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Optical and generalized oscillator strengths for valence and inner-shell excitations on the Mg atom

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Theoretical results for the transition energies involving three Rydberg series, optical oscillator strengths (OOSs), and generalized oscillator strengths (GOSs) for valence and inner-shell electronic excitations are presented for the transitions $^1P \leftarrow X\ ^1S_0(3s \rightarrow np,\ 2s \rightarrow np,\ 1s \rightarrow np\ e\ 2p_z \rightarrow ns)$, $^1S \leftarrow X\ ^1S_0(3s \rightarrow ns,\ 2s \rightarrow ns,\ 1s \rightarrow ns)$, and $^1D \leftarrow X\ ^1S_0(3s \rightarrow 3d)$ in the magnesium atom. The influence of relaxation and correlation effects on the excitation energy and OOS and GOS values is studied. For this purpose, the target wave functions for each electronic state studied is determined independently at the Hartree-Fock and configuration-interaction methods. The first Born approximation is used in the calculation of the GOS and the properties between the nonorthogonal target wave functions are calculated with a biorthogonalization procedure. [S1050-2947(97)03910-3]

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I. INTRODUCTION

A great deal of work has been devoted in the past two decades to the study of valence excitations in the magnesium atom [1–6]. Among the reasons for this effort is the interest related to astrophysical research [7] and the fact that the Mg atom has, in the ground state, two correlated electrons in the $3s$ orbit. When one of the $3s$ electrons is promoted to an excited state, another kind of correlation takes place, such as angular $3snp$, $3s3d$, or radial $3sns$ correlations, depending on the excitation process. This means that the correlation effects act differently for the ground and excited states. For this reason, the Hartree-Fock calculations do not predict correctly the excitation energies and the optical properties. This makes the Mg excitation process interesting for the discussion of the atomic electron correlation [8].

Previous calculations of optical properties for valence excitations have taken into account the correlation by the configuration-interaction (CI) or multiconfiguration methods within the frozen-core approximation, in which the same occupied and virtual orbitals are used to build the ground- and excited-state wave functions. In the present work, we have determined the excitation energy, optical oscillator strength (OOS), and generalized oscillator strength (GOS) from CI calculations with the occupied and virtual orbitals optimized for the ground state and each of the excited states. The following valence excitations were considered: $^1P \leftarrow X\ ^1S_0(3s \rightarrow np)$, $^1S \leftarrow X\ ^1S_0(3s \rightarrow ns)$, and $^1D \leftarrow X\ ^1S_0(3s \rightarrow 3d)$ with $n=4-6$.

Very little effort has been dedicated to inner-shell excitations of the Mg atom. The calculation of inner-shell excitations must take into account the structural changes that occur in all the atomic orbitals when an inner-shell electron is excited [9]. For this reason, relaxation and correlation effects should be considered in the theoretical description of these processes. In this work these effects were taken into account in the calculations of the excitation energy, OOS, and GOS for the following inner-shell excitations of the Mg atom: $^1P \leftarrow X\ ^1S_0(2s \rightarrow np,\ 1s \rightarrow np\ e\ 2pz \rightarrow ns)$ and $^1S \leftarrow X\ ^1S_0(2s \rightarrow ns,\ 1s \rightarrow ns)$ with $n=4-6$.

In order to study the influence of relaxation and correlation effects on the excitation energy and on the optical and generalized oscillator strengths, different levels of calculation were used. The target wave functions were determined at the Hartree-Fock (HF) and CI levels, either using the ''frozen-core approximation'' or allowing all the atomic orbitals to relax for each of the excited states. The electron-atom collision process was described within the frame of the first Born approximation (FBA) [10]. The theoretical values for the excitations energies, OOS, and GOS have been compared to available experimental and theoretical results.

II. THEORETICAL METHOD

The calculations of the excitation energy, optical oscillator strength, and generalized oscillator strength were performed using either HF or CI wave functions expanded on a basis of Gaussian-type orbitals (GTOs). The $(17s,12p,5d)/[4s,3p,2d]$ basis of Widmark *et al.* [11] was uncontracted in order to properly describe the inner-shell excitations, originating an $(17s,12p,2d)$ basis. In order to describe the diffuse excited states, s, p, and d diffuse functions were added, originating the $(20s,13p,6d)$ basis set used in the present calculation.

