Analytical calculations of scattering lengths in atomic physics

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Abstract. We describe a method for evaluating analytical long-range contributions to scattering lengths for some potentials used in atomic physics. We assume that an interaction potential between colliding particles consists of two parts. The form of a short-range component, vanishing beyond some distance from the origin (a core radius), need not be given. Instead, we assume that a set of short-range scattering lengths due to that part of the interaction is known. A long-range tail of the potential is chosen to be an inverse power potential, a superposition of two inverse power potentials with suitably chosen exponents or the Lenz potential. For these three classes of long-range interactions a radial Schrödinger equation at zero energy may be solved analytically with solutions expressed in terms of the Bessel, Whittaker and Legendre functions, respectively. We utilize this fact and derive exact analytical formulae for the scattering lengths. The expressions depend on the short-range scattering lengths, the core radius and parameters characterizing the long-range part of the interaction. Cases when the long-range potential (or its part) may be treated as a perturbation are also discussed and formulae for scattering lengths linear in strengths of the perturbing potentials are given. It is shown that for some combination of the orbital angular momentum quantum number and an exponent of the leading term of the potential the derived formulae, exact or approximate, take very simple forms and contain only polynomial and trigonometric functions. The expressions obtained in this paper are applicable to scattering of charged particles by neutral targets and to collisions between neutrals. The results are illustrated by accelerating convergence of scattering lengths computed for e⁻⁻Xe and Cs-Cs systems.

1. Introduction

In many approaches used to solve collision problems in atomic physics the three-dimensional configuration space is divided into two regions separated by a spherical shell (a core boundary) of radius \( \rho \) [1]. In the inner region \( (r < \rho) \) the short-range interaction between two colliding particles is very complicated and a scattering equation must be solved independently for each combination of particles. In contrast, if \( \rho \) is chosen sufficiently large the scattering problem in the outer region \( (r > \rho) \) may be reduced to potential scattering with the long-range potential accurately approximated by a simple analytical expression. A numerical solution in this region is usually easily approachable. However, if exact or approximate analytical solutions to the Schrödinger equation are available in this region, a general discussion of the dependency of scattering observables on parameters characterizing the long-range part of the interaction is possible. Clearly, such cases always remain of considerable interest.

In this paper we consider a problem of computing long-range contributions to scattering lengths in atomic physics. This problem has recently attracted some interest [2, 3].
We utilize the fact that analytical solutions to the radial Schrödinger equation at zero energy do exist for the most important long-range potentials used in atomic physics. This immediately implies that corresponding long-range contributions to the scattering lengths may be found exactly. In section 2 we derive analytic expressions for scattering lengths for potentials vanishing asymptotically as the inverse power potentials, superpositions of two such potentials with suitably chosen exponents and the Lenz potentials. In section 3 we discuss applications of these results to atomic physics and give illustrative examples.

2. Theory

2.1. Preliminaries

A variety of definitions of the scattering lengths exist. Throughout this paper we use the one which defines an \( l \)th partial wave scattering length \( a_l \) as

\[
a_l = -2(2l - 1)!!(2l + 1)!! \lim_{k \to 0} [k^{2l+1} \cot \delta_l(k)]^{-1}
\]

where \( \delta_l(k) \) is an \( l \)th partial wave phase shift due to the scattering potential and \( k \) is a wavenumber of a scattered particle. Some authors use a definition with an opposite sign while some omit the factor \( (2l - 1)!!(2l + 1)!! \) for \( l = 0 \) our definition agrees with that adopted by Fano and Rau [1]. It may be shown [4] that \( a_l \) exists only for potentials with long-range tails \( V_L(r) \) satisfying a condition

\[
\lim_{r \to \infty} r^{2l+3} V_L(r) = 0.
\]

Numerical computation of the scattering lengths is usually based on numerical integration of the zero-energy Schrödinger equation (e.g. [5]) or a first-order nonlinear differential equation arising in the variable phase method [6]. Alternative approaches have recently been presented by Gribakin and Flambaum [2] and Marinescu [3]. Here we shall use still another method.

The scattering length may be extracted from a solution to a radial Schrödinger equation at an energy \( E = 0 \)

\[
\frac{d^2 u_l(r)}{dr^2} - \frac{l(l + 1)}{r^2} u_l(r) - \frac{2m}{\hbar^2} V_L(r) u_l(r) = 0 \quad r \geq \rho
\]

which for potentials satisfying condition (2) behaves asymptotically as

\[
u_l(r) \xrightarrow{r \to \infty} \text{constant} \times r^{l+1} - a_l r^{-l}.
\]

It follows from (3) and (4) that \( a_l \) is an asymptotic limit of a function \( a_l(r) \),

\[
a_l = \lim_{r \to \infty} a_l(r)
\]

defined as

\[
a_l(r) = r^{2l+1} \frac{rL_l(r) - (l + 1)}{rL_l(r) + l}.
\]

Here

\[
L_l(r) = \frac{1}{u_l(r)} \frac{du_l(r)}{dr}
\]

is a logarithmic derivative of the zero-energy wavefunction \( u_l(r) \).

In the following we shall assume that the interaction potential between a projectile and a target consists of two parts. The form of a short-range component, vanishing beyond the
core radius $\rho$, need not be given. Instead, we suppose that a set of short-range scattering lengths $a_{ls}$ due to that part of the interaction is known. For $r \geq \rho$ the general solution to (3) has the form

$$u_l(r) = A_l f_l(r) + B_l g_l(r) \quad r \geq \rho$$

where $f_l$ and $g_l$ are two linearly independent solutions to this equation. Then the logarithmic derivative $L_l$ is

$$L_l(r) = \frac{f'_l(r) + D_l g'_l(r)}{f_l(r) + D_l g_l(r)}$$

where prime denotes differentiation with respect to the argument and $D_l = B_l / A_l$ is to be determined. This can easily be done and from (6) and (9) used at $r = \rho$ one obtains

$$D_l = -\frac{(\rho^{l+1} - a_{ls}) \rho f'_l(\rho) - [(l + 1) \rho^{l+1} + l a_{ls}] f_l(\rho)}{(\rho^{l+1} - a_{ls}) \rho g'_l(\rho) - [(l + 1) \rho^{l+1} + l a_{ls}] g_l(\rho)}$$

since $a_{ls} = a_l(\rho)$. The method which we shall utilize in this paper employs (5), (6), (9) and (10).

