Electron-photon correlations in electron-impact excitation of alkaline-earth atoms

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Abstract. We present a study of electron-photon correlations for the $ns^2{}^1S$-$nsnp^1P^o$ transitions in Mg, Ca, Sr, and Ba atoms. Effects of inter-channel coupling and approximations in the target wave functions were investigated.

INTRODUCTION

Modern electron-atom scattering theories, such as Convergent Close-Coupling (CCC) method [1] and R-Matrix with Pseudo States (RMPS) method [2], have proved to be very successful in describing electron scattering from hydrogen[1], alkali atoms [3] and helium [4, 5]. The one-electron approximation for target wave functions was mostly adequate in those studies. Electron scattering from alkaline-earth atoms brings the next level of complexity due to substantially more complex target wave functions. Here, two-electron excitations in the target wave functions become progressively more important as we go from light to heavier alkaline-earth atoms. In addition, we observe a breakdown of the nonrelativsitic approximation for heavy alkaline-earth atoms. The ability of electron-atom scattering theories to adequately account for these new features is yet to be systematically demonstrated. Study of electron-photon correlations is known to offer a very sensitive test of various aspects of the scattering process. Here we look at electron-photon coherence parameters for the $ns^2{}^1S$-$nsnp^1P^o$ transitions in Mg, Ca, Sr, and Ba for which a great deal of theoretical and experimental results are available.

THEORETICAL METHOD

We calculate wave functions of the alkaline-earth atoms in a model of two active electrons above an inert Hartree-Fock core. For each of the alkaline-earth atoms the set of one electron orbitals is obtained by diagonalizing the corresponding one-electron positive ion (for example Mg^+) in a Sturmian (Laguerre) basis. Standard configuration-interaction (CI) calculations are then performed in the space of two valence electrons and energy levels and wave functions of the target atom are determined. One and two-electron polarization potential is added to account for polarizability of the core [6]. The set of closed-coupling (CC) equations is obtained by expanding the total wave function

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TABLE 1. Characteristics of the ground state and first excited $^1P^o$ state of alkaline-earth atoms and helium.

	Excitation energy	Oscillator strength		Spectroscopic factors	
		CI	FC	^1S	^1P
He	21.1	0.276	0.282	0.995	0.999
Mg	4.3	1.72	1.89	0.934	0.942
Ca	2.9	1.73	2.17	0.933	0.828
Sr	2.7	1.80	2.21	0.942	0.838
Ba	2.2	1.69	2.39	0.931	0.706

in the target state basis. These equations are formulated and solved in momentum space. The use of a Sturmian basis allow us to perform a discretization of the target continuum and thereby model coupling to the ionization channels in the scattering calculations.

In Table 1 we present some important properties of the first excited $^1P^o$ states of alkaline-earth atoms and compare them with corresponding values in helium. The excitation energies of $nsnp^1P^o$ levels in alkaline-earth atom are about five to six times smaller than in helium. The oscillator strengths are in the range of 1.7 - 1.8 a.u. which is much larger than in helium (0.276 a.u.). This suggests that the $^1P^o$ level is coupled much stronger to the ground state in the alkaline-earth atoms than in helium. In a close-coupling calculation this would manifest itself in a very fast rate of convergence for this alkaline-earth atom transition.

The choice of two-electron configurations is of great importance for an accurate calculation of target wave functions. In helium, we have used the Frozen-Core model where one of the electrons fixed in the He^+ $1s$ orbital. The success of the FC model in the e-He scattering calculations was largely due to the rather small probability of two-electron excitations in helium which are more than ten times smaller than transitions with excitations of only one electron [7]. In the alkaline-earth atoms the two-electron excitations play a much more prominent role. There are two-electron excited states in the discrete spectrum of theses atoms, while there are none in helium. The accuracy of the FC model for the alkaline-earth atoms as opposed to helium can be assessed by comparing the values of oscillator strengths for these transitions calculated in the FC model and in the CI model, see Table 1. For helium there is very little difference while for the alkaline-earth atoms we observe substantial and increasing difference as we progress from the lighter Mg atom to the heavier Ba atom. The relative weight of the FC configurations in the ground state and $^1P^o$ wave functions is given by the spectroscopic factor of the FC configurations [6]. They are presented in Table 1. For helium ground and 2^1P^o states the FC configurations are by far the most important. The ground states of the alkaline-earth atoms have relatively large and very similar FC spectroscopic factors. For the $^1P^o$ states it diminishes from Mg to Ba to a relatively small value (0.706) confirming that two-electron excitations are more important in heavy atoms.

