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Relativistic effects in spin-polarization parameters for low-energy electron–Cs scattering

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Abstract. Based on a recent Dirac R-matrix (close-coupling) calculation, we present results for various spin-polarization parameters for elastic and inelastic scattering of slow ($E_{\mathrm{kin}} \lesssim 2$ eV) polarized electrons from unpolarized and polarized neutral Cs atoms in their ground state. Our results allow for a quantitative estimate of the importance of relativistic effects, and our calculated parameters clearly deviate from predictions obtained by just jj-recoupling the results of a non-relativistic calculation.

1. Introduction

Scattering processes involving spin-polarized electrons have been of great interest for many years (for an introduction, see Kessler 1985). Such interest has, in part, been generated by the possibility of performing so-called 'perfect scattering experiments' (Bederson 1969) in which the maximum available information, namely the magnitudes and the relative phases of the scattering amplitudes, is determined. These experiments allow for a very detailed test of theoretical models (see, for example, Berger and Kessler 1986 and references therein).

So far, experiments for the so-called '*STU* parameters' (Kessler 1985) have been restricted to elastic scattering from targets with total electronic angular momentum $J = 0$. An extension of the general theory has been given by Bartschat and Madison (1988) who introduced the 'generalized *STU* parameters' which were then further discussed by Bartschat (1989). In the latter review (to be referred to as I), it was shown that the seven generalized *STU* parameters S_P, S_A, T_x, T_y, T_z, U_{xz} and U_{zx} reduce to the three parameters S, T and U of Kessler (1985) in the case of scattering from a target without electronic angular momentum in the initial and final states (i.e. especially for elastic scattering from such targets). Furthermore, it was shown that time-reversal invariance of the projectile–target interaction reduces the number of independent generalized *STU* parameters to five for elastic scattering from targets with non-zero but otherwise arbitrary angular momentum. Results for the complete set of these parameters were then presented by Bartschat *et al* (1990) and Goerss *et al* (1991) for elastic electron scattering from thallium and lead atoms. These calculations were based on T-matrix elements calculated by Bartschat and Scott (1984) and

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Bartschat (1985) who applied the semi-relativistic Breit–Pauli R-matrix method of Scott and Burke (1980).

In this paper we follow a similar strategy to obtain differential cross sections and spin-polarization parameters for elastic and inelastic scattering of slow spin-polarized electrons from both unpolarized and polarized caesium atoms. The results presented are based on the Dirac R-matrix calculation of Thumm and Norcross (1991, 1992, the latter paper being referred to as II) and therefore, for the first time, include complete sets of generalized *STU* parameters obtained from a fully relativistic close-coupling calculation. It was shown previously that relativistic interactions can yield a non-statistical branching ratio of inelastic differential cross sections for (6p) $^2P_{1/2}$ and (6p) $^2P_{3/2}$ electron-impact excitation of caesium atoms (Thumm and Norcross 1993). It is of fundamental interest to verify quantitatively to what extent parameters other than cross sections, that contain additional information on the details of the scattering dynamics and are sensitive to the phase information included in the scattering amplitudes, are influenced by relativistic effects. For this purpose, the generalized *STU* parameters are exceptionally well suited due to several simple algebraic relations that must hold if relativistic effects are taken into account only by angular momentum recoupling procedures (Hanne 1983); thus a violation of these relations indicates the importance of a relativistic description of the scattering process.

This paper is organized as follows. In section 2, we will summarize the general theory given in I. Next we briefly outline the main steps of the numerical calculation, while numerical results for elastic and inelastic electron scattering from caesium atoms will be presented and discussed in section 4. Finally, our conclusions are presented in section 5.

2. General theory

As shown in I, the reduced spin density matrix of electrons after scattering from unpolarized targets is given by

$$\begin{aligned}(\rho_{\rm out})_{m_1'm_1} &= \sum_{M_1}\langle J_1M_1;\boldsymbol{k}_1m_1'|T\rho_{\rm in}T^{\dagger}|J_1M_1;\boldsymbol{k}_1m_1\rangle \\ &= \sum_{m_0'm_0}\langle m_1'm_0';m_1m_0\rangle\rho_{m_0'm_0}\end{aligned}\tag{1}$$

where

$$\langle m_1'm_0';m_1m_0\rangle \equiv \frac{1}{2J_0+1}\sum_{M_1M_0} f(M_1m_1';M_0m_0')f^*(M_1m_1;M_0m_0)\tag{2}$$

and T is the transition operator. In (2), the scattering amplitudes

$$f(M_1m_1;M_0m_0) \equiv \langle J_1M_1;\boldsymbol{k}_1m_1|T|J_0M_0;\boldsymbol{k}_0m_0\rangle\tag{3}$$

describe the scattering of electrons with initial linear momentum $\boldsymbol{k}_0$ and spin component m_0 (with regard to a given quantization axis) from a target with total angular momentum J_0 and component M_0 with the final state characterized by the projectile momentum $\boldsymbol{k}_1$, spin component m_1 and the target quantum numbers J_1 and M_1, respectively. Throughout this paper, we refer to the so-called 'collision frame' where the z-axis, as quantization axis,

