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Analytical calculations of scattering lengths in atomic physics

Radosław Szmytkowski

Institute of Theoretical Physics and Astrophysics, University of Gdańsk, Wita Stwosza 57, 80-952 Gdańsk, Poland

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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 ρ [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 ρ 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 lth partial wave scattering length a_l as

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

where $\delta_l(k)$ is an lth 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

$$\lim_{r\to\infty} r^{2l+3}V_L(r) = 0\,. \tag{2}$$

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 $E=0$

$$\frac{d^2u_l(r)}{dr^2} - \frac{l(l+1)}{r^2}u_l(r) - \frac{2m}{\hbar^2}V_L(r)u_l(r) = 0 \qquad r \geqslant \rho \tag{3}$$

which for potentials satisfying condition (2) behaves asymptotically as

$$u_l(r) \overset{r\to\infty}{\longrightarrow} \text{constant} \times (r^{l+1} - a_l r^{-l})\,. \tag{4}$$

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

$$a_l = \lim_{r\to\infty} a_l(r) \tag{5}$$

defined as

$$a_l(r) = r^{2l+1}\frac{rL_l(r) - (l+1)}{rL_l(r) + l}\,. \tag{6}$$

Here

$$L_l(r) = \frac{1}{u_l(r)}\frac{du_l(r)}{dr} \tag{7}$$

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 ρ, 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 $r \geqslant \rho$ the general solution to (3) has the form

$$u_l(r) = A_l f_l(r) + B_l g_l(r) \qquad r \geqslant \rho \tag{8}$$

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

$$L_l(r) = \frac{f_l'(r) + D_l g_l'(r)}{f_l(r) + D_l g_l(r)} \tag{9}$$

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

$$D_l = -\frac{(\rho^{2l+1} - a_{ls})\rho f_l'(\rho) - [(l+1)\rho^{2l+1} + l a_{ls}] f_l(\rho)}{(\rho^{2l+1} - a_{ls})\rho g_l'(\rho) - [(l+1)\rho^{2l+1} + l a_{ls}] g_l(\rho)} \tag{10}$$

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 $V_{\mathrm{L}}(r)$ be the inverse power potential of the form

$$V_{\mathrm{L}}(r) = -\frac{\hbar^2}{2m}\frac{b^2}{r^n} \qquad b > 0 \quad r \geqslant \rho\,. \tag{11}$$

A general solution to the Schrödinger equation

$$\frac{\mathrm{d}^2 u_l(r)}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} u_l(r) + \frac{b^2}{r^n} u_l(r) = 0 \qquad r \geqslant \rho \tag{12}$$

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

$$u_l(r) = A_l r^{1/2} J_\mu(x) + B_l r^{1/2} Y_\mu(x) \qquad r \geqslant \rho \tag{13}$$

where

$$\mu = \frac{2l+1}{n-2} \tag{14}$$

and

$$x \equiv x(r) = \frac{2b}{n-2} r^{-(n-2)/2}\,. \tag{15}$$

Condition (2) requires

$$n > 2l + 3 \qquad \text{or equivalently} \qquad 0 < \mu < 1 \tag{16}$$

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

$$a_l = \pi \left(\frac{b}{n-2} \right)^{2\mu} \frac{\Phi_l + \cot(\pi\mu)}{\Gamma(\mu)\Gamma(\mu+1)} \tag{17}$$

with

$$\Phi_l = -\frac{2\mu\rho^{2l+1} Y_\mu(x_s) - (\rho^{2l+1} - a_{ls}) x_s Y_{\mu+1}(x_s)}{2\mu\rho^{2l+1} J_\mu(x_s) - (\rho^{2l+1} - a_{ls}) x_s J_{\mu+1}(x_s)} \tag{18}$$

where

$$x_s = x(\rho)\,. \tag{19}$$

Similar results have been obtained by Fabrikant [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

$$a_l = \frac{b}{2l+1} \frac{1 + (x_s - y_{ls}) \tan(x_s)}{\tan(x_s) - (x_s - y_{ls})} \tag{20}$$

where

$$y_{ls} = \frac{b}{(2l+1)a_{ls}}. \tag{21}$$

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 ρ. In such a case one gets the following expression correct to the first order in b^2:

$$a_l \simeq a_{ls} - b^2 \theta_l^{(n)} \tag{22}$$

where

$$\theta_l^{(n)} = \frac{1}{2l+1} \rho^{-n-2l+1} \left(\frac{\rho^{2(2l+1)}}{n-2l-3} - \frac{2a_{ls}\rho^{2l+1}}{n-2} + \frac{a_{ls}^2}{n+2l-1} \right) \tag{23}$$

