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Analytic scattering length and critical constants for potential scattering

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Abstract. Two analytic expressions for the scattering length dependent on the coupling constant λ are proposed. These expressions possess an infinite range of convergence unlike previous attempts. As a possible application we discuss the scattering length for collisions of electrons with rare gases, calculation of critical constants for short-range potentials and calculation of Sturmians.

1. Introduction

The scattering length plays an important role in low-energy scattering in a large variety of physical scattering processes. Its dependence on the coupling constant λ is quite complicated. Starting from zero at $\lambda = 0$, it passes through poles and zeros with increasing λ. Appearance of a pole indicates the existence of a new zero-energy bound state. Not only the overall coupling constant dependence of the scattering length is important, but also its dependence on other parameters like the screening parameter which plays a significant role in the scattering of electrons on rare gases where it is related to the Ramsauer-Townsend effect.

There are, of course, numerical methods for evaluation of the scattering length but they do not elucidate its dependence on the various parameters of interest.

An important step forward in the investigation of the analytic dependence of the scattering length on the coupling constant λ has been performed by Patil (1981), who proposed an expansion of the inverse of the scattering length $a^{-1}(\lambda)$ in the form

$$a^{-1}(\lambda) = -\frac{1}{2\lambda\beta} - \frac{1}{2\beta}\sum_{n=1}^{\infty} b_n \lambda^{n-1} \tag{1.1}$$

where β and b_n are certain integrals. He studied a special class of potentials, the screened Coulomb potentials, which can be written in the form

$$V(r) = -(Z/r) f(r/r_0) \tag{1.2}$$

where r_0 is the screening parameter for which the screening becomes significant when $r > r_0$. Although such potentials are functions of the two parameters Z and r_0, the scattering length is a function of essentially only one parameter, namely the effective coupling constant

$$\lambda = Z r_0. \tag{1.3}$$

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The region of convergence of the expansion (1.1) is restricted below the first zero of $a(\lambda)$. This is a rather severe limitation which prevents the method being used, for example, for heavier atoms such as Ar, Kr and Xe.

In this paper we propose two expansions of the scattering length which do not suffer from this restriction. They are valid in principle for any effective coupling constant λ. Both our expressions also prove very effective tools for calculation of the critical constants, i.e. such values of λ for which there exist zero-energy bound states. A knowledge of the critical constants is very important for the study of ionised gases. For example, the partition function for the isolated hydrogen atom

$$Z = \sum_{n=1}^{\infty} 2n^2 \exp\left(\frac{Ry}{n^2 kT}\right) \tag{1.4}$$

diverges. In any real physical situation the electric field is not purely Coulombic but is screened by other atoms. The resulting potential decreases faster and Z is finite containing only a finite number of terms.

As a last application of our formulae we discuss the calculation of Sturmian functions.

The paper is organised as follows. The expansions for the scattering length are developed in § 2. Section 3 contains applications to (i) calculation of the scattering length for the collision of electrons with rare gas atoms, (ii) calculation of the critical constants for some typical short-range potentials and (iii) calculation of Sturmians.

2. Expansions of the scattering length

In this section we develop two expansions for the scattering length. The first expansion is based on a reduction of the Schrödinger equation to a Volterra-type integral equation and the second is based on the Fredholm equation. First we shall discuss the Volterra equation (VE) approach. Let us assume that the potential V is local and satisfies the condition

$$\int_0^{\infty} \mathrm{d}r\, r|V(r)| < \infty.$$

The scattering wavefunction $\psi_l(k, r)$, regular at the origin, is given by the following equation:

$$\psi_l(k, r) = j_l(kr) + \int_0^{\infty} G_l(k; r, r')\, V(r')\psi_l(k, r')\, \mathrm{d}r' \tag{2.1}$$

where

$$G_l(k; r, r') = \begin{cases} j_l(kr)n_l(kr') & r < r' \\ n_l(kr)j_l(kr') & r > r' \end{cases} \tag{2.2}$$

and $j_l(kr)$ and $n_l(kr)$ are Riccatti-Bessel functions. The phase shift $\delta_l(k)$ is given by the standard relation

$$\tan \delta_l(k) = \int_0^{\infty} j_l(kr)\, V(r)\psi_l(k, r)\, \mathrm{d}r. \tag{2.3}$$