2.2. Inverse power potentials

Let $V_L(r)$ be the inverse power potential of the form

$$V_L(r) = -\frac{\hbar^2 b^2}{2 m r^n} \quad b > 0 \quad r \geq \rho$$

A general solution to the Schrödinger equation

$$\frac{d^2 u_l(r)}{dr^2} - \frac{l(l + 1)}{r^2} u_l(r) + \frac{b^2}{r^n} u_l(r) = 0 \quad r \geq \rho$$

may be written in terms of the Bessel and Neumann functions [7–9]

$$u_l(r) = A_l r^{l+1/2} J_\mu(x) + B_l r^{l+1/2} Y_\mu(x) \quad r \geq \rho$$

where

$$\mu = \frac{2l + 1}{n - 2}$$

and

$$x = x(r) = \frac{2b}{n - 2} r^{-(n-2)/2}$$

Condition (2) requires

$$n > 2l + 3 \quad \text{or equivalently} \quad 0 < \mu < 1$$

otherwise $a_l$ does not exist. Utilizing equations (5)–(10) and standard properties of the Bessel and Neumann functions [7] one finds

$$a_l = \pi \left( \frac{b}{n - 2} \right)^{2\mu} \Phi_l + \cot(\pi \mu) \frac{\Phi_l}{\Gamma(\mu) \Gamma(\mu + 1)}$$

with

$$\Phi_l = \frac{2 \mu \rho^{2l+1} J_\mu(x_s) - (\rho^{2l+1} - a_{ls}) x_s J_{\mu + 1}(x_s)}{2 \mu \rho^{2l+1} J_\mu(x_s) - (\rho^{2l+1} - a_{ls}) x_s J_{\mu + 1}(x_s)}$$

where

$$x_s = x(\rho).$$
Similar results have been obtained by Fabrikan [10] and Gribakin and Flambaum [2].

Equations (17) and (18) greatly simplify for those combinations of \( n \) and \( l \) for which \( \mu = \frac{1}{2} \). Then the Bessel and Neumann functions may be expressed in terms of trigonometric functions [7] and one gets

\[
a_l = \frac{b}{2l + 1} \frac{1 + (x_s - y_{ls}) \tan(x_s)}{\tan(x_s) - (x_s - y_{ls})}
\]

where

\[
y_{ls} = \frac{b}{(2l + 1)a_{ls}}.
\]

In many practical applications the long-range potential may be treated as a perturbation of the short-range interaction, which always holds for sufficiently large \( \rho \). In such a case one gets the following expression correct to the first order in \( b^2 \):

\[
a_l \approx a_{ls} + b^2 \theta_l^{(n)}
\]

where

\[
\theta_l^{(n)} = \frac{1}{2l + 1} \rho^{-n-2l+1} \left( \frac{\rho^{2(2l+1)}}{n-2l-3} - \frac{2a_{ls} \rho^{2l+1}}{n-2} + \frac{a_{ls}^2}{n+2l-1} \right)
\]

is independent on \( b \). A condition of applicability of (22) is

\[
b^2 |\theta_l^{(n)}| \ll |a_{ls}|.
\]

2.3. Superposition of two inverse power potentials

Next we consider scattering of an \( l \)th partial wave by the long-range potential [11]

\[
V_L(r) = \frac{\hbar^2}{2m} \frac{b^2}{r^n} + \frac{\hbar^2}{2m} \frac{c^2}{r^{2n-2}} \quad b > 0 \quad r \gg \rho
\]

with a restriction \( n > 2l + 3 \). In applications \( c^2 \) may be positive as well as negative. A general solution to the radial Schrödinger equation

\[
\frac{d^2 u_l(r)}{dr^2} - \frac{l(l+1)}{r^2} u_l(r) + \frac{b^2}{r^n} u_l(r) - \frac{c^2}{r^{2n-2}} u_l(r) = 0 \quad r \gg \rho
\]

may be expressed in terms of the Whittaker functions [12–14]

\[
u_l(r) = A_l r^{(n-1)/2} W_{\kappa,\mu/2}(z) + B_l r^{(n-1)/2} M_{\kappa,\mu/2}(z)
\]

where

\[
\mu = \frac{2l + 1}{n - 2} \quad \kappa = \frac{b^2}{2(n-2)c}
\]

and

\[
z = z(r) = \frac{2c}{n-2} r^{-(n-2)}.
\]

Note that for \( c^2 < 0 \) the index \( \kappa \) and the variable \( z \) are purely imaginary. Utilizing properties of the Whittaker functions [7] the scattering length is found to be

\[
a_l = \left( \frac{2\pi}{n-2} \right)^{\mu} \frac{\rho^{2n+1}(\rho^{2n+1})(2\kappa+\mu+1)M_{\kappa+1/2}(z_s) + (\rho^{2n+1}(\rho^{2n+1})(2\kappa+\mu+1)M_{\kappa+1/2}(z_s))}{\rho^{2n+1}(\rho^{2n+1})(2\kappa+\mu+1)M_{\kappa+1/2}(z_s) + (\rho^{2n+1}(\rho^{2n+1})(2\kappa+\mu+1)M_{\kappa+1/2}(z_s))}
\]

where

\[
z = z(\rho).
\]
We observe that in applications the second term contributing to $V_{L}(r)$ (proportional to $c^2$) might be much smaller than the first one and thus might be treated as a perturbation of the latter. This allows us to apply the perturbation theory to derive an analytical expression which is linear in $c^2$. The substitution

$$u_l(r) = \xi^{-(n-1)/(2n-4)}v_\lambda(\xi)$$

(32)

with

$$\xi \equiv \xi(r) = r^{-(n-2)} \quad \lambda = \frac{1}{2}(\mu - 1)$$

(33)

converts the Schrödinger equation (26) into the well known Coulomb equation

$$\frac{d^2 v_\lambda(\xi)}{d\xi^2} - \frac{\lambda(\lambda + 1)}{\xi^2} v_\lambda(\xi) + \frac{\bar{b}^2}{\xi} v_\lambda(\xi) - c^2 v_\lambda(\xi) = 0 \quad \xi \leq \rho^{-(n-2)}$$

