

Atomic magnesium: Discrete and continuum spectrum properties from a valence-shell L^2 configuration-interaction calculation with polarization potential

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The discrete and continuous spectrum of atomic magnesium below the $3p^2P^o$ ionization threshold has been investigated by a valence-shell frozen-core L^2 configuration-interaction calculation with a phenomenological polarization potential. The results presented include positions of bound and autoionizing levels, oscillator strengths and radiative lifetimes, the ground-state one- and two-photon ionization cross sections, and several observables of interest for long-range interaction and Zeeman-effect studies. In particular, the two-photon ionization cross section is discussed in the near-threshold region, where one experimental result is available for comparison

I. INTRODUCTION

In previous works¹⁻³ we have developed an efficient L^2 technique for the discrete and continuum states of two-valence electron atoms which has been successfully applied to atomic magnesium⁴⁻⁶ (hereafter referred to as I-III).

While accurate enough to be useful in assignment problems, these results presented a few discrepancies with the experimental data which should, at least partially, arise from the complete neglect of the intershell correlation effects (other reasons, e.g., the need to go beyond the lowest-order perturbation theory for the two-photon processes, may also be envisaged). In this work we therefore investigate the possibility of reducing these discrepancies by employing a phenomenological polarization potential.

Unless otherwise specified, all quantities are expressed in atomic units and the energy positions are relative to the ion ground state.

II. METHOD OF CALCULATION

The analytical form of the L^2 variational states employed has been discussed in detail elsewhere,¹⁻⁷ so here only a few details about the polarization potential employed are given.

The valence-shell group functions G_{VI} are the solutions of the eigenvalue problem

$$H_V G_{VI} = E_{VI} G_{VI},$$

where the valence-shell Hamiltonian H_V is

$$H_V = Q(T + V_{NCE} + 1/r_{12} + V_P)Q$$

in which Q is a projector to ensure strong orthogonality to the core self-consistent-field group function, T is the kinetic energy, V_{NCE} is the core (nuclear, Coulomb, and

exchange) potential and the polarization potential V_P is given by

$$V_P(\mathbf{r}, \mathbf{r}') = V_1(\mathbf{r}) + V_1(\mathbf{r}') + V_2(\mathbf{r}, \mathbf{r}').$$

The one-electron term V_1 is

$$V_1(\mathbf{r}) = -\alpha \sum_L P_L [W_6(r/r_L)/2r^4] P_L,$$

$$W_6(x) = 1 - \exp(-x^6),$$

where P_L is the projector for the one-electron angular momentum subspaces, $\alpha = 0.491$, interpreted as the core-dipole polarizability, was taken from Mendoza,⁸ and the cutoff parameters r_L ($r_0 = 1.2$, $r_1 = 1.335$, $r_2 = 1.25$, $r_3 = 1.30$, $r_4 = 1.1$, $r_5 = 1.0$) are chosen to reproduce the position of the lowest 2L level of Mg^+ with respect to the Mg^{2+} ground state. The two-electron term V_2 is

$$V_2(\mathbf{r}, \mathbf{r}') = -\alpha [W_6(r/R)W_6(r'/R)]^{1/2}$$

$$\times \cos \left[\frac{\mathbf{r} \cdot \mathbf{r}'}{rr'} \right] / (rr')^2.$$

The matrix elements of this operator factor in the product of an angular coefficient and two radial one-electron integrals, each of them couples orbitals whose l values differ by one; the parameter R in the cutoff W_6 was chosen as the arithmetic mean of the two r_L involved. Phenomenological corrections of this kind are largely employed in studies on two-valence electron atoms,⁹ but often in connection with not sufficiently correlated valence states. Recently, it has been employed in the eight target states ($3s, 3p, 4s, 3d, 4p, 5s, 4d, 4f$) close-coupling (8CCP) calculations of Mendoza and Zeippen,^{10,11} which appear in many respects equivalent to ours, and in the Fano-configuration-interaction (CI) calculations of Chang.¹²

It is claimed in the literature that, to be consistent with

the polarization potential, the calculation of the oscillator strengths should be performed with a modified transition operator.⁹ In the length gauge (LG) this correction proves to be rather small, while in the velocity gauge (VG) it is expected to introduce some spurious effects due to the phenomenological cutoff. Therefore we have preferred to compute the transition processes with the unmodified operator. On the whole, the introduction of the polarization potential worsens at a very limited extent the gauge invariance of the results.