Since we shall treat zero-energy S-wave scattering only we shall omit all unnecessary indices and write (2.1) explicitly as

$$\psi(r) = r - \int_0^r yV(y)\psi(y)\,dy - r\int_r^\infty V(y)\psi(y)\,dy \tag{2.4}$$

and the scattering length a as

$$a = \int_0^\infty yV(y)\psi(y)\,dy. \tag{2.5}$$

Equation (2.1) is of Fredholm type but can be transformed by a simple transformation of the Green function $G_0 \to g_0$†

$$G_0(0; r, r') \to g_0(0; r, r') = (r - r')\Theta(r - r') \tag{2.6}$$

where Θ is the Heaviside step function, to an equation

$$\psi(r) = r\left(1 - \int_0^\infty V(y)\psi(y)\,dy\right) - \int_0^r (y - r)V(y)\psi(y)\,dy \tag{2.7}$$

which is of Volterra type. The quantity in the bracket on the RHS of (2.7) is of course not known but this provides no problem. Instead of (2.7) the following auxiliary equation is solved first:

$$\varphi(r) = r - \int_0^r (y - r)V(y)\varphi(y)\,dy \tag{2.8}$$

and then ψ and a are expressed by means of φ as

$$\psi = \frac{\varphi(r)}{1 + \int_0^\infty V(y)\varphi(y)\,dy} \tag{2.9}$$

$$a = \frac{\int_0^\infty yV(y)\varphi(y)\,dy}{1 + \int_0^\infty V(y)\varphi(y)\,dy}. \tag{2.10}$$

Let us now explicitly introduce the coupling constant λ into consideration, i.e. we will write λV instead of V in (2.8). Since this equation is a Volterra-type equation its unique solution is given by the series

$$\varphi = f + \lambda g_0 Vf + (\lambda g_0 V)^2 f + \ldots \tag{2.11}$$

which is absolutely and uniformly convergent for any λ (Newton 1982). (f here denotes the first term on the RHS of (2.8).) Denoting by p_n and q_n the integrals

$$p_n = \int_0^\infty yV(y)(g_0 V)^n f(y)\,dy \tag{2.12}$$

$$q_n = \int_0^\infty V(y)(g_0 V)^n f(y)\,dy \tag{2.13}$$

and using (2.10) and (2.11) we obtain the sought-after expansion of the scattering length, namely

$$a(\lambda) = \lambda \frac{\Sigma_0^\infty p_n \lambda^n}{1 + \Sigma_0^\infty q_m \lambda^m} \tag{2.14}$$

† For details of this transformation see Sasakawa (1977).

or, for its inverse,

$$a^{-1}(\lambda)=\frac{1}{\lambda}\frac{1+\Sigma_0^\infty q_m\lambda^m}{\Sigma_0^\infty p_n\lambda^n}. \tag{2.15}$$

This is our first result. The series in (2.14) (resp (2.15)) are convergent for any λ. Equation (2.15) should be compared with Patil's expansion (1.1) which, unlike our expansion, is valid only for $|\lambda|<|\lambda_0|$ where λ_0 is the first zero of $a(\lambda)$. It should be stressed, however, that our statement about the convergence of (2.14) (resp (2.15)) is correct only for local potentials V. If V is a non-local potential, then our expansion also has a limited range of convergence. In order to obtain an expansion which would be convergent for any λ, even in the case of a non-local potential, we must use a completely different approach. Some time ago we proposed the method of continued fractions (MCF) (Horáček and Sasakawa 1983, 1984, 1985). This approach is based on a repeated decomposition of the potential V into two terms, one of which is separable:

$$V=V_1+\frac{V|f\rangle\langle f|V}{\langle f|V|f\rangle} \tag{2.16}$$

$$V_1=V_2+\frac{V_1|f_1\rangle\langle f_1|V_1}{\langle f_1|V_1|f_1\rangle} \tag{2.17}$$

etc, where $|f_1\rangle=G_0V|f\rangle$. We will not go into details of this method here and refer readers to the original papers. Here we quote only some results. This method yields the scattering length (t or K matrix elements) in the form of a continued fraction:

$$a(\lambda)=\cfrac{\lambda d_0^2}{d_0-\lambda d_1-\cfrac{\lambda^2 d_2^2}{d_2-\lambda d_3-\cfrac{\lambda^2 d_4^2}{d_4-\lambda d_5-\ldots}}}. \tag{2.18}$$

This expansion is convergent for any λ provided the operator G_0V is compact. This is our second expression for the scattering length. It is useful for local as well as for non-local potentials and for separable N-term potentials gives exact results.

