J. Phys. B: At. Mol. Opt. Phys. **22** (1989) 3733-3745. Printed in the UK

# Low-energy elastic $e^-$–Xe scattering: the effect of exchange in the polarisation potential

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Received 13 July 1988, in final form 30 June 1989

**Abstract.** Continuum Dirac-Fock equations are solved for elastic scattering of electrons on xenon. The polarisation of the target atom is described by a model polarisation potential with one adjustable parameter $r_0$ in the cut-off function. The electrostatic exchange for both large and small components of the Dirac wavefunction is treated exactly. Moreover, the exchange contribution to the polarisation potential is included and is found to decrease the d-wave phaseshifts by as much as 25% in the energy range 1-25 eV, and thereby to improve the agreement between theory and experiment for the total differential cross sections. However, some discrepancies still remain, particularly for the spin polarisation.

## 1. Introduction

Since the classical work of Ramsauer (1921) and of Townsend and Bailey (1922), who measured total cross sections for electrons elastically scattered from noble gases, and the pioneering calculations of Mott (1929), there has been considerable interest in elastic electron-atom scattering, and a number of new experimental techniques and theoretical methods have been developed (see, for example, Lorents *et al* 1986). The relativistic, exchange, and polarisation effects have been investigated by many authors, including Walker (1971), Sin Fai Lam and Baylis (1981), McEachran and Stauffer (1984), and Sienkiewicz and Baylis (1987). The $R$-matrix method is one widely used approach (see, for example, Bartschat and Burke 1987). Another method, which uses a complex optical potential in order to include inelastic channels, has been discussed by McCarthy *et al* (1977). Also a local-density potential approach with an energy-dependent exchange approximation has been used by Awe *et al* (1983).

Correlation effects between the scattering electron and the target are manifested in the polarisation of the target by the electric field of the incident electron. The importance of such effects for electron scattering on polarisable targets has been well documented. The $R$-matrix method is a powerful coupled-channel approach with which one can treat exchange effects in calculations of both elastic and inelastic scattering. Although it can also handle correlation effects in principle, convergence of the polarisation terms with increasing basis size can be slow, particularly as in the case of closed-shell targets when many virtual excitations (closed channels) make roughly equal contributions, and implementation of the approach for heavy atomic targets with a sufficiently flexible basis can be prohibitive. Polarised-orbital treatments (for example,

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0953-4075/89/223733+13$02.50 

McEachran and Stauffer 1984) give target polarisation effects more efficiently. One makes a first-order adiabatic approximation for the distortion of the target orbitals by the scattering electron. In the usual 'adiabatic exchange' approximation (Dasgupta and Bhatia 1985), contributions to the electron exchange from the polarisation of the target are ignored. In all versions of the polarised-orbital method, the electrons are treated as distinguishable in that the scattering wavefunction has a different Hamiltonian than the target orbitals.

A simple approach to include effects of the target polarisation is to add a model polarisation potential (see, for example, Geltman 1969 or Sienkiewicz and Baylis 1987, 1988). However, applications of this approach to electron scattering have so far also treated the scattering electron as distinguishable from those in the target and have ignored contributions of the polarisation to the exchange interaction. In a polarised-orbital calculation of electron scattering on neon, Dasgupta and Bhatia (1984) investigated the exchange effect with the first-order distortions of the target orbitals and found that the effect can be important. Their approach follows the original polarised-orbital method (Temkin 1957) and sets the adiabatic polarising perturbation equal to zero whenever scatterer lies at smaller $r$ than the target electron.

The purpose of this paper is to use a model polarisation potential in continuum relativistic Dirac–Fock calculations of electron scattering which treat all electrons as indistinguishable. We also investigate the importance of an exact treatment of the exchange, including the exchange term arising from the polarisation potential. To test this approach the $e^-$–Xe system has been chosen because of the severe disagreement existing between experimental and theoretical results, as recently emphasised by Kessler (1986).

In the following sections we briefly describe our approach based on a continuum Dirac–Fock equation which includes the effect of exchange on the polarisation potential. In § 3 we specify our numerical methods, in § 4 we discuss our results and compare them with the available experimental and other theoretical results and in § 5 we summarise our conclusions.

## 2. Theory

The formulation of our scattering problem is based on the Dirac–Fock equation (see Grant 1970) and has been presented in earlier papers (Sienkiewicz and Baylis 1987, 1988), to which we refer the reader for details. Here we stress the modifications made in order to include the exchange contribution to the polarisation potential.

