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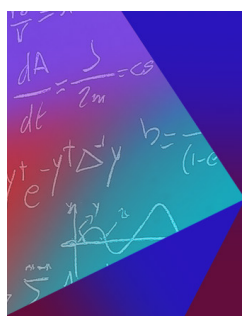
Analytical calculations of scattering lengths for a class of long-range potentials of interest for atomic physics

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ABSTRACT

We derive two equivalent analytical expressions for an l th partial-wave scattering length a_l for central potentials with long-range tails of the form $V(r) = -\frac{\hbar^2}{2m} \frac{Br^{n-4}}{(r^{n-2} + R^{n-2})^2} - \frac{\hbar^2}{2m} \frac{C}{r^2(r^{n-2} + R^{n-2})}$, ($r \geq r_s$, $R > 0$). For $C = 0$, this family of potentials reduces to the Lenz potentials discussed in a similar context in our earlier works [R. Szmytkowski, Acta Phys. Pol. A **79**, 613 (1991); J. Phys. A: Math. Gen. **28**, 7333 (1995)]. The formulas for a_l that we provide in this paper depend on the parameters B , C , and R characterizing the tail of the potential, on the core radius r_s , as well as on the short-range scattering length a_{ls} , the latter being due to the core part of the potential. The procedure, which may be viewed as an analytical extrapolation from a_{ls} to a_l , is relied on the fact that the general solution to the zero-energy radial Schrödinger equation with the potential given above may be expressed analytically in terms of the *generalized* associated Legendre functions.

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I. INTRODUCTION

Scattering lengths are among the most important parameters characterizing atomic collisional processes at ultralow energies.^{1–4} Therefore, there is a need for developing reliable and effective methods for the calculation of these quantities and a variety of such procedures—analytical, numerical, or of a mixed character—have been proposed.^{5–45}

Some time ago, in Ref. 19, we presented analytical formulas for partial-wave scattering lengths a_l for central potentials with the following three types of long-range tails: (i) the inverse power tail

$$V(r) = -\frac{\hbar^2}{2m} \frac{A_n}{r^n} \quad (r \geq r_s), \quad (1.1)$$

(ii) the so-called Lennard-Jones ($n, 2n - 2$) tail

$$V(r) = -\frac{\hbar^2}{2m} \frac{A_n}{r^n} - \frac{\hbar^2}{2m} \frac{A_{2n-2}}{r^{2n-2}} \quad (r \geq r_s), \quad (1.2)$$

and (iii) the so-called Lenz tail

$$V(r) = -\frac{\hbar^2}{2m} \frac{Br^{n-4}}{(r^{n-2} + R^{n-2})^2} \quad (r \geq r_s, R > 0). \quad (1.3)$$

The expressions for a_l provided in Ref. 19 involve parameters characterizing tails of particular potentials, the core radius r_s , the short-range scattering lengths a_{ls} that are due to the core part of the potential and that usually have to be determined numerically, and also some of the well-known special functions of mathematical physics: the Bessel functions for the tail (1.1), the Whittaker functions for the tail (1.2), and the associated Legendre functions for the tail (1.3). In brief, the procedure may be viewed as an analytical extrapolation from a_{ls} to a_l , with the use of the fact that in the region $r \geq r_s$ the general solution to the zero-energy radial Schrödinger equation with the potentials given above are expressible in terms of the afore-mentioned special functions.

In the present paper, we consider a class of central potentials with still another functional form of the long-range tail, which is

$$V(r) = -\frac{\hbar^2}{2m} \frac{Br^{n-4}}{(r^{n-2} + R^{n-2})^2} - \frac{\hbar^2}{2m} \frac{C}{r^2(r^{n-2} + R^{n-2})} \quad (r \geq r_s, R > 0). \tag{1.4}$$

This tail is seen to generalize the Lenz tail (1.3); moreover, asymptotically, it imitates the Lennard-Jones tail (1.2) since it falls off as

$$V(r) \xrightarrow{r \rightarrow \infty} -\frac{\hbar^2}{2m} \frac{B+C}{r^n} - \frac{\hbar^2}{2m} \frac{(-2B-C)R^{n-2}}{r^{2n-2}} + O(r^{-3n+4}). \tag{1.5}$$

In the following, we shall prove that also for potentials with the tail (1.4), it is possible to extrapolate analytically from a_{ls} to a_l , but this time with the use of *generalized* associated Legendre functions.⁴⁶

The paper is structured as follows: In Sec. II, a definition and some basic facts about partial-wave scattering lengths are reminded, and then, a particular method enabling one to calculate these quantities is sketched. This method is then used in Sec. III to derive two equivalent analytical expressions, displayed in Eqs. (3.16a) and (3.16b), for scattering lengths for potentials with the tail given in Eq. (1.4). Special cases when these two formulas simplify are discussed in Sec. IV. Finally, concluding remarks form Sec. V.

