

Satellite lines in the photoionization of ions: The Be isoelectronic sequence

W.-C. Chu,¹ H.-L. Zhou,¹ A. Hibbert,² and S. T. Manson¹

¹*Department of Physics and Astronomy, Georgia State University, Atlanta, Georgia 30303, USA*

²*School of Mathematics and Physics, Queen's University of Belfast, Belfast BT7 1NN, United Kingdom*

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Partial photoionization cross sections from the 1S ground and the 3P metastable states of the Be isoelectronic series to different final states, including a number of satellite (ionization plus excitation) channels are studied using the R -matrix method. As expected, the ratio of each satellite partial cross section to the dominant partial cross section is found to be a monotonic decreasing function of Z for both the ground and the metastable states. The complicated patterns of these ratios as functions of photon energy are analyzed.

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I. INTRODUCTION

As a basic physical process in nature, the photoionization of atoms and ions has been studied intensively over the years. Since electron-electron correlations play an important role in the photoionization process in many-body systems, it is of importance to study correlations to fully understand photoionization cross sections. Ionization plus excitation processes, which are usually referred as “satellite lines,” are of particular interest since they exist only due to correlations; they are forbidden from a single-particle viewpoint. Thus, investigations of photoionization plus excitation processes constitute an ideal “laboratory” to study correlation in the photoionization process. To date, a number of theoretical and experimental studies of satellite lines have been reported for neutral atoms but there are only very few (especially experimental) for positive ions. It is known, however, that in the limit $Z \rightarrow \infty$, satellite lines vanish because the e^2/r_{ij} terms in the Hamiltonian that are the source of correlation become negligible compared with the nuclear Coulomb potential. Thus, while satellite lines for the neutral atom and for infinite Z are known, their evolution with Z has not yet been investigated.

In this article, a theoretical study of a number of the satellite lines in the Be isoelectronic sequence resulting from the photoionization of the $^1S^e$ ground and the $^3P^o$ metastable states is presented. The four-electron Be-like systems are relatively simple systems and can be handled quite well theoretically; excellent agreement with measured total cross sections has been found [1]. In addition, these ions are among the abundant species in astrophysical plasmas. This study includes 14 ions, Be, B⁺, C⁺², N⁺³, O⁺⁴, Ne⁺⁶, Mg⁺⁸, Si⁺¹⁰, S⁺¹², Ar⁺¹⁴, Ca⁺¹⁶, Ti⁺¹⁸, Cr⁺²⁰, and Fe⁺²², the most astrophysically abundant of the sequence. To simplify matters, we ignore the region of autoionizing resonances and focus on the photon energy range above the double ionization threshold. In this report we calculate the partial cross section covering the photon energy range up to $8.0E_{\text{range}}$, where E_{range} is the energy range from the ionization threshold ($2s$) to the $4f$ threshold for each ion. Each satellite line is compared with the dominant partial cross section and these ratios are examined. How the ratios behave as functions of photon energy as well as how these ratios change as functions of Z are studied. The nonrelativistic R -matrix method [2], introduced in the next section, is employed to calculate the partial cross sections. For the photoionization cross sections of these systems, the

nonrelativistic and Breit-Pauli R -matrix methods differ mainly in the splitting of resonances and in threshold energies, but the agreement between the nonresonant cross sections predicted by the two methods is quite good [1]. Thus it is adequate to use a nonrelativistic treatment of the photoionization process.