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

$$b^2 |\theta_l^{(n)}| \ll |a_{ls}|. \tag{24}$$

2.3. *Superposition of two inverse power potentials*

Next we consider scattering of an lth partial wave by the long-range potential [11]

$$V_{\mathrm{L}}(r) = -\frac{\hbar^2}{2m} \frac{b^2}{r^n} + \frac{\hbar^2}{2m} \frac{c^2}{r^{2n-2}} \qquad b > 0 \qquad r \geqslant \rho \tag{25}$$

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

$$\frac{\mathrm{d}^2 u_l(r)}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} u_l(r) + \frac{b^2}{r^n} u_l(r) - \frac{c^2}{r^{2n-2}} u_l(r) = 0 \qquad r \geqslant \rho \tag{26}$$

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

$$u_l(r) = A_l' r^{(n-1)/2} M_{\kappa,\mu/2}(z) + B_l' r^{(n-1)/2} M_{\kappa,-\mu/2}(z) \tag{27}$$

where

$$\mu = \frac{2l+1}{n-2} \qquad \kappa = \frac{b^2}{2(n-2)c} \tag{28}$$

and

$$z \equiv z(r) = \frac{2c}{n-2} r^{-(n-2)}. \tag{29}$$

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

$$a_l = \left(\frac{2c}{n-2}\right)^{\mu} \frac{(\rho^{2l+1} - a_{ls})(2\kappa - \mu + 1) M_{\kappa+1,-\mu/2}(z_s) + [\rho^{2l+1}(z_s - 2\kappa + \mu - 1) - a_{ls}(z_s - 2\kappa - \mu - 1)] M_{\kappa,-\mu/2}(z_s)}{(\rho^{2l+1} - a_{ls})(2\kappa + \mu + 1) M_{\kappa+1,\mu/2}(z_s) + [\rho^{2l+1}(z_s - 2\kappa + \mu - 1) - a_{ls}(z_s - 2\kappa - \mu - 1)] M_{\kappa,\mu/2}(z_s)} \tag{30}$$

where

$$z_s = z(\rho). \tag{31}$$

We observe that in applications the second term contributing to $V_{\mathrm{L}}(r)$ (proportional to c^2) might be much smaller then 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

$$u_l(r) = \xi^{-(n-1)/(2n-4)} v_\lambda(\xi) \tag{32}$$

with

$$\xi \equiv \xi(r) = r^{-(n-2)} \qquad \lambda = \tfrac{1}{2}(\mu - 1) \tag{33}$$

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

$$\frac{\mathrm{d}^2 v_\lambda(\xi)}{\mathrm{d}\xi^2} - \frac{\lambda(\lambda+1)}{\xi^2} v_\lambda(\xi) + \frac{\tilde{b}^2}{\xi} v_\lambda(\xi) - \tilde{c}^2 v_\lambda(\xi) = 0 \qquad \xi \leqslant \rho^{-(n-2)} \tag{34}$$

where

$$\tilde{b} = \frac{b}{n-2} \qquad \tilde{c} = \frac{c}{n-2}. \tag{35}$$

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 $\tilde{c}^2$ one has

$$v_{\lambda\,\mathrm{reg}}(\xi) \simeq x J_\mu(x) + \frac{\tilde{c}^2}{24\tilde{b}^4} x^3 [x J_{\mu+1}(x) - (1-\mu) J_{\mu+2}(x)] \tag{36}$$

$$v_{\lambda\,\mathrm{irr}}(\xi) \simeq x Y_\mu(x) + \frac{\tilde{c}^2}{24\tilde{b}^4} x^3 [x Y_{\mu+1}(x) - (1-\mu) Y_{\mu+2}(x)] \tag{37}$$

