Core-polarization effects on near-threshold photoionization of Mg

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The multiconfiguration relativistic random-phase approximation theory (MCRRPA) is applied to the photoionization processes of Mg. Double-electron excitations as well as core-electron excitations are included. The core-electron excitations account for the core-valence correlations, specifically the core-polarization effects, and the double-electron excitations account for the intravalence correlations. We obtain a prediction of the $3s_{1/2}$ threshold photoionization cross section that is in excellent agreement with experiment. It shows that the core-polarization effects in addition to the double-electron excitations play an important role in the near-threshold photoionization processes of Mg and the MCRRPA provides an accurate account of these effects. [S1050-2947(97)04811-7]

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I. INTRODUCTION

In recent years, photoionization of magnesium has attracted much attention from theoretical and experimental researchers. The magnesium atom with two valence electrons outside a closed core has low-lying doubly excited states. Besides the usual discrete-continuum correlations with singly excited states, the correlation effects due to the presence of doubly excited states are also important in the photoionization processes of valence electrons. Measurements of the photoionization cross section of the magnesium atom [1–6] indicate that the spectrum is dominated by autoionization resonances. Certain features of these structures have also been reported in several theoretical calculations [7–21]. However, only the measurement of Ditchburn and Marr has reported the absolute photoionization cross section of magnesium, and it is found that all available calculations predict much larger near-threshold cross sections in comparison with the data of Ditchburn and Marr [1].

Including doubly excited states in the calculation of the photoionization processes of magnesium is essential for good agreement with experiment. Relativistic effects should also be dealt with to produce fine structures of the autoionization resonances. The generalization of the relativistic random-phase approximation (RRPA) theory [13,22–28] by using a multiconfiguration wave function as the reference state provides the allowance for treating double excitation correlations and is thereby appropriate for this application. This approach is called the multiconfiguration relativistic random-phase approximation (MCRRPA) theory [29,30]. The MCRRPA theory preserves all the advantages of the RRPA approach: First, the MCRRPA results are gauge independent. Second, both discrete and continuum correlations can be dealt with. Third, the initial- and final-state correlations are treated on an equal footing. Fourth, core-polarization effects can be treated readily. Applications of the MCRRPA are to the photoionization of Be, Mg, Zn, and Sr [31–36], and to photoexcitations of ions in the Be, Mg, Zn, Co, Hg, and Pb isoelectronic sequences [37–46]. Most of these MCRRPA results have been reviewed recently [47].

In the present calculation, the MCRRPA theory is applied to photoionization of magnesium with core-polarization effects included. The interplay between the double-excitation effects and core-polarization effects having an influence on the photoelectrons in the photoionization processes of magnesium is investigated.

In Sec. II we review briefly the MCRRPA theory with emphasis on its application to the photoionization of the magnesium atom. The results and discussion are given in Sec. III.

II. THEORY

The MCRRPA theory treats both relativistic and correlation effects in open-shell atoms and has been presented in detail in a previous paper [30]. In the present application, the wave function of the ground reference state of magnesium is described by the admixture

$$\Psi = C_1(3s_{1/2}^2)_0 + C_2(3p_{1/2}^2)_0 + C_3(3p_{3/2}^2)_0, \qquad (1)$$

where $(3l_j^2)_0$ represents a Slater determinant with the total angular momentum $J=0$ and even parity, constructed from the $3l_j$ valence orbitals and ten core orbitals. The ground-state orbitals and weights can be obtained from a MCDF computer code [48]. The weights for configurations $(3s_{1/2}^2)_0$, $(3p_{1/2}^2)_0$, and $(3p_{3/2}^2)_0$ are 0.9617, 0.1586, and 0.2236, respectively. Therefore, the mixing of configurations $(3p_{1/2}^2)_0$ and $(3p_{3/2}^2)_0$ with the dominant configuration $(3s_{1/2}^2)_0$ is significant for the description of the ground state of magnesium. The binding energies for the $3s_{1/2}$, $3p_{1/2}$, and $3p_{3/2}$ orbitals from the Dirac-Fock (DF) and MCDF calculations together with the experimental values are listed in Table I. Since we

TABLE I. Experimental removal energies and theoretical Dirac-Fock (DF) and multiconfiguration Dirac-Fock (MCDF) eigenvalues (in eV) for valence electrons of the neutral magnesium atom.

