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ELECTRON-ARGON SCATTERING: A HIGH ANGLE MINIMUM IN DIFFERENTIAL CROSS SECTIONS

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Abstract: *Ab initio* relativistic calculations of the high angle differential cross section minimum have been presented. Theoretical method is based on the Dirac-Hartree-Fock scattering equation. *Ab initio* polarization and exact exchange have been included. Calculations have been performed for the low energy elastic electron scattering from argon. A very good agreement with the recent experimental data has been found.

Keywords: scattering, atomic physics, relativistic theory

1. Introduction

Since 1921, when Ramsauer published his pioneer work on electron scattering from noble gases, there have been a considerable interest in experimental and theoretical investigation on this subject. A lot of experimental measurements have been published. They include differential and total cross sections and quite recently spin-polarization cross sections. In particular at low energy scattering from noble gases the total cross section (TCS) exhibits well-known minimum called Ramsauer-Townsend minimum. Very recently other features in the elastic scattering of electrons from noble gases attracted attention of experimentalists. These features are the positions of minima in differential cross section (DCS). Because the positions of these minima are very sensitive to both experimental and theoretical methods, they are called critical minima.

From the theoretical point of view the explanation of this sensitivity lies in the fact that positions of DCS minima are influenced by contributions from different electron-atom interaction potentials.

From the experimental point of view the physical interpretation of DCS minima is essential in spin-polarization analysis of scattered electrons. The reason for this is that positions of maxima in spin-polarization cross sections are nearly the same as positions of critical minima in DCS.

The first systematic experimental measurements of critical minima have been reported by Panajatović *et al.* [1] in the elastic scattering of low-energy electrons from argon. This situation provides excellent occasion to test our theoretical approach, which is based on Dirac equation with careful treatment of polarization and exchange potentials [2].

Theoretical calculations of DCS critical minima in argon have been carried out by a few groups. Nahar and Wadhera [3] used non-relativistic Born approximation with a model polarization potential. McEachran and Stauffer [4] solved non-relativistic scattering equations with the adiabatic exchange approximation, including polarization and local exchange interactions. This method has been developed by Bartschat *et al.* [5], where polarization potential has been calculated in non-relativistic polarized orbital approximation. Our fully relativistic approach uses the polarization potential obtained in the relativistic version of polarized orbital method [6] with exact treatment of exchange.

2. Theoretical method

Our theoretical method is based on the radial Dirac-Hartree-Fock equation [7] which can be written in atomic units as:

$$\begin{aligned} \left(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{\kappa}{r}\right)P_\kappa(r) &= \left\{2/\alpha+\alpha\left[E-V_{fc}(r)-V_p(r)\right]\right\}Q_\kappa(r)+X_Q(r), \\ \left(\frac{\mathrm{d}}{\mathrm{d}r}-\frac{\kappa}{r}\right)Q_\kappa(r) &= -\alpha\left[E-V_{fc}(r)-V_p(r)\right]P_\kappa(r)-X_P(r), \end{aligned} \tag{1}$$

where P_κ and Q_κ are radial parts of the large and small components of the Dirac wave-function, the quantum number $\kappa=\pm(j+\frac{1}{2})$ for $l=j\pm\frac{1}{2}$, α is the fine structure constant, E is the energy of the incoming electron, V_{fc} is the relativistic frozen-core potential, V_p is the polarization potential and X_Q and X_P are the exchange terms.

The phase shifts $\delta_l^\pm$ are obtained by comparison of the numerical solutions of Equation (1) to the analytical ones at large r,

$$P_\kappa(r)/r = j_l(kr)\cos\delta_l^\pm - n_l(kr)\sin\delta_l^\pm, \tag{2}$$

where k is the momentum of the incident electron, $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions, respectively. δ_l^+ is the phase shift calculated for $\kappa=-l-1$ in Equation (1) and δ_l^- that for $\kappa=l$. In the case of the relativistic scattering problem we have two scattering amplitudes:
the direct one

$$f(\theta)=\frac{1}{2ik}\sum_l\left\{(l+1)[\exp(2i\delta_l^+)-1]+l[\exp(2i\delta_l^-)-1]\right\}P_l(\cos\theta), \tag{3}$$

and the spin-flip one

$$g(\theta)=\frac{1}{2ik}\sum_l\left[\exp(2i\delta_l^-)-\exp(2i\delta_l^+)\right]P_l^1(\cos\theta), \tag{4}$$

where θ is the scattering angle, $P_l(\cos\theta)$ and $P_l^1(\cos\theta)$ are the Legendre polynomials and the Legendre associated functions, respectively.

