R$, viz. (24).

II. EFFECTIVE-RANGE EXPANSION

A convenient function for an expansion for $|a|/R \ll 1$ is $k^{-1} \tan \delta$ [11], which is the reciprocal of the function...
A Taylor series expansion of the function $k^{-1} \tan \delta$ for small $k^2$ should have the following form

$$k^{-1} \tan \delta = -a + bk^2 + O(k^4) + \ldots, \quad (3)$$

where $b$ is a coefficient of expansion with the dimension of length cubed. If we take the reciprocal of the expansion (1) for $|a|/R \ll 1$ we obtain

$$k^{-1} \tan \delta = -a - \frac{1}{2} a^2 r_0 k^2 + O(k^4) + \ldots \quad (4)$$

Expansion (4) also follows from (2).

Although (4) relates the parameter $b$ of (3) to the parameter $r_0$ of (1) through $b = -a^2 r_0 / 2$, we would like to give a physical interpretation of the parameter $b$ for $|a|/R \ll 1$ by relating it to the range and scattering length of a finite-range interaction potential. We recall that the name effective range was attributed to $r_0$ of expansion (1) after a comparison with the same for a square-well potential with a well-defined range.

The function $k^{-1} \tan \delta$ can be related to the $S$-wave scattering solution of a short-range potential $V(r)$. If we define $u(r) = r \psi(r)$, where $\psi(r)$ is the $S$-wave radial wave function for potential $V(r)$, and $r$ the radial coordinate, then $u(r)$ satisfies

$$u''(r) + [k^2 - V(r)] u(r) = 0, \quad (5)$$

where prime denotes radial derivative. We are using units $\hbar = 2m = 1$. The corresponding free-particle wave function $\psi(r)$ satisfies

$$\psi''(r) + k^2 \psi(r) = 0. \quad (6)$$

We consider the solution

$$v(r) = \frac{\sin(kr)}{k \cos \delta} \quad (7)$$

of (6) and the solution of (5) with the asymptotic behavior

$$\lim_{r \to \infty} u(r) = \frac{\sin(kr + \delta)}{k}, \quad (8)$$

and with property $u(0) = 0$. Multiplying (6) by $u(r)$ and (5) by $v(r)$ and subtracting and integrating over $r$ we get

$$\int_0^\infty dr [v(r)u''(r) - u(r)v''(r)] = \int_0^\infty dr u(r)v(r) V(r), \quad (9)$$

Integrating by parts and using the boundary conditions $u(0) = v(0) = 0$ we get

$$\lim_{r \to \infty} [v(r)u'(r) - u(r)v'(r)] = \int_0^\infty dr u(r)v(r) V(r). \quad (10)$$

Using the asymptotic boundary conditions (7) and (8) on $v(r)$ and $u(r)$, respectively, we get

$$k^{-1} \tan \delta = - \int_0^\infty dr u(r)v(r) V(r). \quad (11)$$

Equation (11) relates the present expansion function to the solution of the scattering problem. Bethe [6] also related the expansion function (11) to the solution of the scattering problem.

To attribute a physical interpretation to the parameter $b$ of (3) for $|a|/R \ll 1$, we consider the analytically known result for $k \cot \delta$ for $S$-wave scattering by an attractive square-well potential of range $R$ and depth $\beta^2$ [10]:

$$k^{-1} \tan \delta = \frac{k \tan \gamma R - \gamma \tan kR}{k^2 \tan \gamma R \tan kR + \gamma k}, \quad (12)$$

where $\gamma = \sqrt{\beta^2 + k^2}$. This result can also be obtained by a direct evaluation of the integral on the rhs of Eq. (11). The scattering length $a$ for this potential is

$$a = - \lim_{k^2 \to 0} k^{-1} \tan \delta - \frac{\tan \beta R}{\beta}. \quad (13)$$

For this square-well potential the scattering wave function of (5) with the asymptotic behavior (8), has the following form for $r < R$

$$u(r) = \frac{\cos(kR + \delta)}{\gamma \cos \gamma R} \sin \gamma r. \quad (14)$$