II. THEORETICAL METHODOLOGY

The photoionization processes for ground and metastable states are given nonrelativistically by

$$1s^2 2s^2 (^1S^e) + h\nu \rightarrow [1s^2 nl + e^-(\epsilon l')](^1P^o) \quad (1)$$

and

$$1s^2 2s 2p (^3P^o) + h\nu \rightarrow [1s^2 nl + e^-(\epsilon l')](^3S^e, ^3P^e, ^3D^e), \quad (2)$$

respectively, where the terms are expressed in the LS framework. In the R -matrix calculation, the so-called target (N -electron) discrete wave functions are constructed, and the photoelectron is added onto the target wave functions to construct the initial- and final-state wave functions of the $(N+1)$ -particle system. To build the target-state wave functions, we used the $1s$ and $2s$ orbital functions from the Hartree-Fock calculations of the Li-like ground states as given by Weiss [3] and by Clementi and Roetti [4]. With this $1s$ function held in common to all states, we constructed nine configurations: $1s^2 2s$, $1s^2 2p$, $1s^2 3s$, $1s^2 3p$, $1s^2 3d$, $1s^2 4s$, $1s^2 4p$, $1s^2 4d$, and $1s^2 4f$. The outer nl orbital function was optimized, using the CIV3 program [5], on the energy of the corresponding 2L state. The nine configurations are taken as the basis for the target wave functions, which are calculated by diagonalizing the N -particle Hamiltonian.

The core idea of the R -matrix method is to partition space into internal and external regions, divide by a spherical shell ($r = a$) centered at the nucleus, and calculate the wave functions in the two regions with the relevant boundary conditions by means of the R matrix at $r = a$. The radius of the sphere a is determined by the condition that all the discrete wave functions are small enough at $r = a$ so that they can be neglected in the external region, which means only the continuum extends to the external region. In the internal region, all the $N+1$ electrons are indistinguishable and all

exchange terms are taken into account. Thus, the total wave function is given by

$$\Psi_k^{LS\pi} = A \sum_{ij} c_{ijk} \bar{\Phi}_i(S_i L_i; x_1, x_2, \dots, x_N, \hat{x}_{N+1}) \times \frac{F_j(r_{N+1})}{r_{N+1}} + \sum_j d_{jk} \chi_j^{SL\pi}, \quad (3)$$

where $\bar{\Phi}_i$ are the target wave functions coupled to the angular and spin parts of the photoelectron wave function, the $F_j(r_{N+1})$ are the continuum radial functions of the photoelectron, and A is the antisymmetry operator. Note that the coupling between the target and the photoelectron must match the total angular momentum and the total spin specified by $LS\pi$ in each calculation. The second term in Eq. (3) is a linear combination of discrete total wave functions to ensure the completeness of the expansion. In the external region, the whole system is viewed as a two-body system where the exchange terms between the photoelectron and any other electron are small enough to be omitted. The total continuum wave function in the outer region is then given by

$$\Psi_k^{SL\pi} = \sum_{ij} c_{ijk} \bar{\Phi}_i(S_i L_i; x_1, x_2, \dots, x_N, \hat{x}_{N+1}) \frac{F_j(r_{N+1})}{r_{N+1}}. \quad (4)$$

Note that there is no antisymmetry operator A in Eq. (4). With the forms of Eq. (3) and Eq. (4), by solving the Schrödinger equation with the boundary conditions at $r = 0$, at $r \rightarrow \infty$, and the continuity at $r = a$, the wave functions in both regions are obtained using the R matrix as the connection between the regions. Thus, we obtain the initial-state wave function with the corresponding initial-state energy and the final-state wave function with any given total energy over all space. The transition matrix elements are then calculated within the framework of the electric dipole approximation to give the photoionization cross sections.

In the cross-section calculation, we consider 400 energy points evenly distributed in the energy range from the ionization threshold to $8E_{\text{range}}$. This energy mesh is good enough to describe the cross sections in this range since we focus on the energy region above the resonances.

III. RESULTS AND DISCUSSION

For both the ground state and the metastable state, above the resonance region, all the partial cross sections from the initial state to the $1s^2 nl$ final states (designated σ_{nl}) are smooth functions of photon energy E_{ph} , and each σ_{nl} as a function of E_{ph} also evolves smoothly with Z . Since the energy scale increases with Z , to analyze the evolution along Z in detail, these ratios are plotted against the energy scaled by the factor E_{range} , the energy between the $2s$ and $4f$ thresholds ($E_{\text{ph}}/E_{\text{range}}$) of each ion, so the ratios for different ions are easily compared.