where

$$x \equiv x(r) = \frac{2b}{n-2} r^{-(n-2)/2} = 2\tilde{b}\xi^{1/2}. \tag{38}$$

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

$$\begin{aligned} u_l(r) \simeq {} & A_l r^{1/2} \left\{ J_\mu(x) + c^2 \frac{(n-2)^2}{24b^4} x^2 [x J_{\mu+1}(x) - (1-\mu) J_{\mu+2}(x)] \right\} \\ & + B_l r^{1/2} \left\{ Y_\mu(x) + c^2 \frac{(n-2)^2}{24b^4} x^2 [x Y_{\mu+1}(x) - (1-\mu) Y_{\mu+2}(x)] \right\} \\ & r \geqslant \rho \end{aligned} \tag{39}$$

and one obtains the following expression for the scattering length:

$$a_l \simeq \pi \left(\frac{b}{n-2} \right)^{2\mu} \frac{\Phi_l + \cot(\pi\mu)}{\Gamma(\mu)\Gamma(\mu+1)} \left[1 + c^2 \frac{(n-2)^2}{24b^4} \left(4\mu(1-\mu^2) + \frac{\phi_l}{\Phi_l + \cot(\pi\mu)} \right) \right] \tag{40}$$

valid to the first order in c^2. Φ_l has been defined by (18) and ϕ_l is given by

$$\begin{aligned} \phi_l = -\Phi_l \, & \frac{x_s^2[\rho^{2l+1} x_s^2 - a_{ls}(2\mu^2 - 2\mu + x_s^2)] J_\mu(x_s) + x_s[\rho^{2l+1}(1+\mu) x_s^2 - a_{ls}(1-\mu)(4\mu^2 + 4\mu + x_s^2)] J_{\mu+1}(x_s)}{2\mu\rho^{2l+1} J_\mu(x_s) - (\rho^{2l+1} - a_{ls}) x_s J_{\mu+1}(x_s)} \\ & - \frac{x_s^2[\rho^{2l+1} x_s^2 - a_{ls}(2\mu^2 - 2\mu + x_s^2)] Y_\mu(x_s) + x_s[\rho^{2l+1}(1+\mu) x_s^2 - a_{ls}(1-\mu)(4\mu^2 + 4\mu + x_s^2)] Y_{\mu+1}(x_s)}{2\mu\rho^{2l+1} J_\mu(x_s) - (\rho^{2l+1} - a_{ls}) x_s J_{\mu+1}(x_s)} \end{aligned} \tag{41}$$

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

$$|c^2| \frac{(n-2)^2}{24b^4} \left| 4\mu(1-\mu^2) + \frac{\phi_l}{\Phi_l + \cot(\pi\mu)} \right| \ll 1. \tag{42}$$

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

$$a_l \simeq \frac{b}{2l+1} \frac{1 + (x_s - y_{ls}) \tan(x_s)}{\tan(x_s) - (x_s - y_{ls})} \left[1 + c^2 \frac{(2l+1)^2}{12b^4} \left(3 + 2\frac{\phi_l}{\Phi_l} \right) \right] \tag{43}$$

where

$$\frac{\phi_l}{\Phi_l} = \frac{1}{2} \frac{(2x_s^4 - 2x_s^3 y_{ls} - 3x_s y_{ls} + 3)\tan(x_s) - x_s(x_s^2 - 3x_s y_{ls} + 3)}{\tan(x_s) - (x_s - y_{ls})} - \frac{1}{2} \frac{(2x_s^4 - 2x_s^3 y_{ls} - 3x_s y_{ls} + 3) + x_s(x_s^2 - 3x_s y_{ls} + 3)\tan(x_s)}{1 + (x_s - y_{ls})\tan(x_s)} \tag{44}$$

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

Finally, for sufficiently large ρ 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

$$a_l \simeq a_{ls} - b^2\theta_l^{(n)} + c^2\theta_l^{(2n-2)} \tag{45}$$

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

$$|b^2\theta_l^{(n)} - c^2\theta_l^{(2n-2)}| \ll |a_{ls}|. \tag{46}$$

2.4. *The Lenz potentials*

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

$$V_L(r) = -\frac{\hbar^2}{2m} \frac{b^2 r^{n-4}}{\left(r^{n-2} + R^{n-2}\right)^2} \qquad b > 0 \qquad R > 0 \qquad r \geqslant \rho \tag{47}$$