Subshell	Expt.[a]	MCDF	DF
$3s_{1/2}$	7.644	7.692	6.88
$3p_{1/2}$	12.069	11.848	10.907
$3p_{3/2}$	12.080	11.861	10.918

[a]Moore [49].

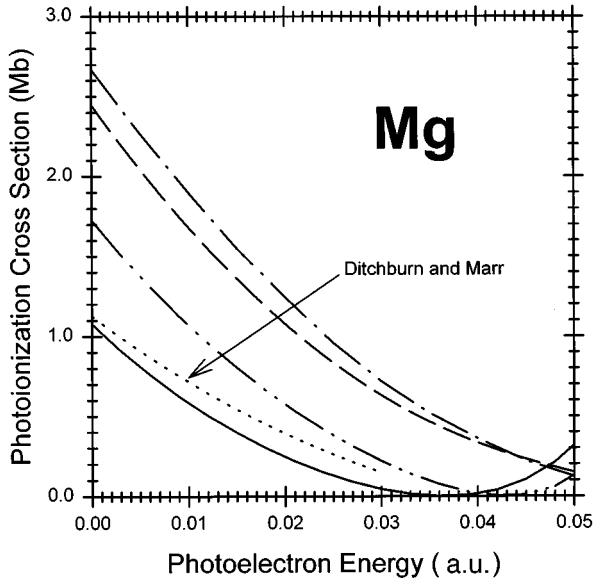

FIG. 1. Comparison of the $3s_{1/2}$ photoionization cross section of magnesium from various theoretical calculations and the experimental measurement. ---------, experimental data of Ditchburn and Marr [1]. ———, present MCRRPA calculation. –––––––-, our previous MCRRPA calculation [35]. –––––––-, eight-state close-coupling calculation of Mendoza and Zeippen [19]. –––––, configuration-interaction calculation of Altick and Bates [9].

are interested in low-energy photoionization, the main contributions to the photoionization amplitudes are predominantly due to electric dipole transitions. Within the electric dipole approximation, the allowed valence excitations of the ground reference state (1) consist of seven interacting channels, denoted symbolically as

$$3s_{1/2}\rightarrow \varepsilon p_{1/2}, \varepsilon p_{3/2},$$

$$3p_{1/2}\rightarrow \varepsilon s_{1/2}, \varepsilon d_{3/2}, \tag{2}$$

$$3p_{3/2}\rightarrow \varepsilon s_{1/2}, \varepsilon d_{3/2}, \varepsilon d_{5/2}.$$

In addition, we have included seven allowed core-excitation channels in the present calculation. The included channels are

$$2s_{1/2}\rightarrow \varepsilon p_{1/2}, \varepsilon p_{3/2},$$

$$2p_{1/2}\rightarrow \varepsilon s_{1/2}, \varepsilon d_{3/2}, \tag{3}$$

$$2p_{3/2}\rightarrow \varepsilon s_{1/2}, \varepsilon d_{3/2}, \varepsilon d_{5/2}.$$

We are concerned with photon energies just above the $3s$ ionization threshold; therefore, only the first two valence-excitation channels are open. A coherence interference among all 14 excitation channels coupled by interelectron Coulomb interactions leads to our MCRRPA results. By omitting the negative-frequency parts in the MCRRPA theory, we obtain our multiconfiguration Tamm-Dancoff approximation (MCTD) results. If the single configuration $(3s^2_{1/2})_0$ is used as the ground reference state in the MCRRPA theory, we have our RRPA and Tamm-Dancoff approximation (TD) results.

TABLE II. Photoionization cross section of magnesium at the $3s_{1/2}$ ionization threshold from various theoretical predictions and experimental measurement.