RESULTS

We present results of our calculations of parameters γ and $L_\perp$ in Figs. 1 and 2 for Mg (40 eV), Ca (45eV), Sr (30.3 eV), and Ba (20 eV). The results of the RDWA calculations [8, 9] and experimental data indicate that relativistic effects are not important for these transitions, since both find that P^+ is approximately unity.

We find very good agreement between all theoretical results and experiment for the γ parameter. For the $L_\perp$ parameter the agreement between the experiment, present CCC, RDWA [8, 9], and DWA [16, 14, 17], and calculations are very good in the forward scattering region for Mg, Ca, and Sr but not for Ba where large differences between theoretical results are apparent. At intermediate scattering angles the CCC method is in a good agreement with experiment for Mg, Ca, and Ba but for Sr we found a large discrepancy at around 50° with the DWA and RDWA results supporting the experiment. This discrepancy is rather unexpected and prompted us to look at the influence of channel coupling effects and the accuracy of the target wave functions on the $L_\perp$ parameter.

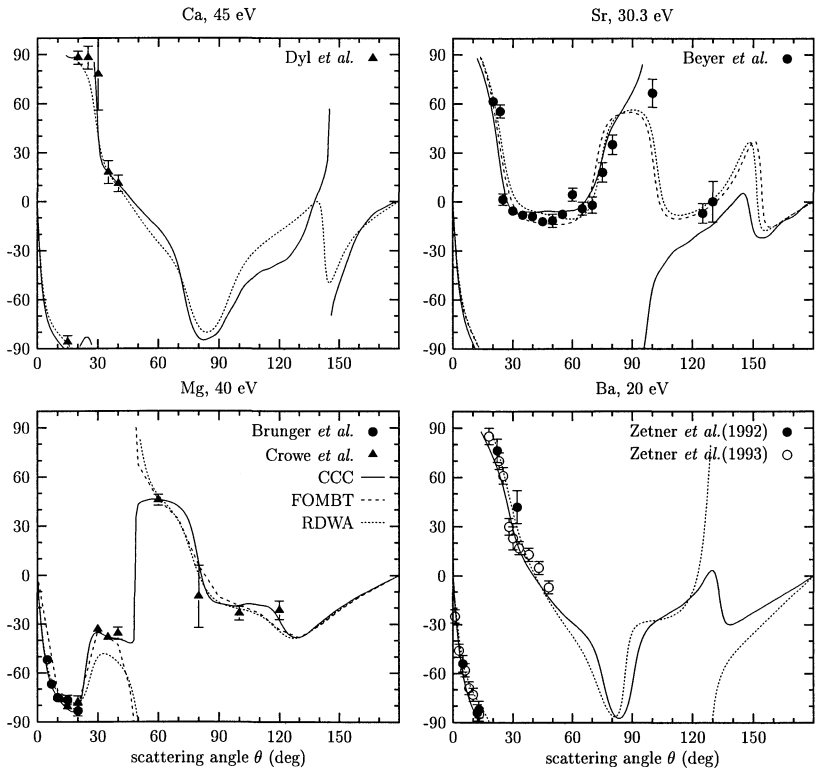

FIGURE 1. The γ parameter for excitation of the $(3s3p)\,^1P^o$ state of Mg at 40 eV, $(4s4p)\,^1P^o$ state of Ca at 45 eV, $(5s5p)\,^1P^o$ state of Sr at 30.3 eV, $(6s6p)\,^1P^o$ state of Ba at 20 eV incident electron energies. The measurements are due to Brunger *et al.*[10] (Mg), Crowe *et al.*[11] (Mg), Law and Teubner [12] (Ca), Dyl *et al.*[13] (Ca) Beyer *et al.*[14] (Sr), Li and Zetner [15] (Ba). The theory is as described in text.