III. ENERGY LEVELS

The term energies of the lowest $3snl$ bound states are reported in Table I, together with their experimental counterparts.¹³ The positions of the lowest $3pnl$ bound ($1,3P^e$ and $1,3D^o$) and autoionizing states are reported in Tables II and III, respectively, together with a few experimental data whose interpretation may be considered definitive.¹³⁻¹⁷ Indeed, the interpretation of the spectral data in the region between the $3s^2S^e$ and $3p^2P^o$ ionization thresholds is confused and often contradictory, as discussed in I to which we refer the reader for more details. The results reported in these tables justify the very simple correction to the wave energies employed in I and show that the polarization potential is a simple and efficient tool for fixing the energy levels. On the whole, it appears that the present calculations may be useful for assignment purposes. It is particularly worth noting the good agreement we found for the $3p^2S^e$ resonance, whose wave energy has proved a delicate matter. For instance, the 8CCP calculations of Mendoza and Zeippen¹¹ place it at 0.0323, indicating that the limited number of configurations which may be employed in a close-coupling calculation is not always sufficient for reproducing correctly the position of highly correlated states such as the $3p^2S^e$ of magnesium or the $2p^2S^e$ in the beryllium isoelectronic sequence. In addition, the recent calculation of Chang¹² yields for this resonance the excitation

energy 0.31042, but does not report the ionization potential necessary to obtain the wave energy.

The effect of the polarization potential upon the autoionizing widths appears to be more dramatic and difficult to assess than that upon the energy levels. For instance, the inclusion of the polarization potential has increased the width of the $3p^2S^e$ resonance (as determined by the phase-shift analysis) from 1.56×10^{-3} to 1.72×10^{-3} , very close, as expected, to the result of Mendoza and Zeippen,¹¹ but in worse agreement with the experimental values^{17,18} $(1.26-1.27) \times 10^{-3}$. A close examination has revealed that, within the limits of the present approach, the width of this resonance becomes stable only if the basis includes many localized ss configurations; for example, when the ss subspace comprised only the $3sns$ configurations we obtained a width of only 0.9×10^{-3} . In terms of the close-coupling calculation, this means that more ns target states should be employed to have a stable result. Indeed, our width is almost identical to the value 1.74×10^{-3} from the 8CCP calculations of Mendoza and Zeippen,¹¹ while the three-target ($3s, 3p, 3d$) close-coupling calculation of Thompson *et al.*¹⁹ yielded only 0.625×10^{-3} . In view of this, the value 1.24×10^{-3} of Chang¹² is probably affected by this deficiency, since all his ss configurations are $3sns$ ones, and should be considered an unconverged result.

Some of the smallest widths were significantly altered by the polarization potential and there is no guarantee that the new results are an improvement upon the previous ones, so we prefer not to report them. For the reader's convenience, we add Refs. 12 and 20 to the widths reported in table 6 of I.

IV. ONE-PHOTON PROCESSES

As discussed in II, our frozen-core oscillator strengths and radiative lifetimes were in good agreement with the experimental data but for the $1D^e$ levels, for which the discrepancies in the lifetimes reached the 20%.

TABLE I. Term energies of $3snl$ levels expressed in a.u. Experimental values (average of multiplet components) from Risberg (Ref. 13).