The FBA [10] was used to calculate the generalized oscillator strength. In the calculations of the OOS and GOS, the matrix elements between nonorthogonal wave functions were done using a biorthogonalization procedure [12]. For this purpose, unitary transformations are applied to the two sets of N nonorthogonal molecular orbitals, turning $N-1$ of them orthogonal.

In order to discuss the influence of different effects involved in the target description when a core or valence electron is excited (i.e., relaxation and electron correlation) four different wave functions were calculated for each excitation process and from these both the optical and the generalized oscillator strengths were computed. Briefly, the wave func-

TABLE I. Excitation energies of the magnesium atom.

Valence excitation	ΔE (eV) HF-FC	CI-FC	HF-RE	CI-RE	Expt. value[a]
$3s\rightarrow 3p_z$	4.19	4.25	3.90	4.25	4.4
$3s\rightarrow 4p_z$	5.52	5.98	5.29	5.96	5.8
$3s\rightarrow 5p_z$	6.36	6.79	6.18	6.78	6.6

[a]Reference [1].

tions used resulted from the following calculations.

(i) The HF-FC is a Hartree-Fock calculation in which the atomic orbitals (AOs) optimized for the ground state are also used for the excited state, that is, a frozen-core (FC) description.

(ii) The HF-RE is a Hartree-Fock calculation with the atomic orbitals for the ground and excited states independently optimized, that is, a description where the orbitals are allowed to relax. In order to obtain the local minimum of energy related to a particular core electron excited state, the following procedure was used. During the calculation we do not allow the simultaneous variation of the following orbitals: $1s$ and $3p$, $2s$ and $3p$, $1s$ and $4s$, $2s$ and $4s$. They are alternatively frozen and optimized up to the convergence of the wave function. After convergence they do not change when simultaneously optimized.

(iii) The CI-FC is a CI calculation with single and double excitations based on the HF-FC orbitals. The occupied atomic orbitals optimized for the ground state of the target are used to generate the improved virtual orbitals (IVOs) [13] for both the ground and excited state.

The IVOs are determined in the self-consistent field of $N-1$ electrons, where N is the number of electrons of the neutral target. The virtual space for the Mg atom in the ground and excited states was formed with 21 IVOs of $s(4)$, $p_x(4)$, $p_y(4)$, $p_z(4)$, $d_{xy}(3)$, $d_{xz}(3)$, $d_{yz}(3)$, $d_{x2}(3)$, and $d_{z2}(3)$ symmetries. The IVOs were calculated independently for each series of excitation process corresponding to a particular Rydberg series. In this sense, nine different set of IVOs were determined to be related to the ground state, the $^1P\leftarrow X\ ^1S_0(3s\rightarrow np,\ 2s\rightarrow np,\ 1s\rightarrow np\ e\ 2pz\rightarrow ns)$ and $^1S\leftarrow X\ ^1S_0(3s\rightarrow ns,\ 2s\rightarrow ns,\ 1s\rightarrow ns)$ Rydberg series, and the $^1D\leftarrow X\ ^1S_0(3s\rightarrow 3d)$ excited state. This calculation takes into account correlation effects directly and relaxation effects indirectly.

(iv) The CI-RE is a single and double (SD) CI calculation with the atomic orbitals and IVOs for the ground and excited states being independently optimized. The HF-RE orbitals are used to build the IVOs of each Rydberg series. The virtual space is formed with the same number of virtual orbitals used in the CI-FC calculation. This calculation takes directly into account both correlation and relaxation effects.

In the determination of the excitation energies, OOS, and GOS for the HF-FC and HF-RE calculations a HF wave function was used for the ground state; for the CI-FC and CI-RE calculations a CI-SD wave function was used for the ground state. By means of this procedure, we try to make a balanced representation between the ground and excited states [14].

TABLE II. OOS for the $3s\rightarrow np_z$ excitation in the magnesium atom.

Excitation	OOS HF-FC	CI-FC	HF-RE	CI-RE	Expt. value
$3s\rightarrow 3p_z$	2.2033	1.7550	2.0133	1.7866	1.86,[a]1.83[b]
$3s\rightarrow 4p_z$	0.3234	0.1146	0.3093	0.1252	0.180,[a]0.107[c]
$3s\rightarrow 5p_z$	0.2545	0.0593	0.3346	0.0720	0.055,[a]0.022[c]

[a]Reference [24].
[b]Reference [17].
[c]Reference [18].