II. THE METHOD

The l th partial-wave scattering length a_l is defined through the limit relation⁴⁷

$$a_l = -(2l-1)!!(2l+1)!! \lim_{k \rightarrow 0} \frac{\tan \delta_l(k)}{k^{2l+1}}, \tag{2.1}$$

[by definition, $(-1)!! = 1$], where $\delta_l(k)$ is the l th partial-wave scattering phase shift at the particle wave number k (notice that some authors prefer a definition of a_l with the double factorials omitted). It can be shown (Ref. 48, Sec. 12) that for potentials that asymptotically fall off as

$$V(r) \xrightarrow{r \rightarrow \infty} \text{const} \times r^{-n} + O(r^{-n-\epsilon}) \quad (n > 3, \epsilon > 0) \tag{2.2}$$

the limit in Eq. (2.1) is finite, and thus, a_l does exist, for partial waves with the angular momentum quantum number l constrained by the inequality

$$2l < n - 3. \tag{2.3}$$

The method of evaluation of a_l based on the direct use of the definition (2.1) is impractical, as it requires prior knowledge of the functional form of $\delta_l(k)$ in the neighborhood of the threshold point $k = 0$. The more convenient approach is the following one (cf. Ref. 19). Let $F_l(r)$ be a solution to the zero-energy radial Schrödinger equation in the outer domain,

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) \right] F_l(r) = 0 \quad (r \geq r_s), \tag{2.4}$$

which at $r = r_s$ matches smoothly onto an inner-domain solution that is regular at $r = 0$. The asymptotic form of $F_l(r)$ is

$$F_l(r) \xrightarrow{r \rightarrow \infty} \mathcal{A}_l \left[r^{l+1} - a_l r^{-l} \right], \tag{2.5}$$

where a_l is the scattering length and \mathcal{A}_l is a multiplicative factor. Guided by the form of the right-hand side of Eq. (2.5), we introduce two auxiliary functions $\mathcal{A}_l(r)$ and $a_l(r)$ such that

$$F_l(r) = \mathcal{A}_l(r) \left[r^{l+1} - a_l(r) r^{-l} \right] \tag{2.6a}$$

and

$$\frac{dF_l(r)}{dr} = \mathcal{A}_l(r) \left[(l+1)r^l + la_l(r)r^{-l-1} \right]. \quad (2.6b)$$

It is evident that asymptotically, the function $a_l(r)$ tends to a_l ,

$$a_l = \lim_{r \rightarrow \infty} a_l(r) \quad (2.7)$$

and that $a_l(r)$ may be expressed as

$$a_l(r) = r^{2l+1} \frac{rL_l(r) - (l+1)}{rL_l(r) + l}, \quad (2.8)$$

where

$$L_l(r) = \frac{1}{F_l(r)} \frac{dF_l(r)}{dr} \quad (2.9)$$

is the logarithmic derivative of $F_l(r)$. If $f_l(r)$ and $g_l(r)$ are any two linearly independent solutions to Eq. (2.4), the physical solution $F_l(r)$ is a linear combination of the two,

$$F_l(r) = \alpha_l f_l(r) + \beta_l g_l(r). \quad (2.10)$$

Hence, the logarithmic derivative $L_l(r)$ is

$$L_l(r) = \frac{f_l'(r) + \gamma_l g_l'(r)}{f_l(r) + \gamma_l g_l(r)}, \quad (2.11)$$

where the prime means differentiation with respect to r , while γ_l is the ratio of the coefficients appearing in Eq. (2.10),

$$\gamma_l = \frac{\beta_l}{\alpha_l}. \quad (2.12)$$

If in Eqs. (2.8) and (2.11) we set $r = r_s$ and solve the resulting system for γ_l , this gives

$$\gamma_l = - \frac{(r_s^{2l+1} - a_{ls}) r_s f_l'(r_s) - [(l+1)r_s^{2l+1} + la_{ls}] f_l(r_s)}{(r_s^{2l+1} - a_{ls}) r_s g_l'(r_s) - [(l+1)r_s^{2l+1} + la_{ls}] g_l(r_s)}, \quad (2.13)$$

where

$$a_{ls} = a_l(r_s) \quad (2.14)$$

is a scattering length due to the core part of the potential. Thus, we see that the scattering length a_l may be found from Eqs. (2.7) and (2.8) augmented with Eqs. (2.11) and (2.13). This method is adopted in the present work.

III. SCATTERING LENGTHS FOR POTENTIALS WITH THE TAIL (1.4)

The zero-energy radial Schrödinger equation with the tail potential (1.4) may be written in the form

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{Br^{n-4}}{(r^{n-2} + R^{n-2})^2} + \frac{C}{r^2(r^{n-2} + R^{n-2})} \right] F_l(r) = 0 \quad (r \geq r_s) \quad (3.1)$$