Method	σ_{TH} (Mb)
Experiment[a]	1.18 ± 0.25
Quantum-defect theory[b]	2.6
Close coupling[c]	1.5
Configuration interaction[d]	2.55
RRPA[e]	4.4
R matrix[f]	4.2
Complex basis expansion[g]	2.3
Quantum-defect theory[h]	2.3
Close coupling[i]	2.67
MCRRPA[j]	1.73
MCRRPA[k]	1.08

[a]Ditchburn and Marr [1].
[b]Burgess and Seaton [7].
[c]Dubau and Wells [8].
[d]Bates and Altick [9].
[e]Amusia, Cherepkov, Zivanovic, and Radojevic [10].
[f]O'Mahony and Greene [15].
[g]Rescigno [16].
[h]Berrington and Seaton [18].
[i]Mendoza and Zeippen [19].
[j]Our previous MCRRPA results without core-polarization effects [35].
[k]Our present MCRRPA results with core-polarization effects.

III. RESULTS AND DISCUSSION

Figure 1 shows the comparison of the experimental photoionization cross section near the $3s_{1/2}$ threshold of magnesium with various theoretical predictions. From this figure, we see that all previous theoretical calculations have overestimated the photoionization cross section. It is found that most approaches predicted a double value of the $3s_{1/2}$ threshold cross section in comparison with the experimental data. In comparison with the RPA calculation, we have obtained improved agreement of the $3s_{1/2}$ threshold cross section with the experiment in our previous MCRRPA calculation. From Table II, we see that the RRPA gives a threshold cross section of 4.4 Mb, and the MCRRPA gives a prediction of 1.73 Mb. It is revealed that a multiconfiguration wave function is important and necessary in describing the photoionization processes of magnesium. The intravalence correlations between the two equivalent valence electrons of magnesium are well accounted for by a multiconfiguration wave function. However, a large discrepancy still exists between our previous MCRRPA calculation and the experimental data. The discrepancy is ascribed to the ignored core-polarization effects arising from excitation of the inner $2s$ and $2p$ core electrons. The relaxation of the core electrons accounts for the core-valence correlations among the photoelectron and the electrons of the residual ion. As we can see from Fig. 1, our present calculation shows that the magnitude of the $3s_{1/2}$ threshold cross section is modified drastically by the core-polarization effects. We have obtained a threshold cross section of 1.08 Mb, which is in excellent agreement with the experimental value 1.18 Mb. Our calculation demonstrates that the core-valence correlations as well as the intravalence correlations play an important role in an accurate description of photoionization processes of magnesium.