The scattering equation we solve is the radial continuum Dirac–Fock equation which can be written (compare Desclaux 1975):

$$\left(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{\kappa}{r}\right)P_\kappa(r)=\left\{2c+\frac{1}{c}[E-V_{\mathrm{fc}}(r)-V_{\mathrm{pol}}(r)]\right\}Q_\kappa(r)+X_Q(r)+X_Q^{\mathrm{pol}}(r)$$
$$\left(\frac{\mathrm{d}}{\mathrm{d}r}-\frac{\kappa}{r}\right)Q_\kappa(r)=-\frac{1}{c}(E-V_{\mathrm{fc}}(r)-V_{\mathrm{pol}}(r))P_\kappa(r)-X_p(r)-X_p^{\mathrm{pol}}(r) \tag{1}$$

where $\kappa=\pm(j+\frac{1}{2})$ for $l=j\pm\frac{1}{2}$, $V_{\mathrm{fc}}(r)$ is the relativistic frozen-core potential between the scattered electron and the target atom, $V_{\mathrm{pol}}(r)$ is the model polarisation potential, $X_{P(\mathrm{or}\,Q)}(r)$ is the exchange contribution of the electrostatic potential on the large $P$ (or small $Q$) component of the Dirac wavefunction and $X^{\mathrm{pol}}(r)$ is the correction to the exchange term due to the polarisation potential.

The polarisation potential arises from the second-order correlation correction to the frozen-core approximation. As shown by Baylis (1986) (see also Bottcher and Dalgarno 1974, Peach 1983), the dipole contribution can be written in the form

$$V_{\text{pol}}(\boldsymbol{r}_1, \ldots \boldsymbol{r}_N, \boldsymbol{r}) = -\tfrac{1}{2}\alpha_d \boldsymbol{E}^2 \tag{2}$$

where $\boldsymbol{r}_1, \ldots \boldsymbol{r}_N$ are the positions of the target electrons relative to the target atom centre, $\boldsymbol{r}$ is the radial coordinate of the scattering electron, and $\alpha_d$ is the static dipole polarisability of the target atom. Here $\boldsymbol{E}$ is the electric field, appropriately averaged over the target-atom core, of the scattering electron plus all $N$ target electrons together; it is approximated by

$$\boldsymbol{E} = \sum_i \boldsymbol{r}_i/(r_i^3 + r_0^3) \tag{3}$$

where $r_0$ is an adjustable parameter and atomic units are used. The approximation (2) is designed to have the correct form both asymptotically ($r \gg r_0$) and as $r \to 0$.

It is possible, by using polarised orbitals, for example, in a first-order inhomogeneous, coupled Hartree-Fock approximation (McEachran and Cohen 1983), to determine *ab initio* numerical values of the $r$ dependence of $\boldsymbol{E}$ (equation (2)) inside the target ($r < r_0$). However, there also exist static multipole terms corresponding to higher multipole moments and non-adiabatic dynamic corrections to each of the static polarisation contributions (Baylis 1986) which are usually ignored in polarised-orbital calculations. Neither the dynamic corrections nor the higher-order polarisabilities are known with much accuracy, but they tend to cancel one another. Thus for example, the asymptotic dependence of the dynamic correction to the dipole polarisation contribution is the same as for the static quadrupole interaction; the two effects are of roughly equal size but have opposite signs.

Because of the difficulty in determining accurately the short-range behaviour of the correlation correction to the frozen-core approximation, it seems reasonable to model it by a single-parameter function (3) with the correct limiting forms and to adjust the parameter to fit experimental data. A similar procedure to represent core-valence correlation has been used with considerable success in a series of publications of bound-state properties of atoms (see, for example, Migdalek and Baylis 1986 and references therein). Model polarisation potentials have also long been used in electron scattering (see, for example, Geltman 1969). The new feature of the approach presented here is to use the potential in a way fully consistent with the indistinguishability of the electrons; i.e. to use the same interaction for all electrons and to include exchange effects in the interaction.

Substituting the approximation (3) into (2) we obtain

$$\begin{aligned} V_{\text{pol}}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N, \boldsymbol{r}) &= -\tfrac{1}{2}\alpha_d \frac{r^2}{(r^3 + r_0^3)^2} - \alpha_d \sum_{i=1}^{N} \frac{\boldsymbol{r} \cdot \boldsymbol{r}_i}{(r^3 + r_0^3)(r_i^3 + r_0^3)} - \tfrac{1}{2}\alpha_d \sum_{i=1}^{N} \frac{r_i^2}{(r_i^3 + r_0^3)^2} \\ &\quad - \alpha_d \sum_{i<j=2}^{N} \frac{\boldsymbol{r}_i \cdot \boldsymbol{r}_j}{(r_i^3 + r_0^3)(r_j^3 + r_0^3)}. \end{aligned} \tag{4}$$

The first term on the right side in the above equation is the model polarisation potential $V_{\text{pol}}(r)$ used in the scattering equation (1). Although the second, 'dielectric', term contributes nothing to the direct interaction when the target atom is spherically symmetric, it does contribute to the exchange interaction and is responsible for what is referred to as 'exchange polarisation' (Temkin 1957). Its effect on the average is to reduce the strength of the polarisation interaction. The third and fourth terms from

(4) are included in the code for calculating the target-atom orbitals. This inclusion ensures orthogonality between the scattered-electron and target-atom wavefunctions, because they are now eigenfunctions of the same Hermitian one-electron operator. Obviously this inclusion also changes the calculated phaseshifts, but this change is found to be minimal and does not exceed 1% of the phaseshift in the 2–75 eV impact-energy range.

