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Short communication

On an improved model of a complex optical potential for electron elastic scattering

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ABSTRACT

Empirical scaling functions of the type suggested by Lee et al. [M.-T. Lee, I. Iga, L.E. Machado, L.M. Brescansin, E.A. y Castro, I.P. Sanches, G.L.C. Souza, J. Electron Spectrosc. Relat. Phenom. 155 (2007) 14] for the quasifree-scattering model are tested. The parameters of the scaling function have been fitted by using the genetic algorithm to reproduce the experimental data for the elastic scattering of electrons by helium, neon and argon atoms at impact energies 20–3000 eV. The results confirm the effectiveness of the model.

1. Introduction

One of methods to describe an elastic scattering of electrons by atoms (molecules) is the method of the effective potential in which a nonlocal optical potential operator is approximated by a local complex potential. The aim of investigations is to find nonempirical models of potentials which would reproduce empirical cross-sections in a wide range of energies and possibly wide range of scattering angles. This aim has not been achieved yet. The existing models of potentials usually give good results within some ranges of energies and angles.

In our previous paper [2] various combinations of nonempirical models of polarization and absorption potentials based on quasifree-scattering model V_f^A [3–6] were tested for e-Ne scattering. The evaluation was performed on the set of 282 experimental data (elastic, absorption, and differential cross-sections) for impact energies in the range of 20–3000 eV and scattering angles 3–150°. Theoretical mean unsigned error (MUE) Δ^{cs} in the cross-sections was compared with an estimated experimental one. The experimental MUE of 5% for total (elastic, absorption) cross-sections and of 10% for differential cross-sections was assumed. The smallest error Δ^{cs}, calculated on the whole data set, exceeded the experimental MUE by 70%. It was achieved for the combination of the polarization potential V_b^P of Buckingham type [7] and original absorption potential V_{fo}^A based on the quasifree-scattering model. (Abbreviations and notation are as in [2].) The versions V_{fv2}^A and V_{fv3}^A [8] of the latter potential gave slightly bigger errors. Nonempirical modifications of the potential V_{fo}^A discussed in [2] improve the model merely for certain ranges of energies and angles, not on the whole data set.

It is known that the potential V_{fo}^A is too strong at high electronic density region and too weak at low density region [8], cf. also [1]. Potentials depending on empirical parameters fitted to experimental data can be helpful in determining the functional form of potentials and indicate the direction of future modifications. Recently Lee et al. [1] have proposed a new empirical correction to the potential V_{fv3}^A [8,2]. The aim of this paper is to extend the previous research [2] by a validation of this empirical model. The model relies on multiplying the absorption potential V_{fv3}^A by a scaling factor SF containing two empirical parameters M and N

$$\mathrm{SF} = 1.0 + Mpr_s - \frac{N}{pr_s}, \tag{1}$$

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where $E = p^2/2$ is the energy of the incident electron, $r_s = [3/4\pi\varrho(\vec{r})]^{1/3}$ and $\varrho(\vec{r})$ is the electronic charge density of a target. The parameters are assumed to be independent of a particular target and the energy of incident electron. Those authors have chosen the parameters to reproduce the absorption cross-section for e-N_2 scattering at 500 eV. For a variety of atomic and molecular targets, they obtained a better agreement with experimental data.

In this paper the parameters appearing in SF have been optimized by minimizing the MUE (defined in [2], Eq. (40)) on the data set containing experimental cross-sections for a wide range of impact energies and scattering angles. The tests have been performed for three targets: He (316 data), Ne (282 data), and Ar (302 data). The minima were determined with the help of the genetic algorithm [9,10].

The intervals in which the parameters M and N are optimized should be carefully chosen. Due to the minus sign appearing in the formula (1) the absorption potential can become positive for some r (and behaves like a source, not an absorber). For the targets considered in this paper, the absorption potentials, with parameters recommended in [1], become positive for certain energies and distances. For He and Ar the error function achieves its minimum for very small values of N (of the order 10^{-4}), setting $N = 0$ practically did not change the error. For Ne keeping $N \neq 0$ together with the condition $V^A(r) < 0\ \forall r$, do not improve the MUE. Therefore, we set $N = 0$ and consider scaling factors in the following forms:

$$\mathrm{SF1} = 1.0 + a_1 p r_s, \tag{2}$$

$$\mathrm{SF2} = c_0 + c_1 p r_s. \tag{3}$$

a_1, c_0, c_1 are empirical parameters.