For the photoionization of the $1S^e$ ground state, σ_{2s} is the largest cross section since it results from a single-electron transition. Thus, the ratio σ_{nl}/σ_{2s} as a function of scaled energy is studied. Figures 1–3 show our results for the ratios σ_{nl}/σ_{2s} for neutral Be, Si^{+10} , and Fe^{+22} , respectively. We first examine

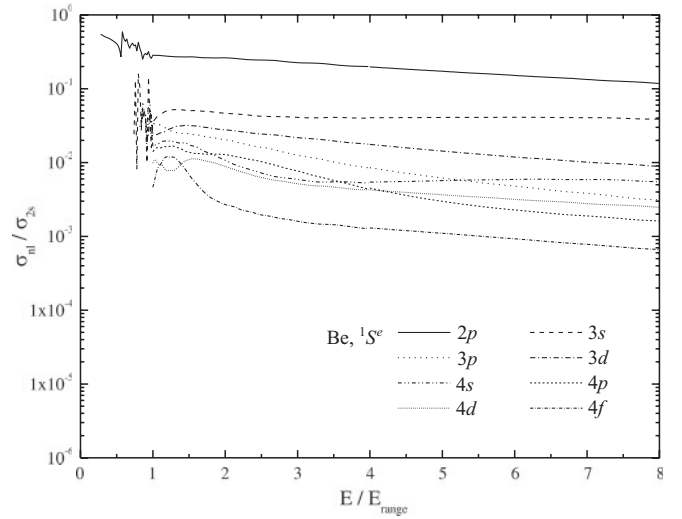


FIG. 1. Ratios of partial cross sections σ_{nl} to the $2s$ partial cross section σ_{2s} for ground-state Be against scaled photon energy.

the overall strength of each σ_{nl} over the whole energy range. As seen in the Fig. 1 for Be, the largest ratio, σ_{2p}/σ_{2s} , varies between 0.1 and 1, while the smallest, σ_{4f}/σ_{2s} , lies between 0.01 and 0.1. For Fe^{+22} , which is the highest- Z ion in this study, σ_{2p}/σ_{2s} varies between 0.01 and 0.1, and σ_{4f}/σ_{2s} is quite small, of the order of 10^{-5} . All ratios decrease with Z , which means σ_{2s} is more and more dominant at high Z 's. This is consistent with what must happen as $Z \rightarrow \infty$, and the system becomes hydrogenic; in that limit, only σ_{2s} is nonzero and all other σ_{nl} , which result from two-electron transitions, vanish. In addition, it is seen that at low Z , all the partial cross section strengths clustered together, while at high Z they are more separated.

Looking at the ratios as a function of energy, it is evident from Figs. 1–3 that the ns ratios, σ_{3s}/σ_{2s} and σ_{4s}/σ_{2s} , are more or less energy independent (horizontal) at the higher energies, indicating that all of the ns cross sections, including the $2s$, have the same energy dependence at the higher energies. We emphasize that transitions to a final ns state have the

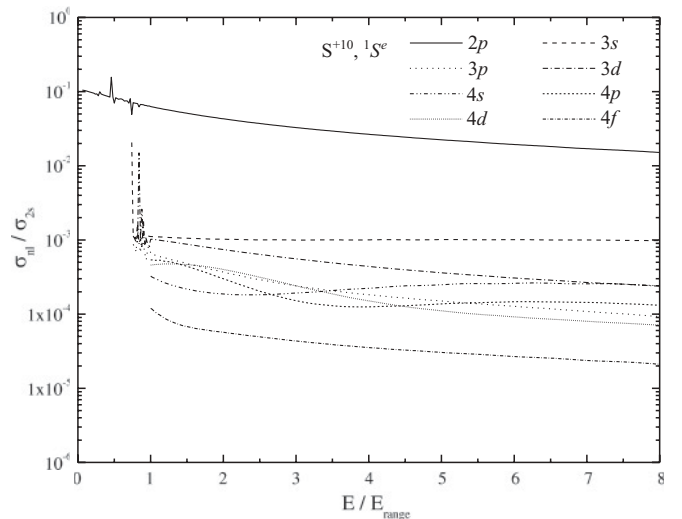


FIG. 2. As in Fig. 1 but for ground-state Si^{+10} .