III. RESULTS

A. Effects of relaxation and correlation on the excitation energies and OOS

1. Valence-shell excitations: Optical excitations

In order to discuss the influence of relaxation and correlation effects on the excitation energy, Table I shows the results obtained with the four different types of calculations for valence excitations, compared with the experimental results. Very few changes occur between the HF-FC and HF-RE results where the differences between these calculations refer basically to relaxation effects. One concludes that relaxation effects are not important in the determination of the excitation energy for valence excitations. On the other hand, comparing the HF-RE and CI-RE results, where the differences refer to correlation effects, one observes that these effects play an important role.

The importance of the correlation effects for these excitation processes was already expected once the magnesium in the ground state possesses two electrons on the $3s$ orbital firmly correlated. This double occupacion comes to an end as we excite one of these electrons. These effects have been discussed extensively in the literature [3,5–8].

Table II shows the OOS values for the $3s\rightarrow np(^1S\text{-}^1P)$ excitation process at various levels of calculation. The difference between the HF-FC and HF-RE results shows that, for OOS values, the inclusion of relaxation effects is important.

TABLE III. Inner-shell excitations energies $2p_z\rightarrow ns$ in the magnesium atom.

Inner-shell excitation	ΔE (eV) HF-FC	CI-FC	HF-RE	CI-RE	Theoretical value[a]
$2p_z\rightarrow 4s$	59.57	58.25	53.88	53.72	54.80
$2p_z\rightarrow 5s$	60.85	59.63	55.21	55.99	56.27
$2p_z\rightarrow 6s$	61.29	60.29	55.78	56.56	56.77

[a]Reference [4].

It is interesting at this point to mention the work of Chang [3], where these effects were analyzed within the frozen-core approximation at HF and CI levels. This work emphasizes the importance of correlation effects for both the excitation energy and the OOS calculations. Nevertheless, this work considered only orthogonal target wave functions (within the

TABLE IV. OOS for the $2p_z \rightarrow ns$ excitations in the magnesium atom.

Inner-shell excitation	OOS			
	HF-FC	CI-FC	HF-RE	CI-RE
$2p_z \rightarrow 4s$	0.0082	0.0165	0.0281	0.0232
$2p_z \rightarrow 5s$	0.0034	0.0039	0.0071	0.0087
$2p_z \rightarrow 6s$	0.0074	0.0013	0.0064	0.0074

TABLE VI. OOS for the $1s \rightarrow np_z$ excitations in the magnesium atom.

Inner-shell excitation	OOS			
	HF-FC	CI-FC	HF-RE	CI-RE
$1s \rightarrow 3p_z$	0.0025	0.0022	0.0233	0.0207
$1s \rightarrow 4p_z$	0.0013	0.0001	0.0016	0.0017
$1s \rightarrow 5p_z$	0.0022	0.0011	0.0011	0.0010

frozen-core approximation) and was not able to separate the relaxation and correlation effects independently. In this sense, once the CI calculations of the frozen-core approximation include indirectly relaxation effects for the excited state, it was concluded that correlation effects were essential to calculate the OOS values correctly. The present work shows that for the calculation of OOS values both relaxation and correlation effects are important.

2. *Inner-shell excitations from n=2 orbitals*

The excitation energies at various levels of calculations are presented in the Table III compared with experimental results. Comparing the HF-FC and CI-FC results with the HF-RE and CI-RE results, one observes that relaxation effects must be included carefully. In this sense, one cannot use for inner-shell excitations predictions obtained with the valence-shell studies, where a CI-FC calculation has been able to recover partially the relaxation effects. This has been observed in other studies [15,16] and shows that for inner-shell excitations it is important to work with independent sets of atomic orbitals for the ground and excited states. Consequently, the atomic orbitals used in the construction of the ground-state CI wave function are not orthogonal to those used for the excited state. The difference between the HF-RE and CI-RE results in Tables I and III show that correlation effects for inner-shell and valence excitations are similar in importance. Table IV presents the OOS results. Comparing the HF-FC and HF-RE results, we notice that for inner-shell excitations both relaxation and correlation effects play an important role.