The polarisation interaction found from a second-order perturbation calculation of the energies is equivalent to that determined from first-order perturbed wavefunctions such as obtained in the polarised-orbital method. Of course matrix elements of the interaction are taken between antisymmetrised states and thereby give rise to both direct and exchange contributions (Baylis 1986). The explicit effect of exchange on the polarisation interaction between the scattering and target electrons is calculated here using the usual Grant (1970) method. Since the angular dependence of the contributing terms is $\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{r}}_i = P_1(\cos\theta) = \cos\theta$, where $\theta$ is the angle between the position vectors $\boldsymbol{r}$ and $\boldsymbol{r}_i$, the exchange term can be written in the following form

$$crX^{\mathrm{pol}}_{P(\mathrm{or}\,Q)} = \sum_{i=1}^{N} b^1(s, i)\, Y_{\mathrm{pol}}(s, i; r) P_i(\mathrm{or}\, Q_i)$$

where the index '$s$' refers to the scattered electron and $b^1$ is an angular coefficient (see Grant 1970). The radial function $Y_{\mathrm{pol}}$ is defined as

$$Y_{\mathrm{pol}}(s, i, r) = -\alpha_{\mathrm{d}} \frac{r^2}{r^3 + r_0^3} \int_0^\infty \frac{q\,\mathrm{d}q}{q^3 + r_0^3} \left(P_s(q)P_i(q) + Q_s(q)Q_i(q)\right) \mathrm{d}q. \qquad (5)$$

## 3. Numerical calculations

We determine the relativistic frozen-core potential $V_{\mathrm{fc}}$ (see equation (1)) which describes the ground state of the target atom using the Desclaux (1975) code with some modifications including a new direct five-point algorithm (Sienkiewicz and Baylis 1987). Having $V_{\mathrm{fc}}$, we solve the scattering equation (1) using the same integration algorithm. We obtain phaseshifts for $l = 0$ up to $l = 6$ by comparing the numerical solutions with the analytical ones at large $r$, and with these phaseshifts, calculate the total, momentum-transfer, differential and spin-polarisation (the Sherman function) cross sections (e.g. Kessler 1976, Sin Fai Lam 1982). We extend the summation in the cross section formulae from $l = 6$ to $l = 50$ by means of the effective formula given by Ali and Fraser (1977).

The dipole polarisability $\alpha_{\mathrm{d}}$ in our model polarisation potential (equation (4)) for Xe is taken to be $26.07a_0^3$ (Johnson and Kolb 1983). The remaining parameter $r_0$ is chosen to reproduce the Ramsauer–Townsend minimum in the total elastic target section for the electron–xenon scattering. The value $r_0 = 2.25a_0$ gives almost exactly the position and depth of the minimum, which was recently measured by Jost *et al* (1983) and Ferch *et al* (1987).

## 4. Results and discussion

We present our results for the phaseshifts $\delta_l^{\pm}$ ($l = 0, 1, \ldots, 5$) and for total elastic and momentum-transfer cross sections in table 1. Figure 1 shows how the omission of the exchange term of the polarisation potential affects phaseshifts. There is no significant

**Table 1.** The phaseshifts $\delta_l^{\pm}$ (for $j = l \pm \frac{1}{2}$) and total ($\sigma_{el}$) and momentum-transfer ($\sigma_m$) cross sections for electrons elastically scattered from xenon. The phaseshifts are in radians and the cross sections are in units of $\pi a_0^2$.