	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.
	$1S^e$		$3S^e$		$1P^o$		$3P^o$	
$3s^2$	-0.280 67	-0.280 99			$3s3p$	-0.121 08	-0.121 29	-0.181 23
$3s4s$	-0.082 63	-0.082 78	-0.093 20	-0.093 28	$3s4p$	-0.055 96	-0.056 15	-0.062 85
$3s5s$	-0.041 46	-0.041 53	-0.044 60	-0.044 64	$3s5p$	-0.031 68	-0.031 73	-0.033 78
$3s6s$	-0.024 95	-0.024 99	-0.026 30	-0.026 33	$3s6p$	-0.020 27	-0.020 30	-0.021 18
$3s7s$	-0.016 66	-0.016 68	-0.017 36	-0.017 38	$3s7p$	-0.014 06	-0.014 08	-0.014 54
$3s8s$	-0.011 91	-0.011 93	-0.012 32	-0.012 34	$3s8p$	-0.010 31	-0.010 33	-0.010 60
$3s9s$	0.008 93	-0.008 94	-0.009 20	-0.009 21	$3s9p$	-0.007 88	-0.007 90	-0.008 07
	$1D^e$		$3D^e$		$1F^o$		$3F^o$	
$3s3d$	-0.069 47	-0.069 57	-0.062 31	-0.062 47				
$3s4d$	-0.038 82	-0.038 89	-0.033 99	-0.034 08	$3s4f$	-0.031 85	-0.031 87	-0.031 85
$3s5d$	-0.024 38	-0.024 43	-0.021 42	-0.021 43	$3s5f$	-0.020 34	-0.020 35	-0.020 34
$3s6d$	-0.016 59	-0.016 62	-0.014 70	-0.014 71	$3s6f$	-0.014 09	-0.014 10	-0.014 09
$3s7d$	-0.011 96	-0.011 98	-0.010 71	-0.010 71	$3s7f$	-0.010 33	-0.010 34	-0.010 33
$3s8d$	-0.009 01	-0.009 03	-0.008 14	-0.008 15	$3s8f$	-0.007 89	-0.007 91	-0.007 89
$3s9d$	-0.007 02	-0.007 03	-0.006 40	-0.006 41	$3s9f$	-0.006 23	-0.006 24	-0.006 23

TABLE II. Term energies of $3pnl$ bound levels, given in a.u.

	Calc.	Expt.	Calc.	Expt.		Calc.	Expt.	Calc.	Expt.
	$^1P^e$		$^3P^e$			$^1D^o$		$^3D^o$	
$3p^2$			-0.017 46	-0.017 39 ^a	$3p3d$	0.086 62	0.086 67 ^a	0.099 63	0.099 58 ^a
$3p4p$	0.092 06	0.092 04 ^b	0.100 84	0.100 82 ^c	$3p4d$	0.124 84		0.128 62	0.128 49 ^b
$3p5p$	0.126 39		0.129 30	0.128 76 ^c	$3p5d$	0.139 70		0.141 35	
$3p6p$	0.140 41		0.141 74		$3p6d$	0.147 25		0.148 12	

^a Risberg, Ref. 13.^b Okasaka and Fukuda, Ref. 14.^c Mehlman-Balloffet and Esteva, Ref. 15.TABLE III. Wave energies of $3pnl$ autoionizing levels, expressed in a.u.

