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LETTER TO THE EDITOR

Characteristics of light emission after low-energy electron impact excitation of caesium atoms

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Abstract. Results of a recent calculation for e–Cs scattering, carried out in a fully relativistic (Dirac R-matrix) framework, are used to calculate the polarization of the light emitted by excited caesium atoms in an energy range from threshold to 2.7 eV. They are compared with previous semirelativistic Breit–Pauli calculations and the available experimental data. The results indicate that the Percival–Seaton theory approximating relativistic scattering amplitudes by recoupling amplitudes from a non-relativistic LS calculation is not valid for low-energy e–Cs scattering.

In this letter, we present the results of a new calculation for the polarization of the light emitted by caesium atoms after low-energy electron impact excitation of the $(6p)^2P^o_{1/2,3/2}$ states. These results have been obtained from scattering amplitudes of a previous relativistic R-matrix calculation (Thumm and Norcross 1992a, b). In this work, the Cs target was described as a quasi one-electron atom by representing the innermost 54 electrons with a semiempirical core potential. Details of this calculation can be found in a recent paper by Thumm and Norcross (1992a) and will not be repeated here.

The main motivation for the present work was twofold: first, to compare the results with those of a previous Breit–Pauli R-matrix calculation (Nagy *et al* 1984, for further details see Scott *et al* 1984a, b) as well as with more recent experimental data (Eschen *et al* 1989, Nass *et al* 1989); and second, to test the validity of the Percival–Seaton hypothesis (Percival and Seaton 1957) which is often used to relate the results obtained for excitation of various fine-structure levels. In this model, it is assumed that the excitation process is essentially independent of the fine (and also the hyperfine) structure. Consequently, scattering amplitudes from a non-relativistic LS calculation are recoupled and transitions to the various members of a multiplet are related by purely algebraic recoupling coefficients. In fact, it was shown by Bartschat (1989a) that the predictions of this hypothesis are fairly well fulfilled in the

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Breit–Pauli calculation of Nagy *et al* (1984), i.e. after integration over all scattering angles the net effect of explicitly spin-dependent forces on the collision was predicted to be rather small.

Since the general theory of 'integrated Stokes parameters' has been described in several previous publications (see Bartschat 1989a and references therein), we will only summarize the most important definitions and equations at this point. Basically, we are interested in the polarization of the light emitted in the optical decay from the $(6p)^2P^o_{1/2,3/2}$ states of atomic caesium back to the ground state $(6s)^2S_{1/2}$, after the caesium atoms have been excited directly (no cascading) by (possibly spin-polarized) electrons. The scattered projectiles are not observed, and the cases of most practical interest are the following.

(i) Unpolarized electrons incident along the z-axis and observation of the light in a direction perpendicular to the incident beam axis. In this case, one can usually observe a non-vanishing degree of linear polarization with respect to the z- and x-axes (if, for example, the light is observed in the y-direction). This is defined as

$$\eta_3^y = P_1^y \equiv \frac{I(0^\circ) - I(90^\circ)}{I(0^\circ) + I(90^\circ)} \tag{1a}$$

where $I(\beta)$ denotes the intensity transmitted by a linear polarizer oriented at an angle β with respect to the z-axis; the superscript on the polarization denotes the direction of light observation.

(ii) Transversely spin-polarized electrons ($\boldsymbol{P} = P_y\hat{e}_y$) incident along the z-axis and observation of the light again in the y-direction defined by the incident electron polarization. In this case, one can generally observe two more non-vanishing 'integrated Stokes parameters', namely

(a) the linear polarization

$$\eta_1^y = P_2^y \equiv \frac{I(45^\circ) - I(135^\circ)}{I(45^\circ) + I(135^\circ)} \tag{1b}$$

and

(b) the circular light polarization

$$\eta_2^y = -P_3^y \equiv \frac{I_+ - I_-}{I_+ + I_-} \tag{1c}$$

where I_+ and I_- are the intensities of light transmitted by polarization filters which only admit photons with positive (I_+) and negative (I_-) helicity, respectively. In (1), the η correspond to the notation used, for example, by Blum (1981) while the P are the light polarizations defined by Born and Wolf (1970). Note that both η_1^y and η_2^y are directly proportional to the electron spin polarization P_y while η_3^y is independent of any electron polarization (for details, see Bartschat and Blum 1982).