[1] R. W. Ditchburn and G. V. Marr Proc. Phys. Soc. London, Sect. A **66**, 655 (1953).
[2] G. Mehlman-Ballofet and J. M. Esteva Astrophys. J. **157**, 945 (1969).
[3] J. M. Esteva, G. Mehlman-Ballofet, and J. Romand, J. Quant. Spectrosc. Radiat. Transf. **12**, 1291 (1972).
[4] M. A. Baig and J. P. Connerade Proc. R. Soc. London, Ser. A **364**, 353 (1978).
[5] J. M. Preses, C. E. Burkhardt, W. P. Garver, and J. J. Leventhal Phys. Rev. A **29**, 985 (1984).
[6] W. Fiedler, Ch. Kortenkamp, and P. Zimmermann, Phys. Rev. A **36**, 384 (1987).
[7] A. Burgess and M. J. Seaton, Mon. Not. R. Astron. Soc. **120**, 121 (1960).
[8] J. Dubau and J. Wells, J. Phys. B **6**, L31 (1973).
[9] P. L. Bates and G. N. Altick, J. Phys. B **6**, 653 (1973).
[10] C. Laughlin and G. A. Victor, *Atomic Physics*, edited by S. J. Smith and G. K. Walters (Plenum, New York, 1973), Vol. 3, p. 247.
[11] M. Ya Amusia, N. A. Cherepkov, Dj. Zivanovic, and V. Radojevic, Phys. Rev. A **13**, 1466 (1976).
[12] C. H. Greene, Phys. Rev. A **23**, 661 (1981).
[13] D. C. Deshmukh and S. T. Manson Phys. Rev. A **28**, 209 (1982).
[14] C. D. Lin, J. Phys. B **16**, 723 (1983).
[15] P. E. O'Mahony and C. H. Greene, Phys. Rev. A **31**, 250 (1985).
[16] T. N. Rescigno, Phys. Rev. A **31**, 607 (1985).
[17] V. Radojevic and W. R. Johnson, Phys. Rev. A **31**, 2991 (1985).
[18] K. A. Berrington and M. J. Seaton, J. Phys. B **18**, 2587 (1985).
[19] C. Mendoza and C. J. Zeippen, Astron. Astrophys. **179**, 346 (1987).
[20] C. Froese Fischer and H. P. Saha, Can. J. Phys. **65**, 772 (1987).
[21] R. Moccia and P. Spizzo, Phys. Rev. A **39**, 3855 (1989).
[22] W. R. Johnson and C. D. Lin, J. Phys. B **10**, L331 (1977).
[23] W. R. Johnson and K. T. Cheng, Phys. Rev. A **20**, 978 (1979).
[24] K.-N. Huang, W. R. Johnson, and K. T. Cheng, Phys. Rev. Lett. **43**, 1658 (1979).
[25] K. T. Cheng, K.-N. Huang, and W. R. Johnson, J. Phys. B **13**, L45 (1979).
[26] K.-N. Huang, W. R. Johnson, and K. T. Cheng, Phys. Lett. **77A**, 234 (1980).
[27] W. R. Johnson, K. T. Cheng, K.-N. Huang, and M. LeDourneuf, Phys. Rev. A **22**, 989 (1980).
[28] K.-N. Huang, W. R. Johnson, and K. T. Cheng, At. Data Nucl. Data Tables **26**, 33 (1981).
[29] W. R. Johnson and K.-N. Huang, Phys. Rev. Lett. **48**, 315 (1982).
[30] W. R. Johnson and K. N. Huang, Phys. Rev. A **25**, 634 (1982).
[31] H.-C. Chi, K.-N. Huang, and K.-T. Cheng, Phys. Rev. A **43**, 2542 (1991).
[32] H.-C. Chi and K.-N. Huang, Phys. Rev. A **43**, 4742 (1991).
[33] C.-Y. Hwang, H.-C. Chi, and K.-N. Huang, Phys. Rev. A **44**, 7189 (1991).
[34] C.-M. Wu, H.-C. Chi, and K.-N. Huang, Phys. Rev. A **46**, 1680 (1992).
[35] H.-C. Chi and K.-N. Huang, Phys. Rev. A **50**, 392 (1994).
[36] C.-M. Wu, H.-C. Chi, and K.-N. Huang, J. Phys. B **27**, 3927 (1994).
[37] K.-N. Huang and W. R. Johnson, Nucl. Instrum. Methods Phys. Res. B **9**, 502 (1985).
[38] H.-S. Chou, K.-N. Huang, and W. R. Johnson, Phys. Rev. A **44**, R2769 (1991).
[39] T.-C. Cheng and K.-N. Huang Phys. Rev. A **45**, 4367 (1992).
[40] H.-S. Chou and K.-N. Huang, Phys. Rev. A **45**, 1403 (1992).
[41] H.-S. Chou and K.-N. Huang, Phys. Rev. A **46**, 3725 (1992).
[42] H.-S. Chou, H.-C. Chi, and K.-N. Huang, Phys. Rev. A **48**, 2453 (1993).
[43] H.-S. Chou and K.-N. Huang, Phys. Rev. A **45**, 1403 (1992).
[44] H.-S. Chou, H.-C. Chi, and K.-N. Huang, J. Phys. B **26**, 2303 (1993).
[45] H.-S. Chou, H.-C. Chi, and K.-N. Huang, Phys. Lett. A **182**, 302 (1993).
[46] H.-S. Chou, H.-C. Chi, and K.-N. Huang, Phys. Rev. A **49**, 2394 (1994).
[47] K.-N. Huang, H.-C. Chi, and H.-S. Chou, Chin. J. Phys. **33**, 656 (1995).
[48] J. P. Desclaux, Comput. Phys. Commun. **9**, 31 (1975).
[49] C. E. Moore, *Atomic Energy Levels*, Natl. Bur Of Stand. (U.S.) National Standard Circ. No. 35 (U.S. GPO, Washington, DC, 1971).