The function (14) is obtained after solving (5) for $r < R$ and matching the wave functions for $r > R$ and $r < R$ and their derivatives at $r = R$ in usual fashion [10]. Using (7) and (13), a low-energy expansion of the rhs of (11) leads to

$$k^{-1} \tan \delta = \left( - R + \frac{\tan \beta R}{\beta} \right) (1 - Rk \tan \delta)
+ \frac{1}{6 \beta^3} \left( \beta R(3 + 4 \beta^2 R^2) - 3(1 + 2 \beta^2 R^2) \tan \beta R
+ 3 \beta R \tan^2 \beta R \right) k^2 + \ldots \quad (15)$$

Now recalling $\lim_{k^2 \to 0} \delta = -ka$ and using (14), (15) can be rewritten as

$$\frac{\tan \delta}{k} = -a + \left[ \frac{a}{2 \beta^2} + \frac{R^3}{6} - \frac{a^2 R}{2} \right] k^2 + O(k^4) + \ldots, \quad (16)$$

consistent with (3). A low-energy expansion of the analytic result (12) also yields (16), which is useful for $|a|/R < 1$.

The analytic expression (12) yields the following low-energy $(k^2 \to 0)$ Taylor series expansion (11):

$$k \cot \delta = - \frac{1}{a} + \frac{R}{2} - \frac{R^3}{6a^2} - \frac{1}{2a^2 \beta^2} \right] k^2 + O(k^4) + \ldots, \quad (17)$$

useful for $|a|/R > 1$. Mathematically, expansion (17) is just the reciprocal of the expansion (10). If we impose the conditions $|a|/R \ll 1$ and $|a|/R \gg 1$ in (16) and (17), we get the lowest-order two-parameter expansions

$$\frac{\tan \delta}{k} = -a + \frac{1}{6} R^3 k^2 + O(k^4) + \ldots, \quad (18)$$

$$k \cot \delta = - \frac{1}{a} + \frac{1}{2} R k^2 + O(k^4) + \ldots, \quad (19)$$
respectively. Keeping the next-order terms in (16), we get the improved two-parameter effective-range expansion for \(|a|/R < 1\):

\[
\tan \frac{\delta}{k} = -a + \left[ \frac{R^3}{6} - \frac{a^2 R}{2} \right] k^2 + O(k^4) + \ldots
\]  

(20)

For \(|a|/R < 1\), the term \(a/(2\beta^2)\) in (10) is found to be much smaller than the other terms and hence is neglected. For \(|a|/R \gg 1\), Eq. (13) yields \(\beta R = \pi/2\). Using this condition in Eq. (17) we get the improved two-parameter effective-range expansion for \(|a|/R > 1\):

\[
k \cot \delta = -\frac{1}{a} + \left[ \frac{R}{2} - \frac{R^3}{6a^2} - \frac{2R^2}{\pi^2 a} \right] k^2 + O(k^4) + \ldots
\]  

(21)

Comparing (11) and (19), we realize that the effective range \(r_0\) is the range of the potential in the limit \(|a|/R \gg 1\). Comparing (3) and (18), we obtain the following:

\[
k^{-1} \tan \delta = -a + \frac{1}{6} r_0^3 k^2 + O(k^4) + \ldots
\]  

(22)

with the identification \(b = r_0^3/6\), where we call \(r_0\) an effective range as in (11), which becomes the actual range \(R\) of the potential well as \(a \to 0\), viz. (18). A consideration of Eq. (20) implies the following improved two-parameter effective-range expansion for \(|a|/R < 1\):

\[
k^{-1} \tan \delta = -a + \left[ \frac{r_0^3}{6} - \frac{a^2 r_0}{2} \right] k^2 + O(k^4) + \ldots
\]  

(23)

Similarly, Eq. (21) suggest the improved two-parameter expansion for \(|a|/R > 1\):

\[
k \cot \delta = -\frac{1}{a} + \left[ \frac{r_0}{2} - \frac{r_0^3}{6a^2} - \frac{2r_0^2}{\pi^2 a} \right] k^2 + O(k^4) + \ldots
\]  

(24)

Expansions (11) and (22) are appropriate for \(|a|/R > 1\) and expansions (22) and (23) for \(|a|/R < 1\).

