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Elastic scattering of electrons from He, Ne and Ar atoms at 35 keV

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Abstract. The eikonal Born series (EBS) method is applied to the elastic scattering of electrons by He, Ne and Ar atoms at 35 keV. The differential cross-sections are compared with the numerical results obtained by the partial-wave analysis. A simple analytical Dirac-Hartree-Fock-Slater (DHFS) field is used for these atoms. The results are also obtained by Wallace, Das and modified Das method. An oscillatory nature and a strong forward peak in the cross-section are not found at 35 keV. The results are nearer to the experimental data of Coffmann and M. Fink as well as numerical results based on relativistic partial-wave treatment.

PACS. 34.80.Bm Elastic scattering of electrons by atoms and molecules

1 Introduction

Elastic electron-atom scattering at intermediate and high energies is studied by combining the Born series and eikonal series. The results should be consistent through order k_i^{-2}[1,2]. The eikonal approximation gives good results for small scattering angle [3], when the magnitude of incident wave vector k_i is large.

Various corrections to the eikonal approximation are used for very small-angle elastic scattering of electrons from He, Ne and Ar atoms. A simple computational scheme which is no more difficult than a second Born computation was described by Das [4]. Further modification in the Das technique was applied successfully by K. Lata [5]. A third-order eikonal term in the place of the third Born term is used to get a consistent result. Thus the Das approach is improved without any additional complexities of the calculations. The computational results are compared with the new experimental data [6]. The exact results are obtained by solving Dirac equation numerically with the code PWADIR [7].

2 Theory

Consider the non-relativistic scattering of a particle of mass m by a real, spherically symmetric potential $V(r)$ of range a. The Glauber eikonal scattering amplitude is

$$f_{\mathrm{E}} = \frac{k}{i}\int_0^\infty \mathrm{d}b\, b J_0(\Delta b)(e^{iX_0(b)/k}-1)\,. \tag{1}$$

The real and the imaginary parts of f_{E} are

$$\mathrm{Re} f_{\mathrm{E}} = k\int_0^\infty \mathrm{d}b\, b J_0(\Delta b)\sin(X_0)\,, \tag{2}$$

$$\mathrm{Im} f_{\mathrm{E}} = k\int_0^\infty \mathrm{d}b\, b J_0(\Delta b)[\cos(X_0)-1]\,, \tag{3}$$

where

$$X_0(b) = -\frac{1}{2}\int_0^\infty U(b,z)\mathrm{d}z\,, \tag{4}$$

and $\Delta = 2k\sin\theta/2$ the magnitude of the momentum transfer. The wave number of the incident particle $|k_i| = k$. The value of $U(r) = 2mV(r)/\hbar^2$. This is the reduced potential. In the case of superposition of Yukawa-type potential

$$U(r) = -U_0\sum_i \gamma_i \frac{e^{-\lambda_i r}}{r}\,. \tag{5}$$

It was shown that by adding the quantity $\mathrm{Re}\bar{f}_{\mathrm{B2}}$, the real part of the second Born amplitude to f_{E}, a marked improvement over the eikonal amplitude was obtained [1]. Thus

$$f_{\mathrm{EBS}} = f_{\mathrm{E}} + \mathrm{Re}\bar{f}_{\mathrm{B2}}\,. \tag{6}$$

Especially in the weak-coupling situation the eikonal Born series amplitude gives a consistent picture of the scattering amplitude through order k_i^{-2}. In the case of potential $U(r)$ we have

$$X_0(b) = -U_0\sum_i \gamma_i K_0(\lambda_i b)\,, \tag{7}$$

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where K_0 is the modified Bessel function of order zero. In this case the real part of the second Born amplitude is evaluated using Dalitz integrals [8],

$$\mathrm{Re}\bar{f}_{\mathrm{B2}} = \sum_{i,j} \frac{U_0^2}{2} \gamma_i \gamma_j \int_0^1 F(\lambda_i, \lambda_j, t) \mathrm{d}t \,, \tag{8}$$