3. *Inner-shell excitations from 1s orbitals*

Table V presents the excitation energies and Table VI the OOS at various levels of calculation. As expected, relaxation effects have a greater influence on this excitation process. The CI-FC calculation was not able to account for the relaxation effects, demonstrating that in this case it is necessary to work in the frame of nonorthogonal orbitals. This table shows that the orthogonal HF calculation presents a value for the excitation process about 26 eV higher than the nonorthogonal one, about three times the ionization potential of the valence electrons.

TABLE V. Inner-shell excitation energies $1s \rightarrow np$ in the magnesium atom.

Inner-shell excitation	ΔE (eV)			
	HF-FC	CI-FC	HF-RE	CI-RE
$1s \rightarrow 3p_z$	1329.51	1326.46	1303.69	1303.25
$1s \rightarrow 4p_z$	1332.16	1329.63	1307.65	1307.86
$1s \rightarrow 5p_z$	1332.75	1329.94	1308.56	1308.80

B. Final results for excitation energies ΔE and OOS

Table VII reports the final CI-RE results for the excitation energies and OOS compared with the available theoretical and experimental results for the $3s \rightarrow np$ excitation process and Table VIII for the other process considered in the present work. The differences between the available experimental values for the $3s \rightarrow np_z$ OOS prevent one from assessing the correctness of the theoretical results, also divergent in some cases, particularly for the $3s \rightarrow 3p_z$ excitation.

It is interesting to note that all the calculations at the Hartree-Fock [17–19] level show OOS values too high in magnitude. As all the previous calculations use the frozen-core approximation, the differences between the OOS

TABLE VII. OOS for the $3s \rightarrow np_z$ excitation in the magnesium atom.

Valence shell excitation	CI-RE	Experimental value	Theoretical value
$3s \rightarrow 3p_z$	1.7866	1.86,[c]1.67[d] 1.83,[h]1.75[i] 1.81[k] 1.76[o]	1.38,[a]1.42,[a]1.67[b] 1.76,[e,f]2.10[g] 1.91,[b]1.73[j] 1.72,[m]1.75[e] 1.66[g],2.36 1.73,[c]1.72,[n]1.56[n]
$3s \rightarrow 4p_z$	0.1252	0.18[j] 0.107[p]	0.092,[a]0.099[a] 0.164,[b]0.11[e] 0.34,[g]0.129[b] 0.125,[f]0.141[q] 0.116,[q]0.114[e]
$3s \rightarrow 5p_z$	0.0720	0.055,[c]0.0227[p]	0.023,[a]0.025[a] 0.041,[b]0.026[e] 0.087,[g]0.036[b] 0.028[f]

[a] Reference [9].
[b] Reference [31].
[c] Reference [24].
[d] Reference [32].
[e] Reference [5].
[f] Reference [19].
[g] Reference [20].
[h] Reference [17].
[i] Reference [22].
[j] Reference [33].
[k] Reference [23].
[l] Reference [34].
[m] Reference [35].
[n] Reference [30]
[o] Reference [36].
[p] Reference [18].
[q] Reference [37].

TABLE VIII. Final results for the excitation energies (ΔE) and optical oscillator strengths (OOS) of the processes considered in this work. * denotes an optically forbidden excitation process and ** denotes no experimental results available to our knowledge.