	Calc.	Expt.	Calc.	Expt.		Calc.	Expt.
	$^1P^o$		$^3P^o$				
$3p4s$	0.0760	0.0774 ^a	0.0698	0.0696 ^a			
$3p5s$	0.1205	0.1202 ^a	0.1184	0.1180 ^a			
$3p6s$	0.1375	0.1377 ^a	0.1366	0.1364 ^a			
	Calc.	Expt.	Calc.		Calc.	Calc.	
	$^1S^e$		$^3S^e$		$^1D^e$	$^3D^e$	
$3p^2$	0.0306	0.0300 ^b					
$3p4p$	0.1116		0.1011		0.1058	0.0951	
$3p5p$	0.1336		0.1295		0.1314	0.1279	
$3p6p$	0.1439		0.1419		0.1422	0.1408	
	Calc.	Expt.	Calc.		Calc.	Calc.	
	$^1P^o$		$^3P^o$		$^1F^o$	$^3F^o$	
$3p3d$	0.1112	0.1105 ^a	0.1024		0.1107	0.0852	
$3p4d$	0.1330	0.1326 ^a	0.1291		0.1332	0.1247	
$3p5d$	0.1435	0.1434 ^a	0.1415		0.1437	0.1396	
$3p6d$	0.1493	0.1492 ^a	0.1482		0.1494	0.1472	

^a Baig and Connerade, Ref. 16.^b Bonanno *et al.*, Ref. 17.TABLE IV. Radiative lifetimes and absorption oscillator strengths from the $3s3p\ ^1P^o$ level for the $3snd\ ^1D^e$ levels.

	Lifetimes (ns)				Expt. Reference 21	$f(3s3p-3snd)$				
	Calculation		Reference 5			Calculation		Reference 5		Expt. Reference 21
	Present work LG	VG	LG	VG		Present work LG	VG	LG	VG	
$3s3d$	82.7	82.0	106	105	81 ± 6	0.236	0.238	0.207	0.209	0.24 ± 0.02
$3s4d$	46.9	47.0	42.3	42.8	57 ± 3	0.126	0.125	0.153	0.151	0.16 ± 0.01
$3s5d$	44.5	45.6	37.9	38.3	50 ± 4	0.112	0.112	0.143	0.141	0.10 ± 0.01
$3s6d$	44.1	43.6	47.6	48.2	54 ± 3	0.105	0.105	0.098	0.097	0.083 ± 0.007
$3s7d$	67.6	68.0	64.6	66.1	70 ± 6	0.062	0.061	0.066	0.064	0.063 ± 0.007
$3s8d$	94.7	91.6	90.4	88.7	93 ± 7	0.042	0.043	0.044	0.045	0.043 ± 0.003
$3s3d$	132	126	123	122	127 ± 8	0.029	0.030	0.031	0.032	

It is therefore very gratifying that, on the whole, only the transition probabilities involving the $^1D^e$ levels have been significantly modified and brought in better agreement with the experimental data,²¹ as may be seen from Table IV. As discussed in II, the lifetime discrepancy arises almost equally from the transition matrix element and the transition energy in the case of the $3s3d$ level, while for the upper $3snd$ levels it should be due essentially to the matrix elements. Indeed, the polarization potential should have the effect of raising the $3p^2^1D^e$ perturber towards the ionization threshold and hence modifies the spreading of this configuration in the $3snd$ series.

The oscillator strengths and radiative lifetimes not involving $^1D^e$ levels have undergone only negligible variations; for instance the oscillator strength for the $3s^2^1S^e-3s3p^1P^o$ transition has changed from 1.761 (1.746) to 1.765 (1.745) in the length gauge (velocity gauge). The radiative lifetime of the $3s3p^1P^o$ level, however, changes to a larger extent from 2.15 (2.17) to 2.08 (2.10) ns in the LG (VG) due to the increase in the transition energy, in better agreement with the experimental data (see II). The reader may find extensive theoretical tabulations in Ref. 10 and 22-24, while the available experimental data and a few other accurate theoretical results are collected in II.