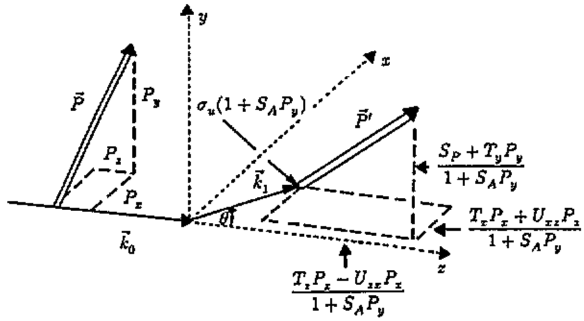

Figure 1. Illustration of the generalized *STU* parameters (see text).

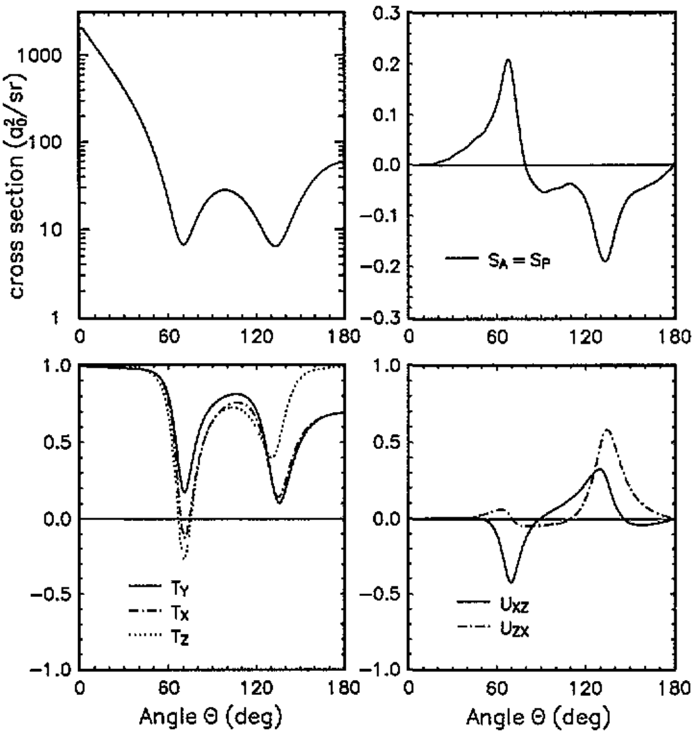

Figure 2. Differential cross section σ_u (in a_0^2 sr^{-1}), Sherman function S ($= S_A = S_P$), contraction parameters T_x, T_y, T_z, and rotation parameters U_{xz} and U_{zx} for elastic elcetron scattering from unpolarized caesium atoms at 1.3 eV.

is chosen parallel to k_0 and the scattering takes place in the xz plane with the scattering angle θ and a vanishing azimuthal angle ϕ.

Using the Hermiticity of the density matrix and assuming parity conservation in the projectile–target interaction, it was shown in I that the spin density matrix (1) can be fully characterized in terms of the eight independent parameters

