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STUDY OF BRANCHING RATIONS OF $3p_{3/2}nd$ (J=1,3) AUTOIONIZING SERIES OF NEUTRAL MAGNESIUM *

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With the K matrix and multichannel quantum defect theory, we have studied the branching ratios of $3p_{3/2}nd$ (J=1,3) autoionizing series of Mg above the $3p_{1/2}$ ion limit. The calculations are compared with the previous experimental spectra, and the unmeasured branching ratios are presented. The conclusion is that $3p_{3/2}nd$ state prepared by the three-step excitation can form population inversion between the $3p_{1/2}$ and $3s_{1/2}$ ionic states.

Keywords: autoionization, branching ratio, configuration interaction.
PACC: 3270, 3120, 3130J

I. INTRODUCTION

In the last two decades, multichannel quantum defect theory(MQDT)[1,2] has been used with remarkable success in analyzing the experimental observables of alkaline-earth atoms, such as energy levels[3], photoionization cross sections[4,5], branching ratios, and angular distributions of photoelectrons.[6,7] Meanwhile, eigenchannel R-matrix calculations have been successfully performed for Mg[8], Ca[9], Sr[10] and Ba[11]. Affiliated with these results, MQDT has become more powerful since less empirical determinations are involved in R-matrix method and the theoretical processes are almost independent of experimental data. With the reaction K matrices obtained from R-matrix calculations, MQDT can be used not only to reproduce the experiment data, but also to provide reliable predictions for the further experimental study.[12]

Spectral line profiles and electron angular distributions of the Mg 3pnd states were extensively measured with detailed MQDT analyses. [8,12,13] However, due to the experimental difficulties, no experimental study on branching ratios of 3pnd autoionizing states has been reported up to now. Unlike Ca, Sr, and Ba, the first excited state of Mg^+ ion is the $3p_{1/2}$ state. There are fewer final ionic states for 3pnd autoionizing states since the lower energy d states of Mg^+ are absent. Thus one should find branching ratios of photoelecrons in the energy range above the $3p_{1/2}$ threshold, where the $3p_{3/2}nd$ ($n > 35$) states may decay to both the $3s_{1/2}$ and $3p_{1/2}$ ionic states. Although experimental data is not available, it is worthwhile to carry out a theoretical study on this subject.

Experimentally, the autoionizing $3p_{3/2}nd$ states are produced using a three-step laser-excitation scheme, the so-called isolated-core excitation (ICE).[14] Namely, the final 3pnd states are excited by resonant excitation of the inner valence electron, from the bound 3snd Rydberg states prepared by the first two lasers. If the three lasers are linearly polarized in the same direction, both J=1 and J=3 states will be formed. And the separate J=3 states may be obtained only if the three lasers are circularly polarized in the same sense. In this work, both J=1 and J=3 states will be calculated, according to the experimental excitation and laser polarization schemes.

II. THEORY

Since the theoretical procedure is well documented in the literature[6,8], we only outline the key expressions here. The partial cross section for photoionization resulting in a particular final ionic state $Mg^+(J_c)$ is given by

$$\sigma_{J_c} = \frac{4\pi^2\alpha\hbar\omega_3}{3} a_0(J_c), \tag{1}$$

where $\hbar\omega_3$ is the photon energy of the third laser, and α is the fine-structure constant; $a_0(J_c)$ can be calculated from

$$a_0(J_c) = \sum_{J_{cs},l,l',J,J'} (-1)^{J_{cs}} [J][J'][l][l'] C D_{J_{cs}lJ} D^*_{J_{cs}l'J'}, \tag{2}$$

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where C is a multiplier of several $3j$ and $6j$ symbols (see Ref.[8]), and $D_{J_{cs}lj}$ is an abbreviation of the reduced dipole matrix element evaluated by

$$D_{J_{cs}lj} = \langle (J_c s)J_{cs}, l, J- \parallel D \parallel J_0\rangle = \mathrm{i}^{-l}\exp(\mathrm{i}\sigma_{l,j_c}) \cdot \sum_{\rho}\langle (J_c s)J_{cs}l|\rho\rangle\exp(\mathrm{i}\pi\tau_\rho)\langle\rho \parallel D \parallel J_0\rangle, \quad (3)$$

where the operator D represents r and $\bigtriangledown/\omega$ in the length and velocity forms of dipole matrix element, respectively, and σ_{l,J_c}=arg$\Gamma(l+1-\mathrm{i}/k_{J_c})$ is the Coulomb phase of the outgoing electron. The wavefunctions and the eigenphase shifts $\pi\tau_\rho$ of the collision eigenchannels ρ, and the reduced dipole matrix elements $\langle\rho \parallel D \parallel J_0\rangle$ are derived from MQDT, which will be described later.