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

$$\frac{d^2 u_l(r)}{dr^2} - \frac{l(l+1)}{r^2} u_l(r) + \frac{b^2 r^{n-4}}{\left(r^{n-2} + R^{n-2}\right)^2} u_l(r) = 0 \qquad r \geqslant \rho \tag{48}$$

has the form [17, 18]

$$u_l(r) = A_l r^{1/2} P_\nu^{-\mu}(t) + B_l r^{1/2} P_\nu^{\mu}(t) \qquad r \geqslant \rho \tag{49}$$

where $P_\nu^{\mp\mu}(t)$ are the Legendre functions of the first kind,

$$\mu = \frac{2l+1}{n-2} \qquad \nu = \frac{1}{2}\left(1 + \frac{4b^2}{(n-2)^2 R^{n-2}}\right)^{1/2} - \frac{1}{2} \tag{50}$$

and

$$t \equiv t(r) = \frac{r^{n-2} - R^{n-2}}{r^{n-2} + R^{n-2}}. \tag{51}$$

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

$$a_l = R^{2l+1} \frac{\Gamma(1-\mu)}{\Gamma(1+\mu)} \frac{[\rho^{2l+1}(\nu t_s + t_s - \mu) - a_{ls}(\nu t_s + t_s + \mu)] P_\nu^{\mu}(t_s) - (\rho^{2l+1} - a_{ls})(\nu - \mu + 1) P_{\nu+1}^{\mu}(t_s)}{[\rho^{2l+1}(\nu t_s + t_s - \mu) - a_{ls}(\nu t_s + t_s + \mu)] P_\nu^{-\mu}(t_s) - (\rho^{2l+1} - a_{ls})(\nu + \mu + 1) P_{\nu+1}^{-\mu}(t_s)} \tag{52}$$

where

$$t_s = t(\rho). \tag{53}$$

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

$$a_l = (2\nu+1)R^{2l+1}\frac{(R^{2(2l+1)} + a_{ls}\rho^{2l+1}) - (2\nu+1)R^{2l+1}(\rho^{2l+1} - a_{ls})\tan\Omega_s}{(R^{2(2l+1)} + a_{ls}\rho^{2l+1})\tan\Omega_s + (2\nu+1)R^{2l+1}(\rho^{2l+1} - a_{ls})} \tag{54}$$

where

$$\Omega_s = (2\nu+1)\arctan\left(\frac{R^{2l+1}}{\rho^{2l+1}}\right). \tag{55}$$

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

$$V_L(r) \simeq -\frac{\hbar^2}{2m}\frac{b^2}{r^n} + \frac{\hbar^2}{2m}\frac{c^2}{r^{2n-2}} \tag{56}$$

where

$$c^2 = 2b^2R^{n-2}. \tag{57}$$

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^2R^{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]

$$V(r) \simeq -\frac{C_4}{r^4} - \frac{C_6}{r^6} + O(r^{-7}) \qquad r\to\infty \tag{58}$$

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

$$V_L(r) = -\frac{\hbar^2}{2m}\frac{b^2}{r^4} \tag{59}$$

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

$$a_0 = b\,\frac{1 + b(1/\rho - 1/a_{0s})\tan(b/\rho)}{\tan(b/\rho) - b(1/\rho - 1/a_{0s})} \tag{60}$$

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

$$a_0 \simeq a_{0s} - \frac{b^2}{\rho}\left(1 - \frac{a_{0s}}{\rho} + \frac{a_{0s}^2}{3\rho^2}\right). \tag{61}$$

This approximate formula has been derived in alternative ways by Temkin and Drukarev [22].