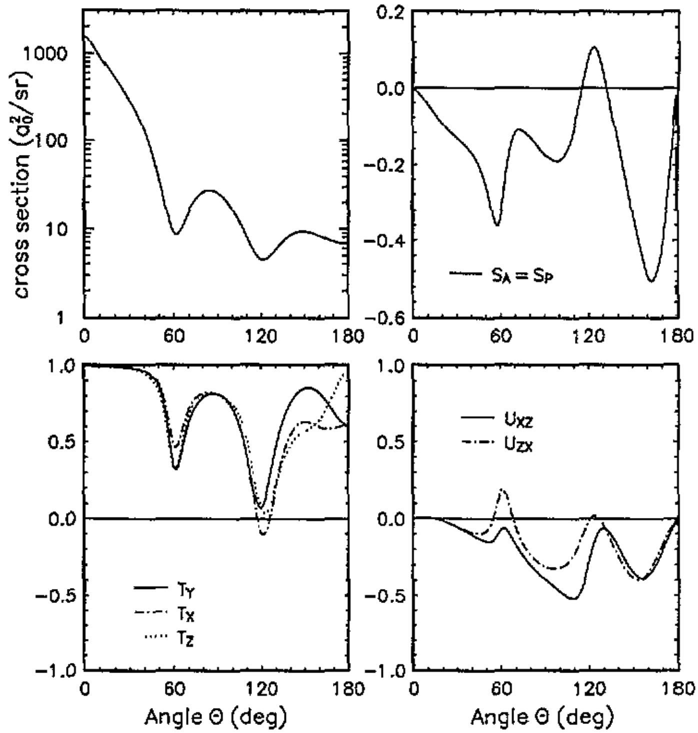

Figure 3. As figure 2 at 1.6 eV.

$$\sigma_u = \frac{1}{2}\sum_{m_1 m_0} \langle m_1 m_0; m_1 m_0 \rangle \tag{4a}$$

$$S_P = -\frac{2}{\sigma_u} \operatorname{Im}\{\langle \tfrac{1}{2}\tfrac{1}{2}; -\tfrac{1}{2}\tfrac{1}{2} \rangle\} \tag{4b}$$

$$S_A = -\frac{2}{\sigma_u} \operatorname{Im}\{\langle \tfrac{1}{2} - \tfrac{1}{2}; \tfrac{1}{2}\tfrac{1}{2} \rangle\} \tag{4c}$$

$$T_x = \frac{1}{\sigma_u}[\langle -\tfrac{1}{2} - \tfrac{1}{2}; \tfrac{1}{2}\tfrac{1}{2} \rangle + \langle -\tfrac{1}{2}\tfrac{1}{2}; \tfrac{1}{2} - \tfrac{1}{2} \rangle] \tag{4d}$$

$$T_y = \frac{1}{\sigma_u}[\langle -\tfrac{1}{2} - \tfrac{1}{2}; \tfrac{1}{2}\tfrac{1}{2} \rangle - \langle -\tfrac{1}{2}\tfrac{1}{2}; \tfrac{1}{2} - \tfrac{1}{2} \rangle] \tag{4e}$$

$$T_z = \frac{1}{\sigma_u}[\langle \tfrac{1}{2}\tfrac{1}{2}; \tfrac{1}{2}\tfrac{1}{2} \rangle - \langle \tfrac{1}{2} - \tfrac{1}{2}; \tfrac{1}{2} - \tfrac{1}{2} \rangle] \tag{4f}$$

$$U_{xz} = \frac{2}{\sigma_u} \operatorname{Re}\{\langle \tfrac{1}{2}\tfrac{1}{2}; -\tfrac{1}{2}\tfrac{1}{2} \rangle\} \tag{4g}$$

$$U_{zx} = -\frac{2}{\sigma_u} \operatorname{Re}\{\langle \tfrac{1}{2} - \tfrac{1}{2}; \tfrac{1}{2}\tfrac{1}{2} \rangle\} \tag{4h}$$

where Re$\{x\}$ and Im$\{x\}$ denote the real and imaginary parts of the complex quantity x. Note that all the T-parameters are real which follows from the Hermiticity of the density matrix.

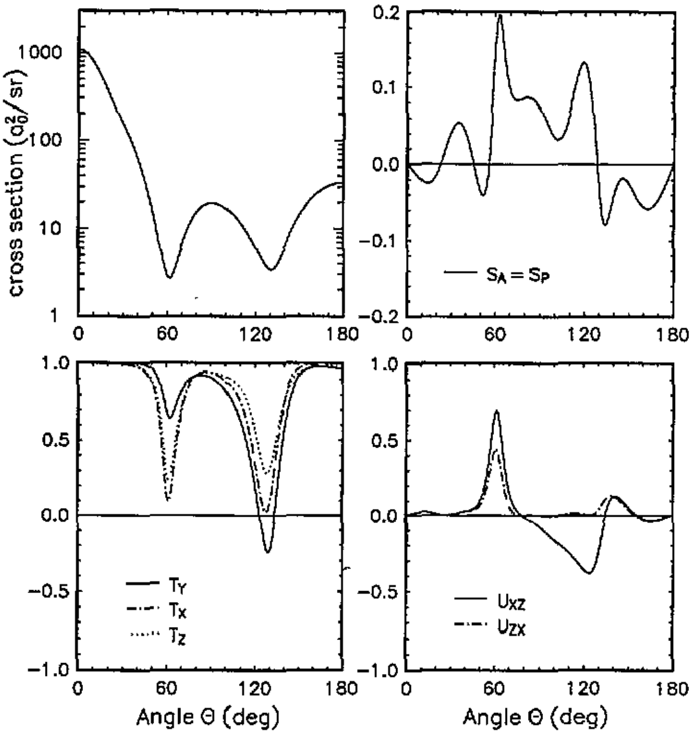

Figure 4. As figure 2 at 2.04 eV.