(the constraint $R > 0$ is assumed to hold throughout the rest of the paper). Below, we shall show that this equation may be solved analytically in terms of known special functions. To this end, we switch from the independent variable r to the new one

$$\rho = \frac{r^{n-2} - R^{n-2}}{r^{n-2} + R^{n-2}} \quad (\rho_s \leq \rho \leq 1), \quad (3.2)$$

with

$$\rho_s = \frac{r_s^{n-2} - R^{n-2}}{r_s^{n-2} + R^{n-2}}, \quad (3.3)$$

and from the function $F_l(r)$ to the function

$$\mathcal{F}_l(\rho) = r^{-1/2} F_l(r). \quad (3.4)$$

The new function $\mathcal{F}_l(\rho)$ is found to be a solution to the equation

$$\left[\frac{d}{d\rho} (1 - \rho^2) \frac{d}{d\rho} + \lambda(\lambda + 1) - \frac{\mu^2}{2(1 - \rho)} - \frac{\nu^2}{2(1 + \rho)} \right] \mathcal{F}_l(\rho) = 0 \quad (\rho_s \leq \rho \leq 1), \quad (3.5)$$

with

$$\lambda = \frac{1}{2} \sqrt{1 + \frac{4B}{(n-2)^2 R^{n-2}}} - \frac{1}{2}, \quad (3.6a)$$

$$\mu = \frac{2l + 1}{n - 2} \quad (3.6b)$$

and

$$\nu = \sqrt{\left(\frac{2l + 1}{n - 2} \right)^2 - \frac{4C}{(n - 2)^2 R^{n-2}}}. \quad (3.6c)$$

It should be observed that, in virtue of the inequality (2.3), the parameter μ defined above is constrained to obey

$$0 < \mu < 1. \quad (3.7)$$

Equation (3.5) is the *generalized* associated Legendre equation. Some investigations concerning its solutions had been carried out by Bateman⁴⁹ in the early 1900's, but systematic studies on the subject began only half a century later with the works of Kuipers and Meulenbeld;^{50,51} a summary of relevant results obtained by various researchers up to the year 2000 may be found in the monograph.⁴⁶ The solution to Eq. (3.5) is

$$\mathcal{F}_l(\rho) = \alpha_l P_\lambda^{\mu,\nu}(\rho) + \beta_l P_\lambda^{-\mu,-\nu}(\rho), \quad (3.8)$$

where

$$P_\lambda^{\mu,\nu}(\rho) = \frac{1}{\Gamma(1 - \mu)} \frac{(1 + \rho)^{\nu/2}}{(1 - \rho)^{\mu/2}} {}_2F_1 \left(-\lambda - \frac{\mu - \nu}{2}, \lambda + 1 - \frac{\mu - \nu}{2}; 1 - \mu; \frac{1 - \rho}{2} \right) \quad (3.9)$$

is the *generalized* associated Legendre function of the first kind on the cross-cut $-1 \leq \rho \leq 1$; here, ${}_2F_1(\dots)$ denotes the hypergeometric function. The functions $P_\lambda^{\mu,\nu}(\rho)$ and $P_\lambda^{-\mu,-\nu}(\rho)$ appearing in Eq. (3.8) are linearly independent since their Wronskian

$$W[P_\lambda^{\mu,\nu}(\rho), P_\lambda^{-\mu,-\nu}(\rho)] = -\frac{2 \sin(\pi\mu)}{\pi(1 - \rho^2)} \quad (3.10)$$

does not vanish by virtue of the constraint (3.7) obeyed by μ . Now, as $\rho \rightarrow 1 - 0$ (which corresponds to $r \rightarrow \infty$), the functions $P_\lambda^{\mu,\nu}(\rho)$ and $P_\lambda^{-\mu,-\nu}(\rho)$ behave as

$$P_\lambda^{\mu,\nu}(\rho) \xrightarrow{\rho \rightarrow 1-0} \frac{2^{\nu/2}}{\Gamma(1 - \mu)} (1 - \rho)^{-\mu/2} + O((1 - \rho)^{-\mu/2+1}) \quad (3.11a)$$

and

$$P_\lambda^{-\mu,-\nu}(\rho) \xrightarrow{\rho \rightarrow 1-0} \frac{2^{-\nu/2}}{\Gamma(1 + \mu)} (1 - \rho)^{\mu/2} + O((1 - \rho)^{\mu/2+1}), \quad (3.11b)$$

respectively. On combining Eqs. (3.4), (3.8) and (3.11), we see that the asymptotic behavior of the radial wavefunction $F_l(r)$ is



$$F_l(r) \xrightarrow{r \rightarrow \infty} \alpha_l \frac{2^{(v-\mu)/2}}{\Gamma(1-\mu)} \frac{r^{l+1}}{R^{l+1/2}} + \beta_l \frac{2^{(\mu-v)/2}}{\Gamma(1+\mu)} \frac{R^{l+1/2}}{r^l} + O((r/R)^{l-n+3}). \quad (3.12)$$

Hence, with the use of the method presented in Sec. II, it is found that the scattering length a_l is

$$a_l = R^{2l+1} 2^{\mu-v} \frac{\Gamma(1-\mu)}{\Gamma(1+\mu)} \frac{(r_s^{2l+1} - a_{ls})(1 - \rho_s^2) [dP_\lambda^{\mu,v}(\rho)/d\rho]_{\rho=\rho_s} - \mu(r_s^{2l+1} + a_{ls}) P_\lambda^{\mu,v}(\rho_s)}{(r_s^{2l+1} - a_{ls})(1 - \rho_s^2) [dP_\lambda^{\mu,-v}(\rho)/d\rho]_{\rho=\rho_s} - \mu(r_s^{2l+1} + a_{ls}) P_\lambda^{\mu,-v}(\rho_s)}, \quad (3.13)$$

where a_{ls} is the short-range scattering length.