### III. NUMERICAL RESULT

To test the performance of the effective-range expansions (22) and (23) we consider a square-well potential of range \(R\) and depth \(\beta^2\). The domain of applicability of this expansion is small energy \(k^2 (k^2 \ll \beta^2)\) and small values of scattering length \(a\) (\(|a| \ll R\)). The depth parameter \(\beta^2\) will be conveniently chosen to satisfy the condition \(|a| \ll R\). In figure 1 we plot dimensionless scattering length \(a/R\) given by (13) versus \(\beta R\). From this figure we find that the scattering length has multiple zeros as a function of \(\beta R\). The zero at the origin for vanishing strength \(\beta R\) of the square well is trivial. The first nontrivial zero of \(a\) appears for \(\beta R \approx 4.4934\); in this case there is a single bound state of the system. We consider four values of \(\beta\) near this zero of \(a\), e. g., \(\beta = 4.4, 4.45, 4.4934\) and 4.515 leading to scattering lengths \(a/R = 0.2963, 0.1633, 0\) and \(-2.1\), respectively, all satisfying (\(|a|/R \ll 1\)). In figure 2 we plot \((kR)^{-1} \tan \delta\) versus \((kR)^2\) as obtained from the analytic expression (12) and also from the effective-range expansions (22) and (23) taking the effective range equal to the range of the square well: \(r_0 = R\). From figure 2 we find that the proposed effective-range expansion (23) gives a good description of low-energy scattering for small positive and negative values of scattering length (\(|a|/R \ll 1\)). Nevertheless, the improved effective-range expansion (23) gives a better account of the actual state of affairs.

In figure (3) we contrast the effective-range expansion (11) with (24) by plotting the function \(k R \cot \delta\) versus \((kR)^2\) for \(a/R = -3.14, 0\) and 2.54. We display the exact result (12), the effective-range expansion (11), and the improved expansion (24) in this figure. We find that although the expansion (11) leads to a good description...
FIG. 3: Exact (ex) dimensionless effective-range function $(kR)\cot\delta$ versus dimensionless energy $(kR)^2$ of (1) for different scattering lengths compared with the same from the effective-range expansions (22) and (24) using the effective range $r_0 = R$. 

of $kR\cot\delta$ at low energies, the improved expansion (24) has better performance compared to the exact result.

Effective-range expansions (22) and (24) on the one hand and (1) and (23) on the other are valid for $|a| < R$ and $|a| > R$, respectively. It is pertinent to investigate the limits of validity of these expansions. To study how well they perform for $|a| \sim R$, we compare in figure 4(a)-(b) the results of effective-range expansions (22) and (24) with the corresponding exact results for $a/R = \mp 1$. The same for the expansions (1) and (23) for $a/R = \mp 1$ are illustrated in figures 4(c)-(d). We find that for both $a/R = \pm 1$ the improved expansions (22) and (24) perform better than the basic expansions (22) and (1). Considering that the expansions of this paper are not appropriate for the condition $a/R = \mp 1$ considered in figure 4 these perform fairly well in all cases with the improved expansions (23) and (24) exhibiting better performance that the basic expansions (22) and (1), respectively.

IV. SUMMARY

We have proposed an effective-range expansion (22) valid for scattering lengths much smaller than the range of the potential: $|a|/R \ll 1$. This should be considered complementary to the textbook expansion (1) valid for $|a|/R \gg 1$. Two improved expansions (23) and (24) are also suggested for $|a|/R < 1$ and $|a|/R > 1$, respectively. We illustrated the usefulness of these expansions with a finite-range square-well potential for both positive and negative scattering lengths. Nevertheless, one should recall that these expansions are valid for short-range potentials. In many problems of physical interest the underlying potential is not of short range and such expansions are not physically meaningful. In these cases such an expansion could involve a linear and a logarithmic term in $k$ [1], viz. (3.39) of [1].

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