3. Applications

3.1. Calculation of the scattering length

First we apply our results to the calculation of the scattering length for the Coulomb screened potential of the form

$$V(r)=-(Z/r)f(r/r_0). \tag{3.1}$$

As noted in the introduction, the scattering length of such potentials depends only on the effective coupling constant λ,

$$\lambda=Zr_0. \tag{3.2}$$

For the sake of comparison we consider the same examples as Patil (1981), namely

(i) the Yukawa potential

$$V(r)=-(Z/r)\exp(-r/r_0) \tag{3.3}$$

and

(ii) a potential describing the polarisation interaction

$$V(r) = -\frac{Z}{r}\left(1 - \frac{r}{(r^3 + r_0^3)^{1/3}}\right) \tag{3.4}$$

which has an asymptotic behaviour

$$V(r) \underset{r\to\infty}{\sim} -Zr_0^3/3r^4. \tag{3.5}$$

First we discuss case (i). The coefficients of the MCF expansion for the scattering length, i.e. of equation (2.18), are shown in table 1 and that of the VE expansion (2.14) in table 2. A comparison of both expressions is shown in tables 3 and 4 where the scattering length is given as a function of the coupling constant λ and the number N of terms of the respective expansions. For the same accuracy, the MCF requires a much smaller number of terms than the VE approach.

Table 1. The coefficients d_i for the continued fraction expansion (2.18) of the scattering length for a Yukawa potential.

i	d_i	i	d_i
1	-2	10	$-2.118\,312\times10^{-9}$
2	-2	11	$-2.320\,415\times10^{-11}$
3	$-3.014\,566\times10^{-1}$	12	$-1.009\,208\times10^{-12}$
4	$-1.154\,714\times10^{-1}$	13	$-8.112\,355\times10^{-15}$
5	$-5.139\,451\times10^{-3}$	14	$-2.594\,356\times10^{-16}$
6	$-8.863\,615\times10^{-4}$	15	$-1.595\,465\times10^{-18}$
7	$-2.197\,874\times10^{-5}$	16	$-3.908\,622\times10^{-20}$
8	$-2.142\,731\times10^{-6}$	17	$-1.898\,278\times10^{-22}$
9	$-3.386\,870\times10^{-8}$	18	$-3.676\,149\times10^{-24}$

Table 2. The coefficients p_i and q_i for the VE expansion (2.14) of the scattering length for a Yukawa potential.

i	p_i	q_i
0	-1	-1
1	0.5	0.306 8528
2	$-0.945\,3491\times10^{-1}$	$-0.452\,2874\times10^{-1}$
3	$0.958\,5373\times10^{-2}$	$0.390\,5938\times10^{-2}$
4	$-0.609\,8587\times10^{-3}$	$-0.221\,3592\times10^{-3}$
5	$0.266\,8709\times10^{-4}$	$0.886\,0573\times10^{-5}$
6	$-0.853\,5578\times10^{-6}$	$-0.263\,7732\times10^{-6}$
7	$0.208\,4031\times10^{-7}$	$0.606\,7522\times10^{-8}$
8	$-0.401\,3496\times10^{-9}$	$-0.111\,0724\times10^{-9}$
9	$0.625\,4395\times10^{-11}$	$0.165\,6487\times10^{-11}$
10	$-0.805\,0213\times10^{-13}$	$-0.205\,1328\times10^{-13}$
11	$0.870\,3897\times10^{-15}$	$0.214\,2970\times10^{-15}$
12	$-0.801\,7377\times10^{-17}$	$-0.191\,3911\times10^{-17}$

Table 3. The scattering length for a Yukawa potential calculated using the continued fraction expansion (2.18) for various values of the coupling constants λ. N denotes the number of terms in the expansion (2.18).

