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Critical minima in elastic scattering of electrons from Ar and Zn

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Abstract

Ab initio relativistic calculations have been carried out to search for critical minima in the angle and energy differential cross-sections for the elastic scattering of electrons from argon and zinc atoms. Theoretical approach is based on the Dirac–Hartree–Fock method. Exchange between incident and target electrons is calculated exactly. Target polarization is described by an ab initio potential taken from relativistic polarized orbital calculations. Comparison is made with experimental data and other theoretical results.
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1. Introduction

The position of *a critical minimum* in differential cross-section (DCS) is the point on the plane constituted by the scattering angle and projectile energy axis where DCS reaches its local minimum.

The first who proposed systematic search for critical points defined by above were Kessler et al. (1976), Lucas (1979), Khare and Raj (1980). Although, Bühring (1968) was the first who brought the attention to critical energies at which critical minima occur, he proved their physical significance due to their sensitivity in experimental methods. The precise measurements of the minima positions are difficult since they require very good angular and energetic resolutions.

The positions of the minima in the differential cross-sections depend very sensitively on the theoretical method used for description. A proper treatment of the exchange potential and careful choice of the target polarization potential is required. A precise knowledge of the critical minima is also important to the region with the highest degree of spin polarization of the scattered electrons. Our relativistic approach allows to calculate both the minima of the differential cross-sections and the degree of spin polarization.

2. Theoretical method

To obtain the wave function for the scattered electron with a given angular symmetry κ and energy E we solve the radial Dirac–Fock equations (Grant, 1970) which can be written in atomic units as

$$\left(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{\kappa}{r}\right)P_\kappa(r) = \{2/\alpha+\alpha[E-V_{\mathrm{fc}}(r)-V_{\mathrm{p}}(r)]\}Q_\kappa(r)+X_Q(r),$$

$$\left(\frac{\mathrm{d}}{\mathrm{d}r}-\frac{\kappa}{r}\right)Q_\kappa(r) = -\alpha[E-V_{\mathrm{fc}}(r)-V_{\mathrm{p}}(r)]P_\kappa(r)-X_P(r), \quad (1)$$

where P_κ and Q_κ are radial parts of the *large* and *small* components of the Dirac wave-function, $\kappa=\pm(j+\frac{1}{2})$ for $l=j\pm\frac{1}{2}$ comprises the total angular momentum j and parity $(-1)^l$, α is the fine structure constant, V_{fc} is the relativistic frozen-core potential, V_{p} is the polarization potential. Two terms X_P and X_Q describe the exchange potential between the incident electron and bound target electrons.

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Both, the exchange terms and the frozen-core potential V_{fc} are calculated from first principles using the one-electron orbitals obtained from the multiconfiguration Dirac–Fock (MCDF) program of Desclaux (1975) with some modifications (Sienkiewicz and Baylis, 1987). These terms are defined as

$$V_{fc} = -\frac{Z}{r} + \frac{1}{r}\sum_{j,k} a^k(s,j)\,Y^k(j,j;r),$$

$$\text{cr } X_{P(\text{or } Q)} = \sum_{j,k} b^k(s,j)\,Y^k(s,j;r)P_j(\text{or } Q_j),$$

where index s refers to the scattered electron, Z is the nuclear charge and the sums run over electrons of the target atom. The radial function Y^k and the angular coefficients a^k and b^k are given by Grant (1970).

The polarization potential V_p can be derived in the perturbation theory as a second-order correction to the frozen-core approximation. In the present approach, it includes the dipole static term and is taken in a numerical form from the ab initio calculations of Szmytkowski (1993) which were done with the relativistic polarized orbital method.