| $E$ (eV) | $\delta_0^+$ | $\delta_1^+$<br>$\delta_1^-$ | $\delta_2^+$<br>$\delta_2^-$ | $\delta_3^+$<br>$\delta_3^-$ | $\delta_4^+$<br>$\delta_4^-$ | $\delta_5^+$<br>$\delta_5^-$ | $\sigma_{el}$ | $\sigma_m$ |
|---|---|---|---|---|---|---|---|---|
| 0.4 | 0.1489 | 0.0483 | 0.0260 | 0.0082 | 0.0042 | 0.0025 | 14.721 | 5.052 |
| | | 0.0604 | 0.0260 | 0.0082 | 0.0042 | 0.0025 | | |
| 0.6 | 0.0729 | 0.0405 | 0.0408 | 0.0123 | 0.0059 | 0.0037 | 6.306 | 1.041 |
| | | 0.0597 | 0.0407 | 0.0123 | 0.0059 | 0.0037 | | |
| 0.8 | 0.0027 | 0.0240 | 0.0570 | 0.0164 | 0.0078 | 0.0049 | 4.870 | 1.676 |
| | | 0.0499 | 0.0568 | 0.0164 | 0.0078 | 0.0049 | | |
| 1.0 | −0.0629 | 0.0024 | 0.0748 | 0.0206 | 0.0098 | 0.0055 | 6.419 | 4.010 |
| | | 0.0342 | 0.0746 | 0.0205 | 0.0098 | 0.0055 | | |
| 2.0 | −0.3338 | −0.1328 | 0.1880 | 0.0424 | 0.0196 | 0.0109 | 29.163 | 24.944 |
| | | −0.0778 | 0.1873 | 0.0423 | 0.0196 | 0.0109 | | |
| 3.0 | −0.5450 | −0.2697 | 0.3434 | 0.0669 | 0.0296 | 0.0164 | 60.552 | 53.478 |
| | | −0.2013 | 0.3435 | 0.0666 | 0.0296 | 0.0164 | | |
| 4.0 | −0.7210 | −0.3967 | 0.5287 | 0.0947 | 0.0396 | 0.0220 | 93.908 | 81.023 |
| | | −0.3185 | 0.5322 | 0.0939 | 0.0396 | 0.0220 | | |
| 5.0 | −0.8730 | −0.5120 | 0.7174 | 0.1269 | 0.0501 | 0.0276 | 121.981 | 97.647 |
| | | −0.4266 | 0.7266 | 0.1256 | 0.0500 | 0.0275 | | |
| 5.5 | −0.9421 | −0.5655 | 0.8028 | 0.1447 | 0.0554 | 0.0303 | 131.871 | 100.351 |
| | | −0.4773 | 0.8152 | 0.1430 | 0.0553 | 0.0303 | | |
| 6.5 | −1.0695 | −0.6656 | 0.9563 | 0.1810 | 0.0666 | 0.0357 | 144.329 | 98.035 |
| | | −0.5726 | 0.9744 | 0.1787 | 0.0664 | 0.0357 | | |
| 7.5 | −1.1847 | −0.7572 | 1.0707 | 0.2244 | 0.0756 | 0.0395 | 147.993 | 88.822 |
| | | −0.6604 | 1.0929 | 0.2213 | 0.0753 | 0.0394 | | |
| 9.0 | −1.3394 | −0.8815 | 1.1907 | 0.2966 | 0.0932 | 0.0476 | 146.205 | 72.805 |
| | | −0.7805 | 1.2166 | 0.2924 | 0.0927 | 0.0476 | | |
| 10.0 | −1.4330 | −0.9570 | 1.2426 | 0.3536 | 0.1052 | 0.0532 | 143.382 | 63.147 |
| | | −0.8539 | 1.2696 | 0.3487 | 0.1047 | 0.0532 | | |
| 12.5 | −1.6402 | −1.1252 | 1.3109 | 0.5108 | 0.1355 | 0.0676 | 136.231 | 45.292 |
| | | −1.0181 | 1.3390 | 0.5049 | 0.1347 | 0.0674 | | |
| 15.0 | −1.8167 | −1.2703 | 1.3303 | 0.7036 | 0.1702 | 0.0827 | 132.867 | 34.515 |
| | | −1.1608 | 1.3584 | 0.6981 | 0.1691 | 0.0824 | | |
| 17.5 | −1.9730 | −1.3982 | 1.3254 | 0.9787 | 0.2048 | 0.0954 | 130.968 | 29.162 |
| | | −1.2871 | 1.3534 | 0.9755 | 0.2033 | 0.0950 | | |
| 20.0 | −2.1126 | −1.5126 | 1.3077 | 1.1568 | 0.2435 | 0.1111 | 128.405 | 28.071 |
| | | −1.4004 | 1.3355 | 1.1573 | 0.2418 | 0.1108 | | |
| 22.5 | −2.2385 | −1.6161 | 1.2823 | 1.4013 | 0.2839 | 0.1278 | 122.026 | 29.991 |
| | | −1.5013 | 1.3105 | 1.4059 | 0.2820 | 0.1273 | | |
| 25.0 | −2.3534 | −1.7088 | 1.8534 | 1.6429 | 0.3211 | 0.1426 | 111.120 | 33.207 |
| | | −1.5953 | 1.2814 | 1.6507 | 0.3192 | 0.1421 | | |
| 27.0 | −2.4589 | −1.7959 | 1.2218 | 1.8696 | 0.3583 | 0.1599 | 97.625 | 35.813 |
| | | −1.6820 | 1.2499 | 1.8793 | 0.3564 | 0.1593 | | |
| 30.0 | −2.5566 | −1.8769 | 1.2559 | 2.0662 | 0.3987 | 0.1774 | 85.358 | 35.574 |
| | | −1.7627 | 1.2855 | 2.0764 | 0.3968 | 0.1767 | | |

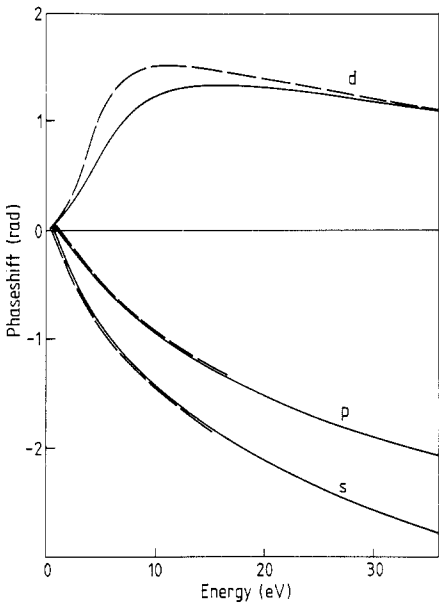


**Figure 1.** Present $\delta_l^+$ phaseshifts for the elastic scattering of electron by xenon with (full curve) and without (broken curve) the exchange term on the polarisation potential.

change in the s- and p-wave shifts, but the d-wave phaseshift calculated with polarisation exchange is considerably lower in the energy range 2–25 eV than that calculated without this exchange. The difference can be as much as 25% of the d-wave phaseshifts as calculated with exchange and reach 0.25 rad at 7.5 eV. Of course, because the exchange polarisation is included not only in the scattering equation (1), but also in the Dirac–Fock equations of the target atom, there may well be some contribution to the d-wave phaseshifts coming from the change in the atomic orbitals. By isolating the polarisation exchange effects between the scattering electron and the target electrons from those within the target xenon atom we find that the latter changes the d-wave phaseshifts by no more than 1% in the energy range 2–25 eV. This means that the exchange-polarisation effect between the scattered electron and the atomic electrons is dominant and obviously plays a significant role in the calculated cross sections.

