

Electron impact excitation of the 4^1P_1 state of calcium

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Abstract

We have used both non-relativistic and relativistic distorted-wave approximation methods to study the excitation of the 4^1P_1 state of calcium from the ground 4^1S_0 state. Calculations have been performed for the differential and integrated cross sections and Stokes parameters. The results are presented for electron impact energies in the range of 10–100 eV. We compare our results with the recently reported experimental measurements of Milisavljevic *et al* (2004 *J. Phys. B: At. Mol. Opt. Phys.* **37** 3571) and discuss the sensitivity of these results to the choice of wavefunctions and approximation method used.

1. Introduction

Recently, there has been increased experimental interest in the electron excitation of the 4^1P_1 state of calcium from the ground 4^1S_0 state. Murray and Cvejanovic (2003) have measured the Stokes parameters using superelastic scattering techniques while Milisavljevic *et al* (2004) reported the experimental differential cross sections (DCS) for this excitation as well as the integrated cross sections. These experimental papers compared their measurements with our earlier relativistic distorted-wave (RDW) calculations (Srivastava *et al* 1992). The comparison of the RDW calculations with these experimental results reveals an interesting feature. While our previous RDW calculations reproduced the measured Stokes parameters of Murray and Cvejanovic (2003) very well at 20, 25 and 35 eV incident electron energies, the RDW calculations for the DCS overestimated the measurements of Milisavljevic *et al* (2004) at 40 and 60 eV. Since we expect our method to become more accurate as the incident electron energy increases clearly there was a problem with our earlier work.

In the present paper, we re-examine theoretically the excitation of the 4^1P_1 state calcium from the ground 4^1S_0 state in the light of this discrepancy. We have carried out two types of calculations by using both relativistic (RDW) and non-relativistic (NDW) distorted-wave approximation methods. The results obtained from these two methods are compared with our earlier work and the recent experiments. Thus we can assess the importance of relativistic effects in electron scattering from this atom as well as investigate the sensitivity of these scattering parameters to the form of the target wavefunctions used.

There have been a number of previous studies on electron inelastic scattering from calcium. Ehlers and Gallagher (1973) have reported values for the integrated cross sections for the excitation of the 4^1P_1 state. Samson and Berrington (2001) have carried out *R*-matrix calculations for the excitation of calcium to various excited states at energies in the threshold region which are too low for the RDW method to be valid. Stokes parameters have been measured for the 4^1P_1 state by El-Fayoumi *et al* (1988), Zhony *et al* (1989), Law and Teubner (1995) and Dyl *et al* (1999). The latter two papers have included comparisons with our earlier RDW calculations. Shafranyosh *et al* (1997) have investigated inelastic electron scattering from the $4s4p^3P$ excited state of calcium both experimentally and theoretically. While they also included some results for excitation from the ground state, the excitation of the 4^1P state of interest here was not among these. We have also calculated the excitation of the $4^{1,3}D$ states of calcium by electron impact using the RDW method (Muktavat *et al* 2002).

In section 2, we briefly outline the distorted-wave approximations used while the form of the wavefunctions is discussed in section 3. Finally, in section 4 the results are presented and discussed.

2. Theory

2.1. Distorted-wave approximation

The distorted-wave *T*-matrix for the electron impact excitation of an atom having *N* electrons and nuclear charge *Z* from an initial state *i* to final state *f* can be written as (Joachain 1983) (atomic units are used throughout)

$$T_{i \rightarrow f}^{\text{DW}} = \langle \chi_f^-(1, 2, \dots, N+1) | V - U_f(N+1) | A \chi_i^+(1, 2, \dots, N+1) \rangle \quad (1)$$

where *V* is the target–projectile interaction given by

$$V = -\frac{Z}{r_{N+1}} + \sum_{j=1}^N \frac{1}{|\mathbf{r}_j - \mathbf{r}_{N+1}|}. \quad (2)$$

Here \mathbf{r}_j ($j = 1, \dots, N$) represent the position coordinates of the target electrons and \mathbf{r}_{N+1} is the position coordinate of the projectile electron with respect to the nucleus of the atom. U_f is the distortion potential which is taken to be a function of the radial coordinates of the projectile electron only, i.e. r_{N+1} . Also U_f is chosen to be the spherically averaged static potential of the excited state of the atom. This choice of U_f has been shown to yield most consistent results (Zuo 1991).