(34)

where

$$\bar{b} = \frac{b}{n-2} \quad \bar{c} = \frac{c}{n-2}$$

(35)

It has been shown in [15] that its regular and irregular solutions may be expanded in series of the Bessel and Neumann functions, respectively, and that to the first order in $c^2$ one has

$$v_{\lambda,\text{reg}}(\xi) \simeq x J_\mu(x) + \frac{c^4}{24\bar{b}^4} x^3 [x J_{\mu+1}(x) - (1 - \mu) J_{\mu+2}(x)]$$

(36)

$$v_{\lambda,\text{irr}}(\xi) \simeq x Y_\mu(x) + \frac{c^2}{24\bar{b}^4} x^3 [x Y_{\mu+1}(x) - (1 - \mu) Y_{\mu+2}(x)]$$

(37)

where

$$x \equiv x(r) = \frac{2\bar{b}}{n-2} r^{-(n-2)/2} = 2\bar{b}^{1/2}$$

(38)

Therefore a general solution to (26) may be written approximately as

$$u_l(r) \simeq A_l r^{1/2} \left\{ J_\mu(x) + c^2 \frac{(n-2)^2}{24\bar{b}^4} x^2 [x J_{\mu+1}(x) - (1 - \mu) J_{\mu+2}(x)] \right\}$$

$$+ B_l r^{1/2} \left\{ Y_\mu(x) + c^2 \frac{(n-2)^2}{24\bar{b}^4} x^2 [x Y_{\mu+1}(x) - (1 - \mu) Y_{\mu+2}(x)] \right\}$$

$$r \geq \rho$$

(39)

and one obtains the following expression for the scattering length:

$$a_l \simeq \pi \left( \frac{b}{n-2} \right)^{2\mu} \frac{\Phi_l + \cot(\pi \mu)}{\Gamma(\mu) \Gamma(\mu + 1)} \left[ 1 + \frac{c^2(n-2)^2}{24\bar{b}^4} \left( 4\mu(1 - \mu^2) + \frac{\phi_l}{\Phi_l + \cot(\pi \mu)} \right) \right]$$

(40)

valid to the first order in $c^2$. $\Phi_l$ has been defined by (18) and $\phi_l$ is given by

$$\Phi_l = -\Phi_l \frac{x_s^2(\rho^{2\mu+1} + 1 - \rho(2\mu - 2x_s^2)) J_{\mu}(x_s) + x_s [\rho^{2\mu+1}(1+\mu)x_s^2 - \rho(1-\mu)4\mu(4\mu(4\mu+4\mu+x_s^2))] J_{\mu+1}(x_s)}{2\mu \rho^{2\mu+1} J_{\mu}(x_s) - (\rho^{2\mu+1} - \rho) x_s J_{\mu+1}(x_s)}$$

$$- \frac{x_s^2(\rho^{2\mu+1} + 1 - \rho(2\mu - 2x_s^2)) Y_{\mu}(x_s) + x_s [\rho^{2\mu+1}(1+\mu)x_s^2 - \rho(1-\mu)4\mu(4\mu(4\mu+4\mu+x_s^2))] Y_{\mu+1}(x_s)}{2\mu \rho^{2\mu+1} J_{\mu}(x_s) - (\rho^{2\mu+1} - \rho) x_s J_{\mu+1}(x_s)}$$

(41)

with $x_s$ defined by (19). A condition of applicability of (40) is

$$|\frac{c^2(n-2)^2}{24\bar{b}^4} \left| \frac{4\mu(1 - \mu^2)}{\Phi_l + \cot(\pi \mu)} \right| \ll 1$$

(42)
A further simplification is possible for those combinations of $n$ and $l$ for which $\mu = \frac{1}{2}$. In such a case one gets

$$a_l \simeq \frac{b}{2l + 1} \frac{1 + (x_s - y_{ls}) \tan(x_s)}{\tan(x_s) - (x_s - y_{ls})} \left[ 1 + c^2 \frac{(2l + 1)^2}{12b^4} \left( 3 + \frac{\Phi_1}{\Phi_l} \right) \right]$$

(43)

where

$$\Phi_l = \frac{1}{2} \frac{(2x_s^2 - 2x_s^3 y_{ls} - 3x_s y_{ls} + 3) \tan(x_s) - x_s(x_s^2 - 3x_s y_{ls} + 3)}{\tan(x_s) - (x_s - y_{ls})}$$

(44)

$$\Phi_1 = \frac{1}{2} \frac{(2x_s^2 - 2x_s^3 y_{ls} - 3x_s y_{ls} + 3) \tan(x_s) + x_s(x_s^2 - 3x_s y_{ls} + 3) \tan(x_s)}{1 + (x_s - y_{ls}) \tan(x_s)}$$

while $y_{ls}$ has been defined by (21).