Consequently, the spin polarizations $\boldsymbol{P}$ and $\boldsymbol{P}'$ of the scattered electrons before and after the interaction with the target are related by

$$P' = \frac{(S_p + T_y P_y)\hat{y} + (T_x P_x + U_{xz} P_z)\hat{x} + (T_z P_z - U_{zx} P_x)\hat{z}}{1 + S_A P_y}. \tag{5}$$

The physical meaning of equation (5) and the generalized *STU* parameters is illustrated in figure 1: σ_u is the differential cross section for the scattering of unpolarized projectiles from unpolarized targets, the polarization function S_P gives the polarization of an initially unpolarized projectile beam after the scattering, and the asymmetry function S_A determines the left–right asymmetry in the differential cross section for scattering of spin-polarized projectiles. Furthermore, the contraction parameters T_x, T_y, T_z describe the change in an initial polarization component along the three Cartesian axes while the parameters U_{xz} and U_{zx} determine the rotation of a polarization component in the scattering plane.

It should be noted that the differential cross section σ_u can be determined in a 'single' scattering experiment, while S_P as well as S_A require 'double' and T_x, T_y, T_z, U_{xz} and U_{zx} even 'triple' scattering experiments corresponding to the production (1), change (2) and analysis (3) of the projectile polarization. Such triple scattering experiments have now become experimentally feasible even at low energies and for physically interesting cases with small cross sections (see, for example, Berger and Kessler 1986).

An interesting special case for the present paper is the elastic scattering from unpolarized targets with arbitrary angular momentum $J_0 = J_1$ where time-reversal invariance of the projectile–target interaction leads to

$$S_P = S_A \tag{6a}$$

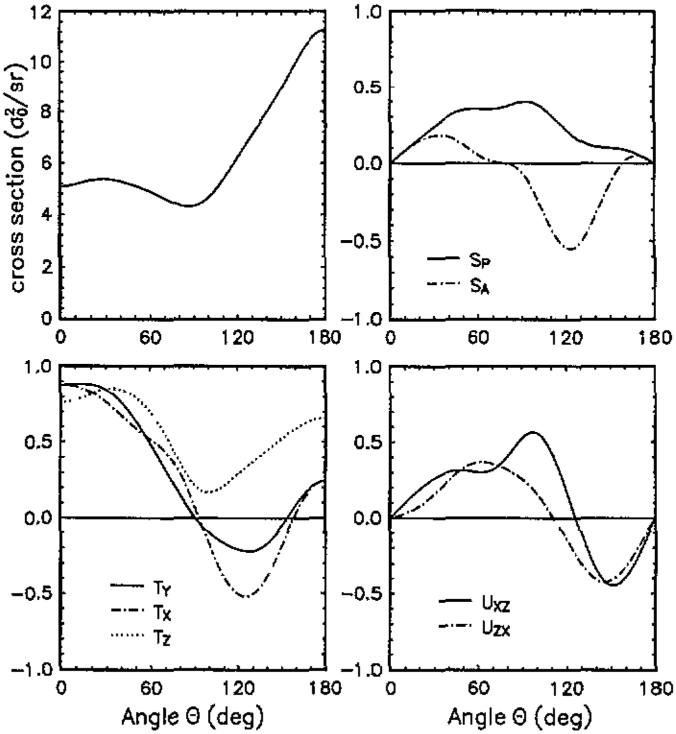

Figure 5. As figure 2 for $(6s)\,^2S_{1/2} \rightarrow (6p)\,^2P_{1/2}$ excitation at 1.6 eV.

and

$$U_{xz} - U_{zx} = (T_z - T_x)\tan\theta \tag{6b}$$

(for details, see I). Hence, the number of independent parameters is reduced to five relative generalized *STU* parameters and one absolute differential cross section σ_u. Although equation (6*b*) also applies to elastic scattering from targets with zero angular momentum, it does not yield any further information in this case since $T_x \equiv T_z$ and $U_{xz} \equiv U_{zx}$ for *all* scattering angles.