where

$$F(\lambda_i, \lambda_j, t) = \frac{\lambda_i^2 t + \lambda_j^2 (1-t)}{\Gamma[\{\lambda_i^2 t + \lambda_j^2 (1-t)\}^2 + 4k^2 \Gamma^2]} \tag{9}$$

and

$$\Gamma = \lambda_i^2 t + \lambda_j^2 (1-t) + t(1-t)\Delta^2 \,. \tag{10}$$

Thus the differential cross-section is obtained as

$$|f_{\mathrm{EBS}}|^2 = |\mathrm{Re}f_{\mathrm{E}} + \mathrm{Re}\bar{f}_{\mathrm{B2}}|^2 + |\mathrm{Im}f_{\mathrm{E}}|^2 \,. \tag{11}$$

We have taken care of zeros of the Bessel function. With the help of Euler's transform [9] the integrals in the equation of $\mathrm{Re}f_{\mathrm{E}}$, $\mathrm{Im}f_{\mathrm{E}}$ are evaluated. Another way of improving eikonal amplitude in potential scattering has been proposed by Wallace [10]. The Wallace-eikonal correction was given as [11]

$$f_{\mathrm{w}} = \frac{k}{i} \int_0^\infty \mathrm{d}b b J_0(\Delta b) \times \left\{ \exp\left[i \left(\frac{X_0}{k}(b) + \frac{X_1}{k^3}(b) \right) \right] - 1 \right\} , \tag{12}$$

where

$$X_1(b) = \sum_{i,j} \frac{U_0^2}{2} \gamma_i \gamma_j \lambda_j K_0((\lambda_i + \lambda_j)b) \tag{13}$$

and $X_0(b)$ is the eikonal phase given by equation (7). We rewrite equation (6) as

$$f_{\mathrm{EBS}} = f_{\mathrm{w}} + \mathrm{Re}\bar{f}_{\mathrm{B2}} \,. \tag{14}$$

A simpler method was suggested by Das [4] in which the second Born term is multiplied by a variationally determined complex number to compensate for the missing higher-order Born terms. The scattering amplitude obtained by Das as

$$f_{\mathrm{D}} = f_{\mathrm{B1}} + (a_{\mathrm{D}} + ib_{\mathrm{D}})(\bar{f}_{\mathrm{B2R}} + \bar{i} f_{\mathrm{B2I}}) \,, \tag{15}$$

where $\bar{f}_{\mathrm{B2R}}$ and $\bar{f}_{\mathrm{B2I}}$ are denoted as real and imaginary parts of $\bar{f}_{\mathrm{B2}}$. The parameters a_{D}, b_{D} are energy dependent. The Das technique was improved further by including the third Born term, the derivation of scattering amplitude [5],

$$f_{\mathrm{MD}} = f_{\mathrm{B1}} + (a_{\mathrm{P}} + ib_{\mathrm{P}})(\bar{f}_{\mathrm{B2}} + \bar{f}_{\mathrm{B3}}) \,. \tag{16}$$

According to the analysis of Byron and Joachain [12] at large energies a_{P} is independent of energy and converge to unity, whereas b_{P} varies with energy as k_i^{-3}. So the terms $\bar{f}_{\mathrm{B3I}}$ and b_{P} which fall faster than k_i^{-2} asymptotically are neglected. Here we replace the $\bar{f}_{\mathrm{B3R}}$ by the equivalent term $\bar{f}_{\mathrm{E3}}$ [13]. Thus f_{MD} corrected up to the order k_i^{-2} is given by

$$f_{\mathrm{MD}} = f_{\mathrm{B1}} + a_{\mathrm{P}}(\bar{f}_{\mathrm{B2R}} + \bar{f}_{\mathrm{E3}}) + i a_{\mathrm{P}} \bar{f}_{\mathrm{B2I}} \,, \tag{17}$$

where

$$a_{\mathrm{P}} = \frac{f_{\mathrm{B1}}}{f_{\mathrm{B1}} - \bar{f}_{\mathrm{E3}}} \,. \tag{18}$$

Fortran 77 code PWADIR [7] gives reliable cross-section data for elastic scattering of electrons by free atoms for K.E. ≥ 1 keV by using the static field approximation with relativistic partial-wave analysis. This code is used to evaluate the exact results. The generalized atomic units are used throughout this paper. We consider a simple analytical approximation $\phi(r)$ for the atomic screening function [14] accounting for relativistic effects distorting the atomic electron cloud and the nuclear screened potential. This is reliable for the large atomic number. The parameters are determined analytically from the results of DHFS self-consistent calculations.