In figure 2 we plot the total elastic cross section calculated with and without the exchange polarisation and compare with other theoretical and experimental results. As may be seen, our results with the exchange polarisation in the region of the maximum agree well with the experimental data of Dababneh *et al* (1980) and Nickel *et al* (1985), whereas our results without the exchange polarisation lie well above but closer to the experimental data of Jost *et al* (1983) and the theoretical results of Sin Fai Lam (1982). At the same time the theoretical curve of McEachran and Stauffer (1984) is well above any of the other results, and it seems that the large values of their d-wave shifts are responsible for this.

In the case of the momentum transfer cross section (figure 3) the situation is not so clear, because the experimental data (Frost and Phelps 1964) lie above all theoretical curves at energies above 8 eV. Once again, among the theoretical curves, ours calculated with the exchange polarisation has the lowest maximum. It is more consistent with the measurements at low energy than any of the other curves.

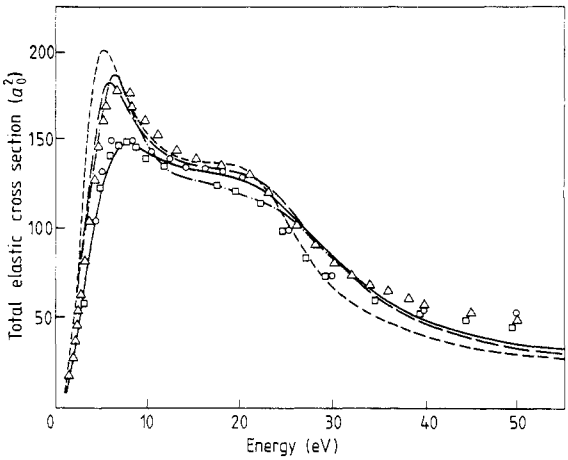


**Figure 2.** Total elastic scattering cross section. Theory: ——, present results with exchange polarisation; — — —, present results without the exchange polarisation; – – –, McEachran and Stauffer (1984); – · – · –, Sin Fai Lam (1982). Experiment: ○, Nickel *et al* (1985); □, Dababneh (1980); △, Jost *et al* (1983).

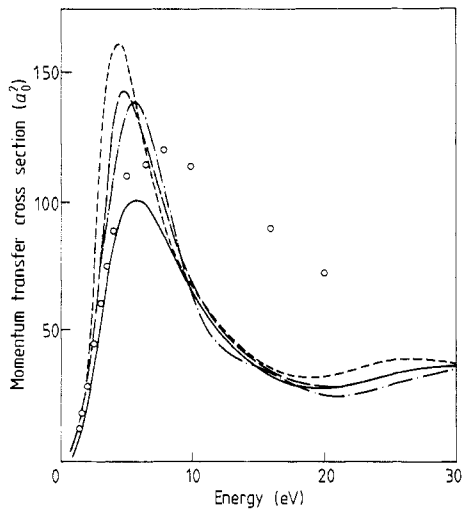


**Figure 3.** Momentum-transfer cross section. Theory: ——, present results with exchange polarisation; — — —, present results without exchange polarisation; – – –, McEachran and Stauffer (1984); – · – · –, Sin Fai Lam (1982). Experiment: ○, Frost and Phelps (1964).

The differential cross sections at 5 eV (figure 4) calculated with the exchange-polarisation contribution are somewhat too small in comparison with the experimental data of Register *et al* (1980) and Jost *et al* (1983) at angles below 120°. At larger angles, our theory appears to give the best results. When the exchange polarisation is omitted we almost reproduce the theoretical values of Sin Fai Lam (1982) (this is the reason the latter is not drawn in figure 4). McEachran and Stauffer (1984) seem to have too shallow a minimum at 120°, at least in comparison with the experimental data of Jost *et al* (1983), the theoretical data of Sin Fai Lam (1982), or our two curves. There is also an interesting feature around 60°, where all the theoretical lines except

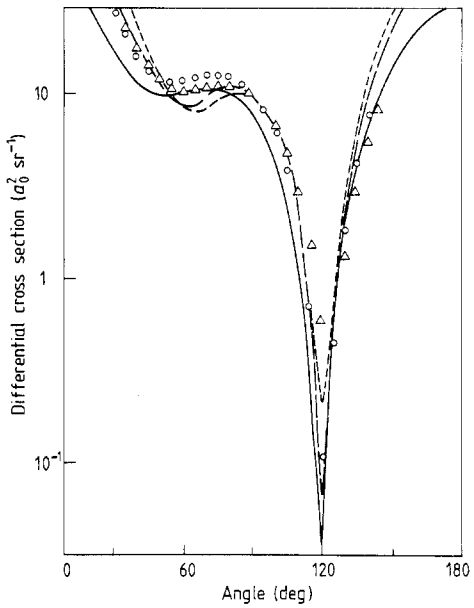


**Figure 4.** Differential cross section at 5 eV. Theory: ——, present results with exchange polarisation; — — —, present results without exchange polarisation; – – –, McEachran and Stauffer (1984). Experiment: ○, Register *et al* (1980); △, Jost *et al* (1983).