In summary, scattering processes involving unpolarized open-shell targets and non-vanishing angular momenta have already become quite complicated for elastic scattering and even more so for inelastic scattering. The determination of the complete set of generalized *STU* parameters in triple scattering experiments can provide one of the most detailed tests of theoretical models for electron–atom collisions.

So far, we have considered the scattering of polarized electrons from unpolarized targets. In contrast, if unpolarized electrons are scattered from spin-polarized targets, the differential cross section can be written as

$$\sigma(\theta) = \sigma_u(\theta)[1 + A(\theta)P_A] \tag{7}$$

where P_A is the component perpendicular to the scattering plane of the target polarization $\boldsymbol{P}_A$ and $A(\theta)$ determines the asymmetry produced by this polarization (Farago 1974). It is interesting to note that non-vanishing values of $A(\theta)$ require both explicitly spin-dependent

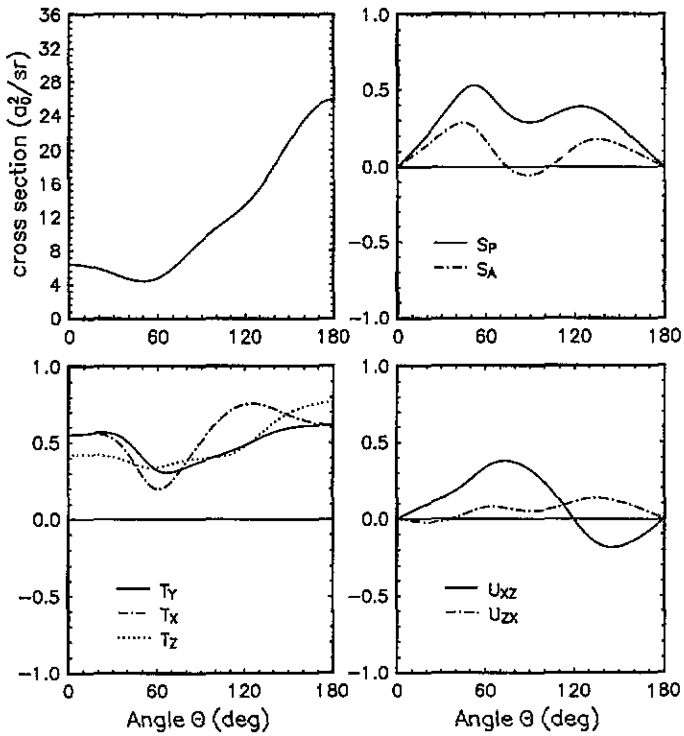

Figure 6. As figure 2 for $(6s)\,^2S_{1/2} \rightarrow (6p)\,^2P_{3/2}$ excitation at 1.6 eV.

projectile–target interactions (the most important one being the spin–orbit interaction) and exchange effects (Raith 1988).

Furthermore, if both the projectile electrons and the target are initially spin-polarized with polarizations $\boldsymbol{P}$ and $\boldsymbol{P}_A$, respectively, and all explicitly spin-dependent effects are neglected, an exchange asymmetry $A_{ex}(\theta)$ can be defined by

$$\sigma(\theta) = \sigma_u(\theta)[1 - A_{ex}(\theta)\boldsymbol{P} \cdot \boldsymbol{P}_A]. \tag{8}$$

The exchange asymmetry parameter can be determined by measuring the differential cross sections $\sigma_{\uparrow\uparrow}$ and $\sigma_{\uparrow\downarrow}$ for parallel and antiparallel polarizations of projectile and target beams. It is independent of the orientation of the polarization vectors with regard to the scattering plane and is given by

$$\frac{\sigma_{\uparrow\downarrow} - \sigma_{\uparrow\uparrow}}{\sigma_{\uparrow\downarrow} + \sigma_{\uparrow\uparrow}} = A_{ex}(\theta)P\ P_A. \tag{9}$$

However, if one allows for explicitly spin-dependent forces, the asymmetry in (8) also depends on the relative orientation of the polarization vectors with respect to the scattering plane. A generalization of (8) leads to the definitions of the asymmetry parameters $A_{\parallel}$ and $A_{\perp}$, where the parallel or antiparallel projectile and target polarizations lie in the scattering plane ($A_{\parallel}$) or perpendicular to the scattering plane ($A_{\perp}$). Without explicitly spin-dependent forces (i.e. for pure exchange scattering), one finds $A_{\parallel} = A_{\perp} = A_{ex}$. Therefore, non-vanishing values for $A_{\parallel} - A_{\perp}$ indicate the presence of explicitly spin-dependent interactions.

