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# Differential cross section minima in elastic scattering of electrons from zinc

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**Abstract**

Ab initio relativistic calculations have been carried out to search for minima in the angle and energy differential cross sections for the elastic scattering of electrons from zinc. Our theoretical approach is based on the Dirac–Fock method including the exchange interaction between the incident and the target electrons. The polarization of the target has been taken into account by ab initio potential from relativistic polarized orbital calculations. The positions of the calculated minima in the differential cross sections agree well with very recent measurements by Predojević et al. © 2002 Elsevier Science B.V. All rights reserved.

## 1. Introduction

Very recent measurements of Predojević et al. [1] provide an excellent data base to test different theoretical methods in their capability to predict the behavior and minima in the differential cross sections for the elastic scattering of electrons from Zn atoms. These cross sections have been analyzed in the energy range from 10 to 40 eV. There are also a number of earlier measurements of such cross sections, including the data by Williams and Bozinis [2], and Trajmar and Williams [3], or even very early measurements by Childs and Massey [4].

Several computations have been performed during the past years to study the elastic scattering from zinc theoretically. Recently, for example, McGarrah et al. [5] obtained the phase shifts for the scattered electrons by solving reduced radial wave equations, based on an static optical potential and including both polarization and exchange terms. A few years later Kumar et al. [6] employed a relativistic approximation which was build on the Dirac equation with some real and complex optical potentials.

In this Letter, we apply a relativistic Dirac–Fock method to study the angle and energy differential cross sections for the scattering of low and medium energy electrons from atomic zinc. By utilizing a previously developed Dirac–Fock approach [7,8], we are able to provide a full relativistic treatment of the elastic scattering at energies of several ten eV. Comparison is made with the recent experiments and previous com-

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putations. Here, we limit ourselves to the experimental energy range of the experiment of Predojević et al. [1].

Minima in the cross sections are found in two dimensions with respect to the electron energy and the angle of scattering. By looking at the minimum position as a function of scattering angle and scattering energy we can introduce so-called *critical* minimum for which the cross section has its minimum in the plane of scattering angle and projectile energy. The definition of *critical* minimum is attractive from an experimental point of view since it allows to focus further experimental effort on certain local areas. In the past, in contrast, comparison between measurements and theory was made for the angular dependence of the cross sections, taken at few selected energies. The precise measurement of the minimum position is difficult since it requires a very good angular and energetic resolution. Here we note that the accurate measurement of the depth of the *critical* minimum is virtually impossible difficult due to the inherit finite resolution of an experimental apparatus.

The use and importance of the *critical* minima for any detailed analysis of the cross sections has been pointed out before by Bühring [9], Kessler et al. [10], Lucas [11], Khare and Raj [12].

The position of the minima depends very sensitively also on the theoretical method which is used for description. Often, a proper treatment of the exchange potential of the incident electron with the bound-state density and a rather 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 (e.g., [13]). Our relativistic approach here allows both to compute the minima of the angle and energy differential cross sections as well as the degree of spin polarization.

## 2. Theoretical method

To obtain the wave function for the scattered electron with a given symmetry $\kappa$ and energy $E$ we solve the radial Dirac–Fock equation [14] which can be written in atomic units as

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

where $P_\kappa$ and $Q_\kappa$ are radial parts of the *large* and *small* components of the Dirac wave function and $\kappa = \pm(j+1/2)$ for $l = j \pm 1/2$ comprises the total angular momentum $j$ and parity $(-1)^l$, $\alpha$ is the fine structure constant. In addition, $V_{\rm fc}$ is the relativistic frozen-core potential, $V_p$ is the polarization potential; the two terms $X_P$ and $X_Q$ describe the exchange potential between the incident electron and bound electrons at the target.

Both the exchange terms and the frozen-core potential $V_{\rm fc}$ are calculated from first principles by using the one-electron orbitals as obtained by the multiconfiguration Dirac–Fock (MCDF) program of Desclaux [15] with some modifications [16]. These terms are defined as

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

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

where index $s$ refers to the scattered electron, $Z$ is the nuclear charge and the sums are over electrons of the target atom. The radial function $Y^k$ and the angular coefficients $a^k$ and $b^k$ are given by Grant [14].

