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CALCULATION OF THE ELECTRON SCATTERING LENGTHS FOR NOBLE ATOMS

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The potentials which fall off asymptotically as const $\cdot\, r^{-s}$, $s > 3$, are considered and the new method of calculating of the scattering lengths for them is presented. This method is especially useful for potentials which behave as $\mp \alpha/(2r^4)$ for large r. The scattering lengths for electron scattering on noble gas atoms have been calculated.

1. Introduction

The scattering length is a very important parameter of low-energy scattering as, for potential $V(r)$ which falls off asymptotically faster then r^{-3}:

$$\lim_{r\to\infty} r^3 \cdot V(r) = 0, \tag{1}$$

it determines values of total and momentum transfer cross sections at zero energy. So it is necessary to develop efficient and accurate methods of its calculation and below we present such method for potential which fall off as r^{-s}, $s > 3$, for large r.

We use a convention which states that the scattering length has a positive value for the repulsive potential. We also assume that the requirement (1) is hold.

Generally, for a given potential $V(r)$, the scattering length a may be found as the asymptotic limit of the function $a(r)$

$$a = \lim_{r\to\infty} a(r), \tag{2}$$

where $a(r)$ satisfies the nonlinear differential equation (in atomic units)[1,2]

$$\frac{\mathrm{d}a(r)}{\mathrm{d}r} = 2 \cdot V(r) \cdot [r - a(r)]^2 \tag{3}$$

with the initial condition $a(0) = 0$.

In numerical calculations one usually integrates (3) from $r = 0$ to $r = \hat{r}$ such that $V(r) \cong 0$ for $r > \hat{r}$. Then from (3) it is clear that $a(r)$ does not change appreciably beyond $\hat{r}$ and one can use (2) to get a: $a \cong a(\hat{r})$. However, for potentials which fall off as r^{-s}, $(s > 3)$, this method requires integration out to large $\hat{r}$ and is impractical in many cases.

2. *Method*

Now we assume that for $r \geq r_0$ the potential $V(r)$ behaves as

$$V^{\mp}(r) \cong \mp \frac{\beta^2}{2 \cdot r^s}, \tag{4}$$

where β is taken to be positive and s may have *not only integer* but also *any real* value greater then 3. The general solutions of the radial Schrödinger equation at $l = 0$ and $E = 0$ (in atomic units)

$$\frac{\mathrm{d}^2 u^{\mp}(r)}{\mathrm{d}r^2} \pm \frac{\beta^2}{r^s} \cdot u^{\mp}(r) = 0 \tag{5}$$

may be written in the form

$$u^{-}(r) = A^{-} \cdot r^{1/2} \cdot J_p(x) + B^{-} \cdot r^{1/2} \cdot N_p(x), \tag{6a}$$

$$u^{+}(r) = A^{+} \cdot r^{1/2} \cdot I_p(x) + B^{+} \cdot r^{1/2} \cdot K_p(x), \tag{6b}$$

where $J_p(x)$ and $N_p(x)$ are cylindrical Bessel and Neumann functions, respectively, $I_p(x)$ and $K_p(x)$ are the modified cylindrical Bessel functions of the first and the second kind, respectively, $p = 1/(s - 2)$, and

$$x = 2p \cdot \beta \cdot r^{-1/(2p)}. \tag{7}$$

It is obvious that $1 > p > 0$ and $x \to 0$ for $r \to \infty$. As one can find in handbooks slightly different definitions of mentioned above functions, so we emphasize that we have used the definitions given in a handbook of Abramowitz and Stegun[3].

Now, let us introduce functions $a^{\pm}(r)$ which are defined in terms of the logarithmic derivative of the radial wave functions

$$\frac{\mathrm{d}}{\mathrm{d}r} \ln u^{\mp}(r) = [r - a^{\mp}(r)]^{-1}, \qquad r \geq r_0. \tag{8}$$

It follows from (5) and (8) that for $r \geq r_0$ $a^{\mp}(r)$ satisfies (3) with $V(r)$ given by (4), so $a^{\mp}(r)$ lead asymptotically to the scattering lengths $a^{\mp}$. On the other hand, from (6a), (6b) and (8) one gets

$$a^{\mp}(r) = r \cdot \frac{1 + \frac{p}{x} \cdot Y_p^{\mp}(x),}{1 - \frac{p}{x} \cdot Y_p^{\mp}(x)} \tag{9}$$

where

$$Y_p^{-}(x) = \frac{J_p(x) + C^{-} \cdot N_p(x)}{J_p'(x) + C^{-} \cdot N_p'(x)}, \tag{10a}$$

$$Y_p^{+}(x) = \frac{I_p(x) + C^{+} \cdot K_p(x)}{I_p'(x) + C^{+} \cdot K_p'(x)}, \tag{10b}$$

$C^{\mp} = B^{\mp}/A^{\mp}$, prime denotes differentiation with respect to x, and x is given by (7).