The wavefunctions $\chi_{\text{ch}}^{+(-)}$, where ‘ch’ refers to the two channels, i.e. initial ‘*i*’ and final ‘*f*’, are represented as a product of the *N*-electron target wavefunctions ϕ_{ch} and a projectile electron distorted wavefunction $F_{i(f)}^{\text{DW}+(-)}$, i.e.

$$\chi_{\text{ch}}^{+(-)}(1, 2, \dots, N+1) = \phi_{\text{ch}}(1, 2, \dots, N) F_{\text{ch}}^{\text{DW}+(-)}(\mathbf{k}_{\text{ch}}, N+1). \quad (3)$$

Here ‘+’ refers to an outgoing wave while ‘−’ denotes an incoming wave. *A* is the antisymmetrization operator that takes into account the exchange of the projectile electron with the target electrons and \mathbf{k}_{ch} are the linear momenta of the projectile electron in the initial and final states.

2.2. Non-relativistic method

In the non-relativistic distorted-wave approximation the target wavefunctions ϕ_i and ϕ_f are taken to be the Hartree–Fock-type solutions of the Schrödinger equation. We expand the distorted wave $F^{\text{DW}+(-)}$ using the following non-relativistic partial wave form,

$$F_{\text{ch}}^{+(-)}(\mathbf{k}_{\text{ch}}, \mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \sum_{\ell=0}^{\infty} (2\ell+1) i^\ell e^{\pm i\delta_\ell} \frac{u_\ell^\pm(k_{\text{ch}}, r)}{r} P_\ell(\hat{\mathbf{k}}_{\text{ch}} \cdot \hat{\mathbf{r}}) \quad (4)$$

where δ_ℓ is the phase shift of the ℓ th partial wave, P_ℓ is the Legendre polynomial of order ℓ and $u_\ell^\pm(k, r)$ is the radial part of the distorted wavefunction. On substituting expression (4) for $F^{+(-)}$ into the Schrödinger equation we get the following equation for the radial functions,

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2} + 2U(r) \right] u_\ell(k, r) = 0 \quad (5)$$

which is solved numerically subject to the following usual boundary conditions,

$$u_\ell(k, r) \underset{r \rightarrow 0}{=} 0 \quad (6)$$

and

$$u_\ell(k, r) \underset{r \rightarrow \infty}{=} \frac{1}{k} \sin \left[kr - \frac{1}{2} \ell \pi + \delta_\ell(k^2) \right]. \quad (7)$$

The potential $U(r)$ is the sum of the distortion potential U_f and the non-local exchange potential of Furness and McCarthy (1973) to take account of the exchange of the projectile with the target electrons.

2.3. Relativistic method

In the relativistic distorted-wave method as described by Zuo *et al* (1991) the wavefunctions ϕ_{ch} of the target atom are taken to be Dirac–Fock-type solutions of the Dirac equations. The projectile electron distorted-wave functions $F_{\text{ch}}^{\text{DW}+(-)}$ are expanded using the following relativistic form,

$$F_{\text{ch}, \mu_{\text{ch}}}^{\text{DW}+(-)}(\mathbf{k}_{\text{ch}}, \mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \sum_{\kappa m} e^{\pm i\eta_\kappa} a_{\text{ch}, \kappa m}^{\mu_{\text{ch}}}(\hat{k}_{\text{ch}}) \frac{1}{r} \begin{pmatrix} f_\kappa(r) \chi_{\kappa m}(\hat{r}) \\ i g_\kappa(r) \chi_{-\kappa m}(\hat{r}) \end{pmatrix} \quad (8)$$

with

$$a_{\text{ch}, \kappa m}^{\mu_{\text{ch}}}(\hat{k}_{\text{ch}}) = 4\pi i^l \left[\frac{E_{\text{ch}} + c^2}{2E_{\text{ch}}} \right]^{1/2} \sum_{m_l} \left(l m_l \frac{1}{2} \mu_{\text{ch}} | j m \right) Y_{l m_l}^*(\hat{k}_{\text{ch}}). \quad (9)$$