For J=1 states, Eq.(3) gives[15]

$$a_0(3s_{1/2}) = \frac{2}{15}\left[|D_{011}|^2 + |D_{111}|^2\right], \quad (4)$$

$$a_0(3p_{1/2}) = \frac{2}{75}|D_{101}|^2 + \sqrt{5}|D_{121}|^2, \quad (5)$$

and for J=3 states we have

$$a_0(3s_{1/2}) = \frac{3}{35}\left[|D_{033}|^2 + |D_{133}|^2\right], \quad (6)$$

$$a_0(3p_{1/2}) = \frac{3\sqrt{5}}{175}|D_{123}|^2. \quad (7)$$

Turning now to the MQDT treatment, according to MQDT, the ith closed dissociation channel yields

$$F_{i\alpha} = \sum_{\alpha} U_{i\alpha}\sin[\pi(\nu_i + \mu_\alpha)]B_\alpha = 0, \quad (8)$$

where ν_i is the effective quantum number related to the corresponding ionization limit, $\nu_i = [R/(I_i - E)]^{1/2}$, and B_α is the coefficient of the close-coupled channel φ_α in the wave function φ. The eigenchannel quantum defects μ_α of the close-coupling channels and the transformation matrix elements $U_{i\alpha}$ are obtained from the K-matrix,

$$KU = U\tan(\pi\mu_\alpha), \quad (9)$$

For the open dissociation channels, the ν_i in Eq.(10) are replaced with $-\tau_\rho$, and the eigenphase shift $\pi\tau_\rho$ of the ρth collision eigen-wavefuntion φ_ρ is obtained by solving the following equation:

$$\det|F_{i\alpha}| = 0, \quad (10)$$

which is required to obtain a non-trivial solution of B_α.

The amplitudes $A_{i\rho}$ of the dissociation channels in the collision eigenstate ρ are determined by

$$A_{i\rho} = \sum_{\alpha} U_{i\alpha}\cos[\pi(-\tau_\rho + \mu_\alpha)]B_\alpha^{(\rho)}, \quad (11)$$

and

$$A_{i\rho} = \sum_{\alpha} U_{i\alpha}\cos[\pi(\nu_i + \mu_\alpha)]B_\alpha^{(\rho)}, \quad (12)$$

for the open and closed dissociation channels, respectively, by which the following expressions in Eq.(3) can be determined:

$$\langle (J_c s)J_{cs}, l|\rho\rangle = \sum_i \langle (J_c s)J_{cs}, l|J_c, (sl)j\rangle A_{i\rho}, \quad (13)$$

where the summation is taken over all open dissociation channels, and

$$\langle\rho \parallel D \parallel J_0\rangle = \sum_k \langle k, J \parallel D \parallel J_0\rangle A_{k\rho}, \quad (14)$$

where the summation is taken over the $3p_{3/2}nd_{5/2}$ and $3p_{3/2}nd_{7/2}$ channels. The reduced matrix element $\langle k, J \parallel D \parallel J_0\rangle$ in Eq.(14) can be expressed as

$$\langle k, J \parallel D \parallel J_0\rangle = \langle 3p_{3/2} \parallel D \parallel 3s\rangle\langle\nu_k'|\nu\rangle, \quad (15)$$

where the dipole matrix element $\langle 3p_{3/2} \parallel D \parallel 3s\rangle$ can be evaluated through both the length and velocity forms, as mentioned before. The two different forms are equivalent but usually give different results if approximate wavefunctions are used. In this work, however, since all matrix elements $D_{J_{cs}lJ}$ contain $\langle 3p_{3/2} \parallel D \parallel 3s\rangle$ as a common factor, the branching ratios do not depend on this matrix element.[8] Therefore, it can be safely considered to be a constant, and excluded from the calculation. $\langle\nu_k'|\nu\rangle$ is the overlap integral defined in Ref.[16]:

$$\langle\nu_k'|\nu\rangle = \frac{2(\nu_k'\nu)\sin[\pi(\nu_k' - \nu)]}{\nu^{3/2}\pi(\nu_k'^2 - \nu^2)}. \quad (16)$$

The K matrices are symmetric matrices and contain the most important dynamical information. Both J=1 and J=3K matrices have been previously published, and the K matrices we use in this work are the same as those in Refs.[8] and [13], for J=1 and J=3 states respectively. We choose a five-channel K matrix for J=3 states, in which the three $3png$ channels are excluded for simplicity, since the g-wave resonances are proved to be negligible.[12] The matrix elements are given at three energies and vary smoothly with energy. Therefore, interpolation is needed to obtain K matrices at all the energies.