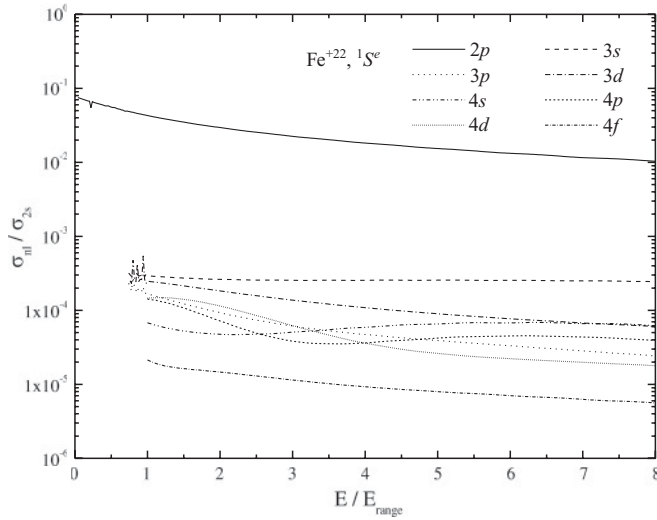


FIG. 3. As in Fig. 1 but for ground-state Fe^{+22} .

same energy dependence, at the higher energies, irrespective of whether the transition is a one-electron or a two-electron transition. For all of the transitions to nl states with $l \neq 0$, the ratios fall off with energy at the higher energies. This shows that ns cross section will become more and more dominant with increasing energy.

To take a closer look at how these overall strengths change with Z , Fig. 4 shows σ_{nl}/σ_{2s} at $E_{\text{ph}} = 8E_{\text{range}}$ vs. $1/Z$. The partial cross sections are examined at an energy much higher than all the thresholds, insuring that only the background cross sections, and no resonance structure, are taken into account. As expected, the high- Z ratios tend toward zero because of the hydrogenic nature of high- Z ions. Note that on this $1/Z$ plot, the ratios for higher Z ions that have not been explicitly calculated in this article are easily obtained by interpolation.

The ratios σ_{nl}/σ_{2p} for the photoionization of the metastable state for neutral Be, Si^{+14} , and Fe^{+22} are shown in Figs. 5–7. For the metastable state, the relative strengths are displayed with respect to σ_{2p} since σ_{2p} is the largest partial cross section

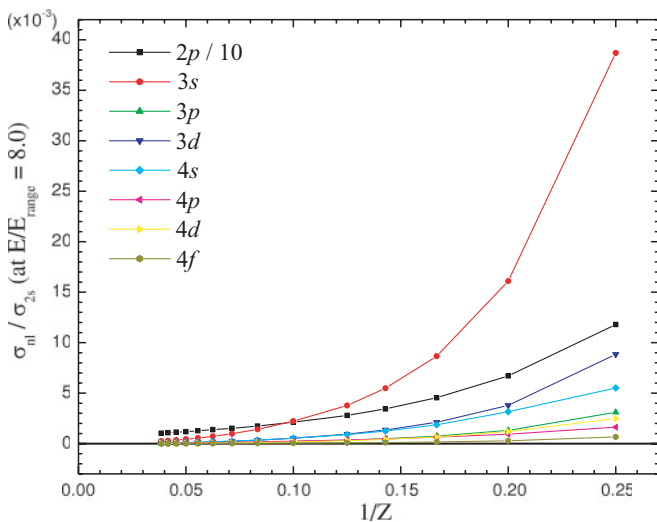


FIG. 4. (Color online) The ratios σ_{nl}/σ_{2s} for all the ground-state ions at the photon energy $E_{\text{ph}} = 8E_{\text{range}}$ vs. $1/Z$.