Using the well known recurrence relations and expansions around $x = 0$ for $J_p(x)$, $N_p(x)$, $I_p(x)$, $K_p(x)$ and their derivatives[3], one finds

$$a^{-} = \lim_{r \to \infty} a^{-}(r) = \frac{\pi \cdot (p \cdot \beta)^{2p} \cdot [1 + C^{-} \cdot \mathrm{ctg}(\pi \cdot p)]}{C^{-} \cdot \Gamma(p) \cdot \Gamma(p+1)}, \tag{11a}$$

$$a^{+} = \lim_{r \to \infty} a^{+}(r) = \frac{\pi \cdot (p \cdot \beta)^{2p} \cdot \left[\frac{C^{+}}{\sin(\pi \cdot p)} - \frac{2}{\pi}\right]}{C^{+} \cdot \Gamma(p) \cdot \Gamma(p+1)}. \tag{11b}$$

We propose the following calculation technique for obtaining the scattering length: integrate (3) from $r = 0$ to $r = r_0$ such that (4) becomes valid — one obtains $a_0^{\mp} = a^{\mp}(r_0)$. Then from (9) one finds

$$C^{-} = -\frac{J_p(x_0) - \frac{x_0}{2p} \cdot \left[1 - \frac{a_0^{-}}{r_0}\right] \cdot J_{p+1}(x_0)}{N_p(x_0) - \frac{x_0}{2p} \cdot \left[1 - \frac{a_0^{-}}{r_0}\right] \cdot N_{p+1}(x_0)}, \tag{12a}$$

$$C^{+} = -\frac{I_p(x_0) + \frac{x_0}{2p} \cdot \left[1 - \frac{a_0^{+}}{r_0}\right] \cdot I_{p+1}(x_0)}{K_p(x_0) - \frac{x_0}{2p} \cdot \left[1 - \frac{a_0^{+}}{r_0}\right] \cdot K_{p+1}(x_0)}, \tag{12b}$$

where $x_0 = x|_{r=r_0}$ and the final result follows immediately from (11a) and (12a) or from (11b) and (12b).

In an important case when $s = 4$,

$$V^{\mp}(r) \cong \mp \frac{\beta^2}{2r^4}, \qquad \text{for } r \geq r_0 \tag{13}$$

$p = 1/2$ and cylindrical Bessel and Neumann functions may be expressed through trigonometric functions, $I_p(x)$ through hyperbolic functions, and $K_p(x)$ through exponential function[3], so formulae (11a), (11b), (12a) and (12b) simplify and yield

$$a^- = \beta \cdot \frac{1 + \beta \cdot \left(\frac{1}{r_0} - \frac{1}{a_0^-}\right) \cdot \tan(\beta/r_0)}{\tan(\beta/r_0) - \beta \cdot \left(\frac{1}{r_0} - \frac{1}{a_0^-}\right)} \tag{14a}$$

$$a^+ = \beta \cdot \frac{1 - \beta \cdot \left(\frac{1}{r_0} - \frac{1}{a_0^+}\right) \cdot \tanh(\beta/r_0)}{\tanh(\beta/r_0) - \beta \cdot \left(\frac{1}{r_0} - \frac{1}{a_0^+}\right)}. \tag{14b}$$

3. *Application*

We have employed above results in order to verify the scattering lengths for electron scattering on noble gas atoms calculated by Czuchaj et al.[4]. As $V(r)$ we have used pseudopotentials proposed by them in the case $l = 0$ which have the form

$$V(r) = g_0 \cdot \exp(-h_0 r^2) - \frac{\alpha_d}{2r^4} \cdot A_4(r) - \frac{\alpha_q - 6\beta}{2r^6} \cdot A_6(r), \tag{15}$$

where

$$A_{2k}(r) = (1 - \exp(-\delta r^2))^{2k} \tag{16}$$

with $k = 2$ or 3. Here α_d and α_q are the dipole and quadrupole polarisabilities of the atom and 6β is a dinamical correction to the dipole polarisability. It is obvious that for sufficiently large r (of order of several dozens au) $V(r) \cong -\alpha_d/(2r^4)$.

We had integrated (3) numerically from $r = 0$ to $r_0 = 100$ au and then we have used (14a). (Larger values of r_0 have given the same results.) Values of α_d, α_q, β, δ, g_0 and h_0 adopted in calculations from Ref. 4 are shown in Table 1. Our results are presented in Table 2 where, for comparison, we also present the results of Czuchaj et al.[4].

