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Spin polarization of slow electrons elastically scattered from xenon atoms

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Abstract. The spin polarization of electrons elastically scattered from Xe atoms was calculated for impact energies up to 10 eV. The calculations were carried out within a relativistic polarized orbital approximation. Our results are in good agreement with recent experimental data.

1. Introduction

Since 1968 more than twenty experimental and theoretical papers concerning spin polarization effects in elastic scattering of slow electrons from xenon atoms have been published. However, until recently the only experimental data available at energies below 10 eV were those of Klewer *et al* (1979). Among a few theoretical papers dealing with this energy range, so far the most sophisticated were polarized orbital calculations of McEachran and Stauffer (1986b). Being generally in qualitative agreement with the data of Klewer *et al*, the calculations of McEachran and Stauffer showed some quantitative deviations from the experimental results. The lack of other independently measured experimental data and other *ab initio* calculations made the explanation of this discrepancy impossible.

Very recent measurements of the Münster group (Dümmler *et al* 1993, Dümmler 1993) have shown that the results of Klewer *et al* (1979) might suffer from larger experimental errors than originally estimated. On the other side, the theoretical approach of McEachran and Stauffer (1986b), although of an *ab initio* form, was not free of shortcomings. One of them was a half-relativistic method: a relativistic approach was used for the description of motion of a continuum electron in an atomic field but a scattering potential was calculated in a hybrid way—its static part was obtained relativistically while a polarization part was found in a non-relativistic manner. Thus an origin of the aforementioned discrepancy might lie on the theoretical side, as well.

Recently, we have developed a fully relativistic version of the polarized orbital approximation, in which a calculated polarization potential is based on the Dirac–Hartree–Fock equations (Szmytkowski 1991, 1993a–c). An application of this method to calculate the spin polarization of slow electrons elastically scattered from zinc, cadmium and mercury atoms (Szmytkowski and Sienkiewicz 1994) has shown that in some cases our fully relativistic results differ significantly from the half-relativistic results of McEachran and Stauffer. This and recent measurements of the Münster group have prompted us to perform new completely relativistic calculations of the spin polarization of slow electrons elastically scattered from xenon atoms in order to verify the results of McEachran and Stauffer and resolve the discrepancy between theory and experiment.

2. Method

Our scattering equation is the radial continuum Dirac–Hartree–Fock equation (Szmytkowski 1991, equation (43))

$$\begin{pmatrix} mc^2 - E + V(r) & -c\hbar\left(\frac{\mathrm{d}}{\mathrm{d}r} - \frac{\kappa}{r}\right) \\ c\hbar\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\kappa}{r}\right) & -mc^2 - E + V(r) \end{pmatrix} \begin{pmatrix} F_\kappa(r) \\ G_\kappa(r) \end{pmatrix} = \begin{pmatrix} X_{F_\kappa}(r) \\ X_{G_\kappa}(r) \end{pmatrix} \tag{1}$$

with an initial condition $F_\kappa(0) = G_\kappa(0) = 0$. Here E is the total energy of the scattered electron (including its rest energy mc^2), $\kappa = \pm(j + \frac{1}{2})$ for $l = j \pm \frac{1}{2}$ and $V(r)$ is a spherically symmetric scattering potential which consists of static and polarization parts. $X_{F_\kappa}(r)$ and $X_{G_\kappa}(r)$ are the exchange terms and have been explicitly given in our previous work (Szmytkowski 1991). The static potential used in the present work has been calculated using the Dirac–Hartree–Fock code of Desclaux (1975) while the polarization potential has been obtained by solving the coupled Dirac–Hartree–Fock equations (Szmytkowski 1993a).

Solving equation (1) we make two simplifications. Firstly, because of the limitations of our computational facilities we are not able to include exchange-polarization terms in our calculations and we omit them. Thus in the present calculations $X_{F_\kappa}(r)$ and $X_{G_\kappa}(r)$ are the static-exchange terms. Secondly, for the reasons explained previously (Szmytkowski 1993a) we retain only the dipole term in the polarization potential. The same two simplifications were made by McEachran and Stauffer (1986b).