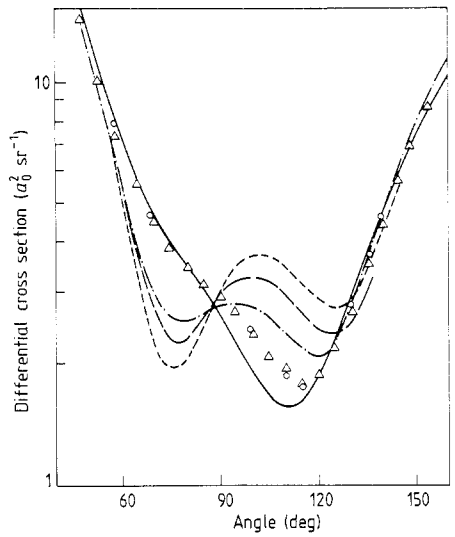


**Figure 5.** Differential cross section at 10 eV. Theory: ——, present results with exchange polarisation; — — —, present results without exchange polarisation; – – –, McEachran and Stauffer (1984); – · – · –, Sin Fai Lam (1982). Experiment: ○, Register *et al* (1980); △, Jost *et al* (1983).

ours calculated with exchange polarisation display a substantial minimum which is not evident in the measurements of Register *et al* (1980) and Jost *et al* (1982). This feature becomes much more pronounced at 10 eV (see figure 5), where only our results with the exchange polarisation agree roughly with the experimental points of Register *et al* (1980) and Jost *et al* (1983) and exhibit a single minimum at around 115°. The other theoretical results of Sin Fai Lam (1982), McEachran and Stauffer (1984) and our calculations without the exchange polarisation show two distinct minima at around 75° and 125°. At 20 eV (figure 6) the experimental and theoretical data including the optical-model results of McCarthy *et al* (1977) give more or less the same shape, but there is quite a discrepancy in the absolute values of the consecutive minima and maxima. We are better satisfied with our results at 30 eV (see figure 7), which are in good agreement with the measurements of Williams and Crowe (1975) and the theoretical results of McCarthy *et al* (1977). The theoretical curve of McEachran and Stauffer significantly underestimates the minimum at 95°. At this energy the difference between our results with and without exchange polarisation is negligible.

We turn now to spin polarisation and compare our results with the recent theoretical work of McEachran and Stauffer (1986) and with the only available experimental work at low energies (up to 30 eV) by Klewer *et al* (1979). Figure 8 displays the spin polarisation results at an impact energy of 5.5 eV. Our curve calculated with the exchange polarisation has pronounced extrema while the curve of McEachran and Stauffer (1986) and our results without the exchange part of the polarisation potential are relatively flat and show better agreement around 110° with the experimental points of Klewer *et al* (1979). At 7.5 eV (see figure 9) our results with exchange polarisation

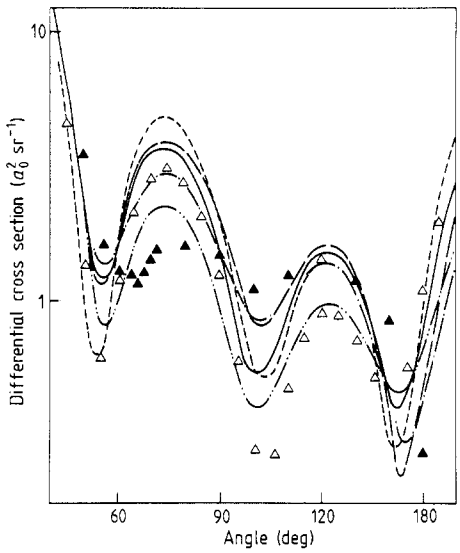


**Figure 6.** Differential cross section at 20 eV. Theory: ——, present results with exchange polarisation; — — —, present results without exchange polarisation; – – –, McEachran and Stauffer (1984); – · – · –, Sin Fai Lam (1982); – · · – · · –, McCarthy *et al* (1977). Experiment: ▲, Williams and Crowe (1975); △, Jost *et al* (1983).