Here E_{ch} is the relativistic energy (including the rest mass of the electron), μ_{ch} is the spin projection of the projectile electron and η_κ is the partial-wave phase shift. f_κ and g_κ are the large and small components of the radial wavefunctions and the $\chi_{\pm\kappa m}$ represent the spin-angular wavefunctions and are given by

$$\chi_{\kappa m}(\hat{\mathbf{r}}, \sigma) = \sum_{\mu\nu} \left(\ell \mu \frac{1}{2} \nu | j m \right) Y_{\ell \mu}(\hat{r}) \psi_{\frac{1}{2}\nu}(\sigma) \quad (10)$$

and

$$\chi_{-\kappa m}(\hat{\mathbf{r}}, \sigma) = \sum_{\mu\nu} \left(\tilde{\ell} \mu \frac{1}{2} \nu | j m \right) Y_{\tilde{\ell} \mu}(\hat{r}) \psi_{\frac{1}{2}\nu}(\sigma), \quad (11)$$

where j is the total angular momentum of the electron, m is the z -component of j , $\tilde{\ell} = 2j - \ell$, $(\ell_1 m_1 \ell_2 m_2 | \ell_3 m_3)$ represents the usual Clebsch–Gordan coefficient, the $Y_{\ell m}(\hat{\mathbf{r}})$ are

spherical harmonics and $\psi_{(1/2)\nu}(\sigma)$ are normalized two-component spin wavefunctions. It should be noted that spin and orbital angular momentum are coupled together. The spin-angular state is characterized by quantum number κ , which is defined as

$$\kappa = \begin{cases} \ell & \text{if } j = \ell - 1/2 \text{ for } \ell > 0 \\ -\ell - 1 & \text{if } j = \ell + 1/2. \end{cases} \quad (12)$$

Substituting expansion (8) into the Dirac equations the following integro-differential equations for the radial parts $f_\kappa(r)$ and $g_\kappa(r)$ are obtained,

$$\left(\frac{d}{dr} + \frac{\kappa}{r} \right) f_\kappa(r) - \frac{1}{c}(c^2 - U_f + E_{\text{ch}})g_\kappa(r) - \frac{1}{cr}W_Q(\kappa; r) = 0 \quad (13)$$

$$\left(\frac{d}{dr} - \frac{\kappa}{r} \right) g_\kappa(r) + \frac{1}{c}(-c^2 - U_f + E_{\text{ch}})f_\kappa(r) + \frac{1}{cr}W_P(\kappa; r) = 0 \quad (14)$$

with the boundary conditions

$$f_\kappa(r) \xrightarrow{r \rightarrow \infty} \frac{1}{k} \sin \left(k_{\text{ch}}r - \frac{l\pi}{2} + \eta_\kappa \right) \quad (15)$$

$$g_\kappa(r) \xrightarrow{r \rightarrow \infty} \frac{c}{c^2 + E_{\text{ch}}} \cos \left(k_{\text{ch}}r - \frac{l\pi}{2} + \eta_\kappa \right). \quad (16)$$

W_P and W_Q are the non-local exchange kernels as discussed by McEachran and Stauffer (1986) and these integro-differential equations are solved numerically as described by Zuo (1991). It should be noted that the spin of the target as well as projectile electrons enters naturally into the description of the scattering through the Dirac equations. Also the spin and orbital angular momentum of the electrons are coupled together to form the spin-angular state which is defined by the total angular momentum j or κ . Therefore, the RDW method gives the scattering amplitudes for the transition from a state having total angular momentum J_i to a state having total angular momentum J_f , i.e. it gives the scattering amplitudes for transitions between fine-structure states of the target atom.

2.4. Scattering parameters

We define the scattering amplitude for the excitation of the 4^1P_1 state with magnetic quantum number M as

$$f(M, \mu_f, \mu_i) = (2\pi)^2 \sqrt{\frac{k_f}{k_i}} T_{i \rightarrow f}^{\text{DW}}(M, \mu_f, \mu_i) \quad (17)$$

where μ_i and μ_f are the spin projections in the initial and final channels, respectively. Note that in the non-relativistic method the T -matrix is independent of the spin of the projectile electron. Then with our normalization the DCS is given by

$$\text{DCS} = \frac{1}{2} \sum_{M, \mu_i, \mu_f} |f(M, \mu_i, \mu_f)|^2 \quad (18)$$

and the corresponding integrated cross section can be obtained by integrating the DCS over the scattering angles.

The detailed expressions for the Stokes parameters in terms of the scattering amplitudes are given by Bartschat *et al* (1981).

Table 1. Calculated energy differences and optical oscillator strengths for the 4^1S_0 – 4^1P_1 transition in Ca. The experimental energy difference is from the NIST Atomic Spectra Database and the OOS was measured by Kelly and Mathur (1980).