Both factors substantially reduce MUEs for He and Ar, the optimal value of the parameters for these targets do not differ much from each other. For Ne the decrease of MUEs is slight and the values of the fitted parameters appearing in scaling factors differ much from those for He and Ar, see Section 4.

The absorption potentials based on the quasifree-scattering model depend on the real part of the potential, V^R. In the model V^A_{fo} this dependence appears in the formula for the local velocity of the incident electron, while for the model V^A_{fv3} it appears also in the conditions resulting from Pauli-blocking restrictions. In the original model V^A_{fo} the real part of the potential is approximated by the sum of the static and exchange potentials: $V^R = V^{SE}$. The absorption potential is often evaluated with $V^R = V^{SEP}$, where the polarization potential V^P is added to V^{SE} [11,1]. Obviously, using V^{SEP} in the absorption potential would make the problem of determining V^P from the dispersion relation (between V^P and V^A) substantially harder. As it is important to know if the inclusion of V^P into V^A is essential, we present the results of computations using both approaches. It is found that for the considered targets the presence of V^P in V^A is rather insignificant.

Altogether, we compare the results of calculations for six versions of the absorption potential for e-He, e-Ne, and e-Ar scattering in a wide range of energies and angles.

2. Theory and calculations

The details concerning the present calculations can be found in [2], where the scattering equation is given by Eq. (1) and the static, exchange and Buckingham polarization potentials for all considered targets are of the form of Eqs. (2)–(4).

The formula for the absorption potential based on the quasifree-scattering model reads

$$V^A_f(\vec{r}, E) = -\frac{2\pi\varrho(\vec{r})u(\vec{r}, E)}{5k_F^3 p^2} H(p^2 + k_F^2 - \alpha - \beta) \times \left[\frac{5k_F^3}{\alpha - k_F^2} - \frac{k_F^3[5(p^2 - \beta) + 2k_F^2]}{(p^2 - \beta)^2} + H(\alpha + \beta - p^2)\frac{2(\alpha + \beta - p^2)^{5/2}}{(p^2 - \beta)^2} \right], \tag{4}$$

where

$$u(\vec{r}, E) = [2(E - V^R)]^{1/2}, \tag{5}$$

$k_F = (3\pi\varrho)^{1/3}$, and H is the Heaviside unit-step function. The quantities α and β come from Pauli blocking conditions [8] and, depending on the model they are different functions of the threshold energy of the atom Δ, the ionization potential I, the Fermi momentum k_F and V^R.

All the models of V^A_f considered in the paper are obtained from Eq. (4) by specifying the quantities V^R, α, β. Moreover, some of the models are multiplied by a scaling factor depending on the adjustable parameters. We have:

V^A_{fo}(SE)—original frivolous model potential

$$V^R = V^{SE}, \quad \alpha = k_F^2 + 2\Delta, \quad \beta = k_F^2; \tag{6}$$

V^A_{fv3}(SE)—frivolous model potential, version 3 with V^{SE}

$$V^R = V^{SE}, \quad \alpha = k_F^2 + 2[\Delta - (I - \Delta)] - V^R, \quad \beta = k_F^2 + 2(I - \Delta) - V^R; \tag{7}$$

V^A_{fv3}(SEP)—frivolous model potential, version 3 with V^{SEP}

$$V^R = V^{SEP}, \quad \alpha \text{ and } \beta \text{ as in (7)}; \tag{8}$$

V^A_{fv3sf1}(SE)—potential (7) multiplied by the scaling factor (2)

$$V^A_{fv3sf1}(\mathrm{SE}) = \mathrm{SF1}\, V^A_{fv3}(\mathrm{SE}); \tag{9}$$

Table 1
The numbers of experimental data

	N_e^{el}	N_e^{abs}	N^{diff}	N	N_e	N_e^{diff}
e-He	20	20	276	316	21	15
e-Ne	17	18	247	282	20	15
e-Ar	17	19	266	302	21	13

Table 2
The optimized parameters for the scaling factors

	a_1	c_0	c_1
e-He			
V^A_{fv3sf1}(SE)	0.1408		
V^A_{fv3sf1}(SEP)	0.1508		
V^A_{fv3sf2}(SE)		1.0198	0.1380
e-Ne			
V^A_{fv3sf1}(SE)	0.01249		
V^A_{fv3sf1}(SEP)	0.02311		
V^A_{fv3sf2}(SE)		0.09949	0.1668
e-Ar			
V^A_{fv3sf1}(SE)	0.1281		
V^A_{fv3sf1}(SEP)	0.1389		
V^A_{fv3sf2}(SE)		1.1161	0.1158