Finally, for sufficiently large $\rho$ the potential (25) may be treated as a perturbation of the short-range interaction and (30) may be replaced by an approximate formula correct to the first order in $b^2$ and $c^2$

$$a_l \simeq a_{ls} - b^2 \theta_l^{(n)} + c^2 \theta_l^{(2n-2)}$$

(45)

with $\theta_l^{(n)}$ defined by (23). A condition of applicability of (45) is

$$|b^2 \theta_l^{(n)} - c^2 \theta_l^{(2n-2)}| \ll |a_{ls}|$$

(46)

2.4. The Lenz potentials

The last family of potentials we discuss are the Lenz potentials [16]

$$V_L(r) = -\frac{n^2}{2m} \frac{b^2 r^{n-4}}{(r^n - R^n)^2} \quad b > 0 \quad R > 0 \quad r \geq \rho$$

(47)

considered here with a restriction $n > 2l + 3$. A general solution to the radial Schrödinger equation

$$\frac{d^2 u_l(r)}{dr^2} - \frac{l(l + 1)}{r^2} u_l(r) + \frac{b^2 r^{n-4}}{(r^n - R^n)^2} u_l(r) = 0 \quad r \geq \rho$$

(48)

has the form [17, 18]

$$u_l(r) = A_l r^{1/2} P_v^{-\mu}(t) + B_l r^{1/2} P_\nu^\mu(t) \quad r \geq \rho$$

(49)

where $P_v^\mu(t)$ are the Legendre functions of the first kind,

$$\mu = \frac{2l + 1}{n - 2} \quad \nu = \frac{1}{2} \left( 1 + \frac{4b^2}{(n - 2)^2 R^{n-2}} \right)^{1/2} - \frac{1}{2}$$

(50)

and

$$t \equiv t(r) = \frac{r^{n-2} - R^{n-2}}{r^{n-2} + R^{n-2}}$$

(51)

Utilizing properties of the Legendre functions [7] we find the following formula for the scattering length:

$$a_l = R^{2l+1} \frac{\Gamma(1-\mu) \zeta(2\nu+1, \nu+n-\mu) - \alpha_0 (\nu+n+\mu) P_\nu^\mu(t) - (\nu+\mu+1) \zeta(-\nu+\nu+\nu+\mu) P_{\nu+\mu}^\nu(\zeta)}{\Gamma(1+\mu) \zeta(2\nu+1, \nu+n-\mu) - \alpha_0 (\nu+n+\mu) P_\nu^\mu(t) - (\nu+\mu+1) \zeta(-\nu+\nu+\nu+\mu) P_{\nu+\mu}^\nu(\zeta)}$$

(52)

where

$$t_s = t(\rho)$$

(53)
As in cases of the potentials discussed previously, a further simplification of this result is possible for those combinations of \(n\) and \(l\) for which \(\mu = \frac{1}{2}\). In such a case one obtains

\[
a_i = (2
u + 1)R^{2l+1} \left( \frac{R^{2l(l+1)}}{R^{2l+1} + a_{ls}\rho^{2l+1}} - (2\nu + 1)R^{2l+1}(\rho^{2l+1} - a_{ls}) \tan \Omega_s \right) \tan \Omega_s + (2\nu + 1)R^{2l+1}(\rho^{2l+1} - a_{ls}) \tan \Omega_s
\]

where

\[
\Omega_s = (2\nu + 1)\arctan \left( \frac{R^{2l+1}}{\rho^{2l+1}} \right).
\]

It may happen in applications that \(R \ll \rho\). Then the Lenz potential (47) may be expanded in an asymptotic series and retaining the first two terms one gets

\[
V_L(r) \simeq -\frac{\hbar^2}{2m} \frac{b^2}{r^n} + \frac{\hbar^2}{2m} \frac{c^2}{r^{n-2}}
\]

where

\[
c^2 = 2b^2 R^{n-2}.
\]

This is the superposition of the inverse power potentials discussed in the previous subsection. Therefore, for \(R \ll \rho\) the exact expression for the scattering length (52) may be replaced by the approximate formula (40). Finally, if the Lenz potential (47) may be treated as a perturbation of the short-range interaction then (52) may be replaced by (45) which is linear in \(b^2\) and \(b^2 R^{n-2}\).

3. Applications to atomic physics

3.1. Scattering of charged particles by neutral targets

The long-range parts of the interactions between charged projectiles and neutral targets have a form \([19, 20]\)

\[
V(r) \simeq -\frac{C_4}{r^4} - \frac{C_6}{r^6} + O(r^{-7}) \quad r \to \infty
\]

and may be approximated by any of the potentials discussed in section 2 with an exponent \(n = 4\). The simplest choice is to approximate the potential (58) by the inverse fourth-power potential

\[
V_L(r) = -\frac{\hbar^2}{2m} \frac{b^2}{r^4}
\]

with \(b^2 = 2mC_4/\hbar^2\). For this potential the scattering length may be calculated exactly from the formula

\[
a_0 = b \frac{1 + b(1/\rho - 1/a_{0s}) \tan(b/\rho)}{\tan(b/\rho) - b(1/\rho - 1/a_{0s})}
\]

which because of its striking simplicity is worthy of remembrance \([21]\). An expression approximating (60), correct to the first order in \(b^2\), is

\[
a_0 \simeq a_{0s} - \frac{b^2}{\rho} \left( 1 - \frac{a_{0s}}{\rho} + \frac{a_{0s}^2}{3\rho^2} \right).
\]

This approximate formula has been derived in alternative ways by Temkin and Drukarev \([22]\).
More accurate results can be obtained by choosing

$$V_L(r) = -\frac{\hbar^2}{2m} \left( \frac{b^2}{r^4} + \frac{c^2}{2m r^6} \right)$$

(62)

with $b^2 = 2mC_4/\hbar^2$ and $c^2 = -2mC_6/\hbar^2$. For this choice an exact expression for the scattering length is [23]

$$a_0 = c^{1/2} \left( \frac{a_0}{c} \left[ \frac{2c}{c-2} + \left( \frac{2c}{c-2} \right)^2 + \left( \frac{2c}{c-2} \right)^3 \right] \right)$$