Transition	$\Delta E_{\text{CI-RE}}$ (eV)	ΔE_{expt} (eV)	CI-RE OOS
$3s\rightarrow 3p_z$	4.25	4.4,[a]4.34[b]	1.7866
$3s\rightarrow 4p_z$	5.96	5.8[a]	0.1252
$3s\rightarrow 5p_z$	6.78	6.6[a]	0.0720
$3s\rightarrow 4s$	4.50	5.3,[a]5.39[b]	*
$3s\rightarrow 5s$	6.30	6.4[a]	*
$3s\rightarrow 6s$	6.87	6.9[a]	*
$3s\rightarrow 3dz^2$	5.90	5.75,[a]5.753[b]	*
$2p_z\rightarrow 4s$	53.72	54.80,[c]54.799[d]	0.0232
$2p_z\rightarrow 5s$	55.99	56.27,[c]56.28[e]	0.0087
$2p_z\rightarrow 6s$	56.56	56.77,[c]56.78[e] 56.8[e]	0.0074
$2s\rightarrow 3p_z$	91.72	**	0.0657
$2s\rightarrow 4p_z$	96.18	**	0.0025
$2s\rightarrow 5p_z$	97.11	**	0.0016
$2s\rightarrow 4s$	94.65	**	*
$2s\rightarrow 5s$	97.07	**	*
$2s\rightarrow 6s$	97.64	**	*
$1s\rightarrow 4s$	1306.29	**	*
$1s\rightarrow 5s$	1308.77	**	*
$1s\rightarrow 6s$	1309.35	**	*
$1s\rightarrow 3p_z$	1303.25	**	0.0207
$1s\rightarrow 4p_z$	1307.86	**	0.0017
$1s\rightarrow 5p_z$	1308.80	**	0.0010

[a] Reference [1].
[b] Reference [38].
[c] Reference [4].
[d] Reference [22].
[e] Reference [39].

obtained with HF wave functions are probably due to the different basis set used.

The OOS values of Martin and Zalubas [4], Amusia *et al.* [20], and Clark, Csanak, and Abdallah [8] were determined with correlated wave functions. The calculations of Amusia and Cherepkov [21] used the random-phase approximation with relativistic effects to determine the target wave functions within the frozen-core approximation and the calculations of Froese Fisher [5] used the multiconfigurational self-consistent field method within the frozen-core approximation to determine the target wave function.

One observes good general agreement among our best results, that is, with the CI-RE wave function (in which relaxation and correlation effects between valence and core electrons are included), the theoretical results of Froese Fisher [5], and the experimental results of Lundin *et al.* [22], Wiese, Smith, and Miles [23] and Smith and Liszt [24].

Table VIII shows good general agreement for the excitation energies between our CI-RE results and the experimental results for several excitation process. The general agreement for both the excitation energies and OOS of very distinct excitation processes (for example, between the $3s\rightarrow 3p_z$ and $2p_z\rightarrow 4s$ excitations [4]) shows that the basis of GTOs used in the present work has the necessary flexibility for non-frozen-core calculations. Unfortunately, there are no experimental results for the OOS of inner-shell excitation processes.

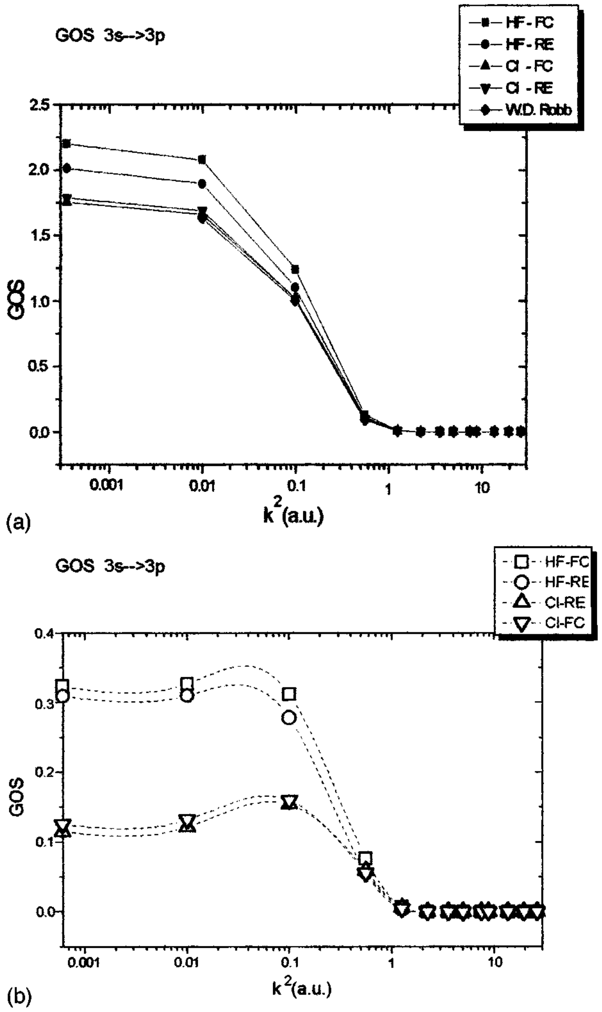

FIG. 1. Generalized oscillator strength (GOS) as a function of k^2 for the (a) $3s\rightarrow 3p_z$ and (b) $3s\rightarrow 4p_z$ transitions in the Mg atom.