Evaluating phaseshifts we divide the configuration space into two regions which are separated by a sphere of radius R. In the inner region ($r < R$), where exchange is important, we perform direct outward integration of the Dirac equation (1) using a modified version of Desclaux's program (Desclaux 1975, Sienkiewicz and Baylis 1987). We stop this integration at the surface of the sphere and extract 'short-range' phaseshifts $\delta_\kappa^{\mathrm{s}}$ from the equation

$$\frac{G_\kappa(R)}{F_\kappa(R)} = \pm\lambda\left(\frac{\hat{j}_{l\mp1}(kR) - \hat{n}_{l\mp1}(kR)\tan\delta_\kappa^{\mathrm{s}}}{\hat{j}_l(kR) - \hat{n}_l(kR)\tan\delta_\kappa^{\mathrm{s}}}\right) \tag{2}$$

where

$$\lambda = \left(\frac{E - mc^2}{E + mc^2}\right)^{1/2} \qquad \text{and} \qquad k^2 = \frac{(E - mc^2)(E + mc^2)}{(c\hbar)^2} \tag{3}$$

while $\hat{j}_l(x)$ and $\hat{n}_l(x)$ are the Riccati–Bessel functions. In equation (2) the upper sign should be taken for $\kappa > 0$ and the lower one for $\kappa < 0$. In the outer region ($r > R$), where the exchange terms on the right-hand side of (1) may be neglected, we use the relativistic version of the variable phase method (Szmytkowski 1993a) solving an equation

$$\frac{\mathrm{d}\delta_\kappa(r)}{\mathrm{d}r} = -\lambda^{-1}\frac{V(r)}{c\hbar}(\hat{j}_l(kr)\cos\delta_\kappa(r) - \hat{n}_l(kr)\sin\delta_\kappa(r))^2 - \lambda\frac{V(r)}{c\hbar}(\hat{j}_{l\mp1}(kr)\cos\delta_\kappa(r) - \hat{n}_{l\mp1}(kr)\sin\delta_\kappa(r))^2 \tag{4}$$

subject to an initial condition

$$\delta_\kappa(R) = \delta_\kappa^{\mathrm{s}} \tag{5}$$

and then obtaining the phaseshift from the formula

$$\delta_\kappa = \lim_{r\to\infty}\delta_\kappa(r)\,. \tag{6}$$

The choice of the sign in (4) is the same as in (2).

Table 1. Summary of experimental work on spin polarization (the Sherman function) of electrons elastically scattered from Xe atoms over the energy range 0–100 eV.

		Fixed angle	
Author	Fixed energy (eV)	Angle (deg)	Energy range (eV)
Schackert (1968)	50, 100		
Klewer *et al* (1979)	5.5, 7.5, 10, 25, 30, 50, 100		
Berger *et al* (1982)	50, 60, 65, 70, 80, 100		
Wübker *et al* (1982)		60	0–360
Möllenkamp *et al* (1984)		80	0–360
Berger and Kessler (1986)	40, 50, 60, 80, 100		
Dümmler *et al* (1993) and Dümmler (1993)	1.5, 2, 3, 4, 5, 6, 7, 8, 9, 10		

We calculate the relativistic phaseshifts from $l = 0$ to $l_0 = 5$. For higher partial waves we estimate their values using the non-relativistic Born approximation (Mott and Massey 1965)

$$\delta_{-l-1} \approx \delta_l \approx \delta_l^{\mathrm{B}} = \pi \left(\frac{me^2\alpha_1}{\hbar^2}\right) \frac{k^2}{(2l-1)(2l+1)(2l+3)} \qquad l > l_0 \tag{7}$$

where $\alpha_1 = 26.97\, a_0^3$ is the relativistic dipole polarizability of the xenon atom extracted from the long-range part of the polarization potential. This leads to the following expressions for the direct $f(\theta)$ and spin-flip $g(\theta)$ scattering amplitudes