	HF	SCGS	MCGS	Expt
Energy (eV)	3.07	2.944	2.829	2.933
OOS	1.671	1.692	1.683	1.79 ± 0.03

3. Theoretical calculations

3.1. The DW calculation

The ground 4^1S_0 state of Ca is represented by the non-relativistic configuration $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$ while for the excited 4^1P_1 state the valence shell becomes $4s4p$. Hartree–Fock (HF) wavefunctions based on these minimal configurations have been used to represent the bound states of the atoms. These wavefunctions are obtained numerically using Froese Fischer’s (1969) code as well as analytically from Hibbert’s (1975) CIV3 code. We found these codes both give very similar results for the wavefunctions. The calculated energy difference and optical oscillator strength (OOS) for this transition are shown in table 1. From these wavefunctions we calculate the distortion potential U_f as the spherically-averaged static potential of the final state. The distorted-wave radial functions are obtained from (5) and used to calculate the T -matrix. The details of these calculations for atoms having two valence electrons are given in Verma and Srivastava (1998). Finally we evaluate the cross sections and Stokes parameters as outlined in section 2.4.

3.2. The RDW calculation

In the relativistic j – j coupling notation, the ground-state configuration of Ca ($Z = 20$) is $1s^2 2s^2 2\bar{p}^2 2p^4 3s^2 3\bar{p}^2 3p^4 4s^2$ where \bar{p} and p indicate p -electrons with total angular momenta j of $1/2$ and $3/2$, respectively. Therefore the ground state of Ca has total angular momentum $J_i = 0$. We consider excitations where the valence $4s^2$ shell is excited to $4s4\bar{p}$ or $4s4p$ with the total angular momentum $J_f = 1$. These were the configurations included in the original calculation of Srivastava *et al* (1992) which we presently denote as the single-configuration ground-state (SCGS) calculation. In detail, we can represent the initial and excited states as

$$\varphi_i = (4s^2)_{J=0} \quad (19)$$

and

$$\varphi_f = b_1(4s4\bar{p})_{J=1} + b_2(4s4p)_{J=1} \quad (20)$$

where the coefficients $(b_1, b_2) = (0.5809, 0.8139)$.

In order to improve on our previous results we have carried out a more elaborate calculation in which we use a multi-configuration ground state (MCGS). In this calculation we added additional configurations to both the ground and excited states. In this case the wavefunctions are expressed as

$$\varphi_i = a_1(4s^2)_{J=0} + a_2(4\bar{p}^2)_{J=0} + a_3(4p^2)_{J=0} + a_4(4s5s)_{J=0} \quad (21)$$

and

$$\begin{aligned} \varphi_f = & c_1(4s4\bar{p})_{J=1} + c_2(4s4p)_{J=1} + c_3(4s5\bar{p})_{J=1} + c_4(4s5p)_{J=1} + c_5(3\bar{d}4\bar{p})_{J=1} + c_6(3\bar{d}4p)_{J=1} \\ & + c_7(3d4p)_{J=1} + c_8(4\bar{p}5s)_{J=1} + c_9(4p5s)_{J=1} \end{aligned} \quad (22)$$

where the Dirac–Fock orbitals and configuration mixing coefficients (CI coefficients) were determined using the GRASP92 code of Parpia *et al* (1996). The energy differences and

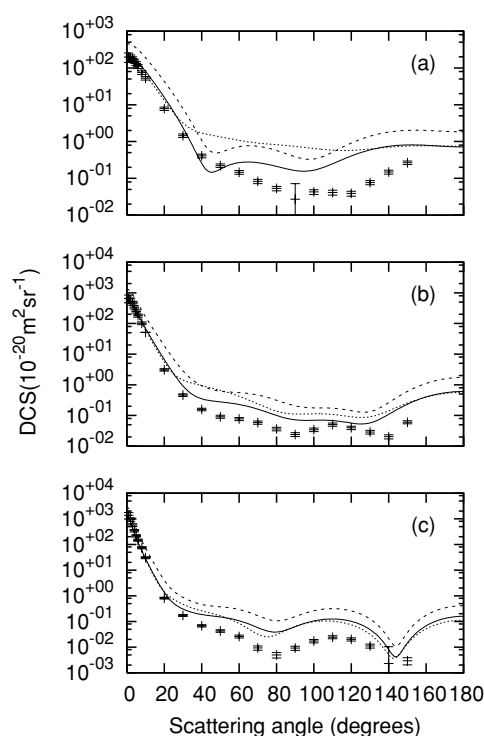


Figure 1. DCS for the excitation of the 4^1P_1 state of calcium at a projectile energy of: (a) 10 eV, (b) 20 eV, (c) 40 eV. The experimental points with error bars are from Milisavljevic *et al* (2004). Solid curve, RDW-MCGS; long-dashed curve, RDW-SCGS, short-dashed curve, NDW.