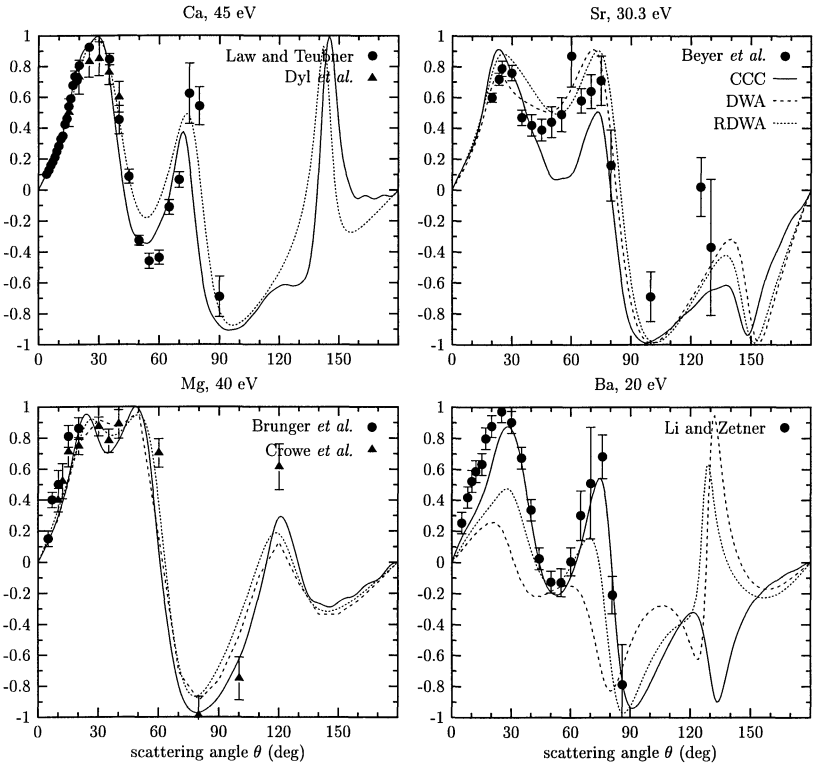

FIGURE 2. Same as in Fig. 2 but for the $L_\perp$ parameter.

In Fig. 3 we present results of 2-state CC calculations performed using the same CI wave function model as in the CCC calculations. The difference between the CCC and CC(2) calculations provides an estimate of importance of inter-channel coupling. We generally observe little difference between CCC and CC(2) results for all four alkaline-earth atoms. This is consistent with the noted very large values of oscillator strengths for these transitions.

We have also performed 2-state CC calculations using the FC model (CC(2)-FC) for the description of the ground and ^1P states (see Fig. 3). The difference between the two CC(2) calculations provides us with an estimate of importance of electron correlations effects in the target wave functions. We find little difference between the results of the two models, though the differences are larger for heavier atoms (Sr and Ba) which is expected as the FC model becomes less accurate for the heavier atoms, see Table 1.

The observed lack of sensitivity of the $L_\perp$ parameter to the details of the inter-channel coupling and the accuracy of the target wave functions can be partially explained by noting that incident electron energies of 40 eV in Mg, 45 eV in Ca, 30.3 eV in Sr, and 20 eV in Ba when measured in the threshold units (see Table 1) are in the range of 10 to 16. In helium the 10 times of the 2^1P^o excitation threshold corresponds to 200 eV incident

electron energy which is considered to be a large energy where good agreement between experiment and various theoretical methods was found [4].