(63)

where the index $\kappa$ is given by

$$\kappa = \frac{b^2}{4c}.$$  

(64)

The simpler formula, valid to the first order in $c^2$, is

$$a_0 \sim b \frac{1 + b(1/\rho - 1/a_{0s}) \tan(b/\rho)}{\tan(b/\rho) - b(1/\rho - 1/a_{0s})} \left[ 1 + \frac{c^2}{12b^4} \left( 3 + 2\frac{\Phi_0}{\Phi_0} \right) \right]$$

(65)

with

$$\Phi_0 = \frac{1}{2} \left[ \frac{2b^4}{b^4} + \frac{b^4}{a_{0s}} \right] \tan(b/\rho) - b(1/\rho - 1/a_{0s})$$

(66)

while the approximate formula valid to the first order in $b^2$ and $c^2$ is

$$a_0 \approx a_{0s} - \frac{b^2}{\rho} \left( 1 - \frac{a_{0s}}{\rho} + \frac{a_{0s}^2}{3\rho^2} \right) + \frac{c^2}{3\rho^2} \left( 1 - \frac{3a_{0s}}{2\rho} + \frac{3a_{0s}^2}{5\rho^2} \right).$$

(67)

Finally, we may approximate the potential (58) by the Buckingham polarization potential [24]

$$V_L(r) = -\frac{\hbar^2}{2m} \frac{b^2}{(r^2 + R^2)^3}$$

(68)

with $b^2 = 2mC_4/\hbar^2$ for which an exact expression for the scattering length has also a very simple form

$$a_0 = \left( b^2 + R^2 \right)^{1/2} \left( \frac{R^2 + \rho a_{0s}}{R^2} \right) \frac{\tan \Omega_s}{(R^2 + \rho a_{0s}) \tan \Omega_s + \left( b^2 + R^2 \right)^{1/2} (\rho - a_{0s})}$$

(69)

with

$$\Omega_s = \left( 1 + \frac{b^2}{R^2} \right) \arctan \left( \frac{R}{\rho} \right).$$

(70)

The appropriate approximate expressions correct to the first orders in $b^2 R^2$ or $b^2$ and $b^2 R^2$ may be obtained from (65)–(67) replacing $c^2$ by $2b^2 R^2$.

3.2. Collisions between neutral particles

If two neutral particles collide, the long-range tail of the interaction potential is often approximated by [19]

$$V(r) \approx -\frac{C_6}{r^6} - \frac{C_8}{r^8} - \frac{C_{10}}{r^{10}} + O(r^{-12}).$$

(71)

Many other analytical formulae are also used [25]. Their common feature is that the leading terms in their asymptotic expansions fall off as $r^{-6}$. Therefore to approximate the potential
(71) we may use any of the potentials discussed in section 2 with an exponent \( n = 6 \). The simplest choice is

\[ V_L(r) = -\frac{\hbar^2}{2m} \frac{b^2}{r^6} \]  

(72)

with \( b^2 = 2mC_6/\hbar^2 \) for which exact expressions for s and p partial wave scattering lengths, obtained from (17) and (18), are

\[ a_0 = \frac{2\pi b^{1/2}}{[\Gamma(1/4)]^2} \left[ 1 - \frac{\rho Y_{1/4}(b/\rho^2) - (b/\rho^2)(\rho - a_0) Y_{5/4}(b/2\rho^2)}{\rho J_{1/4}(b/\rho^2) - (b/\rho^2)(\rho - a_0) J_{5/4}(b/2\rho^2)} \right] \]  

(73)

\[ a_1 = -\frac{\pi b^{3/2}}{6[\Gamma(3/4)]^2} \left[ 1 + \frac{3\rho^2 Y_{3/4}(b/2\rho^2) - (b/\rho^2)(\rho^3 - a_{1s}) Y_{7/4}(b/2\rho^2)}{3\rho^2 J_{3/4}(b/2\rho^2) - (b/\rho^2)(\rho^3 - a_{1s}) J_{7/4}(b/2\rho^2)} \right]. \]  

(74)

Approximate formulae, correct to the first order in the potential strength \( b^2 \), are

\[ a_0 \simeq a_0 = -\frac{b^2}{3\rho^3} \left( 1 - \frac{3a_{0s}}{2\rho} + \frac{3a_{0s}^2}{\rho^2} \right) \]  

(75)

\[ a_1 \simeq a_{1s} = -\frac{b^2}{3\rho} \left( 1 - \frac{a_{1s}}{2\rho^3} + \frac{a_{1s}^2}{7\rho^6} \right). \]  

(76)

Another possibility is to choose

\[ V_L(r) = -\frac{\hbar^2}{2m} \frac{b^2}{r^6} + \frac{\hbar^2}{2m} \frac{c^2}{r^{10}} \]  

(77)

with \( b^2 = 2mC_6/\hbar^2 \) and \( c^2 = -2mC_{10}/\hbar^2 \). For this potential exact expressions for the scattering lengths are

\[ a_0 = (c/2)^{1/4} \frac{(\rho - a_0)(\rho^2/\rho^3 M_{e+1/2} + \rho^4 M_{e+1})}{[\Gamma(1/4)]^2} \left[ \rho + \frac{\rho^2}{7}\left( \frac{15}{16} + \frac{\rho}{\Phi_0 + 1} \right) \right] \]  

(78)

\[ a_1 = (c/2)^{3/4} \frac{(\rho^2 - a_0)(\rho^2/\rho^3 M_{e+1/2}) + (\rho^4 M_{e+1})}{[\Gamma(1/4)]^2} \left[ \rho + \frac{\rho^2}{7}\left( \frac{15}{16} + \frac{\rho}{\Phi_0 + 1} \right) \right] \]  

(79)

where

\[ k = \frac{b^2}{8c}. \]  

(80)