$$\begin{aligned} f(\theta) \approx{}& \frac{1}{2ik}\sum_{l=0}^{l_0}((l+1)(\mathrm{e}^{2\mathrm{i}\delta_{-l-1}}-1) + l(\mathrm{e}^{2\mathrm{i}\delta_l}-1))P_l(\cos\theta) \\ & -\pi\left(\frac{me^2\alpha_1}{\hbar^2}\right)k\left(\frac{1}{2}\sin\frac{\theta}{2} + \sum_{l=0}^{l_0}\frac{P_l(\cos\theta)}{(2l-1)(2l+3)}\right) \end{aligned} \tag{8}$$

$$g(\theta) \approx \frac{1}{2ik}\sum_{l=1}^{l_0}(\mathrm{e}^{2\mathrm{i}\delta_{-l-1}} - \mathrm{e}^{2\mathrm{i}\delta_l})P_l^1(\cos\theta)\,. \tag{9}$$

Given the scattering amplitudes, we calculate the Sherman function $S(\theta)$ (Kessler 1985) describing the spin polarization of initially unpolarized electrons after scattering from an unpolarized target:

$$S(\theta) = \frac{2\,\mathrm{Im}(f^*(\theta)g(\theta))}{|f(\theta)|^2 + |g(\theta)|^2}\,. \tag{10}$$

3. Results

For convenience we present summaries of experimental and theoretical works on the spin polarization of slow electrons elastically scattered from Xe atoms in tables 1 and 2, respectively.

In the present work we perform two types of calculations of the spin polarization: fully relativistic, with relativistically obtained both static and polarization potentials, and,

Table 2. Summary of theoretical work on spin polarization (the Sherman function) of electrons elastically scattered from Xe atoms over the energy range 0–100 eV.

Author	Method	Energy (eV)
Coulthard (1968)	Static	50, 100
Meister and Weiss (1968)	Static	20
Fink and Yates (1970a)	Static	100
Fink and Yates (1970b)	Static	25, 50
Walker (1971)	Static-exchange	2, 10, 20, 30, 60, 75
McCarthy *et al* (1977)	Optical model	50, 100
Walker (1981)	Simplified relativistic Polarized orbital theory	30
Sin Fai Lam (1982)	Pople–Schofield polarization potential	25, 30
Awe *et al* (1983)	Local-density approximation	25, 30, 50, 60, 65, 70, 80, 100
Fritsche *et al* (1984)	Kohn–Sham theory	25, 50
Kemper *et al* (1985)	Two-channel close-coupling theory	25, 30, 50, 60, 80, 100
Haberland and Fritsche (1986)	Kohn–Sham theory	40
Haberland *et al* (1986)	Kohn–Sham theory	50, 60, 100
McEachran and Stauffer (1986a)	Polarized orbital theory	4
McEachran and Stauffer (1986b)	Polarized orbital theory	5.5, 7.5, 10, 20, 50, 60, 80, 100
Jaskólski *et al* (1987)	Quasi-relativistic approach plus model polarization potential	5.5, 7.5, 10, 25, 30, 50
Sienkiewicz and Baylis (1989)	Model polarization potential	5.5, 7.5, 10, 25, 30
Sienkiewicz and Baylis (1991)	Model polarization potential	50, 60, 80, 100
Yuan and Zhang (1991)	Model polarization potential	0.15, 0.5, 10
Yuan and Zhang (1992)	Model polarization potential	0.5, 1, 2, 5, 10, 15, 25, 50, 75, 100
Yuan and Zhang (1993)	Model polarization potential	0.1–1.5
This work	Relativistic polarized orbital theory	2, 4, 5.5, 6, 7.5, 10

for the aim of comparison with similar calculations of McEachran and Stauffer (1986b), half-relativistic, with relativistic static and non-relativistic polarization potentials. Our fully relativistic results are shown in figure 1 over the energy range from 2 to 10 eV along with the experimental data of Klewer *et al* (1979) and the Münster group (Dümmler *et al* 1993, Dümmler 1993). Present half-relativistic results and those of McEachran and Stauffer (1986a, b) (who performed calculations at 4, 5.5, 7.5 and 10 eV) agree exactly and differ from the fully relativistic calculations only very slightly at extrema. We do not show these results for clarity of our graphs. For comparison between present results and those of other groups, which are not of an *ab initio* form, we refer the reader to the original papers (see table 2).