From the solutions of the Dirac–Fock equations given above, we obtain the phase shifts $\delta_l^{\pm}$ by comparison with the analytical form of $P_\kappa(r)$ 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. Here, δ_l^+ is the phase shift calculated for $\kappa = -l-1$ in Eq. (1) and δ_l^- that for $\kappa = l$. In the case of a relativistic scattering problem we have two scattering amplitudes: the direct one

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

and the spin-flip one

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

In Eqs. (3) and (4) θ is the scattering angle, while $P_l(\cos\theta)$ and $P_l^1(\cos\theta)$ are the Legendre polynomials and the Legendre associated functions, respectively. With these two scattering amplitudes, differential cross-section for elastic scattering is defined by

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

while the spin polarization is given by

$$S(\theta) = \frac{i[f(\theta)g^*(\theta) - f^*(\theta)g(\theta)]}{\sigma_{\text{diff}}(\theta)}. \tag{6}$$

3. Results and discussion

3.1. Electron scattering from argon

In our recent work (Sienkiewicz et al., 2001) we have calculated phase shifts for elastic scattering of electrons from argon in the energy range of 10–160 eV to cover all energies used in measurements of Panajotović et al. (1997).

The three-dimensional plot our DCS is shown in Fig. 1. The low-angle critical minimum has been found by Panajotović et al. (1997) at 68.5° and 41.30 eV, while ours is at 68.0° and 39.30 eV. Angular positions are almost the same, while our scattering energy is 2 eV lower. In the case of the high-angle minimum, Panajotović et al. (1997) have localized it at 143.5° and 37.3 eV, while ours is at 141.0° and 39.5 eV.

Angular position of low-angle minimum along incident electron energy is given in Fig. 2. There is a very good agreement between our theoretical results and experimental data of Panajotović et al. (1997). Results of McEachran and Stauffer (1983), who solved the Schrödinger equation with an adiabatic exchange, cover the energy range up to 50 eV and agree well with the experiment. The theoretical line of Fon et al. (1987) who used the R-matrix approach, quite closely follows experimental data in the whole energy region, while the model results of Nahar and Wadhera (1987) fit even better the experimental points, particularly at small scattering energies. Kessler et al. (1976) measurement of the critical minimum position does not agree very well with the experimental point of Panajatović et al., neither with our predictions, although his point lies quite closely to both results.

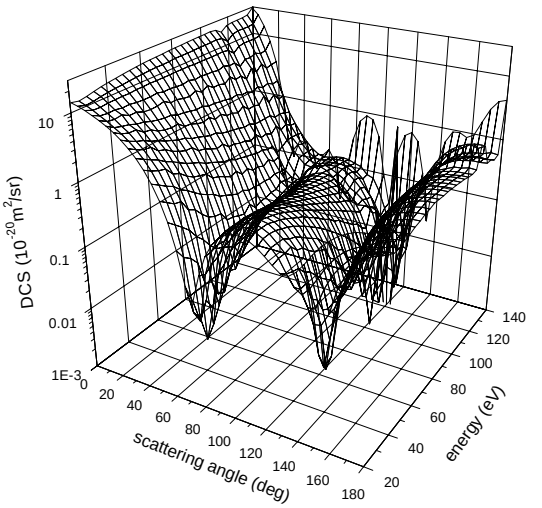

Fig. 1. Three-dimensional plot of the differential cross-section for elastic electron scattering from argon.

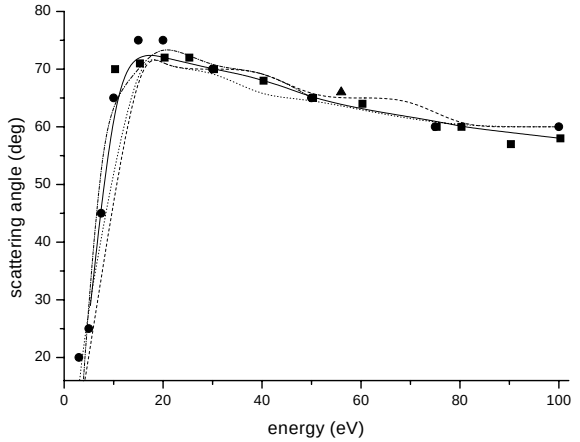

Fig. 2. Position of low-angle differential cross-section minimum versus incident energy for elastic electron scattering from argon. Experiment: ▲, Kessler et al. (1976); ●, Srivastava et al. (1981); □, Panajotović et al. (1997). Theory: ——, present results; ···, Nahar and Wadhera (1987); - - -, Fon et al. (1983); · — · — ·, McEachran and Stauffer (1983).