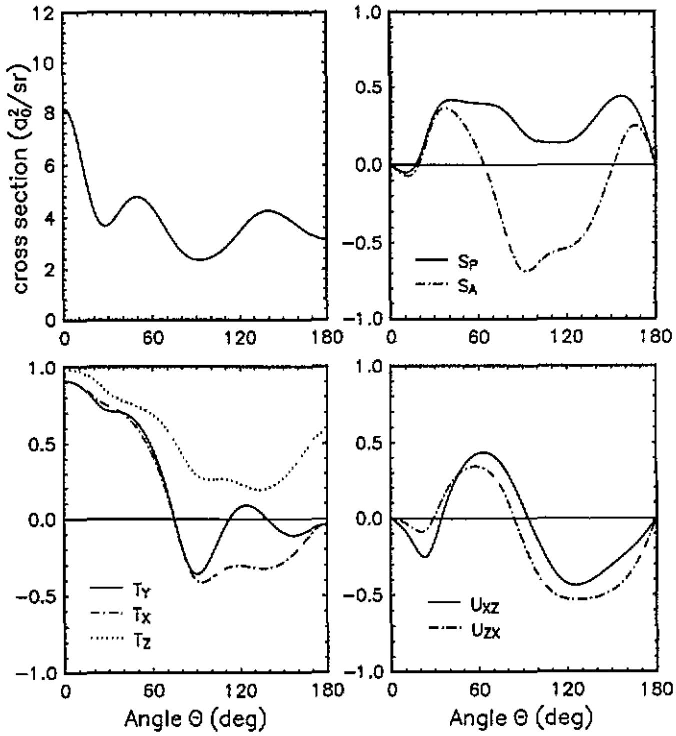

Figure 7. As figure 5 at 2.04 eV.

3. Numerical method

An R-matrix theory based on the Dirac Hamiltonian theory has been formulated and specialized to the case of electron scattering by alkali-like targets in II. In this approach, the many-electron scattering system is approximated by a two-electron model that includes the interaction between the scattered and the valence electron and the interaction between these two active electrons with the noble-gas-like core explicitly. The core electrons, on the other hand, are accounted for through semiempirical, adjustable effective Thomas–Fermi-type and (induced dipole and quadrupole) polarization potentials. These potentials influence the two active electrons separately (from the viewpoint of an independent-electron approach) and, by virtue of the so-called dielectronic polarization potential, their mutual interaction.

The present work has been carried out using the results of the Dirac R-matrix calculation in II where close-coupling between the $(6s)\,^2S_{1/2}$, $(6p)\,^2P_{1/2,3/2}$ and $(5d)\,^2D_{3/2,5/2}$ states of Cs was taken into account. The adjustable parameters in the semi-empirical core potentials were chosen such that the most reliable available binding energies of the lowest caesium states were reproduced. The fundamental dynamical data of this calculation are given in terms of the energy-dependent reactance matrices (also referred to as K matrices). These matrices were transformed into spin-dependent scattering amplitudes f by using the code developed by Thumm and Norcross (1993). Further details of the recoupling calculation and the convergence of the partial wave decomposition can be found in this reference.

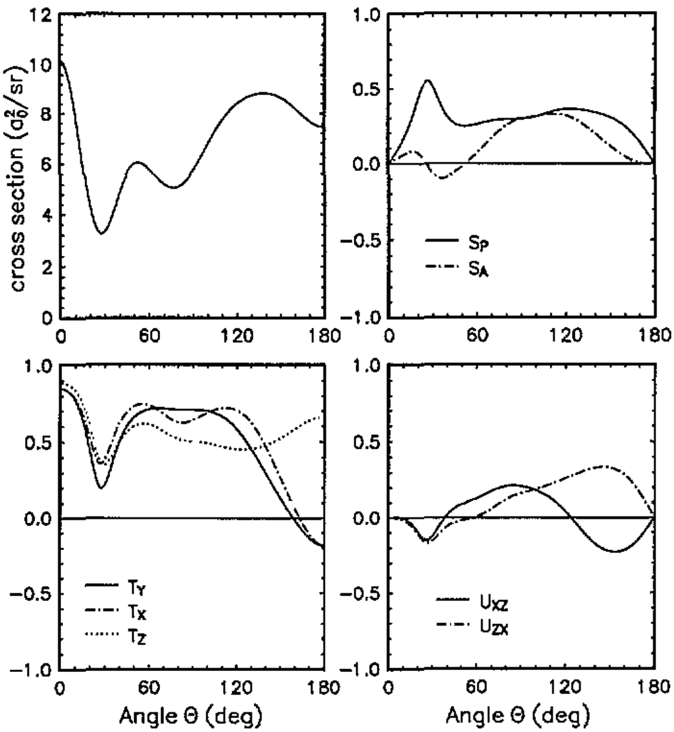

Figure 8. As figure 6 at 2.04 eV.

