

## *Comment*

# Analytical Independent-Particle Model for Electron Scattering by Argon at Low Energy

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**Abstract.** We show that values of the electron-argon scattering lengths and very low-energy phase shifts computed by Endrédi and Apagyí [Few-Body Systems **17**, 199 (1994)] in two variants of the analytical independent-particle model are not converged. To prove this we employ an accurate method of calculating the scattering lengths we proposed previously. Applied to the model used by Endrédi and Apagyí, the method combines numerical computation of a short-range contribution to the scattering length and analytical evaluation of a long-range contribution due to the electron-atom polarization interaction. Outside the low-energy domain the models of Endrédi and Apagyí appear reliable and the corresponding results are not invalidated by the present findings.

In a recent paper [1], Endrédi and Apagyí applied a model potential approach to describe the elastic scattering of electrons by argon atoms in the energy range 0–3 eV. Two models were used. In the first model the electron-atom interaction was approximated by a spherically symmetric potential

$$V_{M1}(r) = V_{\text{BPG}}(r) + V_{\text{pol}}(r, d). \quad (1)$$

In the second model the interaction was approximated by another spherically symmetric potential

$$V_{M2}(r) = \begin{cases} V_{\text{BPG}}(r) + V_{\text{pol}}(d, d) & \text{for } r < d, \\ V_{\text{BPG}}(r) + V_{\text{pol}}(r, d) & \text{for } r \geq d. \end{cases} \quad (2)$$

The Berg-Purcell-Green potential  $V_{\text{BPG}}(r)$  used in Eqs. (1) and (2) is defined as

$$V_{\text{BPG}}(r) = -\frac{Ze^2}{r} \Omega(r). \quad (3)$$

Here  $Z$  is the nuclear charge of the target atom and the exponentially vanishing

two-parameter screening function  $\Omega(r)$  has the form

$$\Omega(r) = \frac{1}{H[\exp(r/D) - 1] + 1}. \quad (4)$$

In both models the long-range part of the interaction between the projectile and the target, due to the deformation of the target's electronic cloud, was taken into account by using the so-called Buckingham polarization potential

$$V_{\text{pol}}(r, d) = -\frac{\alpha_p e^2}{2(r^2 + d^2)^2}, \quad (5)$$

where  $\alpha_p$  is the target static dipole polarizability and  $d > 0$  is an adjustable parameter. For the considered electron-argon system the following values of parameters were adopted (in atomic units):

$$H = DZ^{0.4}, \quad Z = 18, \quad D = 0.862, \quad \alpha_p = 11.08. \quad (6)$$

The parameter  $d$  differs for both models considered and is also  $l$ -dependent. For the partial wave  $l = 0$  the following values were used (in atomic units)

$$d_1 = 0.5352, \quad d_2 = 1.32 \quad (7)$$

(the index refers to the model).

To solve the radial Schrödinger equation, Endrédi and Apagyi employed Ladányi's least-squares variational method. They expanded a radial wave function in a basis set and solved the resulting system of linear inhomogeneous algebraic equations obtaining finally energy-dependent phase shifts  $\delta_l$ . The parameters  $d_1$  and  $d_2$  were adjusted so that the phase shifts computed at a single energy  $E = 3$  eV fitted the best available experimental and theoretical data. This single adjustment resulted in a rather satisfactory agreement also with other available data over a broader energy range 0–3 eV. Additionally, the electron-argon scattering length  $a$  was determined calculating the quantity

$$A(k) = -\frac{\tan \delta_0(k)}{k} \quad (8)$$

at a sequence of scattering energies  $E = \hbar^2 k^2 / 2m = 10^{-3}, 10^{-4}, 10^{-5}$  eV and extrapolating the sequence of values  $A(k)$  to  $A(k = 0) = a$ .

In this Comment we question the reliability of scattering lengths and very low-energy phase shifts computed in ref. [1]. We shall utilize results we have obtained considering scattering lengths for various long-range potentials important in atomic physics [2–6]. In particular, we have shown in refs. [4, 6] that for a potential of the form

$$V(r) = \begin{cases} V_s(r) & \text{for } r < \rho, \\ -\alpha_p e^2 / 2(r^2 + d^2)^2 & \text{for } r \geq \rho, \end{cases} \quad (9)$$

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

$$a = (b^2 + d^2)^{1/2} \frac{(d^2 + \rho a_s) - (b^2 + d^2)^{1/2}(\rho - a_s) \tan \Theta}{(d^2 + \rho a_s) \tan \Theta + (b^2 + d^2)^{1/2}(\rho - a_s)}. \quad (10)$$

Here  $b = (\alpha_p/a_0)^{1/2}$ ,  $a_0$  is the Bohr radius,

$$\Theta = \left(1 + \frac{b^2}{d^2}\right)^{1/2} \arctan\left(\frac{d}{\rho}\right) \quad (11)$$

and  $a_s$  is the scattering length related to the short-range part ( $V_s$ ) of the potential.