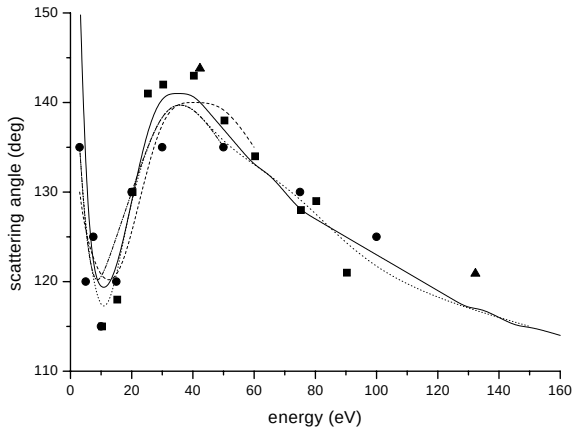

Fig. 3. The same as in Fig. 2 but for high-angle differential cross-section minimum.

In the case of the high-angle minimum (Fig. 3) the biggest discrepancy between our theoretical results and experimental ones occurs at low energies, 10–15 eV. Here, only model calculations (Nahar and Wadhera, 1987) show good agreement with the experiment. At higher energies, all displayed points and lines show better and more consistent agreement between themselves. Experimental points are well described by our theoretical results and results of Fon et al. (1983). It occurs that two other minima pointed out by Kessler et al. (1976) as separate critical minima are lying very close to our high-angle minima position curve. Our calculations of minima depths show that the first one is deeper, which means that this one is more significant.

We have also studied the connection between positions of critical minima and spin polarisation features of a scattered electron beam, which is unpolarised before scattering (Sienkiewicz et al., 2001). The chosen energy of 39.4 eV is very close to energies of low- and high-angle critical minima, which are 39.3 and 39.5 eV, respectively. The angular positions of critical minima very well coincide with positions of spin-polarization maxima. This fact, is explained by the relative weakness of the spin–orbit interaction (e.g. Kessler, 1985).

3.2. Electron scattering from zinc

We have calculated (Sienkiewicz et al., 2002) phase shifts for elastic scattering of electrons from zinc in the energy range of 10–40 eV to cover all energies used in the work of Predojević et al. (2000), who measured differential cross-sections for elastic scattering at 10, 15, 20, 25 and 40 eV. The scattering angle θ varied from 20° to 150°. In their experiment they used a crossed beam technique where a mono-energetic electronic beam crosses perpendicularly an atomic beam. Both, energy and angular resolutions, which were respectively 0.1 eV and 1.5°, assured accurate measurements of minima positions.

Fig. 4 shows a three-dimensional plot of the calculated differential cross-section. Two characteristic features of this surface are the minima which are situated at small and large angles. For large angles, in fact, the minimum splits into two branches at the *critical* minimum. The position of the *critical* minimum with depth of around 0.007×10^{-20} m^2/sr is at an electron energy of 26.0 eV and a scattering angle of 116°. These data agree well with the experimental values which are equal to 25.0 eV and 105°, respectively.