The Dirac radial wave equation is used in the computation of the differential scattering amplitudes for incident electrons of 35 keV. The radial equations are solved using the Buhring power series method [15]. The Dirac phase shifts are determined by solving the Dirac radial wave equation with a central field

$$V(r) = -\frac{Z}{r}\phi(r) + V_{\mathrm{EX}}(r) \,. \tag{19}$$

The exchange effect is included by the local exchange potential of McCarthy $V_{\mathrm{EX}}(r)$ [16]. The charge cloud polarization is neglected. There is at present no experimental evidence that the charge cloud polarization plays a noticeable role at the incident electron energy considered here [17]. For high-energy particles large number of terms are required in the partial-wave series. Here the phase shifts of order l less than a finite value NDELTA=1000 is computed. The value of NDELTA is large enough to enable convergence of the partial-wave series. The accuracy of the computed phase shift is controlled through the input parameter $\epsilon = 1 \times 10^{-8}$.

3 Result and discussion

A systematic study of the differential cross-sections for the inert gas atoms He, Ne, and Ar is reported here for the non-relativistic potential scattering. The differential cross-sections for elastic scattering of electrons from these target atoms are studied for energies in the range of 15 keV to 35 keV. We did not find any strong peak in the forward direction or an oscillatory nature in differential cross-sections as reported by Geiger *et al.* [18]. Our results are close to the new experimental data [6]. The results are exhibited graphically in Figures 1-3. We see that, according to the EBS method, the differential cross-sections for He, Ne, Ar atoms at very small scattering angle differ from

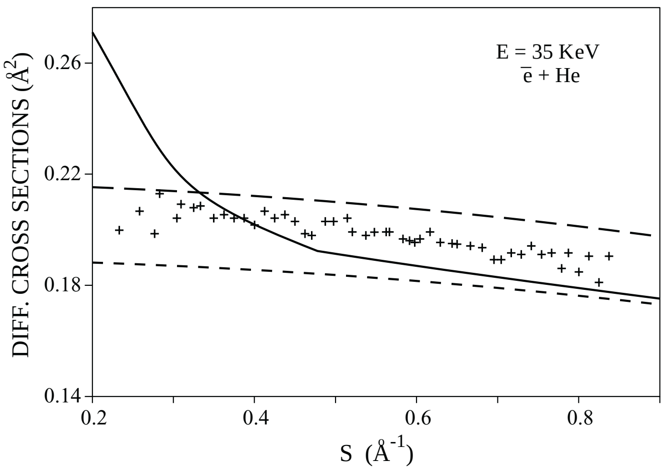

Fig. 1. Differential cross-sections for the elastic scattering of 35 keV electrons by the helium atoms. —-: present EBS results (see Eq. (11)); + + +: experimental data of Coffmann *et al.* (Ref. [6]); — —: numerical data (Ref. [7]);– – – : Das method (see Eq. (15)).