optical oscillator strengths are included in table 1. The coefficient a_i , $i = 1, \dots, 4$, are (0.9432, 0.1707, 0.2162, -0.1858) while c_i , $i = 1, \dots, 9$, are (0.5035, 0.7368, -0.1016 , -0.1043 , -0.2547 , 0.1135, -0.3228 , 0.0124, -0.0175).

Thus after having obtained the ground- and excited-state wavefunctions, the distortion potential U_f is calculated as the spherically-averaged static potential of the final state and equations (13) and (14) are solved for the radial functions. From these the T -matrices can be constructed and the cross sections and Stokes parameters calculated.

4. Results and discussion

From table 1 we note that all three wavefunctions give reasonable results for the energy differences and oscillator strengths. In fact, the best agreement with the experimental results is obtained with the SCGS wavefunction which produces the worst agreement with the experimental DCS as we shall see below. While the results of the SCGS wavefunction may be fortuitous, this is contrary to expectation and indicates that energies and oscillator strengths are not by themselves accurate indicators of the reliability of scattering energies, at least for lower energies where the Born approximation is not valid. Furthermore, we note from the CI coefficients for the MCGS wavefunction that a number of configurations make a significant contribution to the description of the atom and these are important to the description of the scattering problem even if they do not necessarily improve the atomic energy levels.

In figures 1 and 2 we present the results for the DCS for the excitation of the 4^1P_1 state of Ca for projectile electron energies of 10, 20, 40, 60 and 100 eV in the RDW approximation

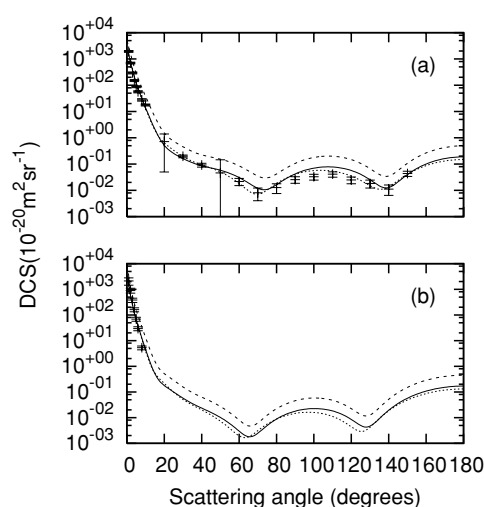


Figure 2. As for figure 1 but at an energy of (a) 60 eV, (b) 100 eV.

Table 2. Integrated cross sections in units of 10^{-20} m^2 for the excitation of the 4^1P_1 state of Ca. The RDW results are from our MCGS calculation. Expt(EG) denotes the results obtained by interpolating the published data of Ehlers and Gallagher (1973) which have quoted errors of 0.1. Expt(M) are the data from Milisavljevic *et al* (2004).

Energy (eV)	NDW	RDW	Expt (EG)	Expt (M)
10	31.6	30.5	26.3	20.0 ± 4.8
20	26.7	28.2	26.1	25.2 ± 6.1
40	18.4	19.6	21.3	23.1 ± 6.1
60	14.3	15.1	17.8	14.7 ± 2.6

using both the SCGS and MCGS wavefunctions as well as the NDW results and experimental measurements of Milisavljevic *et al* (2004). There are a number of features of these graphs worth pointing out. First of all, the SCGS and MCGS have very similar shapes over the whole angular range and while the MCGS results agree well with the experimental data particularly for small scattering angles, the SCGS results are a factor of two or three times larger in all cases. The NDW results also agree very well with the experimental measurements and MCGS results at smaller scattering angles but are less accurate at larger angles, especially at lower energies. As the energy increases both the MCGS and NDW results converge to the experimental results over the whole angular range.