A more detailed comparison with the experiments by Predojević et al. (2000) and Childs and Massey (1933) is

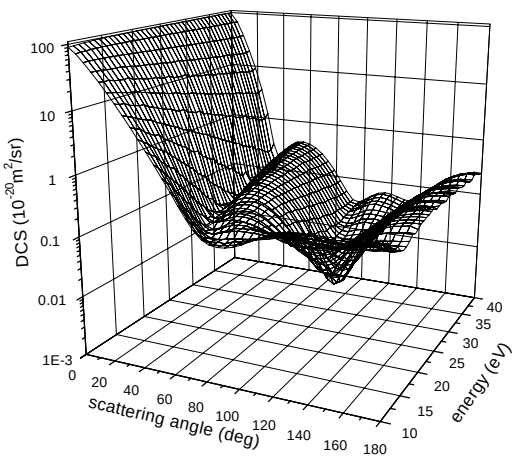

Fig. 4. Three-dimensional plot of the differential cross-section for elastic electron scattering from zinc.

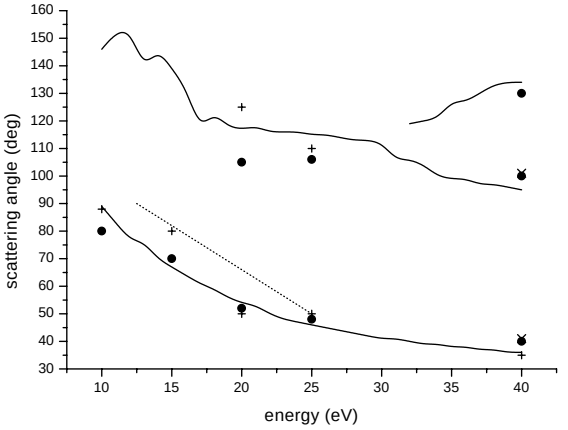

Fig. 5. Positions of differential cross-section minima in elastic electron scattering from zinc. Theory: ——, present; - - -, McGarrah et al. (1991). Experiment: •, Predojević et al. (2000); ×, Williams and Bozinis (1975); +, Childs and Massey (1933).

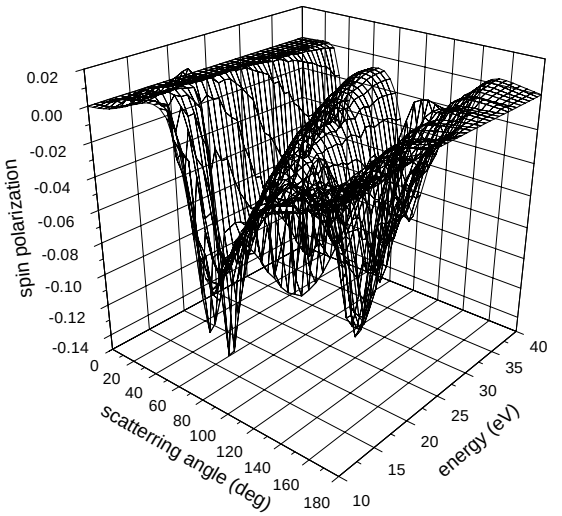

Fig. 6. Three-dimensional plot of the spin polarization cross-section for elastic electron scattering from zinc.

made in Fig. 5 where we also show the positions of small angle minima coming from the theoretical work of McGarrah et al. (1991).

In Fig. 6, we present the spin polarization in a three-dimensional plot. As it is seen from the figure, the highest degree of the spin polarization agrees very well with the minima in differential cross sections. In the case of zinc the highest achieved degree of spin polarization is 15% and occurs in the vicinity of the *critical* minimum.

4. Conclusion

The angle and the energy dependance of the differential cross-sections have been calculated for the elastic electron scattering from argon and zinc. In particular for the cross-section minima, very good agreement is found when compared with the very recent experimental data of Panajotović et al. (1997) and Predojević et al. (2000).

In addition, we present the spin polarization as a function of the energy and scattering angle which confirms the earlier prediction that the highest degree of polarization occurs near the minima of the differential cross sections.

We conclude that our fully relativistic, ab initio method, which incorporates target polarization and exchange effects, gives proper description of minima positions in differential cross-section for elastic scattering of electrons from argon and zinc.

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