N/λ	2	4	6	8
0.5	−2.206 803	−2.206 918	—	—
1.5	2.179 976	2.128 413	2.128 412	—
2.5	−3.793 267	−1.115 844	−1.116 159	−1.116 159
3.5	−8.138 038	10.571 002	10.526 576	10.526 575
4.5	13.962 126	2.975 252	2.946 516	2.946 512
5.5	6.509 792	1.141 251	1.024 770	1.024 724
6.5	4.964 558	−1.737 672	−2.928 304	−2.929 859

Table 4. The same quantity as in table 3 but calculated using the VE expansion (2.14).

N/λ	5	10	15	20
0.5	−2.207 087	−2.206 918	−2.206 918	−2.206 918
1.5	2.154 397	2.128 412	2.128 412	2.128 412
2.5	0.995 715	−1.116 202	−1.116 159	−1.116 159
3.5	2.635 549	10.519 69	10.526 58	10.526 578
4.5	2.959 359	2.951 658	2.946 513	2.946 513
5.5	2.965 683	1.168 734	1.024 724	1.024 725
6.5	2.948 192	−0.018 007	−2.929 919	−2.929 856

Case (ii) is a little more complicated because of the long-range behaviour of the interaction (3.4). The variable phase equation for the scattering length

$$\frac{\mathrm{d}}{\mathrm{d}r}a(r) = -2\lambda V(r)(r+a(r))^2 \tag{3.6}$$

indicates that for the interaction (3.4), $a(r)$ behaves as r^{-1} for large r and therefore must be calculated to very large distances. This is very impractical. To avoid this complication we propose the following. We calculate the scattering length by means of equation (2.14) or (2.18) on a finite large interval $(0, R)$ and obtain a scattering length a_R which corresponds to a cutted potential (3.4), i.e. $V(r)=0$ for $r>R$. For sufficiently large R the neglected remainder $a-a_R$ is small and may be treated as a perturbation. By expanding the remainder $a-a_R$ in powers of $1/R$ and keeping only a few terms we arrive at an approximate expression for a:

$$a(\lambda) \sim \frac{a_R + 2\lambda/3R - 8\lambda^2/27R^3}{1-2\lambda/3R^2-(2\lambda/9R^3)(a_R+2\lambda/3R)} \tag{3.7}$$

which is good for sufficiently large R. We tested this expression for several values of R ranging from 50 to 500 and various λ. In table 5 we show the results obtained by nine iterations of the MCF together with the results of numerical solution of the Schrödinger equation. From this table we conclude that nine terms in the MCF expansion (2.18) yield results useful for λ as large as 20. This allows us to apply our formula also to other noble gases like argon where $\lambda = 17.52$ and, with somewhat lesser accuracy, to krypton with $\lambda = 31.92$.

Table 5. The scattering length a calculated using the continued fraction expansion (2.18) with $N = 9$ for the long-range polarisation potential (3.4). The last column contains values of the scattering length obtained from numerical solution of the Schrödinger equation in its differential form.

	a_{MCF}	a_{NUM}
2	−1.398 168	−1.398 168
4	2.297 449	2.297 449
6	−2.506 499	−2.506 499
8	−0.526 868	−0.526 868
10	7.907 807	7.907 807
12	−4.200 643	−4.200 643
14	−0.450 298	−0.450 297
16	2.437 755	2.437 761
18	18.349 36	18.350 311
20	−6.509 230	−6.508 468
24	0.966 369	0.969 615
28	31.128	32.601 6
32	−3.284 712	−3.080 77

3.2. Calculation of critical constants

Next we apply our results to the calculation of the critical constants, i.e. to the determination of such values of λ for which a zero-energy bound state exists. Such a calculation is usually done in the following way. The bound-state energy is calculated for various values of λ and by interpolating in energy and in λ the critical value is found. Such an approach is time consuming and not very accurate. Our approach allows one to evaluate the critical constants without solving any bound-state problem. This is simply done by finding zeros of the denominators of (2.14) (resp (2.18)). The use of an expression similar to (2.14) for the calculation of the critical values was proposed recently by Buendia and Guardiola (1985) who, however, write this expansion for the zero-energy Jost function instead of $a(\lambda)$ and determine its zeros. To determine the critical values one must solve a polynomial equation in the case of (2.14), namely