The presence of derivatives of the generalized Legendre functions makes the formula displayed in Eq. (3.13) impractical for use in actual applications. However, at this moment, we may exploit either the relation [Ref. 52, Eq. (25)]

$$(\lambda + 1)(1 - \rho^2) \frac{dP_\lambda^{\mu,v}(\rho)}{d\rho} = \left[(\lambda + 1)^2 \rho + \frac{\mu^2 - v^2}{4} \right] P_\lambda^{\mu,v}(\rho) - \left(\lambda + 1 - \frac{\mu - v}{2} \right) \left(\lambda + 1 + \frac{\mu + v}{2} \right) P_{\lambda+1}^{\mu,v}(\rho) \quad (3.14a)$$

or the relation

$$\lambda(1 - \rho^2) \frac{dP_\lambda^{\mu,v}(\rho)}{d\rho} = - \left(\lambda^2 \rho + \frac{\mu^2 - v^2}{4} \right) P_\lambda^{\mu,v}(\rho) + \left(\lambda + \frac{\mu - v}{2} \right) \left(\lambda + \frac{\mu + v}{2} \right) P_{\lambda-1}^{\mu,v}(\rho), \quad (3.14b)$$

where the latter emerges when the expression in Eq. (3.14a) is combined with the identity [Ref. 52, Eq. (7)]

$$(2\lambda + 1) \left[\lambda(\lambda + 1)\rho + \frac{\mu^2 - v^2}{4} \right] P_\lambda^{\mu,v}(\rho) = \lambda \left(\lambda + 1 - \frac{\mu - v}{2} \right) \left(\lambda + 1 + \frac{\mu + v}{2} \right) P_{\lambda+1}^{\mu,v}(\rho) + (\lambda + 1) \left(\lambda + \frac{\mu - v}{2} \right) \left(\lambda + \frac{\mu + v}{2} \right) P_{\lambda-1}^{\mu,v}(\rho). \quad (3.15)$$

This allows us to replace the formula in Eq. (3.13) with either of the following two:

$$a_l = R^{2l+1} 2^{\mu-v} \frac{\Gamma(1-\mu)}{\Gamma(1+\mu)} \frac{\left\{ \begin{array}{l} r_s^{2l+1} [(\lambda + 1)^2 \rho_s - \mu(\lambda + 1) + (\mu^2 - v^2)/4] \\ - a_{ls} [(\lambda + 1)^2 \rho_s + \mu(\lambda + 1) + (\mu^2 - v^2)/4] \end{array} \right\} P_\lambda^{\mu,v}(\rho_s)}{\left\{ \begin{array}{l} r_s^{2l+1} [(\lambda + 1)^2 \rho_s - \mu(\lambda + 1) + (\mu^2 - v^2)/4] \\ - (r_s^{2l+1} - a_{ls}) [\lambda + 1 - (\mu - v)/2] [\lambda + 1 - (\mu + v)/2] \end{array} \right\} P_{\lambda+1}^{\mu,v}(\rho_s)} \quad (3.16a)$$

or

$$a_l = R^{2l+1} 2^{\mu-v} \frac{\Gamma(1-\mu)}{\Gamma(1+\mu)} \frac{\left\{ \begin{array}{l} r_s^{2l+1} [\lambda^2 \rho_s + \mu\lambda + (\mu^2 - v^2)/4] \\ - a_{ls} [\lambda^2 \rho_s - \mu\lambda + (\mu^2 - v^2)/4] \end{array} \right\} P_\lambda^{\mu,v}(\rho_s)}{\left\{ \begin{array}{l} r_s^{2l+1} [\lambda^2 \rho_s + \mu\lambda + (\mu^2 - v^2)/4] \\ - (r_s^{2l+1} - a_{ls}) [\lambda + (\mu - v)/2] [\lambda + (\mu + v)/2] \end{array} \right\} P_{\lambda-1}^{\mu,v}(\rho_s)}. \quad (3.16b)$$

Equations (3.16a) and (3.16b) constitute the main result of this paper. In Sec. IV, we shall investigate particular cases when these two expressions may be simplified.