If the second term contributing to \( V_L(r) \) may be treated as a perturbation, the following formulae correct to the first order in the potential strength \( c^2 \) hold

\[ a_0 \simeq \frac{2\pi b^{1/2}}{[\Gamma(1/4)]^2} (\Phi_0 + 1) \left[ 1 + \frac{c^2}{3\rho^4} \left( \frac{15}{16} + \frac{\rho}{\Phi_0 + 1} \right) \right] \]  

(81)

with

\[ \Phi_0 = -\frac{\rho Y_{1/4}(b/2\rho^2) - (b/\rho^2)(\rho - a_0) Y_{5/4}(b/2\rho^2)}{\rho J_{1/4}(b/2\rho^2) - (b/\rho^2)(\rho - a_0) J_{5/4}(b/2\rho^2)} \]  

(82)

\[ \phi_0 = -\frac{1}{16} \frac{\rho Y_{1/4}(b/2\rho^2) - (b/\rho^2)(\rho - a_0) Y_{5/4}(b/2\rho^2)}{\rho J_{1/4}(b/2\rho^2) - (b/\rho^2)(\rho - a_0) J_{5/4}(b/2\rho^2)} \]  

(83)

and

\[ a_1 \simeq \frac{\pi b^{3/2}}{6[\Gamma(3/4)]^2} (\Phi_1 - 1) \left[ 1 + \frac{c^2}{3b^4} \left( \frac{21}{16} + \frac{\rho}{\Phi_1 + 1} \right) \right] \]  

(84)
with
\[
\Phi_1 = -\frac{3\rho^3 Y_{3/4}(b/2\rho^2) - (b/\rho^2)(\rho^3 - a_{1s}) Y_{1/4}(b/2\rho^2)}{3\rho^3 Y_{3/4}(b/2\rho^2) - (b/\rho^2)(\rho^3 - a_{1s}) J_{3/4}(b/2\rho^2)}
\]
\[
\phi_1 = -\frac{1}{16} \Phi_1 \frac{(\rho^3/\rho^2)^2 (b^2/\rho^2 - a_{1s}(2b^2/\rho^2 - 3)) J_{3/4}(b/2\rho^2) + (b/\rho^2)(7b^2/\rho^2 - a_{1s}(b^2/\rho^2 + 21)) J_{4/4}(b/2\rho^2)}{3\rho^3 J_{4/4}(b/2\rho^2) - (b/\rho^2)(\rho^3 - a_{1s}) J_{3/4}(b/2\rho^2)}
\]
\[
- \frac{1}{16} \frac{(b^2/\rho^2)^2 (b^2/\rho^2 - a_{1s}(2b^2/\rho^2 - 3)) J_{4/4}(b/2\rho^2) + (b/\rho^2)(7b^2/\rho^2 - a_{1s}(b^2/\rho^2 + 21)) J_{4/4}(b/2\rho^2)}{3\rho^3 J_{4/4}(b/2\rho^2) - (b/\rho^2)(\rho^3 - a_{1s}) J_{3/4}(b/2\rho^2)} .
\]

Finally, the expressions correct to the first order in the potential strengths \(b^2\) and \(c^2\) are
\[
a_0 \simeq a_{0s} - \frac{b^2}{3\rho^3} \left( 1 - \frac{3a_{0s}}{2\rho} + \frac{3a_{0s}^2}{5\rho^2} \right) + \frac{c^2}{7\rho^3} \left( 1 - \frac{7a_{0s}}{4\rho} + \frac{7a_{0s}^2}{9\rho^2} \right)
\]
\[
a_1 \simeq a_{1s} - \frac{b^2}{3\rho^2} \left( 1 - \frac{a_{1s}}{2\rho} + \frac{a_{1s}^2}{7\rho^6} \right) + \frac{c^2}{15\rho^3} \left( 1 - \frac{5a_{1s}}{4\rho^3} + \frac{5a_{1s}^2}{11\rho^6} \right)
\]

The last possibility we discuss is to approximate the long-range part of the interaction by the Lenz potential
\[
V_L(r) = -\frac{\hbar^2}{2m} \frac{b^2r^2}{(r^4 + R^4)^2}
\]
with \(b^2 = 2mC_6/\hbar^2\) for which exact expressions for the scattering lengths are
\[
a_0 = \frac{4\pi\sqrt{2}R}{[\Gamma(1/4)]^2} \frac{[\rho(4\nu_1 + 4\nu_2 - 1) - a_{0s}(4\nu_1 + 4\nu_2 + 1)]P_{-1/4}^{1/4}(t_s) - (\rho - a_{0s})(4\nu_1 + 5)P_{-1/4}^{1/4}(t_s)}{[\rho(4\nu_1 + 4\nu_2 - 1) - a_{0s}(4\nu_1 + 4\nu_2 + 1)]P_{-1/4}^{1/4}(t_s) - (\rho - a_{0s})(4\nu_1 + 5)P_{-1/4}^{1/4}(t_s)}
\]
\[
a_1 = \frac{4\pi\sqrt{3}R^3}{3[\Gamma(3/4)]^2} \frac{[\rho^3(4\nu_1 + 4\nu_2 - 3) - a_{1s}(4\nu_1 + 4\nu_2 + 3)]P_{-3/4}^{3/4}(t_s) - (\rho - a_{1s})(4\nu_1 + 7)P_{-3/4}^{3/4}(t_s)}{[\rho^3(4\nu_1 + 4\nu_2 - 3) - a_{1s}(4\nu_1 + 4\nu_2 + 3)]P_{-3/4}^{3/4}(t_s) - (\rho - a_{1s})(4\nu_1 + 7)P_{-3/4}^{3/4}(t_s)}
\]
with
\[
t_s = \frac{\rho^4 - R^4}{\rho^4 + R^4} = \frac{1}{2} \left( 1 + \frac{b^2}{4R^4} \right)^{1/2} - \frac{1}{2}.
\]

The appropriate approximate expressions correct to the first orders in \(b^2R^4\) or \(b^2\) and \(b^2R^4\) may be obtained from (81)–(88) replacing \(c^2\) by \(2b^2R^4\).