The ground-state photoionization cross section has been thoroughly investigated both theoretically^{11,25-29}

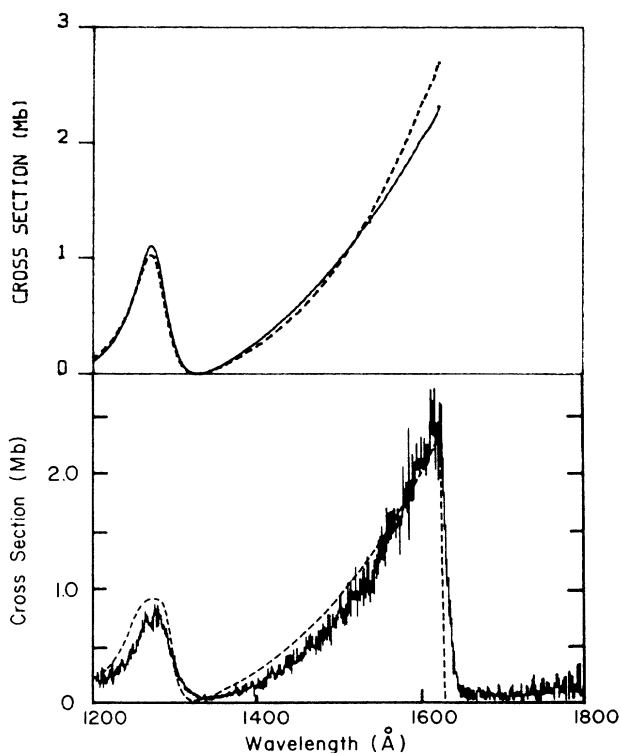


FIG. 1. One-photon ground-state photoionization cross section between 180 and 120 nm. Upper figure: present calculations, LG (dotted line) and VG (solid line) results. Lower figure: experimental results of Preses *et al.* (Ref. 32) normalized against the close-coupling calculations of Bates and Altick (Ref. 25) (broken line).

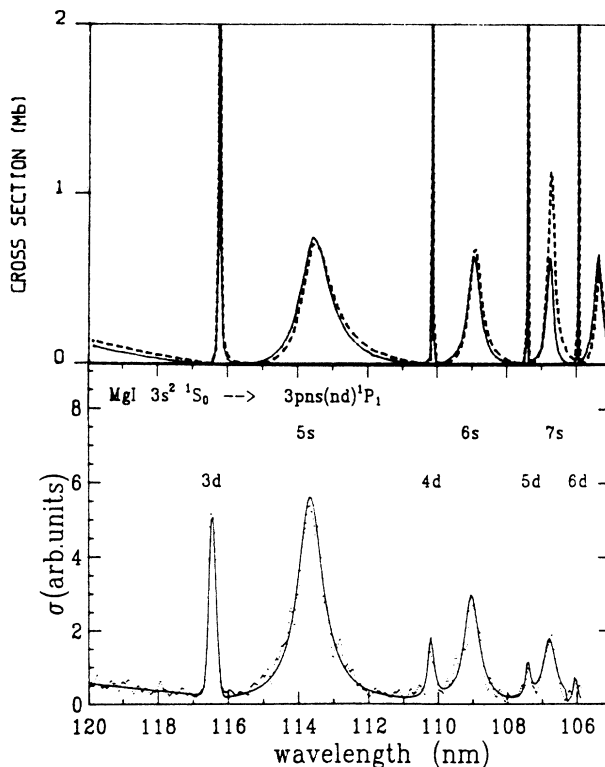


FIG. 2. One-photon ground-state photoionization cross section between 120 and 105 nm. Upper figure: present calculations, LG (dotted line) and VG (solid line) results. At the narrow $3pnd$ resonances the cross section is cut at figure top. Lower figure: experimental results of Fiedler *et al.* (Ref. 33). The width of the narrow $3pnd$ resonances reflects the laser bandwidth 0.2 nm.

and experimentally.^{15,30-33} In Figs. 1 and 2 we report our calculated photoionization cross section together with the recent experimental results of Preses *et al.*³² and of Fiedler *et al.*³³ The present calculations predict a cross section of 2.70 (2.30) Mb at the threshold and of 1.02 (1.10) Mb [LG-(VG)] at the $3p4s$ absorption peak, while place the first minimum at 0.0624 (0.0623) [LG (VG)], which are in excellent agreement with the 8CCP results of Mendoza and Zeippen¹¹ (compare with the data of II and Ref. 11).