IV. CASES WHEN EQS. (3.16a) AND (3.16b) SIMPLIFY

A. The case of $B = 0$

For $B = 0$, the tail potential (1.4) is

$$V(r) = -\frac{\hbar^2}{2m} \frac{C}{r^2(r^{n-2} + R^{n-2})} \quad (r \geq r_s), \tag{4.1}$$

and it holds that

$$\lambda = 0 \tag{4.2}$$

[cf. Eq. (3.6a)]. As a consequence, Eq. (3.16a) becomes

$$a_l = R^{2l+1} 2^{\mu-\nu} \frac{\Gamma(1-\mu)}{\Gamma(1+\mu)} \frac{\left\{ \begin{array}{l} r_s^{2l+1} [\rho_s - \mu + (\mu^2 - \nu^2)/4] \\ - a_{ls} [\rho_s + \mu + (\mu^2 - \nu^2)/4] \end{array} \right\} P_0^{\mu,\nu}(\rho_s) - \left(r_s^{2l+1} - a_{ls} \right) [1 - (\mu - \nu)/2] [1 - (\mu + \nu)/2] P_1^{\mu,\nu}(\rho_s)}{\left\{ \begin{array}{l} r_s^{2l+1} [\rho_s - \mu + (\mu^2 - \nu^2)/4] \\ - a_{ls} [\rho_s + \mu + (\mu^2 - \nu^2)/4] \end{array} \right\} P_0^{-\mu,-\nu}(\rho_s) - \left(r_s^{2l+1} - a_{ls} \right) [1 + (\mu - \nu)/2] [1 + (\mu + \nu)/2] P_1^{-\mu,-\nu}(\rho_s)}, \tag{4.3}$$

while Eq. (3.16b) leads to an expression for a_l of the 0/0 type since it holds that

$$P_{-1}^{\pm\mu,\pm\nu}(\rho_s) = P_0^{\pm\mu,\pm\nu}(\rho_s). \tag{4.4}$$

B. The case of $C = 0$

For $C = 0$, the tail potential (1.4) reduces to the Lenz one displayed in Eq. (1.3),

$$V(r) = -\frac{\hbar^2}{2m} \frac{Br^{n-4}}{(r^{n-2} + R^{n-2})^2} \quad (r \geq r_s). \tag{4.5}$$

From Eqs. (3.6b) and (3.6c), one infers that now the parameters μ and ν are equal,

$$\nu = \mu. \tag{4.6}$$

Since it holds that

$$P_\lambda^{\mu,\mu}(\rho) = P_\lambda^\mu(\rho), \tag{4.7}$$

where $P_\lambda^\mu(\rho)$ is the well-known associated Legendre function of the first kind on the cross-cut $-1 \leq \rho \leq 1$ (Ref. 53, Sec. 4.3), in the case under study, Eq. (3.16a) and (3.16b) simplify and go over into

$$a_l = R^{2l+1} \frac{\Gamma(1-\mu)}{\Gamma(1+\mu)} \frac{\left\{ r_s^{2l+1} [(\lambda+1)\rho_s - \mu] - a_{ls} [(\lambda+1)\rho_s + \mu] \right\} P_\lambda^\mu(\rho_s) - \left(r_s^{2l+1} - a_{ls} \right) (\lambda+1-\mu) P_{\lambda+1}^\mu(\rho_s)}{\left\{ r_s^{2l+1} [(\lambda+1)\rho_s - \mu] - a_{ls} [(\lambda+1)\rho_s + \mu] \right\} P_\lambda^{-\mu}(\rho_s) - \left(r_s^{2l+1} - a_{ls} \right) (\lambda+1+\mu) P_{\lambda+1}^{-\mu}(\rho_s)} \tag{4.8a}$$

and

$$a_l = R^{2l+1} \frac{\Gamma(1-\mu)}{\Gamma(1+\mu)} \frac{\left[r_s^{2l+1} (\lambda\rho_s + \mu) - a_{ls} (\lambda\rho_s - \mu) \right] P_\lambda^\mu(\rho_s) - \left(r_s^{2l+1} - a_{ls} \right) (\lambda+\mu) P_{\lambda-1}^\mu(\rho_s)}{\left[r_s^{2l+1} (\lambda\rho_s + \mu) - a_{ls} (\lambda\rho_s - \mu) \right] P_\lambda^{-\mu}(\rho_s) - \left(r_s^{2l+1} - a_{ls} \right) (\lambda-\mu) P_{\lambda-1}^{-\mu}(\rho_s)}, \tag{4.8b}$$

respectively. Up to notational differences, Eq. (4.8a) coincides with Eq. (52) in Ref. 19.

C. The hard-core potential

The next class of potentials we wish to consider are those with hard cores,

$$V(r) = \begin{cases} +\infty & \text{for } r < r_s, \\ -\frac{\hbar^2}{2m} \frac{Br^{n-4}}{(r^{n-2} + R^{n-2})^2} - \frac{\hbar^2}{2m} \frac{C}{r^2(r^{n-2} + R^{n-2})} & \text{for } r \geq r_s. \end{cases} \quad (4.9)$$

Then, the short-range scattering length is simply

$$a_{ls} = r_s^{2l+1} \quad (4.10)$$

so that either of Eq. (3.16a) or Eq. (3.16b) reduces to

$$a_l = R^{2l+1} 2^{\mu-v} \frac{\Gamma(1-\mu)}{\Gamma(1+\mu)} \frac{P_\lambda^{\mu,v}(\rho_s)}{P_\lambda^{-\mu,-v}(\rho_s)}. \quad (4.11)$$

