

Calculation of the electron-scattering lengths for rare-gas atoms

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In a recent paper, Reisfeld and Asaf [Phys. Rev. A **49**, 348 (1994)] suggested a simple model explaining an observed correlation between the electron scattering lengths and electric polarizabilities of rare-gas atoms. They proposed an electron-target interaction potential consisting of a short-range hard-core repulsive part plus a long-range dipole polarization potential, and used the Born approximation to evaluate the scattering length. We show that for this model the scattering length may be evaluated analytically and that theoretical predictions based on an exact expression disagree with experimental data.

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In a recent paper [1], Reisfeld and Asaf attempted to explain an experimentally established correlation between electron-rare-gas atoms scattering lengths and electric polarizabilities of targets. The electron-target interaction potential was approximated by the short-range hard-core repulsive part plus the long-range dipole polarization potential

$$V(r) = \begin{cases} +\infty & \text{for } r < R \\ -\alpha e^2/2r^4 & \text{for } r > R, \end{cases} \quad (1)$$

where R is the radius of the core and α is the dipole polarizability of the target. Using the Born approximation it was shown [2] that the scattering length A for the potential (1) might be approximately expressed in terms of R and α as follows:

$$A \simeq R - \frac{\alpha}{3a_0R}, \quad (2)$$

where a_0 is the Bohr radius. Reisfeld and Asaf suggested that as the hard-core radii R , the atomic radii, calculated from the van der Waals equations of state, might be used.

Values of the scattering lengths calculated from Eq. (2) are shown in Table I. It is seen that the theoretical results are in disagreement with experimental data. There are two possible explanations that should be examined, (i) the proposed physical model is reliable but an application of the Born approximation to the evaluation of the scattering lengths is unjustified and (ii) the proposed

physical model is incorrect.

We start an examination of these two possibilities discussing a condition of applicability of the Born approximation. It is clear that such a condition is that a contribution to the scattering length due to the long-range part of the interaction potential should be small compared to the hard-sphere scattering length R . This leads to an inequality

$$\alpha \ll a_0 R^2. \quad (3)$$

We see that the Born approximation may fail for scatterers with greater polarizabilities, such as Ar, Kr, and Xe, for which the condition (3) is not satisfied. Thus the examination of the reliability of the model has to be based on its exact, numerical or analytical, solution. Below we shall utilize a fact that an analytical solution to the model does exist.

In our studies of scattering lengths for various long-range potentials [3–5] we have shown that for a potential of the form

$$V(r) = \begin{cases} V_s(r) & \text{for } r < R \\ -\alpha e^2/2r^4 & \text{for } r > R, \end{cases} \quad (4)$$

where $V_s(r)$ is a short-range part of the interaction, the scattering length may be found analytically and is given by

$$A = \beta \frac{1 + \beta(1/R - 1/A_s) \tan(\beta/R)}{\tan(\beta/R) - \beta(1/R - 1/A_s)}. \quad (5)$$

Here $\beta = (\alpha/a_0)^{1/2}$ and A_s is the scattering length related to the short-range part (V_s) of the potential. For the hard-sphere $A_s = R$ and thus for the potential given by Eq. (1) we have an exact expression

$$A = \beta \cot \frac{\beta}{R}. \quad (6)$$

For $\beta/R \ll 1$ [which is just condition (3) of the applicability of the Born approximation] we may expand the cotangent function in a series [6] and, retaining the first two terms only, we obtain the same result as in Eq. (2).

Results calculated from Eq. (6) are presented in the last column of Table I. It is seen that for He and Ne

TABLE I. Polarizabilities, the van der Waals radii, and electron scattering lengths for rare-gas atoms (in atomic units). For references to sources of swarm data see Ref. [1].

Atom	Polarizability	van der Waals radius	Scattering length		
			Experimental (swarm)	Born Eq. (2)	Exact Eq. (6)
He	1.384	2.51	1.19	2.33	2.32
Ne	2.663	2.25	0.214	1.86	1.84
Ar	11.08	2.79	-1.492	1.47	1.32
Kr	16.734	2.99	-3.32	1.12	0.84
Xe	27.292	3.26	-6.0	0.47	-0.17

atoms the exact results almost coincide with values obtained using the Born approximation but, as might be expected, for Ar, Kr, and Xe differences between the two sets of results are distinct. The most important is that for all targets the exact results are in complete disagreement with experimental data, which provides a proof of

unreliability of the physical model suggested by Reisfeld and Asaf.

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- [1] G. Reisfeld and U. Asaf, *Phys. Rev. A* **49**, 348 (1994); *A* **50**, 4428(E) (1994).
- [2] Reisfeld and Asaf made an error in their considerations leading to an approximate expression for the scattering length and, instead of Eq. (2), obtained an expression in which a factor of 3 in a denominator of the second term was omitted [see Eq. (6) of their paper]. The error was corrected in an Erratum to their paper [1]. Incidentally, theoretical predictions based on this erroneous expression were in quite satisfactory agreement with available experimental data which might suggest, in fact incorrectly, that the physical model proposed by Reisfeld and Asaf was reliable.
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- [5] R. Szmytkowski, *Acta Phys. Pol. A* **79**, 613 (1991).
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