For the photoionization of the $3s3p^1P^o$ level around the $3p^2^1S^e$ region, we obtain $\sigma_{\max} \sim 376$ (378) Mb [LG (VG)], the contributions σ_S and σ_D of the s and d waves are 304 (306) Mb and 72 (72) Mb, respectively [LG (VG)], for a ratio $\sigma_S/\sigma_D = 4.2$. The polarization potential leaves, therefore, almost unaltered σ_D , while it reduces σ_S of about the 10%. The localized representation of the $3p^2^1S^e$ resonance gives an f value almost unaltered [0.1992 (0.2011) versus 0.2010 (0.2014)], so the reduction of σ_{\max} appears due to the increase of the width. From the f value and the width, indeed, one may estimate for σ_S a peak value of 302 Mb (see II).

Our calculated cross section is almost identical to the 8CCP results of Mendoza and Zeippen,¹¹ 297 and 71 Mb for σ_S and σ_D , respectively. The experimental results of

Bradley *et al.*¹⁸ give 800 ± 400 Mb for the absorption maximum and 14 for the ratio σ_S/σ_D . The value $q^2 I_R/I_0 = 29.6$ of Bonanno *et al.*¹⁷ appears to be the ratio σ_S/σ_D for a target at least partially z polarized; assuming complete polarization it corresponds to a value of 11.8 for random orientation. A lower bound for the σ_S/σ_D ratio at the $3p^2 1S^e$ absorption peak may be obtained from a result of Bradley *et al.*¹⁸ It may be easily shown that the ratio $R(z/x)$ for the ionization signals from a P level with z and x polarized lights is obviously 1 if the target is randomly oriented, while, when the sample is completely z polarized, it takes its maximum value $R(z/x)_{\max}$ given by $R(z/x)_{\max} = (10\sigma_S + 4\sigma_D)/3\sigma_D$ or $\sigma_S/\sigma_D = 0.3R(z/x)_{\max} - 0.4$. Thus the ratio $R(z/x)_{\max}$ is not equivalent to the ratio σ_S/σ_D as assumed by Bradley *et al.*¹⁸ and their value $R(z/x) = 5$ gives, according to the above relation, the lower bound $\sigma_S/\sigma_D > 1.1$.

The Fano q value, obtained by fitting the s -wave contribution, is 26.20 (26.74) [LG (VG)]. For comparison, the frozen-core results were 28.26 (28.31) while the experimental result of Bonanno *et al.*¹⁷ is 24.4 ± 1 .

Finally, for the photoionization of the $3s3p^3P^o$ level the present calculations give the threshold value 15.0 (14.7) Mb, with s - and d -wave contributions, respectively, of 1.37 (1.22) and 13.6 (13.5) Mb [LG (VG)].

V. TWO-PHOTON PROCESSES

As observed in III, an accurate reproduction of the structured low-energy region of the single-beam two-photon ionization cross section depends critically on the relative closeness of the $3p^2 1S^e$ autoionizing state and of the $3s3p$ intermediate state resonance. Our frozen-core results,⁷ indeed, are in relatively poor agreement with the experimental data. The present results (Fig. 3) are in better qualitative agreement, but significant discrepancies still remain. In particular, the ratio of the absorptions at the $3p^2$ peak and at the minimum is about 1.5 according to the experimental data (Fig. 4 of Ref. 17), 3.3 in our

frozen-core calculations⁷ and 2.3 in the present ones. In this limited energy range, the contribution of the $3s3p$ intermediate state clearly dominates the cross section and indeed our calculations yield almost identical results if only the $3s3p$ state is retained in the resolvent; therefore the two-photon cross section should be quite well reproduced by the Fano profile for the one-photon ionization times $(\omega - \omega_{3p})^{-2}$. This analysis was indeed performed by Bonanno *et al.*¹⁷ to show that the one-photon Fano profile may be recovered from the two-photon signal; however, when their Eq. (5) is employed to estimate this ratio, it yields the value 3.8 instead of the above mentioned value 1.5. A deeper investigation of this energy region appears therefore of great interest; from a theoretical viewpoint this calls for a more accurate treatment of the intershell correlation effects and the inclusion of higher-order corrections for the photonic interaction.