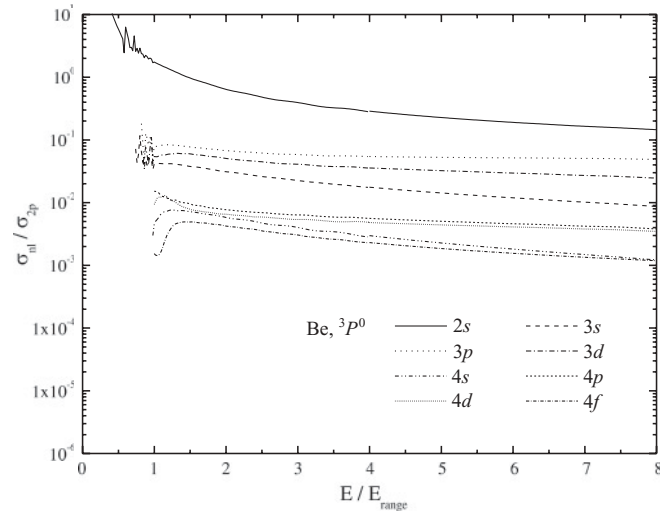


FIG. 5. Ratios of partial cross sections σ_{nl} to the $2p$ partial cross section σ_{2p} for metastable-state Be against scaled photon energy.

at high energies. However, differing from the ground-state case, the single-electron ionization process in the metastable state gives rise to both σ_{2s} and σ_{2p} partial cross sections; thus, as seen in Figs. 5–7, σ_{2s}/σ_{2p} does not decrease much with Z . On the contrary, the whole σ_{2s}/σ_{2p} curve stays almost the same from Si^{+14} to Fe^{+22} , which indicates the ratio between σ_{2s} and σ_{2p} is almost constant with Z (at any specific scaled energy) at high Z 's, although at really high energy, the $2s$ cross section will dominate [6]. Other than these two single-electron-excitation partial cross sections, all other cross sections decrease monotonically with Z , just as in the case of the ground state. For the metastable state, the strengths of all σ_{nl} are well aligned in the order of n for the same l . For example, $\sigma_{2s} > \sigma_{3s} > \sigma_{4s}$ for ns states. This regularity is mostly true for ground-state partial cross sections, except σ_{4p} climbs across σ_{3p} and is higher than σ_{3p} at high energies, as seen in Figs. 2 and 3.

Looking at the cross-section ratios as a function of energy, it is noted that all σ_{nl}/σ_{2p} decrease with energy except σ_{3p}/σ_{2p}