C. Effects of relaxation and correlation on the GOS

Figure 1 shows the results for the GOS as a function on the squared transferred momentum k^2 at various levels of calculations for the valence $3s\rightarrow 3p_z$ together with the available theoretical [2] results. Figure 2 shows the results for the GOS as a function of the squared transferred momentum k^2 at various levels of calculations for the valence $3s\rightarrow 4p_z$ excitation and Fig. 3 for the inner-shell $2s\rightarrow 3p_z$ excitation. The transferred momentum $\vec{k}$ is defined as $\vec{k}=\vec{k}_i-\vec{k}_f$, $\vec{k}_i$ being the momentum of the incident electron and $\vec{k}_f$ the momentum of the scattered electron. Figure 4 shows the differential cross section at 1 keV impact energy as a function of the scattering angle at various levels of calculations for the valence $3s\rightarrow 3p_z$ excitation. Comparing the various levels of calculations, one observes that, also for the GOS, it is important to describe the correlation and relaxation effects correctly, particularly for the inner-shell excitation process.

Figure 1 shows that for the valence $3s$-$3p_z$ excitation process, the CI-FC results for the GOS includes indirectly the

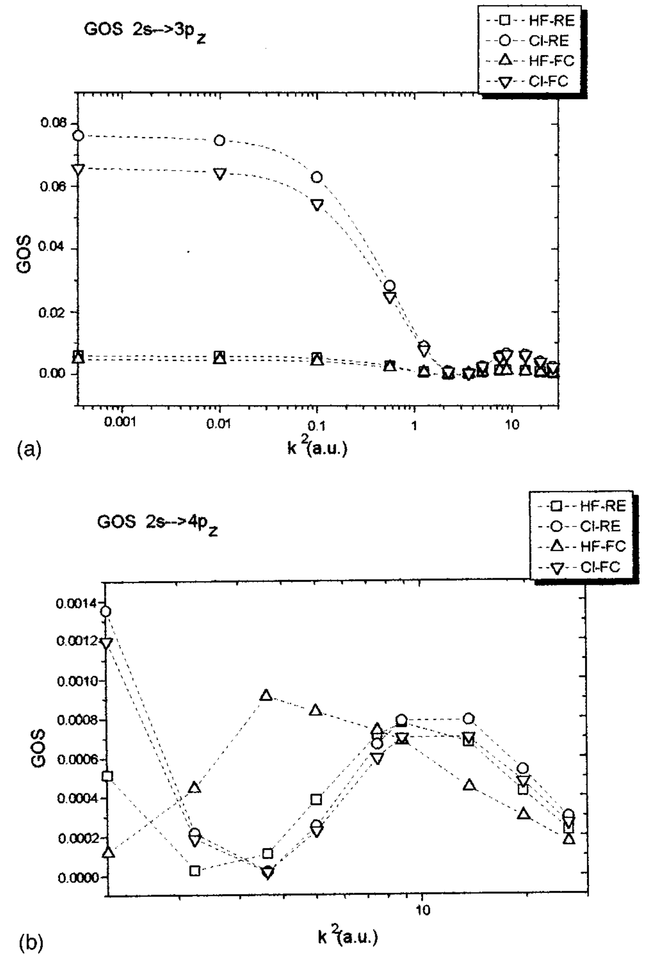

FIG. 2. GOS as a function of k^2 for the (a) $2s\rightarrow 3p_z$ and (b) $2s\rightarrow 4p_z$ transitions in the Mg atom.

relaxation effects, a behavior discussed previously in Sec. III A 1 for the OOS results. This explains the agreement between the present CI-RE results with the FBA results of Robb [2] and Kim and Bagus [6], both using CI-FC target wave functions.