Comparison of present results with the data of Klewer *et al* (1979) shows some quantitative disagreement, the most pronounced at 7.5 eV, where our theoretical curve always lies behind the error bars. In contrast, our results agree much better with the data of the Münster group with differences occurring mainly in the vicinities of extrema. It should be stressed that at an energy of 10 eV where we may simultaneously compare our results with both sets of experimental data, our curve is very close to the experimental points of the Münster group,

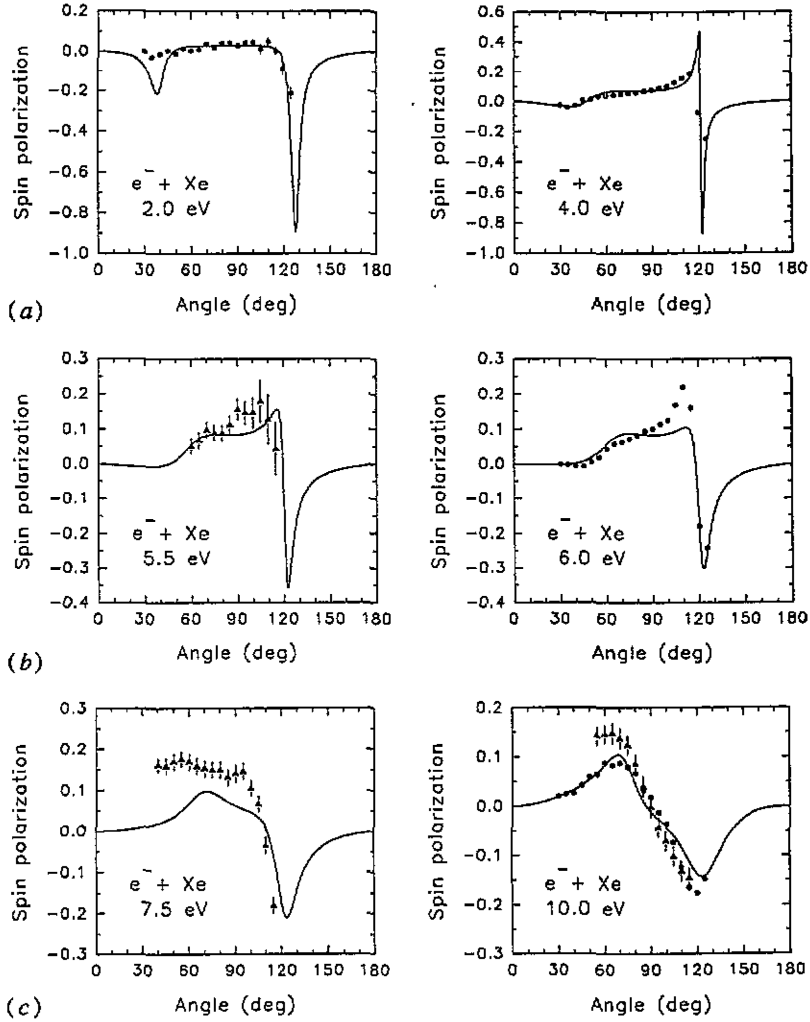

Figure 1. Spin polarization of electrons elastically scattered from xenon atoms over the energy range 2–10 eV: ——, present calculations; •, measurements of the Münster group (Dümmler *et al* 1993, Dümmler 1993); △, measurements of Klewer *et al* (1979).

especially at angles below 100°. Such good agreement suggests that the data of Klewer *et al* (1979) probably suffer from larger experimental errors than originally estimated.

4. Conclusions

We have shown that inclusion of relativity in calculations of the polarization potential within the polarized orbital approximation practically has no influence on the resulting spin polarization of slow electrons elastically scattered from xenon atoms. This effect may be qualitatively explained by a very compact structure of the xenon atom (Desclaux 1973). Comparison of present results with earlier experimental data of Klewer *et al* (1979) shows some discrepancies. In turn, comparison with very recent experimental data of the Münster group shows better agreement over the whole energy range from 2 to 10 eV. We conclude that the results of Klewer *et al* probably suffer from larger experimental errors than originally estimated.

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