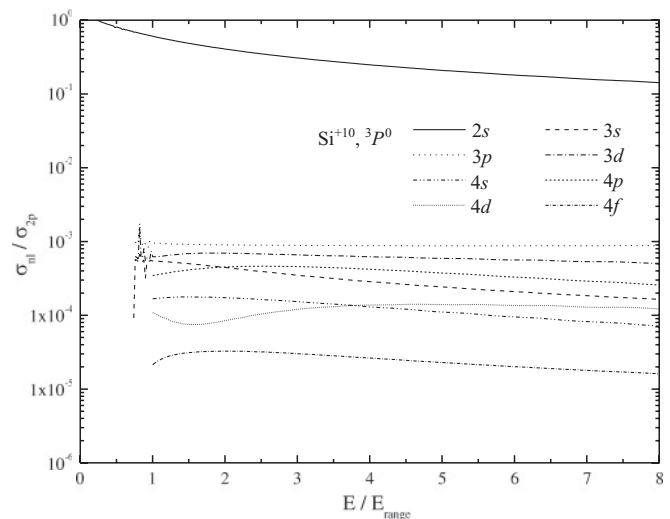
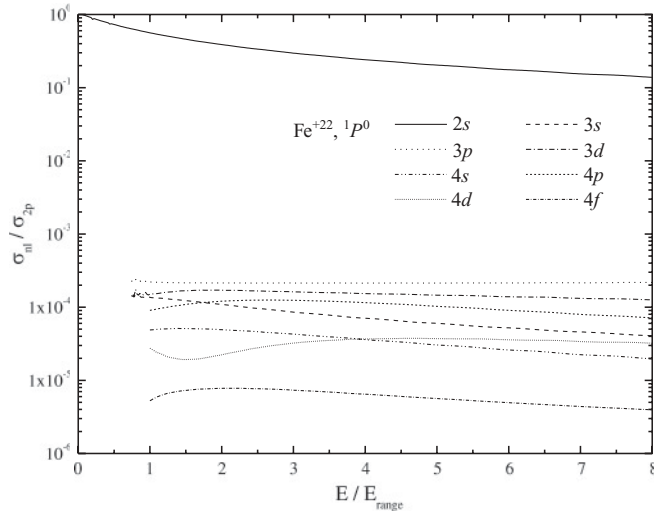


FIG. 6. As for F but for metastable-state Si^{+10} .

FIG. 7. As for F but for metastable-state Fe^{+22} .

which becomes constant (horizontal) at the higher energies for all three metastable cases. In other words, at the higher energies considered here, the $2p$ and $3p$ cross sections have the same energy dependence, but the $4p$ cross section does not. This differs from the ground-state results where all ns cross sections exhibited the same energy dependence at the higher energies. The reason for this difference is interchannel coupling; the $4p$ and $4d$ cross sections are about the same order of magnitude and their thresholds are quite close in energy. Since the strength of interchannel coupling falls off with increasing energy [7], it is expected that σ_{4p}/σ_{2p} will become constant at much higher energies. We note further that for metastable-state photoionization, the three ns cross sections are parallel at the higher energies, i.e., σ_{3s}/σ_{2s} and σ_{4s}/σ_{2s} are constant, as a function of energy, at the higher energies; evidently interchannel coupling is much less important for these ns cross sections.

It is of interest to inquire, quantitatively, as to the role of interchannel coupling in some of these satellite lines. To do this, we look at the ratios of cross sections going to a final ionic state of the same symmetry, e.g., $1s^22s$ and $1s^23s$, in a single-particle formulation with relaxation, the so-called shake-up approximation. In this approximation, for ground-state photoionization to a $1s^2ns$ final state, the cross section

$$\sigma_{ns} \propto \langle 2s_i | ns_f \rangle \langle 2s_i | r | \varepsilon p_f \rangle \quad (5)$$

where the subscripts refer to initial- (i) and final- (f) state orbitals and the overlap of initial- and final-state $1s$ orbitals is so close to unity that it is omitted. Then looking at the ratio σ_{ns}/σ_{2s} at an energy well above the thresholds, the one-electron dipole matrix element should be essentially the same for all ns transitions because the small difference in photoelectron energy is unimportant at high energy, as is the difference in fields experienced by the photoelectrons in the various ns transitions. In that case

$$\frac{\sigma_{ns}}{\sigma_{2s}} = \frac{|\langle 2s_i | ns_f \rangle|^2}{|\langle 2s_i | 2s_f \rangle|^2}, \quad (6)$$

which is independent of energy. The same considerations can be applied to the metastable-state photoionization, and the