There are no experimental results for the GOS at an impact energy where the FBA is expected to describe the collision process properly. The comparison between the theoretical and experimental GOS results for electronic excitations in other targets [14] shows that the first Born approximation properly describes the collision between the electron and the target for large values of impact energy, except in the neighborhood of the minimum of the GOS. The minimum of the GOS is related to the nodal structure of the radial part of the atomic orbitals of the ground and excited states. This effect has been observed before in several different electron-impact valence excitation process [25–29]. In particular, we have shown previously [25] that, at the minimum of the GOS, higher-order terms in the Born expansion become important and, consequently, the minimum is overestimated in the first Born approximation calculations. As far as we know, this is the first time that such a minimum has been predicted for the inner-shell processes.

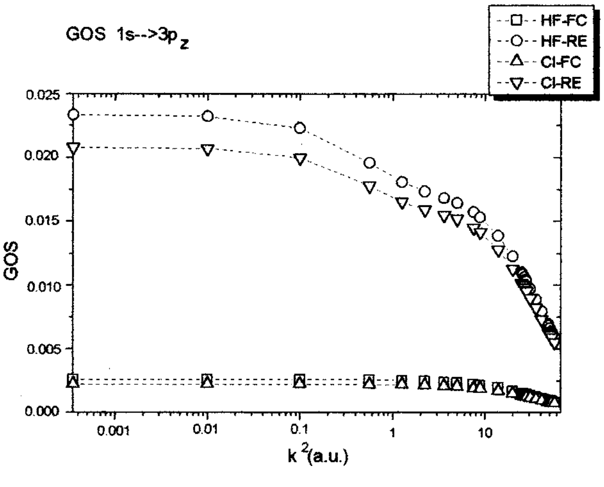

FIG. 3. GOS as a function of k^2 for the $1s\rightarrow 3p_z$ transition in the Mg atom.

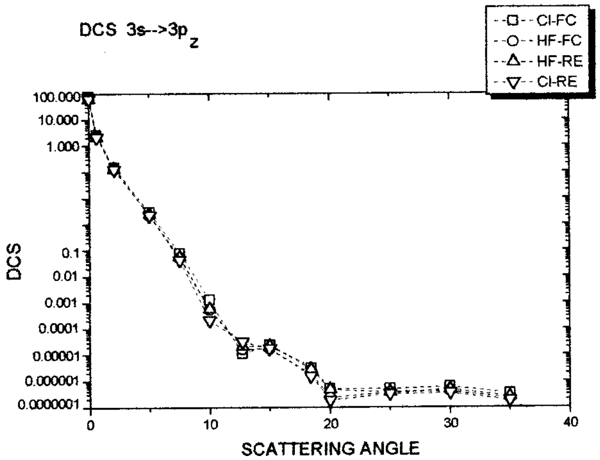

FIG. 4. Differential cross section (DCS) as a function of the scattering angle for the $3s\rightarrow 3p_z$ excitation in the Mg atom at 1 keV impact energy.

IV. CONCLUSION

Theoretical values for the excitation energy, OOS, and GOS related to inner- and valence-shell excitations were determined at four different levels of calculation for the atomic wave functions, with the electron-target collision process being described by the FBA. The comparison of the results obtained with the different target wave functions shows clearly the importance of correlation and relaxation effects on each property for each excitation process considered.

As for the excitation energy for valence-shell electronic excitations, correlation effects seemed to be the most important effect. For the valence excitations the orthogonal CI calculations were able to recover the minor relaxation effects indirectly. In all cases of inner-shell excitation, relaxation seemed to be the most important effect and orthogonal CI calculations did not properly account for this effect.

The present results show that one must be careful in treating the excited state. If important effects such as relaxation and correlation are not taken into account, the ground- and excited-state wave functions may be treated in an unbalanced way. As a consequence, for instance, one may obtain results in a poorer agreement with the experiment at the CI level than at the HF level. This occurs, for instance, in the HF-FC and CI-FC calculations.

When a comparison between the theoretical and experimental results was possible, good general agreement was found. This shows that when the frozen-core approximation is not used, a Gaussian basis set can be sufficiently flexible to describe very different processes, such as the $3s \rightarrow 6p_z$ and the $2s \rightarrow 3p_z$ excitations.

Unfortunately, most of the results obtained in this work cannot be compared with other experimental or theoretical results. The good agreement that we obtained in the different cases where the comparison was possible makes us believe that the methodology used in the present work is sufficient to describe the process considered. In this sense, they can be used as reference whenever necessary.

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