Differential cross section for elastic scattering is defined by the relation:

$$\sigma_{diff}(\theta)=|f(\theta)|^2+|g(\theta)|^2, \tag{5}$$

Our calculations were performed by means of the modified version [2] of the relativistic numerical code “MCDF” written by J. P. Desclaux [8]. *Ab initio* polarization potential

V_p was taken from the calculations of R. Szmytkowski done with relativistic version of polarized orbital method [6].

3. Results and discussion

We performed calculations concerning the position of high-angle minimum. The energy range covered in our investigation is 10–100 eV. Our results are shown in Table 1 along with experimental data of Panajatović *et al.* [1]. It allows for a direct comparison of our numerical results with the measurements. One can see that the biggest discrepancy between two sets of data occurs at 90.3 eV. Our points at 20.3 eV, 30.3 eV, 75.3 eV and 100.3 eV are almost identical with the experimental ones.

Table 1. Position of high angle electron-argon elastic scattering DCS minimum versus electron energy

energy (eV)	θ (present) (*deg*)	θ (Panajatović *et al.*) (*deg*)
10.3	115	117
15.3	122	118
20.3	131	130
25.3	138	141
30.3	141	142
40.3	140	143
50.3	136	138
60.3	132	134
75.3	128	128
80.3	127	129
90.3	125	121
100.3	123	123

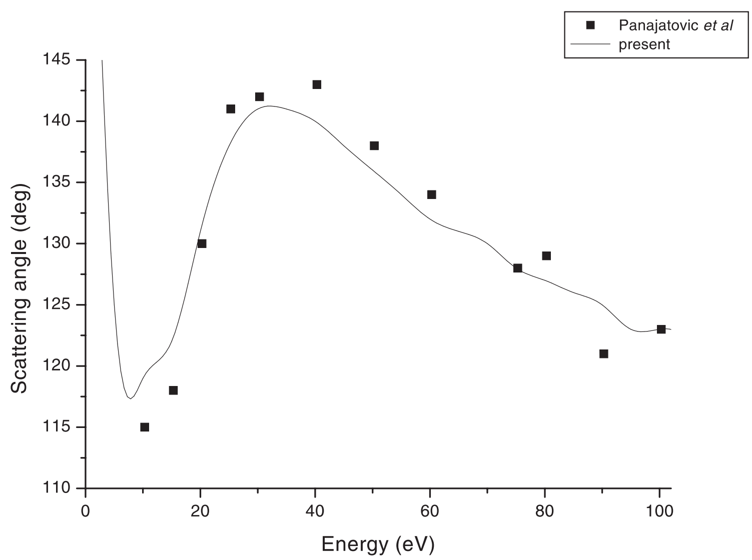

Figure 1. Position of high angle electron-argon elastic scattering DCS minimum versus electron energy

We also display our theoretical curve in Figure 1. As it can be noticed the position of the high-angle minimum reaches its maximal value at scattering angle of 142° at energy around 30 eV. This disagrees with the experiment which shows the position of maximum at 40 eV. At the same time the value of scattering angle is almost the same. As electron energy increases above 30 eV, the position of our minimum decreases almost monotonically, which shows a good agreement with experimental points. There is an exception at 90.3 eV, where the experimental point lies below our curve. At low energies of 10–20 eV our curve lies above the experimental points. This discrepancy may be caused either by lower accuracy of energy resolution or lower sensitivity of our calculations.

4. Conclusions

We performed *ab initio* calculations for low-energy elastic scattering of electrons from argon. Our attention has been focused on the position of high-angle minimum in differential cross section. Overall very good agreement has been found with experimental data recently reported by Panajatović *et al.* [1]. This indicates that our theoretical approach gives proper description of DCS minima in electron-argon scattering, which is very sensitive to proper description of electron-atom interactions. In our future work we plan to perform more exhaustive calculations to take into account other minima in DCS.

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