It follows from Eqs. (1)–(5) that both potentials  $V_{M1}$  and  $V_{M2}$  are of the form as given by Eq. (9), i.e. there exists such a radius  $\rho$ , we shall call it the “core radius”, that for  $r \geq \rho$  the interaction between the scattered electron and the target atom may be approximated by the Buckingham potential (5). This suggests that computations of the electron-argon scattering lengths in the models  $M1$  and  $M2$  may proceed in two steps:

- *numerical* determination of the short-range scattering length  $a_s$  due to that part of the potential that is enclosed by the spherical shell of radius  $\rho$ ,
- *analytical* extrapolation of  $a_s$  to infinity with the aid of Eq. (10).

Advantages of this approach will become clear below.

To determine the electron-argon scattering lengths in the models  $M1$  and  $M2$  we integrated numerically a system of two first-order differential equations,

$$\begin{aligned} \frac{d}{dr}P(r) - \frac{1}{r}P(r) - \frac{2m}{\hbar^2}Q(r) &= 0, \\ \frac{d}{dr}Q(r) + \frac{1}{r}Q(r) - V_M(r)P(r) &= 0, \end{aligned} \quad (12)$$

subject to an initial condition  $P(0) = Q(0) = 0$  using the extremely stable and accurate Sienkiewicz-Baylis algorithm [7]. This system is equivalent to a zero-energy radial Schrödinger equation

$$\frac{d^2}{dr^2}P(r) - \frac{2m}{\hbar^2}V_M(r)P(r) = 0. \quad (13)$$

The short-range scattering length  $a_s$  was determined at various trial values of the core radius  $\rho$  from the formula

$$a_s(\rho) = \rho - \frac{P(\rho)}{dP(\rho)/d\rho} = \rho \frac{(2m/\hbar^2)\rho Q(\rho)}{P(\rho) + (2m/\hbar^2)\rho Q(\rho)} \quad (14)$$

and next extrapolated analytically to its asymptotic value  $a$  using Eq. (10).

In order to check accuracy of our numerical code, we first performed test calculations for the case  $Z = 0$  when the scattering lengths are given by exact analytical expressions

$$M1 : \quad a = (b^2 + d^2)^{1/2} \cot \theta, \quad (15)$$

$$M2 : \quad a = (b^2 + d^2)^{1/2} \frac{d(d + a_d) - (b^2 + d^2)^{1/2}(d - a_d) \tan(\theta/2)}{d(d + a_d) \tan(\theta/2) + (b^2 + d^2)^{1/2}(d - a_d)} \quad (16)$$

with

$$\theta = \frac{\pi}{2d}(b^2 + d^2)^{1/2}, \quad a_d = d \left(1 - \frac{\tan(b/2d)}{b/2d}\right). \quad (17)$$

**Table 1.** Convergence of the scattering length  $a$  for the  $e^-$ -Ar collision in the model  $M1$ . All values are in atomic units. The present value  $a = -1.89$  computed for  $Z = 18$  is to be compared with the value  $a = -1.15$  obtained in ref. [1] within the same model

Core radius $\rho$	Scattering length $a$				
	Test calculations $Z = 0$			Model calculations $Z = 18$	
	Short-range $a_s(\rho)$	Extrapolated Eq. (10)	Exact Eq. (15)	Short-range $a_s(\rho)$	Extrapolated Eq. (10)
5.0	7.1874	6.6226		0.6028	-1.6396
7.5	7.1464	6.6226		-0.2417	-1.8733
10.0	7.1344	6.6226		-0.6630	-1.8924
15.0	7.0715	6.6226		-1.0868	-1.8938
20.0	7.0074	6.6226		-1.2976	-1.8939
50.0	6.8156	6.6226		-1.6645	-1.8939
100.0	6.7261	6.6226		-1.7810	-1.8939
$\infty$			6.6226		

Results obtained for different values of the core radius  $\rho$  are shown in the second, third, and fourth columns of Tables 1 and 2. The remarkable agreement between the extrapolated values given in the third columns and the exact values given in the fourth columns confirms the correctness and accuracy of our computer code.