It can be seen that our results differ signifficantly from those of Czuchaj et al. although we have used pseudopotentials proposed by them. A reason of this discrepancy is that their results were obtained by numerical integration of the radial Schrödinger equation at $l = 0$ and $E = 0$ from $r = 0$ to $r_0 = 50$ au[5], where, against their incorrect assumption, the potential $V(r)$ cannot be neglected.

TABLE 1.

Atom	α_d	α_q	β	δ	g_0	h_0
He	1.3834	2.3265	0.706	1.5	2.08	0.468
Ne	2.663	6.458	1.27	2.0	27.20	1.600
Ar	11.08	48.237	8.33	0.8	29.20	0.900
Kr	16.734	78.762	14.5	0.38	71.50	1.000
Xe	27.292	128.255	29.2	0.28	306.00	1.000

Pseudopotential parameters taken from the work of Czuchaj et al.[4] (in au; for α_d 1 au = $= 1.420 \cdot 10^{-31}$ m^3; for α_q and β 1 au = $4.143 \cdot 10^{-52}$ m^5; for δ and h_0 1 au = $3.573 \cdot 10^{20}$ m^{-2}; for g_0 1 au = $4.357 \cdot 10^{-18}$ J).

TABLE 2.

Atom	present results	Czuchaj et al.
He	1.1869	1.22
Ne	0.2208	0.305
Ar	−1.5121	−1.28
Kr	−3.0080	−2.69
Xe	−4.9530	−4.40

Scattering lengths for noble gas atoms (in au; 1 au = $0.529 \cdot 10^{-10}$ m).

For helium our result ($1.187a_0$) agrees excellently with theoretical values of Nesbet[6] ($1.184a_0$), of O'Malley et al.[7] ($1.189a_0$) and of McEachran and Stauffer[8] ($1.158a_0$), and with the experimental value of Crompton et al.[9] ($1.20a_0$) but is slightly higher than the experimental value of Bullis[10] ($1.145a_0$).

In the case of neon present result ($0.221a_0$) agrees with the theoretical value obtained by McEachran and Stauffer[11] ($0.201a_0$) and with the experimental value of O'Malley and Crompton[12] ($0.214a_0$) but disagrees with the experimental value of Salop and Nakano[13] ($0.30a_0$).

For argon our result ($-1.512a_0$) agrees excellently with the theoretical value of McEachran and Stauffer[14] ($-1.506a_0$) and with the experimental value of Haddad and O'Malley[15] ($-1.492a_0$) but differs slightly from the theoretical value of Plenkiewicz et al.[16] ($-1.4a_0$), and from the experimental values of Ferch et al.[17] ($-1.449a_0$), and of McDowell[18] ($-1.65a_0$). Petrović and Crompton[19] analysed all available data and suggested the value -1.49 $(+0.01-0.02)$ a_0.

For krypton our result ($-3.008a_0$) agrees with the theoretical value of McEachran and Stauffer[20] ($-3.103a_0$) and with the experimental value reported by Buckman and Lohmann[21] ($-3.19a_0$) but differs from values obtained by them from a MERT fit to the cross sections of Sin Fai Lam[22] ($-3.34a$) (theoretical), of Fon et al.[23] ($-3.79a_0$) (theoretical), and to those of Jost et al.[24] ($-2.43a_0$) (experimental).

In the case of xenon our result ($-4.953a_0$) differs slightly from the value calculated by McEachran and Stauffer[20] ($-5.232a_0$).

4. Conclusion

We have developed the new method of calculating of the scattering lengths for long range potentials. We used this method in order to calculate the scattering lengths for electron scattering on noble gas atoms. In spite of using in our calculations pseudopotentials proposed by Czuchaj et al., we found a significant discrepancy between our and their results. Comparison of our results with those of other authors shows a good agreement for helium, neon and argon. In the cases of krypton and xenon further both theoretical and experimental determinations of the scattering lengths are needed.

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PRORAČUN DULJINE RASPRŠENJA ZA ELEKTRONE U PLEMENITIM METALIMA

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Razmatrani su potencijali koji asimptotski opadaju kao *konst* $\cdot\, r^{-s}$, $s > 3$, te je za njih predstavljen novi način proračuna duljine raspršenja. Nova metoda je posebno korisna za potencijale koji se ponašaju kao $\pm\alpha/(2r^4)$ za velike r. Izračunata je duljina raspršenja za raspršenje elektrona na atomima plemenitih plinova