VI. MISCELLANEOUS OBSERVABLES

Some ground state expectation values appear of interest in the context of the long-range interaction.³⁴ The present calculations yield 10.75 (10.62) \AA^2 [LG (VG)] for the static ground-state dipole polarizability, 642 (627) for the C_6 van der Waals coefficient, 28.1 (of which 4.8 from the core) for r^2 and 480 (of which 6 from the core) for r^4 .

Finally, the expectation value of $r^2 Y_{20}$ for the $3s3p^3P^o$ level has proved of interest for the diamagnetic contribution to the Zeeman effect.³⁵ The present calculations yield the value 1.489 \AA^2 for the $M_L = 0$ state. The experimental Zeeman data are often interpreted in terms of $\langle r^2 \rangle$ for the outer electron, for which our results is equivalent to 5.902 \AA^2 . As far as we know, the only theoretical value available for this quantity, 5.319 \AA^2 , has been obtained from the $3p$ natural orbital of a CI calculation including single, double, triple, and quadruple excitations (SDTQ-CI).³⁵ These authors have also obtained 5.299 \AA^2 with the HF orbital and 5.317 \AA^2 at SD-CI lev-

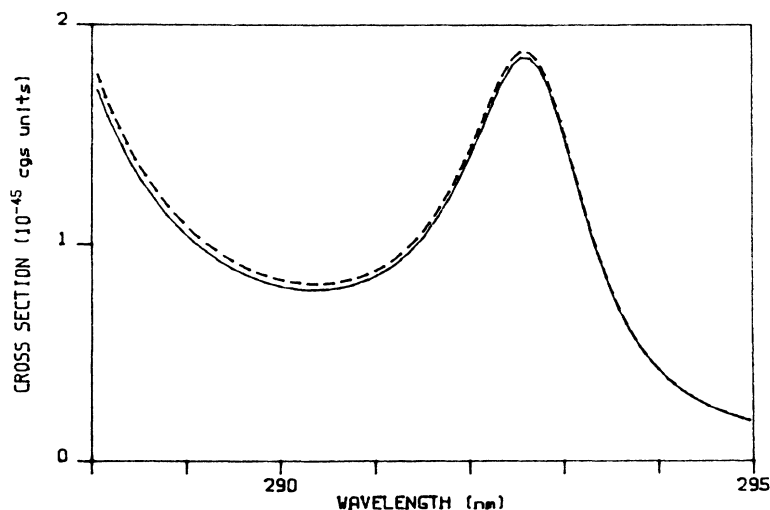


FIG. 3. Two-photon ground-state ionization cross section in the region of the $3p^2 1S^e$ autoionizing state. LG (dotted line) and VG (solid line) results.

el, while we find 5.426 \AA^2 employing only sp configurations.

VII. CONCLUSIONS

The use of a phenomenological polarization potential in connection with highly correlated valence-shell wave functions appears capable of reproducing correctly many delicate features of an interesting system like the magnesium atom. In this context, our L^2 CI technique allows

to include easily a large number of configurations and hence allows to treat efficiently the correlation effects without leading to a large number of coupled radial equations as the more usual close-coupling techniques require. For the autoionizing widths, however, the polarization potential proves unsatisfactory and a more refined treatment of the intershell correlation effects appears desirable. The two-photon ionization cross section reserves open problems in the region of the $3p^2 1S^e$ resonance which call for a more thorough analysis.

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