Ⅲ. RESULT AND DISSCUSSION

In this work, the J=1 and J=3 manifolds are calculated individually, and the results are added up to form the total cross sections σ, as well as the autoionizing branching ratios:

$$BR_{J_c} = \sum_J \sigma^J_{J_c} \Big/ \sum_J \sum_{J_c} \sigma^J_{J_c}, \tag{17}$$

First to verify the correctness of the theoretical model, we have calculated some spectra of 3pnd (J=1,3) autoionizing states, which are comparable with the existing experimental spectra. Two examples are shown in Fig.1, for the 3p11d (J=1,3) and 3p38d (J=3) states, respectively. Good agreement can be seen in Fig.1 between the calculated spectra and the experimental spectra reported in Refs.[4] and [17], indicating that the K matrices used here are accurate enough to obtain reliable predictions of branching ratios of 3pnd states.

Figure 2 shows an example of our calculations of branching ratios, which is for the $3p_{3/2}44d$ (J=3) state, together with spectra of the spectral densities A_4^2 and A_5^2 (corresponding to the $3p_{3/2}nd_{5/2}$ and $3p_{3/2}nd_{7/2}$ channels, respectively), overlap integral, and total cross section. Note that in our case all the closed dissociation channels converge to the $3p_{3/2}$ threshold, making the overlap integral common to all of dipole matrix elements and the partial cross section σ_{J_c}. Therefore, unlike the cross section, the branching ratios are independent of the overlap integral, as seen in Fig.2. When the energy is away from the peak of overlap integral, the amplitude of the branching ratio does not decrease with the autoionizing spectrum. On the other hand, the spectral densities play the crucial roles in branching ratio so that the branching ratio has the same periodicity as the spectral densities. Furthermore, based on many calculations for different states, we conclude that the branching ratios only depend on energy, not on particular n values. For instance, the branching ratios shown in Fig.2 can be corresponding to different autoionizing states in the same series. This particular property is due to the isolated $3p_{3/2}nd$ autoionizing series.

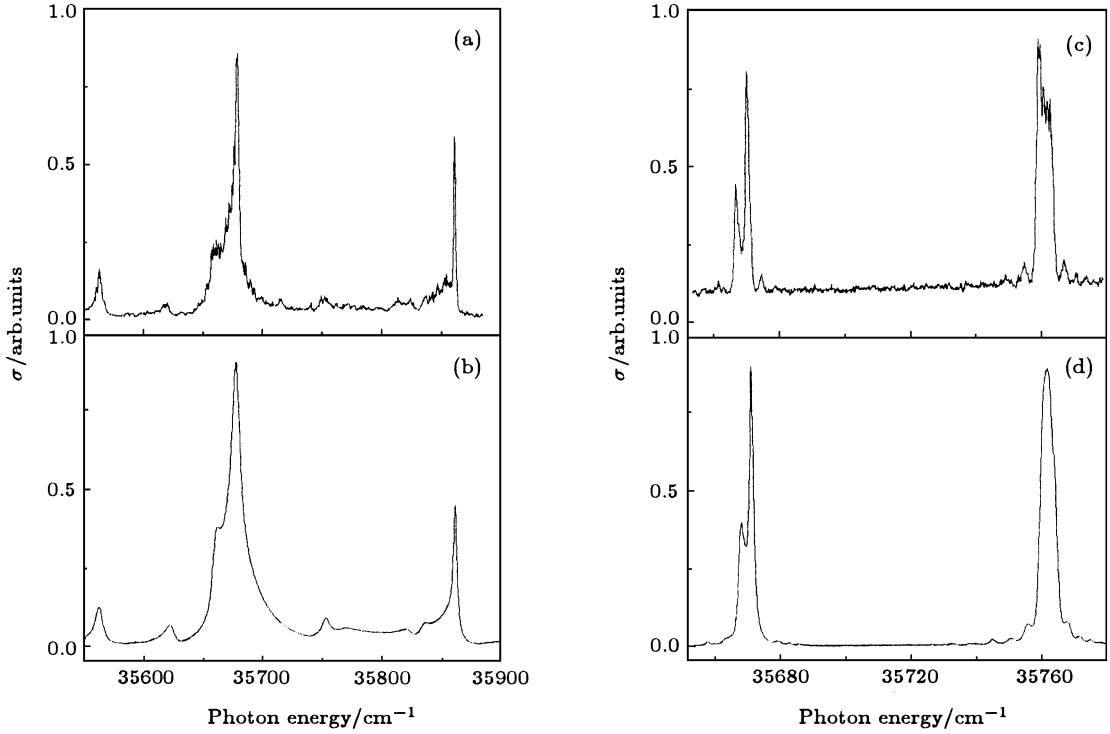


Fig.1. Comparisons of (a) experimental (Ref.[4]) and (b) theoretical spectra of the 3p11d (J=1,3) autoionization state, and (c) experimental (Ref.[17]) and (d) theoretical spectra of the 3p38d (J=3) autoionizing state.