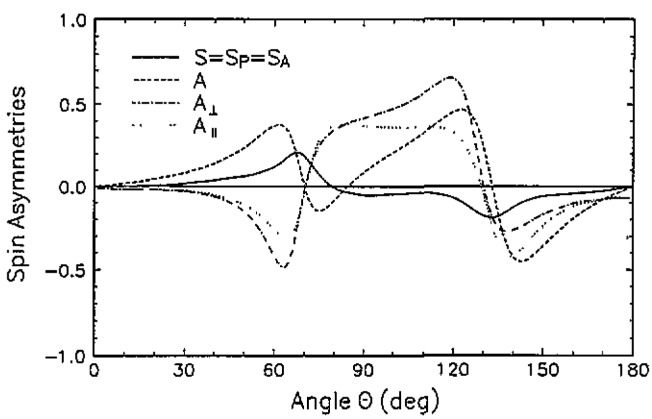

Figure 9. The Sherman function S $(= S_P = S_A)$ (see also figures 2–4) and the spin-asymmetry parameters A, $A_\perp$, $A_\parallel$ for elastic scattering of spin-polarized electrons from spin-polarized caesium atoms at 1.3 eV.

4. Results and discussion

In figures 2–8, we display the differential cross section and the generalized *STU* parameters for elastic and inelastic electron scattering from unpolarized caesium atoms. For elastic

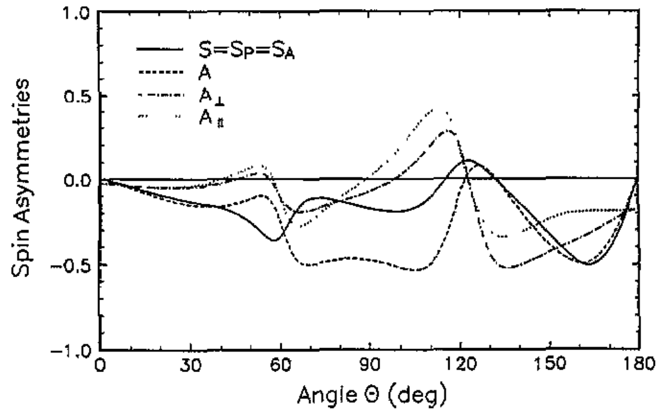

Figure 10. As figure 9 at 1.6 eV.

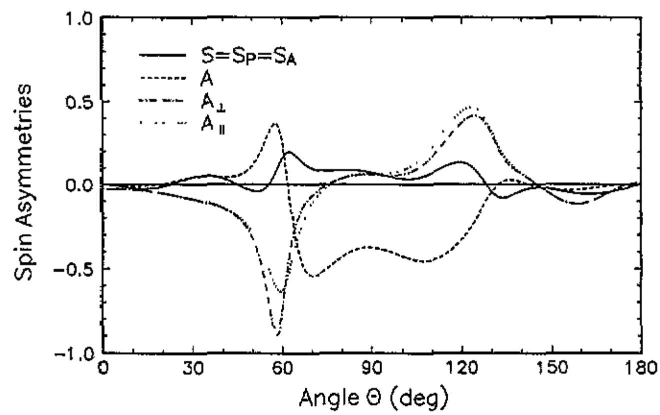

Figure 11. As figure 9 at 2.04 eV.

scattering at 1.3, 1.6 and 2.04 eV (figures 2–4), the differential cross sections are forward peaked and show a characteristic double-minimum structure due to dominant admixtures of p-wave scattering. For a more extensive discussion of differential cross sections in low-energy e^-–Cs scattering, we refer to Thumm and Norcross (1993).

The same double-minimum structure can be observed in the contraction parameters ($T_{x,y,z}$) and also appears to strongly influence the θ dependence of both S_P and the generalized U parameters. In the results for the S_P parameter, this feature is increasingly hidden by additional structures in the angle dependence, as the collision energy increases. To a lesser degree this is also true for the rotation parameters U_{xz} and U_{zx}. The generalized T and U parameters are related by (6*b*), as is illustrated in the plots (e.g. $U_{xz} = U_{zx}$ where $T_x = T_z$).