Next we performed calculations for the case  $Z = 18$ . Corresponding results are shown in the last two columns of Tables 1 and 2. It is seen that, although in both cases the numerically determined short-range scattering length  $a_s(\rho)$  converges, with increasing  $\rho$ , to its asymptotic value  $a_s(\infty)$  extremely slowly, the values

**Table 2.** Convergence of the scattering length  $a$  for the  $e^-$ -Ar collision in the model  $M2$ . All values are in atomic units. The present value  $a = -1.69$  computed for  $Z = 18$  is to be compared with the value  $a = -1.11$  obtained in ref. [1] within the same model

Core radius $\rho$	Scattering length $a$				
	Test calculations $Z = 0$			Model calculations $Z = 18$	
	Short-range $a_s(\rho)$	Extrapolated Eq. (10)	Exact Eq. (16)	Short-range $a_s(\rho)$	Extrapolated Eq. (10)
5.0	5.5767	4.9050		0.6668	-1.4469
7.5	5.5653	4.9050		-0.0994	-1.6683
10.0	5.5203	4.9050		-0.4911	-1.6866
15.0	5.4126	4.9050		-0.8948	-1.6880
20.0	5.3264	4.9050		-1.0990	-1.6880
50.0	5.1049	4.9050		-1.4596	-1.6880
100.0	5.0104	4.9050		-1.5754	-1.6880
$\infty$			4.9050		

extrapolated with the aid of Eq. (10) converge to  $a$  rapidly. This is the main virtue of using the analytical formula.

Now we are prepared to compare our results with those obtained by Endrédi and Apagyi. For the model  $M1$ , the scattering length given by these authors,  $a = -1.15 a_0$ , disagrees seriously with the present value  $a = -1.894 a_0$ . Similarly, in the model  $M2$  the value computed in ref. [1],  $a = -1.11 a_0$ , differs significantly from the present value  $a = -1.688 a_0$ . Since Endrédi and Apagyi calculated scattering lengths extrapolating a sequence of phase shifts [more precisely, a sequence  $A(k) = -\tan \delta_0(k)/k$ ] to an energy  $E = 0$ , we conclude that their phase shifts suffer from large uncertainties at very low energies.

To clarify the situation further we solved numerically a system of two coupled equations

$$\begin{aligned} \frac{d}{dr} P(r) - \frac{1}{r} P(r) - \frac{2m}{\hbar^2} Q(r) &= 0, \\ \frac{d}{dr} Q(r) + \frac{1}{r} Q(r) + (E - V_M(r)) P(r) &= 0, \end{aligned} \quad (18)$$

equivalent to the radial Schrödinger equation

$$\frac{d^2}{dr^2} P(r) + \frac{2m}{\hbar^2} (E - V_M(r)) P(r) = 0, \quad (19)$$

at an energy  $E = 3$  eV. We obtained the following values of the phase shifts

$$\delta_0^{(M1)} = -0.453, \quad \delta_0^{(M2)} = -0.451, \quad (20)$$

which agree satisfactorily with the corresponding results given in ref. [1]

$$\delta_0^{(M1)} = -0.455, \quad \delta_0^{(M2)} = -0.454. \quad (21)$$

Therefore the quality of the results of Endrédi and Apagyi worsens as the energy decreases.

The most probable explanation of the errors occurring in ref. [1] is as follows. It is well known that for long-range potentials the partition of the projectile's configuration space into an interaction region and an asymptotic region (i.e. the region where the scattered particle may be considered to be free) strongly depends on the scattering energy. In particular, at very low energies the asymptotic region is rapidly pushed away towards infinity as the energy decreases. In other words, the lesser the scattering energy, the more important is the long-range tail of the scattering potential. Encouraged by a successful application of their method to electron-hydrogen scattering at the static-exchange level (i.e., for *short-range* potentials), Endrédi and Apagyi used a rather small basis set consisting of approximately 20 Slater functions and two (regular and regularized irregular) Riccati-Bessel functions. It is clear that although this basis set may be capable to provide quite accurate results at an energy  $E = 3$  eV, it must fail to span the reaction region at near-zero energies (for argon the radius of this region is approximately  $1000 a_0$ !). As a consequence, at very low energies, the results of Endrédi and Apagyi are not converged. It must be emphasized here that our conclusion does not invalidate the models discussed by these authors. The models

may give reliable results provided the calculations are performed with the necessary care, especially towards extremely low energies.

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