The application of the identity [Ref. 46, Eq. (4.2)]

$$P_\lambda^{\mu,v}(\rho) = 2^v P_\lambda^{\mu,-v}(\rho) \quad (4.12)$$

casts Eq. (4.11) into

$$a_l = R^{2l+1} 2^\mu \frac{\Gamma(1-\mu)}{\Gamma(1+\mu)} \frac{P_\lambda^{\mu,-v}(\rho_s)}{P_\lambda^{-\mu,-v}(\rho_s)}. \quad (4.13)$$

The latter formula will be used in Sec. IV D.

D. The pure potential with $C < 0$

Finally, we wish to consider a potential that is of the form (1.4) throughout the whole space \mathbb{R}^3 , i.e., such that

$$V(r) = -\frac{\hbar^2}{2m} \frac{Br^{n-4}}{(r^{n-2} + R^{n-2})^2} - \frac{\hbar^2}{2m} \frac{C}{r^2(r^{n-2} + R^{n-2})} \quad (r \geq 0), \quad (4.14)$$

under an additional constraint that it is repulsive near the origin,

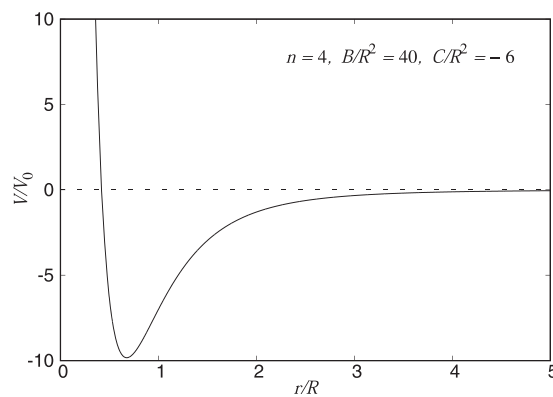


FIG. 1. A sample pure potential (4.14) with $n = 4$, $B/R^2 = 40$, and $C/R^2 = -6$. The potential normalization parameter V_0 equals $\hbar^2/2mR^2$.

$$C < 0 \quad (4.15)$$

(a sample potential function of that sort is depicted in Fig. 1). An expression for the scattering length for such a potential may be derived most conveniently from Eq. (4.13) by taking the limit $\rho_s \rightarrow -1 + 0$ (which corresponds to the limit $r_s \rightarrow 0$). On using Eq. (3.9) and the Gauss' identity (Ref. 53, p. 40)

$${}_2F_1(a_1, a_2; b; 1) = \frac{\Gamma(b)\Gamma(b-a_1-a_2)}{\Gamma(b-a_1)\Gamma(b-a_2)} \quad [\operatorname{Re}(b-a_1-a_2) > 0], \quad (4.16)$$

we eventually find that the l th partial-wave scattering length for the pure potential (4.14) constrained by Eq. (4.15) is

$$a_l = R^{2l+1} \frac{\Gamma(1-\mu)\Gamma(\lambda+1+\frac{\mu+\nu}{2})\Gamma(-\lambda+\frac{\mu+\nu}{2})}{\Gamma(1+\mu)\Gamma(\lambda+1-\frac{\mu-\nu}{2})\Gamma(-\lambda-\frac{\mu-\nu}{2})}. \quad (4.17)$$

V. CONCLUDING REMARKS

The aim of this paper has been to show that there exists still another class of central potentials—those with the long-range tails (1.4) and the asymptotic representation (1.5)—for which partial-wave scattering lengths a_l may be obtained in analytical forms. Whilst expressions for a_l for potentials with the tails (1.1)–(1.3) considered earlier in Ref. 19 contain Bessel, Whittaker, and the associated Legendre functions, respectively, the present case involves lesser-known *generalized* associated Legendre functions.

In two particular cases, namely, for $n = 4$ and for $n = 6$, the potentials (1.4) may find applications in atomic physics. If $n = 4$, the resulting tail potential

$$V(r) = -\frac{\hbar^2}{2m} \frac{B}{(r^2 + R^2)^2} - \frac{\hbar^2}{2m} \frac{C}{r^2(r^2 + R^2)} \quad (r \geq r_s) \quad (5.1)$$

may be used to model a long-range polarization interaction between a charged particle and an atom. On the other hand, with $n = 6$ one obtains the potential function

$$V(r) = -\frac{\hbar^2}{2m} \frac{Br^2}{(r^4 + R^4)^2} - \frac{\hbar^2}{2m} \frac{C}{r^2(r^4 + R^4)} \quad (r \geq r_s), \quad (5.2)$$

which may imitate the van der Waals attraction between two atoms.