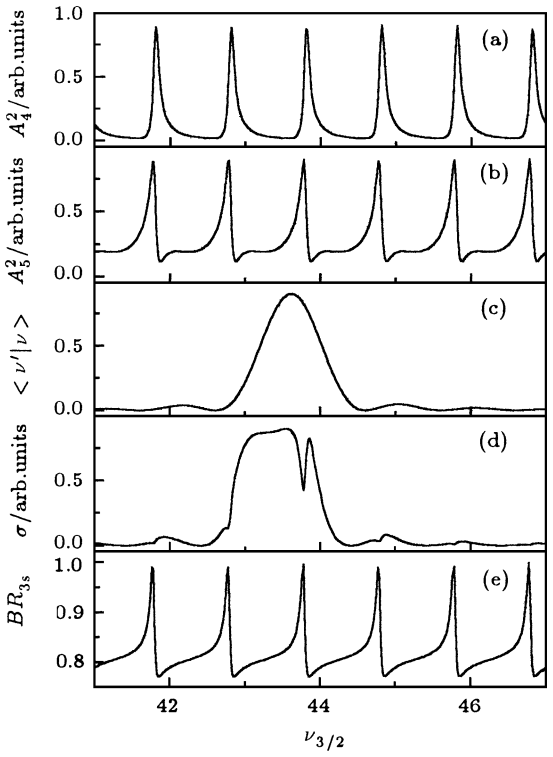


Fig.2. Comparison among (a) spectral density of $3p_{3/2}nd_{3/2}$ channel, (b) spectral density of $3p_{3/2}nd_{5/2}$ channel, (c) overlap integral, (d) total cross section, and (e) branching ratio for the $3p_{3/2}44d$ (J=3) autoionizing state.

Figure 3 shows the total cross sections and the branching ratios of the $3p_{3/2}39d$ and $3p_{3/2}48d$ states. As can be seen from Fig.3, corresponding to the peaks of different autoionizing states, the branching ratios have almost the same amplitude and spectral width relative to the effective quantum number. This means that the branching ratios reflect the properties of the $3p_{3/2}nd$ autoionizing series, which is unperturbed above the $3p_{1/2}$ threshold.

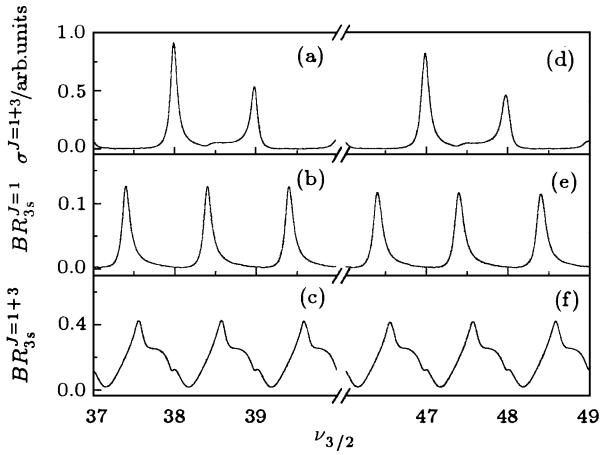


Fig.3. Total cross sections and branching ratios of the $3p_{3/2}39d$ state (a)–(c) and the $3p_{3/2}48d$ state (d)–(e).

From the branching ratios of autoionizing $3p_{1/2}nd$ (J=1,3) states shown in Fig.3, we may find that in the vicinity of the peaks of the autoionizing spectra, the branching ratios is much less than 0.1. This indicates that most of the atoms excited will finally decay to $3p_{1/2}$ ionic states, and thus form population inversion between the $3s_{1/2}^+$ and $3p_{1/2}^+$ states. Therefore, it is possible to generate lasing based on the excitation of Mg 3pnd states. Namely, the Mg atoms are excited from $3s^2$ ground states to $3p_{1/2}nd$ (J=1,3) autoionizing states by three-step excitation, from which they decay to the $3s^+$ and $3p^+$ metastable states, and form population inversion. In principle, a four-energy-level laser may be made based on this physical mechanism.

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