Table 2 contains the results for the integrated cross section in both the NDW and RDW approximations as well as the values measured by Ehlers and Gallagher (1973) and calculated from the measured DCS of Milisavljevic *et al* (2004). The measurements of Ehlers and Gallagher include cascade contributions but are normalized to theoretical values at high energies. These cascade contributions are estimated to produce an error of approximately 25% in the region of the peak of the cross section. Taking this into account, the agreement between our calculations and these experimental results are satisfactory except possibly at 10 eV. To obtain integrated cross sections, Milisavljevic *et al* (2004) had to extrapolate their DCS values to small and large angles. This results in rather large errors quoted for their results and both the NDW and RDW results lie within their error bars except at the lowest

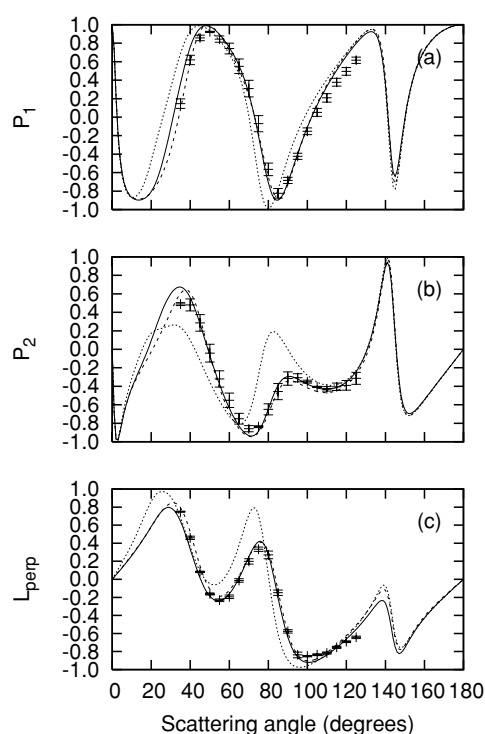


Figure 3. Differential Stokes parameters for the 4^1P_1 state of calcium excited by 35 eV electrons: (a) P_1 , (b) P_2 , (c) L_{\perp} . The experimental points with error bars are from Murray and Cvejanovic (2003). The legends for the experimental curves are as in figure 1.

energy of 10 eV. The agreement between theory and experiment improves as the energy increases.

In figure 3 we show the results for the Stokes parameters P_1 , P_2 and L_{\perp} at 35 eV from our three methods along with the experimental data of Murray and Cvejanovic (2003). Here we note that both the MCGS and SCGS methods give very similar results which are in excellent agreement with the experiment while the NDW results are in poorer agreement with the experimental data. The same general result holds true at 20 and 25 eV where Murray and Cvejanovic also made measurements.

The Stokes parameters depend on ratios of the cross sections for the excitation of the individual magnetic substates of the 4^1P_1 state while the DCS is a sum of these individual cross sections. From our results we can conclude that:

- (i) the MCGS cross sections for the excitation of individual magnetic substates are quite accurate in both absolute and relative magnitudes;
- (ii) the ratios of the individual SCGS cross sections are accurate but the magnitudes are systematically too large;
- (iii) the relative magnitudes of the NDW cross sections are less accurate than the RDW ones but their sum is more accurate than the individual cross sections.

These conclusions apply particularly at higher energies and tend to break down as the energy of the projectile electron decreases. This is particularly noticeable at 10 eV, which is a rather

low energy for a distorted-wave method and where there are larger differences between the MCGS, NDW and experimental data. In comparing the cross sections for the scattering of spin-polarized electrons (not shown in this paper), it appears that there are larger differences between the MCGS and SCGS results so that an experiment using spin-polarized electrons would be an even more stringent test of the theory.

5. Conclusion

This paper reports calculations for the excitation of Ca using a non-relativistic distorted-wave approximation as well as a relativistic version involving both a simple and a more elaborate wavefunction. While the NDW method produces rather good results for the DCS it is less successful in calculating the Stokes parameters which require accurate results for the excitation of individual magnetic substates. Both relativistic methods produce very good results for the Stokes parameters and for the shape of the DCS, but it requires elaborate bound state wavefunctions to obtain the correct magnitudes for the DCS.

Our study also indicates that neither the energy levels nor the optical oscillator strengths for the bound states are accurate predictors for the accuracy of scattering calculations involving these states. It would be of some interest to extend these studies to other alkaline earth atoms, since these atoms have nominally closed valence shells which nevertheless are more sensitive to inter-electronic correlations than the noble gases.

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