It might seem that since some of the expressions presented contain the special functions, their practical importance is very limited. This is not so since with the aid of available software, e.g. the Mathematica system [26], numerical evaluation of all the special functions used in this paper (at least for real values of arguments and indices) is no more difficult or time consuming than evaluation of the trigonometric functions. Examples of applications of the derived formulae in numerical work are given in the following subsection.

### 3.3. Numerical illustrations

We have already utilized (61) and (69) to point out errors in calculations of the electron-scattering lengths for noble-gas atoms performed by other authors [27]. Here we illustrate the applicability of our formulae for computing scattering lengths for the e⁻–Xe and Cs–Cs systems.

As a first example we consider electron scattering by xenon atoms. We approximate the interaction potential by a simple model potential proposed by Czuchaj et al [28]
\[
V(r) = V_0 \exp(-\gamma r^2) - \frac{a_1 e^2}{2r^4} W_4(r) - \frac{(a_2 - 6\beta_1) e^2}{2r^5} W_5(r)
\]
where $\alpha_1$ and $\alpha_2$ are the dipole and quadrupole polarizabilities of the target atom and $6\beta_1$ is the dynamical correction to the dipole polarizability. The cut-off functions $W_n(r)$ have been chosen in the form

$$W_n(r) = \left[ 1 - \exp \left( -\frac{r^2}{r_c^2} \right) \right]^n$$

(94)

with $r_c$ being a cut-off radius. The values of constants appearing in (93) and (94) are (in atomic units): $V_0 = 306.0$, $\gamma = 1.0$, $\alpha_1 = 27.292$, $\alpha_2 = 128.255$, $\beta_1 = 29.2$ and $r_c = 1.89$. Results of our studies of convergence of the computed scattering length are presented in table 1. The short-range contribution $a_{0s}$ to the scattering length has been found numerically for different values of the core radius $\rho$. It is seen that $a_{0s}$ converges to $a_0$ extremely slowly while applications of various analytical formulae, especially more sophisticated ones, accelerate convergence significantly.

<table>
<thead>
<tr>
<th>Core radius $\rho$</th>
<th>Short-range $a_0(\rho)$</th>
<th>Extrapolated (61)</th>
<th>Extrapolated (60)</th>
<th>Extrapolated (67)</th>
<th>Extrapolated (65)</th>
<th>Extrapolated (63)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$5.0 \times 10^0$</td>
<td>1.09714</td>
<td>-3.25115</td>
<td>-5.18890</td>
<td>-3.16355</td>
<td>-4.94998</td>
<td>-4.95477</td>
</tr>
<tr>
<td>$5.5 \times 10^0$</td>
<td>-0.37802</td>
<td>-4.20344</td>
<td>-5.01864</td>
<td>-4.16349</td>
<td>-4.95253</td>
<td>-4.95281</td>
</tr>
<tr>
<td>$1.0 \times 10^1$</td>
<td>-1.45790</td>
<td>-4.60433</td>
<td>-4.98752</td>
<td>-4.38306</td>
<td>-4.95277</td>
<td>-4.95281</td>
</tr>
<tr>
<td>$2.0 \times 10^1$</td>
<td>-3.30875</td>
<td>-4.91155</td>
<td>-4.95546</td>
<td>-4.90908</td>
<td>-4.95281</td>
<td>-4.95281</td>
</tr>
<tr>
<td>$5.0 \times 10^1$</td>
<td>-4.35381</td>
<td>-4.95058</td>
<td>-4.95295</td>
<td>-4.95044</td>
<td>-4.95281</td>
<td>-4.95281</td>
</tr>
<tr>
<td>$1.0 \times 10^2$</td>
<td>-4.66670</td>
<td>-4.95255</td>
<td>-4.95282</td>
<td>-4.95253</td>
<td>-4.95281</td>
<td>-4.95281</td>
</tr>
<tr>
<td>$1.0 \times 10^3$</td>
<td>-4.92538</td>
<td>-4.95280</td>
<td>-4.95281</td>
<td>-4.95280</td>
<td>-4.95281</td>
<td>-4.95281</td>
</tr>
<tr>
<td>$1.0 \times 10^4$</td>
<td>-4.95007</td>
<td>-4.95281</td>
<td>-4.95281</td>
<td>-4.95281</td>
<td>-4.95281</td>
<td>-4.95281</td>
</tr>
<tr>
<td>$\infty$</td>
<td>-4.95281</td>
<td>-4.95281</td>
<td>-4.95281</td>
<td>-4.95281</td>
<td>-4.95281</td>
<td>-4.95281</td>
</tr>
</tbody>
</table>

As a second example we consider Cs–Cs scattering in the $^3\Sigma_u$ state. This system has been studied recently by Gribakin and Flambaum [2] and Marinescu [3] who approximated the interaction potential by

$$V(r) = \frac{1}{2} Br^\alpha \exp(-\beta r) - \left( \frac{C_6}{r^6} + \frac{C_8}{r^8} + \frac{C_{10}}{r^{10}} \right) f_c(r).$$

(95)

The cut-off function $f_c(r)$ has been chosen in a form

$$f_c(r) = \Theta(r - r_c) + \Theta(r_c - r) \exp \left( - \left( 1 - \frac{r_c}{r} \right)^2 \right)$$

(96)

where $\Theta(x)$ is the Heaviside function and $r_c$ is a cut-off radius. The values of constants appearing in (95) and (96) are (in atomic units): $B = 1.6 \times 10^{-3}$, $\alpha = 5.53$, $\beta = 1.072$, $C_6 = 7.02 \times 10^3$, $C_8 = 1.1 \times 10^6$, $C_{10} = 1.7 \times 10^8$ and $r_c = 23.165$. The value of the cesium mass used in the present calculations is (in atomic units) $m_{\text{Cs}} = 2.422 \times 10^5$. Note that for the system considered $m = m_{\text{Cs}}/2$. Results of our calculations are presented in table 2 from which it is evident that also in this case application of analytical formulae improves convergence [29, 30].