REFERENCES

- ¹U. Fano and A. R. P. Rau, *Atomic Collisions and Spectra* (Academic, Orlando, FL, 1986).
- ²H. R. Sadeghpour, J. L. Bohn, M. J. Cavagnero, B. D. Esry, I. I. Fabrikant, J. H. Macek, and A. R. P. Rau, "Collisions near threshold in atomic and molecular physics," *J. Phys. B: At. Mol. Opt. Phys.* **33**, R93 (2000).
- ³M. Borkowski, R. Muñoz Rodriguez, M. B. Kosicki, R. Ciurylo, and P. S. Żuchowski, "Optical Feshbach resonances and ground-state-molecule production in the RbHg system," *Phys. Rev. A* **96**, 063411 (2017).
- ⁴A. Guttridge, M. D. Frye, B. C. Yang, J. M. Hutson, and S. L. Cornish, "Two-photon photoassociation spectroscopy of CsYb: Ground-state interaction potential and interspecies scattering lengths," *Phys. Rev. A* **98**, 022707 (2018).
- ⁵A. Temkin, "Polarization and the triplet electron–hydrogen scattering length," *Phys. Rev. Lett.* **6**, 354 (1961).
- ⁶T. Tietz, "Elastic scattering of low-energy electrons and the periodic system of elements," *J. Chem. Phys.* **38**, 1027 (1963).
- ⁷T. Tietz and C. Malinowska, "Note concerning the elastic scattering of low-energy electrons in Thomas–Fermi theory," *J. Chem. Phys.* **39**, 2778 (1963).
- ⁸T. Tietz, "Pressure shift of the high series of the alkali metals," *Nuovo Cimento* **28**, 1509 (1963).
- ⁹T. Tietz, "Low energy electron–atom scattering cross-section in Thomas–Fermi theory," *Z. Naturforsch. A* **21**, 360 (1966).
- ¹⁰T. Tietz, "The elastic scattering of low energy electrons in Thomas–Fermi theory," in: *VII International Conference on the Physics of Electronic and Atomic Collisions*, edited by L. M. Branscomb *et al.* (North-Holland, Amsterdam, 1971), Vol. 1, p. 81.
- ¹¹S. H. Patil, "Analytic scattering length for potential scattering," *Phys. Rev. A* **24**, 3038 (1981).
- ¹²J. Horaček, "Analytic scattering length and critical constants for potential scattering," *J. Phys. A: Math. Gen.* **20**, 2699 (1987).
- ¹³R. Szymtkowski, "Calculation of the electron scattering lengths for noble atoms," *Fizika* **22**, 481 (1990).
- ¹⁴R. Szymtkowski, "On the exact calculation of the scattering lengths for long range potentials. I. The inverse power potentials," *Acta Phys. Pol.* **A 78**, 517 (1990).
- ¹⁵R. Szymtkowski, "On the exact calculation of the scattering lengths for long range potentials. II. Lenz potentials," *Acta Phys. Pol.* **A 79**, 613 (1991).
- ¹⁶G. F. Gribakin and V. V. Flambaum, "Calculation of the scattering length in atomic collisions using the semiclassical approximation," *Phys. Rev. A* **48**, 546 (1993).
- ¹⁷M. Marinescu, "Computation of the scattering length and effective range in molecular physics," *Phys. Rev. A* **50**, 3177 (1994).
- ¹⁸R. Szymtkowski, "Calculation of the electron-scattering lengths for rare-gas atoms," *Phys. Rev. A* **51**, 853 (1995).
- ¹⁹R. Szymtkowski, "Analytical calculations of scattering lengths in atomic physics," *J. Phys. A: Math. Gen.* **28**, 7333 (1995).
- ²⁰R. Szymtkowski, "Analytical independent-particle model for electron scattering by argon at low energy," *Few-Body Syst.* **20**, 175 (1996).