More accurate results can be obtained by choosing

$$V_{\mathrm{L}}(r) = -\frac{\hbar^2}{2m}\frac{b^2}{r^4} + \frac{\hbar^2}{2m}\frac{c^2}{r^6} \tag{62}$$

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]

$$a_0 = c^{1/2}\frac{(\rho-a_{0s})(b^2/c+1)M_{\kappa+1,-1/4}(c/\rho^2)+[\rho(2c/\rho^2-b^2/c-1)-a_{0s}(2c/\rho^2-b^2/c-3)]M_{\kappa,-1/4}(c/\rho^2)}{(\rho-a_{0s})(b^2/c+3)M_{\kappa+1,1/4}(c/\rho^2)+[\rho(2c/\rho^2-b^2/c-1)-a_{0s}(2c/\rho^2-b^2/c-3)]M_{\kappa,1/4}(c/\rho^2)} \tag{63}$$

where the index κ is given by

$$\kappa = \frac{b^2}{4c}. \tag{64}$$

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

$$a_0 \simeq b\,\frac{1+b(1/\rho-1/a_{0s})\tan(b/\rho)}{\tan(b/\rho)-b(1/\rho-1/a_{0s})}\left[1+\frac{c^2}{12b^4}\left(3+2\frac{\phi_0}{\Phi_0}\right)\right] \tag{65}$$

with

$$\frac{\phi_0}{\Phi_0} = \frac{1}{2}\,\frac{[2b^4/\rho^4-2b^4/(\rho^3a_{0s})-3b^2/(\rho a_{0s})+3]\tan(b/\rho)-(b/\rho)[b^2/\rho^2-3b^2/(\rho a_{0s})+3]}{\tan(b/\rho)-b(1/\rho-1/a_{0s})}$$
$$-\frac{1}{2}\,\frac{[2b^4/\rho^4-2b^4/(\rho^3a_{0s})-3b^2/(\rho a_{0s})+3]+(b/\rho)[b^2/\rho^2-3b^2/(\rho a_{0s})+3]\tan(b/\rho)}{1+b(1/\rho-1/a_{0s})\tan(b/\rho)} \tag{66}$$

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

$$a_0 \simeq a_{0s} - \frac{b^2}{\rho}\left(1-\frac{a_{0s}}{\rho}+\frac{a_{0s}^2}{3\rho^2}\right) + \frac{c^2}{3\rho^3}\left(1-\frac{3a_{0s}}{2\rho}+\frac{3a_{0s}^2}{5\rho^2}\right). \tag{67}$$

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

$$V_{\mathrm{L}}(r) = -\frac{\hbar^2}{2m}\frac{b^2}{(r^2+R^2)^2} \tag{68}$$

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

$$a_0 = (b^2+R^2)^{1/2}\frac{(R^2+\rho a_{0s}) - (b^2+R^2)^{1/2}(\rho-a_{0s})\tan\Omega_{\mathrm{s}}}{(R^2+\rho a_{0s})\tan\Omega_{\mathrm{s}} + (b^2+R^2)^{1/2}(\rho-a_{0s})} \tag{69}$$

with

$$\Omega_{\mathrm{s}} = \left(1+\frac{b^2}{R^2}\right)^{1/2}\arctan\left(\frac{R}{\rho}\right). \tag{70}$$

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

3.2. *Collisions between neutral particles*

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

$$V(r) \simeq -\frac{C_6}{r^6} - \frac{C_8}{r^8} - \frac{C_{10}}{r^{10}} + \mathrm{O}(r^{-12}). \tag{71}$$

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

$$V_{\mathrm{L}}(r) = -\frac{\hbar^2}{2m}\frac{b^2}{r^6} \tag{72}$$

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

$$a_0 = \frac{2\pi b^{1/2}}{[\Gamma(1/4)]^2}\left[1 - \frac{\rho Y_{1/4}(b/2\rho^2) - (b/\rho^2)(\rho - a_{0\mathrm{s}})Y_{5/4}(b/2\rho^2)}{\rho J_{1/4}(b/2\rho^2) - (b/\rho^2)(\rho - a_{0\mathrm{s}})J_{5/4}(b/2\rho^2)}\right] \tag{73}$$

$$a_1 = -\frac{\pi b^{3/2}}{6[\Gamma(3/4)]^2}\left[1 + \frac{3\rho^3 Y_{3/4}(b/2\rho^2) - (b/\rho^2)(\rho^3 - a_{1\mathrm{s}})Y_{7/4}(b/2\rho^2)}{3\rho^3 J_{3/4}(b/2\rho^2) - (b/\rho^2)(\rho^3 - a_{1\mathrm{s}})J_{7/4}(b/2\rho^2)}\right]. \tag{74}$$