(iii) Longitudinally spin-polarized electrons ($\boldsymbol{P} = P_z\hat{e}_z$) and observation of the light along the z-direction. For symmetry reasons, only the circular light polarization $\eta_2^z = -P_3^z$ can be different from zero in this case (Bartschat and Blum 1982).

Using the general equations (13) and the selection rules (31) of Bartschat *et al* (1981), the integrated Stokes parameters for our case of interest can be expressed in terms of 'integrated state multipoles'

$$\langle \mathcal{T}^{+}_{KQ}(J_1)\rangle = \sum_{M_1' M_1} (-1)^{M_1'-M_1}\sqrt{2K+1}\begin{pmatrix} J_1 & J_1 & K \\ M_1' & M_1 & Q \end{pmatrix} \times \langle \mathcal{F}(M_1', m_0')\mathcal{F}^*(M_1, m_0)\rangle \tag{2}$$

which contain angle-integrated bilinear products of scattering amplitudes defined by

$$\langle \mathcal{F}(M_1', m_0')\mathcal{F}^*(M_1, m_0)\rangle \equiv \frac{1}{2J_0+1}\sum_{m_1}\int \mathrm{d}\Omega_{k_1} f(J_1 M_1' m_1 \boldsymbol{k}_1, J_0 M_0 m_0' \boldsymbol{k}_0) \times f^*(J_1 M_1 m_1 \boldsymbol{k}_1, J_0 M_0 m_0 \boldsymbol{k}_0)\,\rho_{m_0' m_0} \tag{3}$$

where $f(J_1 M_1 m_1 \boldsymbol{k}_1, J_0 M_0 m_0 \boldsymbol{k}_0)$ is the scattering amplitude for the transition from an initial atomic level with total electronic angular momentum J_0 and z-component M_0 to a final state with quantum numbers (J_1, M_1) by electrons with initial (final) linear momentum $\boldsymbol{k}_0$ $(\boldsymbol{k}_1)$ and spin angular momentum component m_0 (m_1). In (3) we have assumed that the target is initially unpolarized while the spin polarization of the incident electrons is described by the density matrix elements $\rho_{m_0' m_0}$. Furthermore, the sum over m_1 and the integral $\int \mathrm{d}\Omega_{k_1}$ corresponds to the construction of the 'reduced density matrix' which accounts for the non-observation of the scattered projectiles (Bartschat 1989b).

The integrated state multipoles can either be calculated directly from the K-matrices of the scattering calculation (for details, see Bartschat *et al* 1984), or by numerical integration of the scattering amplitudes. The latter method was used in the present work, since it does not depend on the details of the angular momentum coupling scheme used in the scattering calculation. Note, however, that only products of scattering amplitudes with the same value of the final orbital angular momentum component m_{ℓ_1} can contribute ($m_{\ell_0} = 0$ in our coordinate system which is the 'collision frame'). This is a result of the integration over the spherical harmonics (see section 6.3 of Bartschat *et al* 1981). Finally, it is also necessary to account for hyperfine depolarization effects through 'perturbation coefficients' (Steffen and Alder 1975) by which the various state multipoles (2) must be multiplied.

An important simplification is obtained if one neglects all explicitly spin-dependent forces during the collision as well as the energy splitting between the $(6p)^2P^o_{1/2}$ and the $(6p)^2P^o_{3/2}$ fine-structure states. This procedure reduces the number of independent Stokes parameters to three (Bartschat 1989a) and also predicts $\eta_1^y/P_y \equiv 0$. The latter result was already derived in a general form by Bartschat and Blum (1982) and allows for a test of the importance of explicitly spin-dependent effects.