It is interesting to note that there is a striking similarity between helium 200 eV $L_\perp$ parameter and corresponding $L_\perp$ values in the alkaline-earth atoms. In Fig. 3 we presented in addition the e-He 20 eV CCC results [4]. For forward scattering, up to 40°, there is virtually no differences between the $L_\perp$ parameter in the helium and alkaline-earth atoms. Comparing helium and alkaline-earth atoms $L_\perp$ values at intermediate scattering angles we see that an additional maximum starts to develop at about 50° in Mg and becomes very pronounced in Ca, Sr, and Ba at 75°. In the backward angles one more maximum develops in Mg and Ca which becomes inverted in Sr and Ba. The nature of these structures in the $L_\perp$ parameter is not understood and requires further investigation.

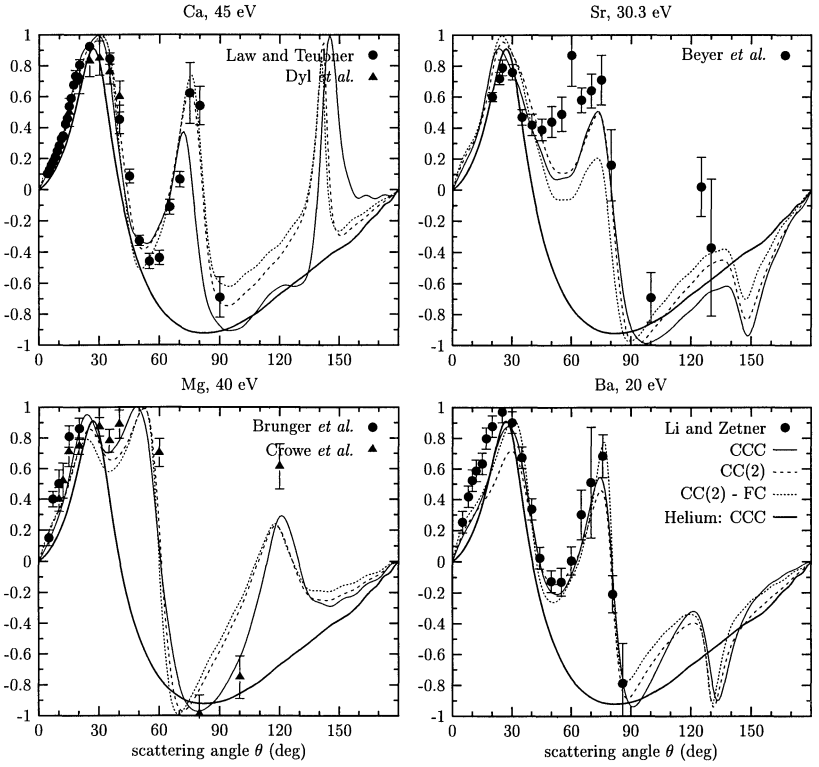

FIGURE 3. Same as in Fig. 2. In addition the results of the 2-state CC calculations in the CI and frozen-core models are presented. The CCC calculation is for helium $2\,^1P$ excitation by 200 eV electrons.

CONCLUSIONS

We have found that the EICP parameters for the $ns^2 {}^1S$-$nsnp\,{}^1P^o$ transitions in Mg, Ca, Sr, and Ba are largely insensitive to the electron correlations in the target wave functions and the details of channel coupling in the scatetring calculations, at least at the considered (relatively large) incident electron energies. We observed a striking similarity between the $L_\perp$ parameter for helium and for alkaline-earth atoms. The "non-helium" features of the $L_\perp$ parameter in the alkaline-earth atoms, in our opinion, deserve a careful study. Clearly, in order to test modern theoretical methods the experimental acitivity should be directed to lower energies and large scattering angles. Note, however, that other transitions involving target states which are strongly affected by electron correlations and break-down of the nonrelativistic approximation in the target wave functions might provide a better testing ground for the theoretical methods.

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