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

$$a_0 \simeq a_{0\mathrm{s}} - \frac{b^2}{3\rho^3}\left(1 - \frac{3a_{0\mathrm{s}}}{2\rho} + \frac{3a_{0\mathrm{s}}^2}{5\rho^2}\right) \tag{75}$$

$$a_1 \simeq a_{1\mathrm{s}} - \frac{b^2}{3\rho}\left(1 - \frac{a_{1\mathrm{s}}}{2\rho^3} + \frac{a_{1\mathrm{s}}^2}{7\rho^6}\right). \tag{76}$$

Another possibility is to choose

$$V_{\mathrm{L}}(r) = -\frac{\hbar^2}{2m}\frac{b^2}{r^6} + \frac{\hbar^2}{2m}\frac{c^2}{r^{10}} \tag{77}$$

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

$$a_0 = (c/2)^{1/4}\frac{(\rho-a_{0\mathrm{s}})(b^2/c+3)M_{\kappa+1,-1/8}(c/2\rho^4)+[\rho(2c/\rho^4-b^2/c-3)-a_{0\mathrm{s}}(2c/\rho^4-b^2/c-5)]M_{\kappa,-1/8}(c/2\rho^4)}{(\rho-a_{0\mathrm{s}})(b^2/c+5)M_{\kappa+1,1/8}(c/2\rho^4)+[\rho(2c/\rho^4-b^2/c-3)-a_{0\mathrm{s}}(2c/\rho^4-b^2/c-5)]M_{\kappa,1/8}(c/2\rho^4)} \tag{78}$$

$$a_1 = (c/2)^{3/4}\frac{(\rho^3-a_{1\mathrm{s}})(b^2/c+1)M_{\kappa+1,-3/8}(c/2\rho^4)+[\rho^3(2c/\rho^4-b^2/c-1)-a_{1\mathrm{s}}(2c/\rho^4-b^2/c-7)]M_{\kappa,-3/8}(c/2\rho^4)}{(\rho^3-a_{1\mathrm{s}})(b^2/c+7)M_{\kappa+1,3/8}(c/2\rho^4)+[\rho^3(2c/\rho^4-b^2/c-1)-a_{1\mathrm{s}}(2c/\rho^4-b^2/c-7)]M_{\kappa,3/8}(c/2\rho^4)} \tag{79}$$

where

$$\kappa = \frac{b^2}{8c}. \tag{80}$$

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

$$a_0 \simeq \frac{2\pi b^{1/2}}{[\Gamma(1/4)]^2}(\Phi_0 + 1)\left[1 + \frac{2c^2}{3b^4}\left(\frac{15}{16} + \frac{\phi_0}{\Phi_0 + 1}\right)\right] \tag{81}$$

with

$$\Phi_0 = -\frac{\rho Y_{1/4}(b/2\rho^2) - (b/\rho^2)(\rho - a_{0\mathrm{s}})Y_{5/4}(b/2\rho^2)}{\rho J_{1/4}(b/2\rho^2) - (b/\rho^2)(\rho - a_{0\mathrm{s}})J_{5/4}(b/2\rho^2)} \tag{82}$$

$$\begin{aligned}\phi_0 = -\tfrac{1}{16}\Phi_0\,&\frac{(b^2/\rho^4)[2b^2/\rho^3-a_{0\mathrm{s}}(2b^2/\rho^4-3)]J_{1/4}(b/2\rho^2)+(b/\rho^2)[5b^2/\rho^3-3a_{0\mathrm{s}}(b^2/\rho^4+5)]J_{5/4}(b/2\rho^2)}{\rho J_{1/4}(b/2\rho^2)-(b/\rho^2)(\rho-a_{0\mathrm{s}})J_{5/4}(b/2\rho^2)}\\ &-\frac{1}{16}\,\frac{(b^2/\rho^4)[2b^2/\rho^3-a_{0\mathrm{s}}(2b^2/\rho^4-3)]Y_{1/4}(b/2\rho^2)+(b/\rho^2)[5b^2/\rho^3-3a_{0\mathrm{s}}(b^2/\rho^4+5)]Y_{5/4}(b/2\rho^2)}{\rho J_{1/4}(b/2\rho^2)-(b/\rho^2)(\rho-a_{0\mathrm{s}})J_{5/4}(b/2\rho^2)}\end{aligned} \tag{83}$$