- ²¹J. A. Kunc, “Low-energy electron–atom scattering in a field of model potentials,” *J. Phys. B: At. Mol. Opt. Phys.* **32**, 607 (1999).
- ²²C. Eltschka, M. J. Moritz, and H. Friedrich, “Near-threshold quantization and scattering for deep potentials with attractive tails,” *J. Phys. B: At. Mol. Opt. Phys.* **33**, 4033 (2000).
- ²³B. Gao, “Zero-energy or quasibound states and their implications for diatomic systems with an asymptotic van der Waals interaction,” *Phys. Rev. A* **62**, 050702 (2000).
- ²⁴M. J. Jamieson and B. Zygelman, “Mass dependence of scattering lengths for hydrogen atoms,” *Phys. Rev. A* **64**, 032703 (2001).
- ²⁵G. Jacoby and H. Friedrich, “Near-threshold properties of a $1/r^4$ plus $1/r^5$ potential tail,” *J. Phys. B: At. Mol. Opt. Phys.* **35**, 4839 (2002).
- ²⁶B. Gao, “Effective potentials for atom–atom interactions at low temperatures,” *J. Phys. B: At. Mol. Opt. Phys.* **36**, 2111 (2003).
- ²⁷H. Ouerdane, M. J. Jamieson, D. Vrinceanu, and M. J. Cavagnero, “The variable phase method used to calculate and correct scattering lengths,” *J. Phys. B: At. Mol. Opt. Phys.* **36**, 4055 (2003).
- ²⁸B. Gao, “Binding energy and scattering length for diatomic systems,” *J. Phys. B: At. Mol. Opt. Phys.* **37**, 4273 (2004).
- ²⁹R. Szymtkowski and K. Mielewczyk, “Exact analytical scattering lengths for a class of long-range potentials with r^{-4} asymptotics,” *Phys. Rev. A* **69**, 064701 (2004).
- ³⁰A. Crubellier and E. Luc-Koenig, “Threshold effects in the photoassociation of cold atoms: R^{-6} model in the Milne formalism,” *J. Phys. B: At. Mol. Opt. Phys.* **39**, 1417 (2006).
- ³¹J. Pade, “Exact scattering length for a potential of Lennard-Jones type,” *Eur. Phys. J. D* **44**, 345 (2007).
- ³²A. S. Dickinson, “Semiclassical approximation for the scattering volume in cold-atom collisions,” *J. Phys. B: At. Mol. Opt. Phys.* **41**, 175302 (2008).
- ³³H. Friedrich and P. Raab, “Near-threshold quantization and scattering lengths,” *Phys. Rev. A* **77**, 012703 (2008).
- ³⁴M. S. Hussein, W. Li, and S. Wüster, “Canonical quantum potential scattering theory,” *J. Phys. A: Math. Gen.* **51**, 475207 (2008).
- ³⁵P. Raab and H. Friedrich, “Near the threshold of potentials—Quantization rules and scattering lengths,” *J. Phys.: Conf. Ser.* **99**, 012015 (2008).
- ³⁶J. Pade, “Exact solutions of the Schrödinger equation for zero-energy,” *Eur. Phys. J. D* **53**, 41 (2009).
- ³⁷P. Raab and H. Friedrich, “Quantization function for potentials with $-1/r^4$ tails,” *Phys. Rev. A* **80**, 052705 (2009).
- ³⁸S. Gautam and D. Angom, “Scattering length for fermionic alkali atoms,” *Eur. Phys. J. D* **56**, 173 (2010).
- ³⁹M. J. Jamieson, A. S. C. Cheung, and H. Ouerdane, “Dependence of the scattering length for hydrogen atoms on effective mass,” *Eur. Phys. J. D* **56**, 181 (2010).
- ⁴⁰H. Ouerdane and M. J. Jamieson, “Comment on “Scattering length for fermionic alkali atoms,”” *Eur. Phys. J. D* **57**, 325 (2010).
- ⁴¹M. J. Jamieson and H. Ouerdane, “Error cancellation in the semiclassical calculation of the scattering length,” *Eur. Phys. J. D* **61**, 373 (2011).
- ⁴²V. V. Meshkov, A. V. Stolyarov, and R. J. Le Roy, “Rapid, accurate calculation of the s -wave scattering length,” *J. Chem. Phys.* **135**, 154108 (2011).
- ⁴³T.-O. Müller, A. Kaiser, and H. Friedrich, “ s -wave scattering for deep potentials with attractive tails falling off faster than $-1/r^2$,” *Phys. Rev. A* **84**, 032701 (2011).
- ⁴⁴F. J. Gómez and J. Sesma, “Scattering length for Lennard-Jones potentials,” *Eur. Phys. J. D* **66**, 6 (2012).
- ⁴⁵B. Gao, “Quantum-defect theory for $-1/r^4$ -type interactions,” *Phys. Rev. A* **88**, 022701 (2013).
- ⁴⁶N. Virchenko and I. Fedotova, *Generalized Associated Legendre Functions and Their Applications* (World Scientific, Singapore, 2001).
- ⁴⁷We follow the terminology adopted in Ref. 19 and call a_l the scattering length whatever the value of l is. However, it is evident from the definition (2.1) that the physical dimension of a_l is (length)^{2l+1}, i.e., a_0 has the physical dimension of length, a_1 has the physical dimension of volume, and so on.
- ⁴⁸V. V. Babikov, *Method of Phase Functions in Quantum Mechanics*, 3rd ed. (Nauka, Moscow, 1988) (in Russian).
- ⁴⁹H. Bateman, “A generalisation of the Legendre polynomial,” *Proc. London Math. Soc.* **3**, 111 (1905).
- ⁵⁰L. Kuipers and B. Meulenbeld, “On a generalisation of Legendre’s associated differential equation. I,” *Indag. Math.* **19**, 436 (1957).
- ⁵¹L. Kuipers and B. Meulenbeld, “On a generalisation of Legendre’s associated differential equation. II,” *Indag. Math.* **19**, 444 (1957).
- ⁵²L. Kuipers, “Relations between contiguous generalized Legendre associated functions (recurrence formulas),” *Math. Scand.* **6**, 200 (1958).
- ⁵³W. Magnus, F. Oberhettinger, and R. P. Soni, *Formulas and Theorems for the Special Functions of Mathematical Physics*, 3rd ed. (Springer, Berlin, 1966).