We emphasize that applicability of our analytical results is not restricted to such simple choices of the short-range parts of the interaction potentials as used above. The interaction between colliding particles inside the core might be described to any degree of sophistication.
Table 2. Convergence of the scattering length $a_0$ for the Cs–Cs collision in the $^3\Sigma_u$ state (the interaction potential given by (95)). All values are in atomic units [29, 30].

<table>
<thead>
<tr>
<th>Core radius $\rho$</th>
<th>Scattering length $a_0$</th>
<th>Short-range extrapolated (75)</th>
<th>Short-range extrapolated (73)</th>
<th>Short-range extrapolated (87)</th>
<th>Short-range extrapolated (81)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1.0 \times 10^2$</td>
<td>118.93602</td>
<td>82.263 85</td>
<td>68.550 17</td>
<td>82.262 74</td>
<td>68.547 74</td>
</tr>
<tr>
<td>$2.0 \times 10^2$</td>
<td>100.385 85</td>
<td>72.171 29</td>
<td>68.295 25</td>
<td>72.171 15</td>
<td>68.295 05</td>
</tr>
<tr>
<td>$5.0 \times 10^2$</td>
<td>71.850 70</td>
<td>68.237 85</td>
<td>68.219 57</td>
<td>68.237 85</td>
<td>68.219 57</td>
</tr>
<tr>
<td>$1.0 \times 10^3$</td>
<td>68.728 38</td>
<td>68.218 45</td>
<td>68.218 28</td>
<td>68.218 45</td>
<td>68.218 28</td>
</tr>
<tr>
<td>$1.0 \times 10^4$</td>
<td>68.218 79</td>
<td>68.218 23</td>
<td>68.218 23</td>
<td>68.218 23</td>
<td>68.218 23</td>
</tr>
<tr>
<td>$\infty$</td>
<td>68.218 23</td>
<td>68.218 23</td>
<td>68.218 23</td>
<td>68.218 23</td>
<td>68.218 23</td>
</tr>
</tbody>
</table>

The only requirement for our formulae to be applicable is that the short-range scattering lengths at the core boundary should be known.

Acknowledgments

I am grateful to Professor I I Fabrikan and Dr G F Gribakin for commenting on the manuscript. This work was supported by the University of Gdansk under grant no BW-5400-50064-5.

References

Calogero F 1967 Variable Phase Approach to Potential Scattering (New York: Academic)
[8] Szymkowksi R 1990 Acta Phys. Pol. A 78 517. Note that equations (20) and (21) in that paper were misprinted; they were corrected in [17].
[9] Since $\mu$ is not an integer, instead of $r^{1/2} F_\mu(x)$ we could use $r^{1/2} J^-_\mu(x)$ as a second particular solution to (12).
We wished to avoid negative indices we decided to use the solution with the Neumann function.
[11] Zero-energy bound states in the pure (i.e., with $\rho = 0$) long-range potential (25) with an exponent $n = 6$ are studied by Makan G D and Lapp M 1969 Phys. Rev. 179 19
[14] Since $0 < \mu < 1$ the solutions $x_\mu = p_\mu(z)$ are linearly independent. Instead of $x_\mu = p_{\mu}(z)$ we could use $W_\mu,_{\mu}(z)$, the Whittaker function of the second kind, but this would needlessly complicate the expression (30) for the scattering length.
Hull M H and Breit G 1959 Handbuch der Physik vol XL/1 ed S Flügge (Berlin: Springer) p 408
[17] Smytkowski R 1991 Acta Phys. Pol. A 79 613. In that paper we solved equation (48) in terms of the Gauss hypergeometric function. In the present work we prefer to use the Legendre functions. For relations between these functions see [7], ch 2.4.3, 4.1 and 4.3.

[18] The Legendre functions $P_\mu^\pm(t)$ are not linearly independent if $\mu$ is equal to an integer. In the case considered here, however, $0 < \mu < 1$ and we may safely use these two functions. Instead of $P_\mu^\pm(t)$ we could use $Q_\mu^\pm(t)$, the Legendre function of the second kind, but this would lead to an expression for the scattering length slightly more complicated than (52).


[21] Equation (60) resembles an expression derived by Holzwarth N A W 1973 J. Math. Phys. 14 191, equation (45). In fact, equation (60) may be obtained from Holzwarth's formula noting that his logarithmic derivative, $R_0(\rho)$, is related to the one we use, $L_0(\rho)$, by $R_0(\rho) = L_0(\rho) - \rho^{-1}$ and that he defines the scattering length with an opposite sign.


[23] The functions $z^{-1/2}M_{\nu \pm1/2}(z)$ are linear combinations of the parabolic cylinder functions $D_{2\nu -1/2}(\mp 2z^{1/2})$, see [13], ch 3.3.


Joachain C J 1975 Quantum Collision Theory (Amsterdam: North-Holland) p 611

Both monographs refer to a paper Buckingham R A 1937 Proc. R. Soc. A 160 94 which does not contain any mention about this potential.


[29] For the potential given by (95) Marinescu [2] reports an 'exact' numerical value of the scattering length $68.21596$ au which slightly differs from our 'exact' value $68.21823$ au. This small difference is presumably due to different numerical algorithms applied to solve the zero-energy Schrödinger equation in the inner region.

[30] We do not present results of application of (78) since the Mathematica system [26] which we used to obtain values of the special functions, failed to evaluate the Whittaker function $M_{\kappa,m}(\kappa)$ for those imaginary values of $\kappa$ and $z$ which we needed.