$$\sum_{0}^{N} q_n \lambda^n = -1 \tag{3.8}$$

or the equation

$$d_0 - \lambda d_1 - \cfrac{\lambda^2 d_2^2}{d_2 - \lambda d_3 - \cfrac{\lambda^2 d_4^2}{d_n - \lambda d_5 - \ldots}} = 0 \tag{3.9}$$

in the case of (2.18). Since the results obtained by the VTE approach are similar to those of Buendia and Guardiola we will discuss only the MCF results which again show much faster convergence. In table 6 we show the results of the calculation of the first few critical constants calculated for various interactions. The second column contains the critical constants for the exponential potential $-\exp(-x)$, the third that for the Yukawa potential $-\exp(-x)/x$ and the last that for the Reid ^{1}S soft core potential (Reid 1968). The Reid soft core potential is widely used in nuclear physics and its typical feature is a strong short-range repulsion which results in small negative critical constants.

Table 6. S-wave critical constants for some typical short-range potentials (exponential, Yukawa and Reid).

i	Exponential λ_i	Yukawa λ_i	Reid λ_i
1	1.445 7965	1.679 8078	−0.062 8772
2	7.617 8156	6.447 2603	−0.253 2902
3	18.721 7517	14.342 0279	−0.576 2825
4	34.760 5209	25.372 4359	−1.031 534
5	55.933 9442	39.758 7794	1.082 1808

3.3. Calculation of Sturmians

As a last application we mention the calculation of Sturmians. These states, also called Weinberg states (Rawitscher 1982), are eigenfunctions of the operator $G_0(E)V$, i.e.

$$G_0(E)V\psi_i(E) = \eta_i(E)\psi_i(E) \tag{3.10}$$

and are of great importance in scattering theory. Once these functions are determined, one can express all important quantities by means of these functions. For example, the T matrix defined as

$$T(E) = V + VG_0(E)T(E) \tag{3.11}$$

is given as

$$T(E) = \sum_{i=0}^{\infty} \frac{V|\psi_i\rangle\langle\psi_i|V}{\eta_i - 1} \tag{3.12}$$

where we have normalised the Sturmians as

$$\langle\psi_i|V|\psi_j\rangle = -\delta_{ij}. \tag{3.13}$$

In fact, the critical constants λ calculated above are a special case of (3.10) because

$$\lambda_i = \eta_i^{-1}(0). \tag{3.14}$$

Once the eigenvalues $\eta_i(E)$ and the critical values $\lambda_i(E)$ are determined by solving the algebraic equation (3.9), the corresponding (unnormalised) Sturmian $\bar{\psi}_i$ is immediately obtained in the following continued fraction form:

$$\bar{\psi}_i(E) = u_1(E) + \varphi_1(E)\frac{\langle u_1|V_1|u_1\rangle}{\langle u_1|V_1|u_1\rangle - \langle u_1|V_1|u_2\rangle - \langle u_2|V_2|\varphi_2\rangle} \tag{3.15}$$

where again

$$\varphi_2 = u_2 + \varphi_3\frac{\langle u_2|V_2|u_2\rangle}{\langle u_2|V_2|u_2\rangle - \langle u_2|V_2|u_3\rangle - \langle u_3|V_3|\varphi_4\rangle} \tag{3.16}$$

etc. In equations (3.15) and (3.16) u_i means

$$u_i = G_0V_{i-1}u_{i-1}. \tag{3.17}$$

In the VE approach the (unnormalised) Sturmian is simply given by (2.11). A detailed discussion of calculation of Sturmians will be given elsewhere.

4. Conclusion

Two analytic expressions for the scattering length $a(\lambda)$ have been proposed. The first expression represents the scattering length in the form of a rational fraction in the coupling constant λ, the second in the form of a continued fraction. Both expansions are convergent under very general conditions for any λ. We discuss three applications of our formulae: (i) elastic scattering of electrons with rare gas atoms in a simple model, (ii) calculation of the critical constants (critical screening parameters) for some local potentials, and (iii) calculation of Sturmians. A typical feature of our approach is that only a few iterations of the operator G_0V are needed to obtain all necessary results. No bound-state energy calculation is required. The resulting scattering length and critical constants are very accurate and stable.

Finally we note that our results are not restricted to zero energy but are equally applicable at any energy, including complex energies of resonances.

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