When this simplified Percival–Seaton model of neglecting all explicitly spin-dependent forces is finally transformed into the language of state multipoles, all non-vanishing Stokes parameters can be expressed in terms of three independent quantities, namely the ratios between total magnetic sublevel cross sections and the relative contribution of direct and exchange processes to the excitation process (Bartschat 1989a, equation (8)). Hence, any three Stokes parameters can be used to obtain the independent ratios which, in turn, can then be employed to predict other

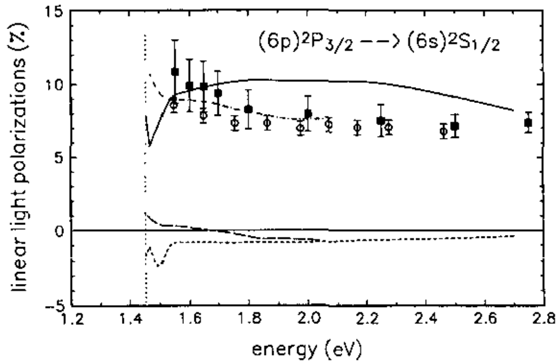

Figure 1. Linear light polarizations for the transition $(6p)^2P^o_{3/2} \rightarrow (6s)^2S_{1/2}$ in caesium after electron impact excitation. The individual curves are: ——, present result for η_3^y; – – –, present result for η_1^y/P_y; — · —, Breit–Pauli result of Nagy *et al* (1984) for η_3^y; — — —, Breit–Pauli result for η_1^y/P_y. The experimental data for η_3^y are taken from Eschen *et al* (1989) (○) and from Chen and Gallagher (1978) (■); the experimental results of Eschen *et al* (1989) for η_1^y/P_y are omitted, since they were zero within the statistical error bars of ±1%. The dotted line in the figure marks the excitation threshold of the $(6p)^2P^o_{3/2}$ state.

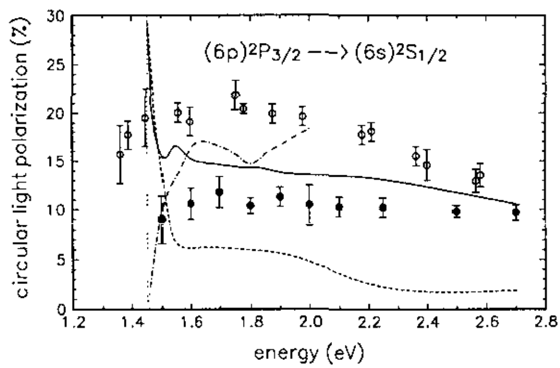

Figure 2. Circular light polarizations for the transition $(6p)^2P^o_{3/2} \rightarrow (6s)^2S_{1/2}$ in caesium after impact excitation by spin-polarized electrons. The individual curves are: ——, present result for η_2^y/P_y; – – –, present result for η_2^z/P_z; — · —, Breit–Pauli result of Nagy *et al* (1984) for η_2^y/P_y. The experimental data for η_2^y/P_y (○) are taken from Eschen *et al* (1989) while the data for η_2^z/P_z (●) are taken from Nass *et al* (1989). The dotted line in the figure marks the excitation threshold of the $(6p)^2P^o_{3/2}$ state.

light polarizations. In a calculation, like the present one, that is not based on this approximation, the results obtained by direct calculation from scattering amplitudes and from the predictions of the simplified model can then be used to provide an explicit test of the Percival–Seaton hypothesis (Bartschat 1989a) for excitation of various fine-structure levels.

In figures 1–3 we show our results for the various Stokes parameters in comparison with those from the semirelativistic Breit–Pauli R-matrix calculation by Nagy *et al* (1984) and with experimental data obtained by Chen and Gallagher (1978), Eschen *et al* (1989) and Nass *et al* (1989). Note that only the circular light polarizations can

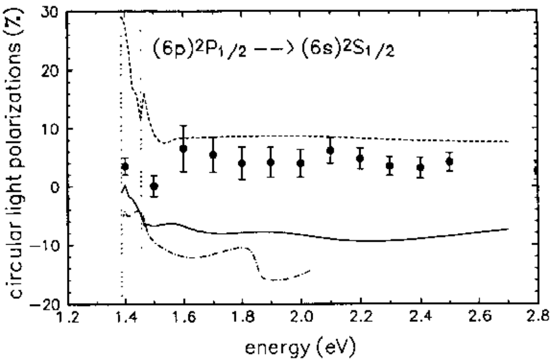

Figure 3. Circular light polarizations for the transition $(6p)^2P^o_{1/2} \rightarrow (6s)^2S_{1/2}$ in caesium after impact excitation by spin-polarized electrons. The individual curves are: ——, present result for η_2^y/P_y; – – –, present result for η_2^z/P_z; — · —, Breit–Pauli result of Nagy *et al* (1984) for η_2^y/P_y. The experimental data for η_2^z/P_z (●) are taken from Nass *et al* (1989). The dotted lines in the figure mark the excitation thresholds of the $(6p)^2P^o_{1/2}$ and the $(6p)^2P^o_{3/2}$ states, respectively.