and

$$a_1 \simeq \frac{\pi b^{3/2}}{6[\Gamma(3/4)]^2}(\Phi_1 - 1)\left[1 + \frac{2c^2}{3b^4}\left(\frac{21}{16} + \frac{\phi_1}{\Phi_1 - 1}\right)\right] \tag{84}$$

with

$$\Phi_1 = -\frac{3\rho^3 Y_{3/4}(b/2\rho^2) - (b/\rho^2)(\rho^3 - a_{1s})Y_{7/4}(b/2\rho^2)}{3\rho^3 J_{3/4}(b/2\rho^2) - (b/\rho^2)(\rho^3 - a_{1s})J_{7/4}(b/2\rho^2)} \tag{85}$$

$$\phi_1 = -\frac{1}{16}\Phi_1 \frac{(b^2/\rho^4)[2b^2/\rho - a_{1s}(2b^2/\rho^4 - 3)]J_{3/4}(b/2\rho^2) + (b/\rho^2)[7b^2/\rho - a_{1s}(b^2/\rho^4 + 21)]J_{7/4}(b/2\rho^2)}{3\rho^3 J_{3/4}(b/2\rho^2) - (b/\rho^2)(\rho^3 - a_{1s})J_{7/4}(b/2\rho^2)}$$
$$- \frac{1}{16}\frac{(b^2/\rho^4)[2b^2/\rho - a_{1s}(2b^2/\rho^4 - 3)]Y_{3/4}(b/2\rho^2) + (b/\rho^2)[7b^2/\rho - a_{1s}(b^2/\rho^4 + 21)]Y_{7/4}(b/2\rho^2)}{3\rho^3 J_{3/4}(b/2\rho^2) - (b/\rho^2)(\rho^3 - a_{1s})J_{7/4}(b/2\rho^2)}. \tag{86}$$

Finally, the expressions correct to the first order in the potential strengths b^2 and c^2 are

$$a_0 \simeq a_{0s} - \frac{b^2}{3\rho^3}\left(1 - \frac{3a_{0s}}{2\rho} + \frac{3a_{0s}^2}{5\rho^2}\right) + \frac{c^2}{7\rho^7}\left(1 - \frac{7a_{0s}}{4\rho} + \frac{7a_{0s}^2}{9\rho^2}\right) \tag{87}$$

$$a_1 \simeq a_{1s} - \frac{b^2}{3\rho}\left(1 - \frac{a_{1s}}{2\rho^3} + \frac{a_{1s}^2}{7\rho^6}\right) + \frac{c^2}{15\rho^5}\left(1 - \frac{5a_{1s}}{4\rho^3} + \frac{5a_{1s}^2}{11\rho^6}\right). \tag{88}$$

The last possibility we discuss is to approximate the long-range part of the interaction by the Lenz potential

$$V_L(r) = -\frac{\hbar^2}{2m}\frac{b^2 r^2}{(r^4 + R^4)^2} \tag{89}$$

with $b^2 = 2mC_6/\hbar^2$ for which exact expressions for the scattering lengths are

$$a_0 = \frac{4\pi\sqrt{2}R}{[\Gamma(1/4)]^2}\frac{[\rho(4\nu t_s + 4t_s - 1) - a_{0s}(4\nu t_s + 4t_s + 1)]P_\nu^{1/4}(t_s) - (\rho - a_{0s})(4\nu + 3)P_{\nu+1}^{1/4}(t_s)}{[\rho(4\nu t_s + 4t_s - 1) - a_{0s}(4\nu t_s + 4t_s + 1)]P_\nu^{-1/4}(t_s) - (\rho - a_{0s})(4\nu + 5)P_{\nu+1}^{-1/4}(t_s)} \tag{90}$$