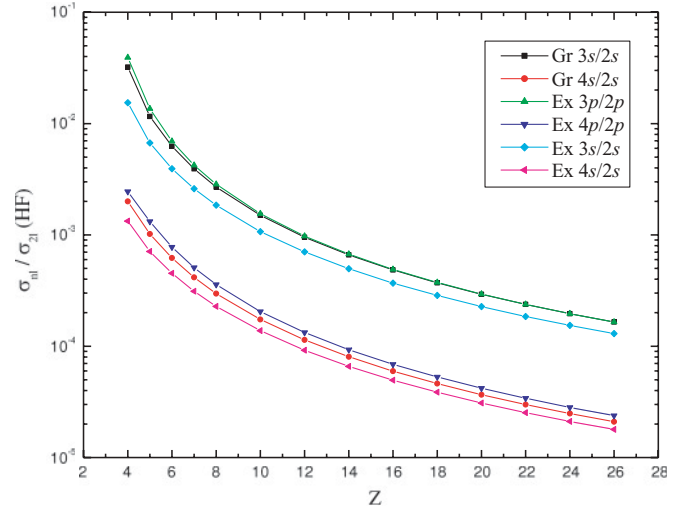


FIG. 8. (Color online) Relaxed Hartree-Fock (HF) values of $|\langle P_{2s}^{(i)} | P_{ns}^{(f)} \rangle| / |\langle P_{2s}^{(i)} | P_{ns}^{(f)} \rangle|$ for ground-state photoionization $|\langle P_{2p}^{(i)} | P_{np}^{(f)} \rangle| / |\langle P_{2p}^{(i)} | P_{np}^{(f)} \rangle|$ and $|\langle P_{2s}^{(i)} | P_{ns}^{(f)} \rangle| / |\langle P_{2s}^{(i)} | P_{ns}^{(f)} \rangle|$ and for metastable-state photoionization vs. Z , where (i) and (f) indicate the radial functions in the initial- and final-state HF wave functions, respectively. In the legend “Gr” denotes ground state, “Ex” denotes metastable state, and “ $nl/2l$ ” means the value of $|\langle P_{2l}^{(i)} | P_{nl}^{(f)} \rangle| / |\langle P_{2l}^{(i)} | P_{2l}^{(f)} \rangle|$.

ratios of the cross sections leaving the ion in the various ns states are also given by Eq. (5) in this approximation, and the np ratios are given by the same expression with all of the ns 's replaced by np 's. In any case, the ratio should be energy-independent as long as interchannel coupling among the photoionization channels is not significant. This implies that interchannel coupling is not important for the ratios σ_{3s}/σ_{2s} and σ_{4s}/σ_{2s} which were seen to be constant, as a function of energy, at the higher energies for both ground- and excited-state photoionization, and the same is true for the σ_{3p}/σ_{2p} ratio in metastable-state photoionization.

The results of the present shake-up calculations of the ratios using relaxed Hartree-Fock (HF) wave functions are presented in Fig. 8 and the R -matrix ratios at $E_{\text{ph}} = 8E_{\text{range}}$ are shown in Fig. 9. Comparing the ratios in the two figures, it is seen that only the ratios σ_{3s}/σ_{2s} for ground-state photoionization and σ_{3p}/σ_{2p} for metastable-state photoionization are in good agreement with the shake-up model. This shows that the other ratios that are constant at the higher energies, and thus unaffected by interchannel coupling, are nevertheless altered by other multiparticle effects not included in the single-particle shake-up model; this means that configuration interaction in the initial or final discrete state (or both) are important for these transitions. In any case, it is clear that the shake-up model is not very accurate, even for the photoionization of a four-electron system. Furthermore, agreement does not appear to get better with increasing Z . In other words, multiparticle effects persist, in general, to satellite lines in the photoionization of highly charged ions as well.