The polarization potential $V_p$ can be derived in perturbation theory as a second-order correction to the frozen-core approximation. In our present approach, it includes the dipole static term and is taken in a numerical form from the ab initio calculations of Szmytkowski [17] which were done with the relativistic version of the polarized orbital method.

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

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

and the spin-flip one,

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

In Eqs. (3) and (4), $\theta$ 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

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

while the spin polarization cross section is given by

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

## 3. Results and discussion

We calculate phase shifts for elastic scattering of electrons from zinc in the energy range of 10–40 eV to cover all energies used in work of Predojević et al. [1], who measured differential cross sections for elastic scattering at 10, 15, 20, 25 and 40 eV. The scattering angle $\vartheta$ varied from 20 to 150°. In their experiment they used a crossed beam technique where a monoenergetic 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.

The position of the *critical* minimum with depth of around $0.007 \times 10^{-20}\ \text{m}^2/\text{sr}$ had been determined before in preliminary computations [16] at an electron energy of 26.0 eV and a scattering angle of 116°. These data agree well with the experimental values [1] which are equal to 25.0 eV and 105°, respectively.

Fig. 1 shows a three-dimensional plot of the calculated differential cross section. Two characteristic features of this landscape 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.

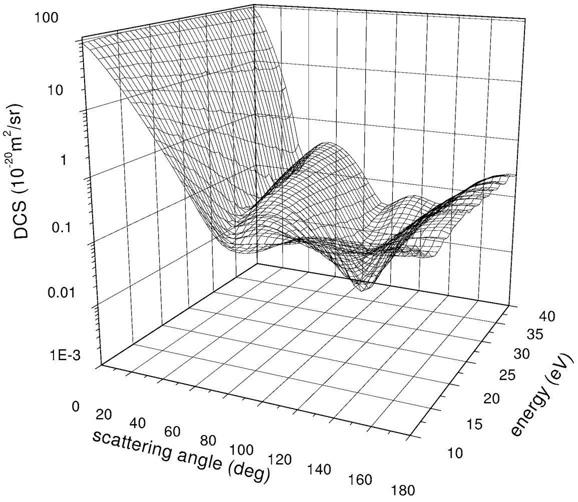


Fig. 1. Three-dimensional plot of the differential cross section for elastic electron scattering from zinc.

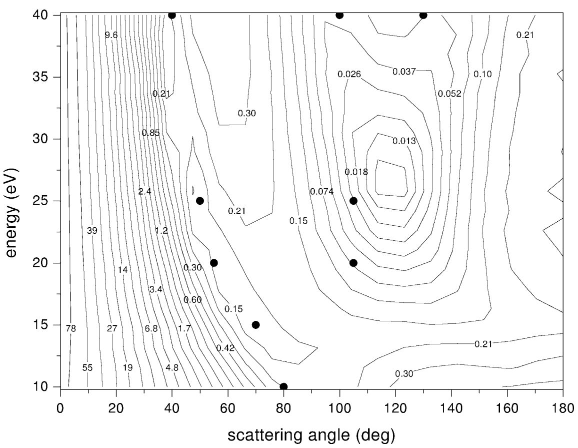


Fig. 2. Contour plot of the present differential cross section for elastic electron scattering from zinc. • indicate positions of experimental minima by Predojević et al. [1].

A contour map of our theoretical cross sections with the experimental points of Predojević et al. is displayed in Fig. 2. As one can notice the five experimental points indicating the the minima position are placed exactly along the small angle valley. Two other points at larger angles do not fit exactly into theoretical valley, but the two points at the top of figure confirm our results showing the split of the large angle valley into two branches.