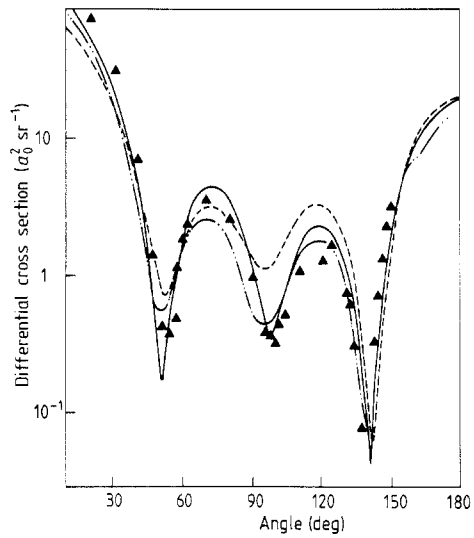


**Figure 7.** Differential cross section at 30 eV. Theory: ——, present results; – – –, McEachran and Stauffer (1984), – · · – · · –, McCarthy *et al* (1977). Experiment: ▲, Williams and Crowe (1975).

have moved the maximum from about 70° to about 110° in comparison with both McEachran and Stauffer (1986) and our results without the polarisation exchange. Our results thus give a closer fit to data near 100°, but none of the theories shows the broad plateau at the forward angles which was measured by Klewer *et al* (1979). A more satisfactory situation occurs at 10 eV (figure 10). Our results with and without the exchange polarisation slowly converge, and at 25 eV there is practically no difference, so we draw only one curve in figure 11. Both McEachran and Stauffer (1986) and our results show some agreement with the experimental data of Klewer *et al* (1979). However, at an energy of 30 eV (figure 12) there is little agreement between theory and experiment. The theoretical results of Walker (1977) (not drawn in the figure) also follow our curve. In view of the good agreement obtained for the differential cross section at the same energy with the measurements of Williams and Crowe (1975), the situation is intriguing and needs further investigation.

## 5. Conclusions

The results for total and differential cross sections show our relativistic Dirac-Fock calculations with a relatively simple model of the polarisation interaction to be comparable with or in somewhat better agreement with experiment than previous calculations. They also show the sizable influence of treating all the electrons as indistinguishable. In particular, the inclusion of exchange in the polarisation interaction lowers the d-wave phaseshifts by as much as 25% for the xenon target in the 1-25 eV energy range. It also lowers the total cross section and generally gives better agreement with

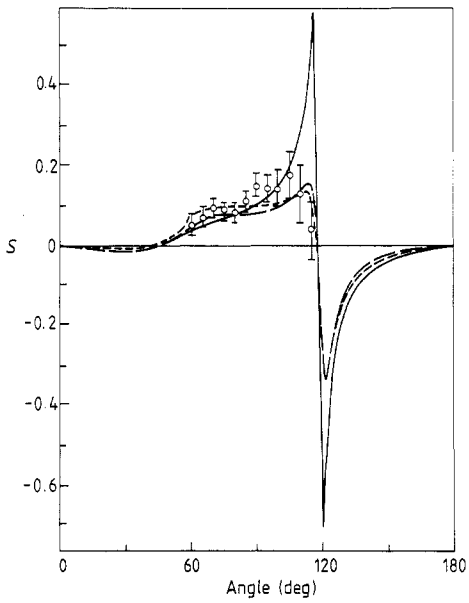


**Figure 8.** Spin polarisation $S$ as a function of the scattering angle at an electron impact energy of 5.5 eV. Theory: ——, present results with exchange polarisation; — — —, present results without exchange polarisation; – – –, McEachran and Stauffer (1986). Experiment: ⊙, Klewer *et al* (1979).