Finally, it is of interest to note that the σ_{nl} for the same n but different l show a variety of patterns as functions of energy. For ground-state photoionization, σ_{3s} and σ_{4s} are always the largest partial cross sections in the $n = 3$ and $n = 4$ manifolds,

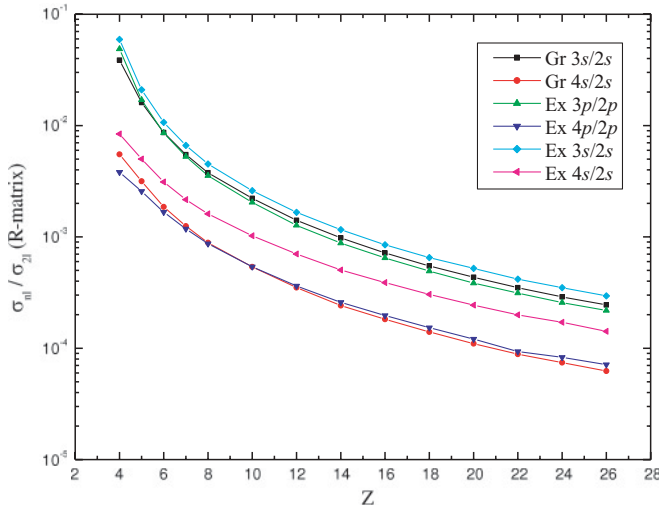


FIG. 9. (Color online) As Fig. 8 except that the ratios are from the R -matrix calculation. The legend is the same as for Fig. 8 but “ $nl/2l$ ” stands for σ_{nl}/σ_{2l} .

respectively, but the comparison between σ_{np} and σ_{nd} are more complicated. For $n = 3$, $\sigma_{3p} < \sigma_{3d}$ is true at the higher energies for all of the ions studied. For $n = 4$, σ_{4p} is above σ_{4d} near threshold but σ_{4d} becomes greater than σ_{4p} at some (Z -dependent) energy E_1 ; and at some higher (Z -dependent) energy E_2 , they reverse again and $\sigma_{4p} > \sigma_{4d}$ at the highest energies. The calculations show that E_1 is about $4E_{\text{range}}$ for Be, $1.5E_{\text{range}}$ for Si^{+10} , and $1E_{\text{range}}$ for Fe^{+22} , while E_2 is above our energy range for Be, $4.5E_{\text{range}}$ for Si^{+10} , and $4E_{\text{range}}$ for Fe^{+22} . For the metastable state σ_{nl} , similar relations are found: $\sigma_{3p} > \sigma_{3d} > \sigma_{3s}$, $\sigma_{4p} > \sigma_{4d} > \sigma_{4s}$ in the higher energy range, and $\sigma_{4p} > \sigma_{4s} > \sigma_{4d}$ in the lower energy range. The priority of the σ_{ns} cross sections for the ground state and σ_{np} for the metastable state is explained qualitatively by the shake-up model in terms of the relaxation of the excited orbitals [8].

IV. CONCLUSIONS

The partial cross sections for photoionization of ground state and metastable state Be-like ions have been calculated using the nonrelativistic R -matrix method; the total cross sections obtained, reported earlier [1], were in good agreement with available experiments. The photon energy range in this study is up to eight times the energy range from the ionization threshold to $4f$ threshold for each ion. The calculated partial cross sections cover the energy range high enough to represent their general behaviors well above the region dominated by autoionizing resonances, with respect to photon energy and Z .

To understand the relative strengths of the partial cross sections for the various satellite lines to the main lines, σ_{2s} for the ground state and σ_{2p} and σ_{2s} for the metastable state, the ratios σ_{nl}/σ_{2s} and σ_{nl}/σ_{2p} for the ground and metastable states, respectively, were studied. These ratios are found to be smooth monotonic functions of Z and approach zero asymptotically at $Z \rightarrow \infty$, as predicted from general considerations. The ratios as functions of photon energy are much more complicated. A simple single-particle shake-up model failed to explain the details of most of the satellite cross sections, indicating that even in the photoionization of a four-electron system, multiparticle effects over and above relaxation are important. This leads us to infer that the behavior of satellite (photoionization plus excitation) cross sections for systems with more electrons will be at least as complicated as the present case.

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