A more detailed comparison with the experiments by Predojević et al. [1] and Childs and Massey [4] is

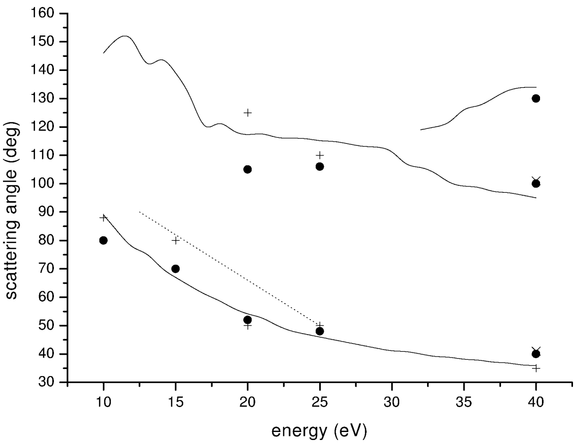


Fig. 3. Positions of differential cross section minima in elastic electron scattering from zinc. Theory: (—) present Letter; (- - -) McGarrah et al. [5]. Experiment: (•) Predojević et al. [1]; (×) Williams and Bozinis [2]; (+) Childs and Massey [4].

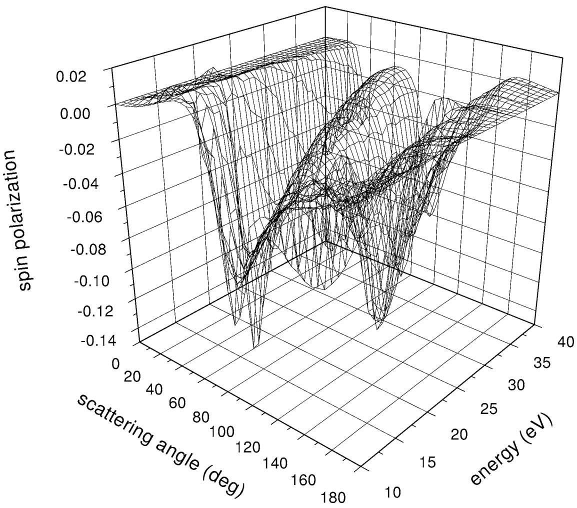


Fig. 4. Three-dimensional plot of the spin polarization cross section for elastic electron scattering from zinc.

made in Fig. 3 where we also draw the positions of small angle minima coming from the theoretical work of McGarrah et al. [5].

For small angles, our results cross the experimental data point of Childs and Massey [4] at 10 eV and come very closely to the data point of Predojević et al. at 20 eV. Overall, this yields a much better agreement with experiment than it was obtained by McGarrah et al. before.

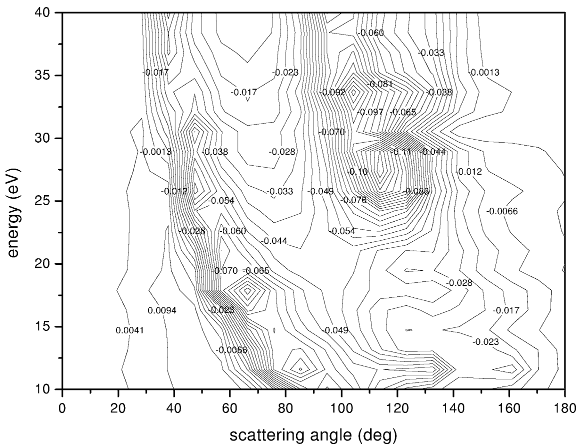


Fig. 5. Contour plot of the spin polarization cross section for elastic electron scattering from zinc.

At 40 eV, we find a slightly larger spread of the cross sections along the two valleys than in experiment by Predojević et al.

In Figs. 4 and 5, we also present the cross sections for the spin polarization in a three-dimensional plot and contour map, respectively. As seen from these figures, the highest degree of the spin polarization agree very well with the minima in differential cross sections. This has been explained before by the relative weakness of the spin–orbit interaction in atoms (e.g., [13]), which is responsible for spin polarization of scattered electronic beam. In the case of zinc the highest achieved degree of spin polarization is 15% and occurs in the vicinity of the *critical* minimum (Fig. 5).

## 4. Conclusion

The angle and the energy differential cross sections have been calculated for the elastic scattering from zinc. In particular for the cross section minima, very good agreement is found when compared with the very recent experimental data of Predojević et al. and quite old measurements of Childs and Massey.

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

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

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