Table 1. Comparison of Stokes parameters for e–Cs

Energy (eV)	Direct		*LS* model	
	$\eta_2^z\left(\frac{3}{2}\right)/P_z[\%]$	$\eta_2^z\left(\frac{1}{2}\right)/P_z[\%]$	$\eta_2^z\left(\frac{3}{2}\right)/P_z[\%]$	$\eta_2^z\left(\frac{1}{2}\right)/P_z[\%]$
1.7000	6.26	12.71	8.56	0.97
1.7308	6.20	12.56	8.59	1.22
1.7615	6.10	12.90	8.62	0.91
1.8000	5.97	13.55	8.66	0.17
1.8692	5.78	13.23	8.71	0.17
1.9000	5.63	12.89	8.72	0.52
2.0231	4.52	11.85	8.70	2.40
2.1462	3.07	10.90	8.45	4.41
2.3000	2.00	9.94	8.08	5.37
2.4846	1.70	9.08	7.80	4.95
2.7000	1.88	8.22	7.60	3.94

be non-zero for the $(6p)^2P^o_{1/2}$ state, since a linear polarization requires components of an alignment tensor of rank $K = 2$ which, in turn, requires an electronic angular momentum of $J \geqslant 1$ (see, for example, Blum 1981). The overall agreement between the two calculations and experiment is quite satisfactory in some cases while severe discrepancies remain in others. We point out, however, that the experimental error bars are fairly large and that there are additional uncertainties in the absolute value of the electron polarization. Note that any change in the latter polarization would either stretch or shrink the curves that are normalized to a polarization of 100%. It is also interesting to point out that the Stokes parameter η_1^y/P_y is indeed very small, in agreement with experiment and qualitatively supporting the non-relativistic model.

On the other hand, table 1 displays theoretical results obtained for the Stokes parameter η_2^z/P_z of the light emitted in the transitions $(6p)^2P^o_{3/2} \rightarrow (6s)^2S_{1/2}$ (denoted as $\eta_2^z(\frac{3}{2})/P_z$) and $(6p)^2P^o_{1/2} \rightarrow (6s)^2S_{1/2}$ (denoted as $\eta_2^z(\frac{1}{2})/P_z$) in caesium after excitation by polarized electrons. The column labelled 'direct' corresponds to the results obtained directly from the scattering amplitudes of Thumm and Norcross (1992a, b), while the column labelled 'LS model' contains the results obtained by determining the parameters X, Y and Z (defined in equations (7*a*)–(7*c*) of Bartschat 1989a), which parametrize the Stokes parameters under the assumption of pure LS coupling, and using these parameters to calculate the above light polarizations from equations (7*d*) and (7*e*) of Bartschat (1989a).

It can be seen that the deviations between the 'direct' and the 'LS-model' values are very large in most cases. In fact, they are much more significant than in the Breit–Pauli R-matrix calculation (cf Bartschat 1989a). This feature was also found in other parameters such as branching ratios of cross sections and spin polarizations for the fine-structure levels. It indicates that the Dirac approach indeed includes important additional relativistic effects that are left out in the Breit–Pauli method. This might be expected for this collision system and will be further discussed in a separate publication (Thumm *et al* 1992). These results indicate that the widely used conceptions of 'singlet' and 'triplet' or 'direct' and 'exchange' scattering, and hence the Percival–Seaton hypothesis for excitation of fine-structure levels, may only be valid to a very limited extent for the electron–caesium collision system—at least at these very low energies where threshold and resonance effects are so important.

In conclusion, we would like to encourage new measurements of all integrated Stokes parameters in a single apparatus, so that a completely analogous experimental test, along the same lines as was carried out here with the theoretical data, can easily be performed. This should provide new insights into the scattering dynamics for this collision system.

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