Our results for inelastic scattering are contained in figures 5–8 for two collision energies (1.6 and 2.04 eV). The comparison of figures 5 with 6 and 7 with 8 shows that all displayed quantities are fine-structure sensitive. The inelastic cross sections for $(6s)\,^2S_{1/2} \rightarrow (6p)\,^2P_{1/2}$ and $(6s)\,^2S_{1/2} \rightarrow (6p)\,^2P_{3/2}$ excitation clearly differ by more than the statistical branching ratio which would predict $\sigma[2P_{3/2}] = 2\,\sigma[2P_{1/2}]$ (cf Thumm and Norcross 1993). It is therefore not surprising that the more sensitive generalized *STU* parameters also depend on the J value of the final $(6p)\,^2P_J$ state of the target. For pure exchange scattering (and degenerate fine-structure levels), it is was shown by Hanne (1983) that the parameters S_A for the two fine-structure levels are related by

$$S_A[^2P_{1/2}] = -2\, S_A[^2P_{3/2}]. \qquad (12a)$$

Furthermore, Goerss *et al* (1991) found that in this approximation

$$U_{xz} = U_{zx} \qquad (12b)$$

and

$$T_x = T_y = T_z. \qquad (12c)$$

Our results for both energies show significant deviations from these predictions. Therefore, additional evidence is given for the importance of relativistic interactions in the scattering of slow electrons from heavy atomic targets. These deviations are more pronounced than those found in the corresponding Breit–Pauli calculation (Bartschat and Burke 1988).

We finish by showing in figures 9–11 our results for elastic electron scattering from spin-polarized Cs atoms. Due to the inclusion of relativistic interactions, including explicitly spin-dependent effects, we, in general, find non-zero values both for A and $A_\parallel - A_\perp$. For forward and backward scattering ($\theta = 0°$ and $180°$), however, the axial symmetry of the scattering system requires identical (but possibly non-zero) values of $A_\parallel$ and $A_\perp$.

The double minimum (or p-wave) structure seen in the elastic differential cross sections is also reflected in the angle dependence of S, A, $A_\parallel$ and $A_\perp$. However, it appears that additional structures, possibly due to the coherent superposition of different scattering amplitudes (which is not relevant for the differential cross sections) are of importance. We also point out that the predicted magnitudes of up to 50% for the parameter A clearly exceed the predictions of the corresponding Breit–Pauli calculation (cf Bartschat 1990). Such large values should indeed allow for an experimental test of our prediction.

5. Conclusions

In this paper, we have presented and discussed a complete set of results for the generalized *STU* parameters in elastic and inelastic scattering of spin-polarized electrons from unpolarized caesium atoms. Furthermore, we have shown selected results for some spin-polarization parameters for elastic scattering of polarized electrons from polarized targets. The predictions of the general theory regarding the symmetry relationships between some of these parameters have been verified, and the importance of the atomic fine-structure and relativistic effects on the outcome of the collision process has been demonstrated. In particular, we predict large values for the asymmetry parameter A. This, together with our other findings, makes a detailed test of our theory through comparison with experimental data for all these spin-polarization parameters highly desirable.

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References

Bartschat K 1985 *J. Phys. B: At. Mol. Phys.* **18** 2519
—— 1989 *Phys. Rep.* **180** 1
—— 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** 2341
Bartschat K and Burke P G 1988 *Coherence in Atomic Collision Physics* ed J Beyer, K Blum and R Hippler (New York: Plenum)
Bartschat K, Goerss H-J and Nordbeck R P 1990 *Z. Phys.* D **17** 25
Bartschat K and Madison D H 1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 2621
Bartschat K and Scott N S 1984 *J. Phys. B: At. Mol. Phys.* **17** 3787
Bederson B 1969 *Comm. At. Mol. Phys.* **1** 71; **2** 65
Berger O and Kessler J 1986 *J. Phys. B: At. Mol. Phys.* **19** 3539
Farago P S 1974 *J. Phys. B: At. Mol. Phys.* **7** L28
Goerss H-J, Nordbeck R-P and Bartschat K 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 2833
Hanne G F 1983 *Phys. Rep.* **95** 95
Kessler J 1985 *Polarized Electrons* 2nd edn (Berlin: Springer)
Raith W 1988 *Fundamental Processes in Atomic Dynamics* ed J S Briggs, H Kleinpoppen and H O Lutz (New York: Plenum)
Scott N S and Burke P G 1980 *J. Phys. B: At. Mol. Phys.* **13** 4299
Thumm U and Norcross D W 1991 *Phys. Rev. Lett.* **67** 3495
—— 1992 *Phys. Rev.* A **45** 6349
—— 1993 *Phys. Rev.* A **47** 305