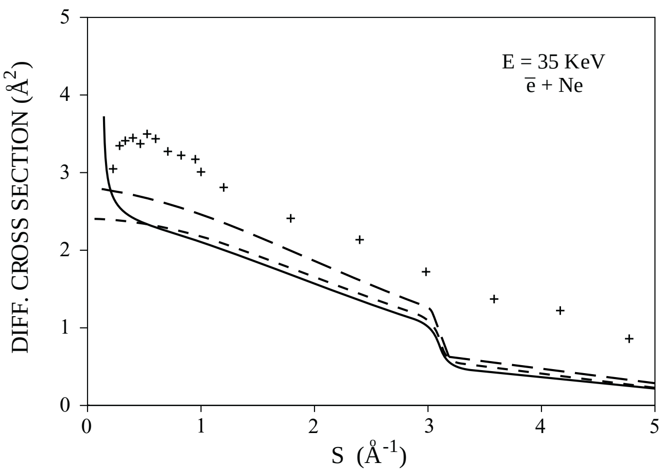

Fig. 2. Electron-neon elastic differential cross-sections at 35 keV. Different symbols have the same meaning as in fig. 1.

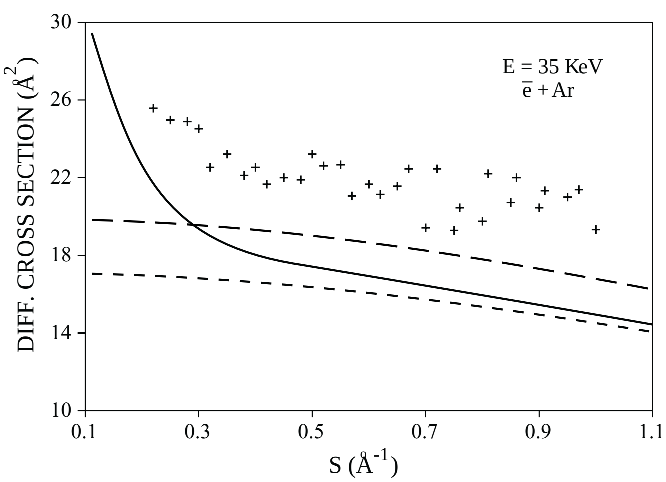

Fig. 3. Electron-argon elastic differential cross-sections at 35 keV. Different symbols have the same meaning as in fig. 1.

Table 1. E = 35 keV. Differential cross-sections in atomic units.

He-atom θ (deg.)	W	MD	Ar-atom W	MD
0.20	0.753	0.669	65.607	62.262
0.30	0.688	0.659	63.004	60.283
0.40	0.662	0.647	60.196	58.249
0.50	0.641	0.631	57.350	55.996
0.60	0.619	0.612	54.504	53.505
0.70	0.597	0.592	51.593	50.805

W: DCS using the Wallace method (see Eq. (14)).
MD: DCS using the Modified Das method (see Eq. (17)).

Table 2. E = 35 keV. Differential cross-sections in atomic units.

Ne-atom θ (deg.)	W	MD
0.20	10.257	8.763
0.40	8.754	8.420
0.60	8.189	8.026
0.80	7.640	7.535
1.00	7.046	6.968
1.20	6.420	6.357
1.40	5.786	5.734
1.60	5.166	5.121
1.80	4.578	4.539
2.00	4.032	3.998

W: DCS using the Wallace method (see Eq. (14)).
MD: DCS using the Modified Das method (see Eq. (17)).

exact results (numerical) in the range 0.2 to 0.3 Å^{-1}. The EBS amplitude reproduce the exact results for momentum transfer greater than 0.3 Å^{-1}. For He-atom (Fig. 1), differential cross-section obtained by the numerical and Das methods have similar nature but they are on either side of the experimental data which cover all points. The EBS results are close to the experimental data compared to the numerical and Das results beyond 0.3 Å^{-1}. In the case of Ne-atom (Fig. 2), differential cross-sections resulting from EBS and Das methods are in excellent agreement with the partial-wave calculations. These results differ from the experimental results. In the case of Ar-atom (Fig. 3), the results obtained by the numerical method are closer to the experimental results.

We have also reported differential cross-sections by Wallace and modified Das method at 35 keV. These results give nearly the same values as those given by EBS and Das methods, respectively. The strong forward peak and oscillating features in differential cross-sections are lacking. The results are shown in Tables 1 and 2 . The differential cross-sections calculated by Wallace method are in close agreement with the EBS results and modified Das results.

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