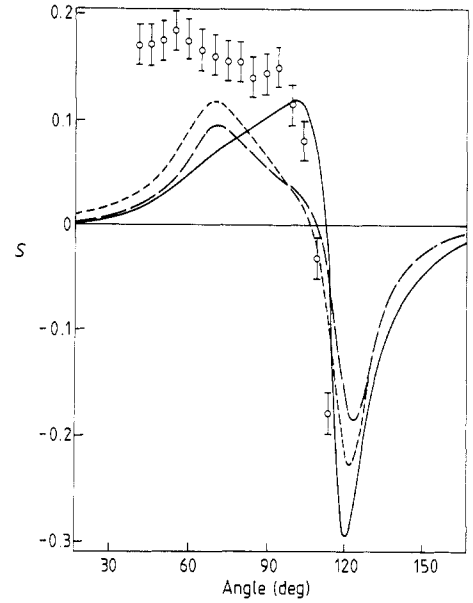


**Figure 9.** As in figure 8 but at 7.5 eV.

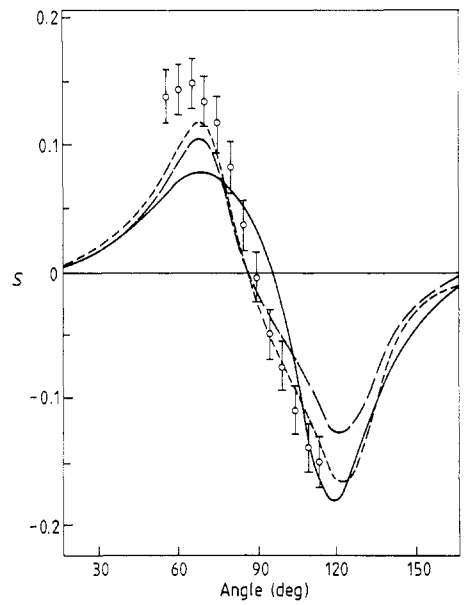


**Figure 10.** As in figure 8 but at 10 eV.

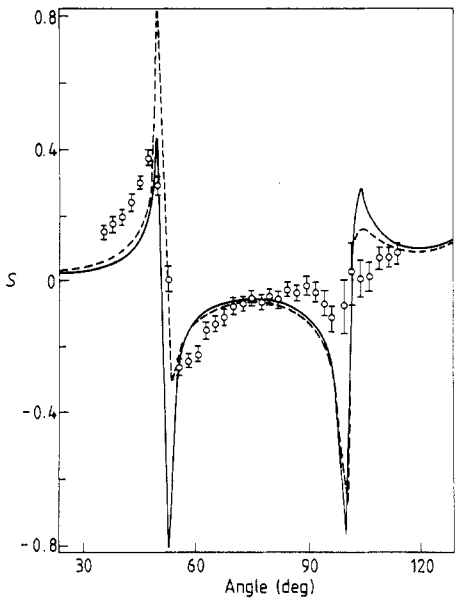


**Figure 11.** Spin polarisation $S$ as a function of the scattering angle at an electron impact energy of 25 eV. Theory: ——, present results; – – –, McEachran and Stauffer (1986). Experiment: ○, Klewer *et al* (1979).

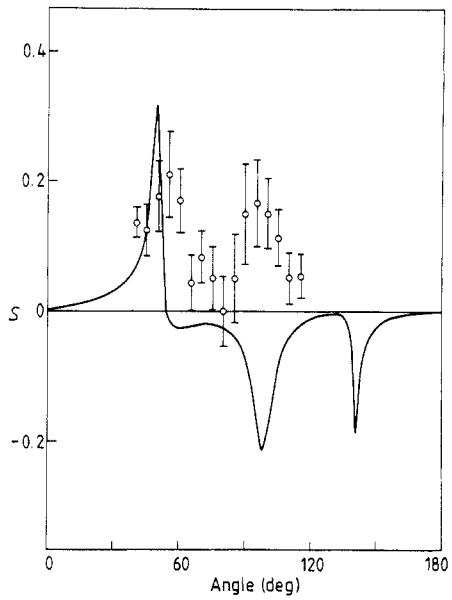


**Figure 12.** Spin polarisation $S$ as a function of the scattering angle at an electron impact energy of 30 eV: ——, present theoretical results; ○, experimental results of Klewer *et al* (1979).

the experimental data. Improvement is also noted for the differential cross sections, especially at the energy of 10 eV, where the spurious minimum has been eliminated. On the other hand, the exchange polarisation does not improve the rather poor agreement for the spin polarisation. The marked disagreement at 30 eV, where the exchange term for the polarisation potential is negligible is especially puzzling since at the same energy there still is good agreement between our theoretical values and experimental ones for the differential cross section.

The effects of exchange polarisation found here for scattering from xenon are consistent with those found by Dasgupta and Bhatia (1984) in the case of neon; in both cases changes of a few per cent were observed in the s and p phaseshifts at low energy. With neon, the change for p waves is greater than for s waves, whereas with xenon, the greatest change occurs for d waves. The overall effect of exchange polarisation is greater for xenon, as one would expect since the polarisation interaction itself is much larger than in neon.

Discrepancies which remain can probably be blamed, at least partially, on an inadequate model for the short-range part of the polarisation potential. The evidence from the total and differential cross sections suggests that the short-range potential should be slightly more attractive so that the final interaction with exchange polarisation is somewhat more like the interaction without it.

Our method, which starts with a frozen-core approximation for the target and adds corrections in the form of polarisation terms, is restricted to calculations of elastic scattering and is best suited to closed-shell targets. For inelastic scattering including exchange interactions, the $R$-matrix method can be used, although as indicated in the introduction, it may be difficult to reproduce polarisation effects adequately in heavy atoms.

The model polarisation potentials in our calculation could be replaced by *ab initio* functions, but unless these functions, which should include higher-order multipoles and non-adiabatic effects, are determined with great care, it is somewhat doubtful that they would represent a real improvement. Indeed, this conclusion seems confirmed by a comparison of our results with those of McEachran and Stauffer (1984, 1986), who calculated such a function by the polarised-orbital method. Nevertheless, in demonstrating the sensitivity of the low-energy results to exchange polarisation, we have also shown their sensitivity to that part of the polarisation potential inside the target, because it is this region that contributes to the exchange. The accurate determination of polarisation potentials is thus a valuable step in improving computations of low-energy elastic scattering on heavy atoms. The evidence presented here shows that in applying such potentials at low energies, the contributions of exchange polarisation must not be ignored.

Model polarisation potentials such as used here will prove useful in many calculations, even those for inelastic scattering. For example, in $R$-matrix calculations they can represent theat part of the correlation interaction involving the frozen inner cores of the target, in analogy with recent multiconfiguration calculations of atomic properties (Migdalek and Baylis 1986).

## Acknowledgments

This work has been supported by the Natural Sciences and Engineering Research Council of Canada.

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