$$a_1 = \frac{4\pi\sqrt{2}R^3}{3[\Gamma(3/4)]^2}\frac{[\rho^3(4\nu t_s + 4t_s - 3) - a_{1s}(4\nu t_s + 4t_s + 3)]P_\nu^{3/4}(t_s) - (\rho^3 - a_{1s})(4\nu + 1)P_{\nu+1}^{3/4}(t_s)}{[\rho^3(4\nu t_s + 4t_s - 3) - a_{1s}(4\nu t_s + 4t_s + 3)]P_\nu^{-3/4}(t_s) - (\rho^3 - a_{1s})(4\nu + 7)P_{\nu+1}^{-3/4}(t_s)} \tag{91}$$

with

$$t_s = \frac{\rho^4 - R^4}{\rho^4 + R^4} \qquad \nu = \frac{1}{2}\left(1 + \frac{b^2}{4R^4}\right)^{1/2} - \frac{1}{2} \tag{92}$$

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]

$$V(r) = V_0 \exp(-\gamma r^2) - \frac{\alpha_1 e^2}{2r^4}W_4(r) - \frac{(\alpha_2 - 6\beta_1)e^2}{2r^6}W_6(r) \tag{93}$$

where α_1 and α_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

$$W_n(r) = \left[1 - \exp\left(-\frac{r^2}{r_c^2}\right)\right]^n \tag{94}$$

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 ρ. 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 1. Convergence of the scattering length a_0 for the e^-–Xe collision (the interaction potential given by (93)). All values are in atomic units.

	Scattering length a_0					
Core radius ρ	Short-range $a_{0s}(\rho)$	Extrapolated (61)	Extrapolated (60)	Extrapolated (67)	Extrapolated (65)	Extrapolated (63)
5.0×10^0	1.097 14	−3.251 15	−5.188 90	−3.163 55	−4.949 98	−4.954 77
7.5×10^0	−0.378 02	−4.203 44	−5.018 64	−4.163 49	−4.952 53	−4.952 81
1.0×10^1	−1.457 90	−4.604 33	−4.978 52	−4.585 06	−4.952 77	−4.952 81
2.0×10^1	−3.308 75	−4.911 55	−4.955 46	−4.909 08	−4.952 81	−4.952 81
5.0×10^1	−4.355 81	−4.950 58	−4.952 95	−4.950 44	−4.952 81	−4.952 81
1.0×10^2	−4.666 70	−4.952 55	−4.952 82	−4.952 53	−4.952 81	−4.952 81
1.0×10^3	−4.925 38	−4.952 80	−4.952 81	−4.952 80	−4.952 81	−4.952 81
1.0×10^4	−4.950 07	−4.952 81	−4.952 81	−4.952 81	−4.952 81	−4.952 81
∞	−4.952 81	−4.952 81	−4.952 81	−4.952 81	−4.952 81	−4.952 81

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

$$V(r) = \frac{1}{2}Br^{\alpha}\exp(-\beta r) - \left(\frac{C_6}{r^6} + \frac{C_8}{r^8} + \frac{C_{10}}{r^{10}}\right) f_c(r) . \tag{95}$$

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

$$f_c(r) = \Theta(r - r_c) + \Theta(r_c - r)\exp\left(-\left(1 - \frac{r_c}{r}\right)^2\right) \tag{96}$$

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) $m_{Cs} = 2.422 \times 10^5$. Note that for the system considered $m = m_{Cs}/2$. 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].

Core radius ρ	Scattering length a_0 Short-range $a_{0s}(\rho)$	Extrapolated (75)	Extrapolated (73)	Extrapolated (87)	Extrapolated (81)
1.0×10^2	118.936 02	82.263 85	68.550 17	82.262 74	68.547 74
2.0×10^2	100.385 85	72.171 29	68.295 25	72.171 15	68.295 05
5.0×10^2	71.850 70	68.237 85	68.219 57	68.237 85	68.219 57
1.0×10^3	68.728 38	68.218 45	68.218 28	68.218 45	68.218 28
1.0×10^4	68.218 79	68.218 23	68.218 23	68.218 23	68.218 23
∞	68.218 23	68.218 23	68.218 23	68.218 23	68.218 23

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

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[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 $M_{\kappa,\mu}(z)$ for those imaginary values of κ and z which we needed.