Photoionization of Be, B⁺, C²⁺, N³⁺, O⁴⁺, and F⁵⁺ in the MCRRPA theory

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Abstract. The multiconfiguration relativistic random-phase approximation theory is applied to the valence-shell photoionization along the Be isoelectronic sequence. Photoionization cross sections between \((1s^22s)^2S_{1/2}\) and \((1s^22p)^2P_{1/2}\) ionization thresholds are calculated. There are five Rydberg series of doubly excited states that manifest themselves as autoionization resonances in the photoionization cross section. A comparative study of Be, B⁺, C²⁺, N³⁺, O⁴⁺, and F⁵⁺ is presented.

1. Introduction

Photoionization spectra of atoms or ions have attracted much attention in recent years because of the interplay between correlation and relativistic effects plays an important role. Double-excitation resonances in the photoionization spectrum provide a stringent testing ground for the accuracy of theoretical models, while experimental studies have gained considerable momentum due to the rapidly evolving experimental techniques.

Atomic systems in the Be isoelectronic sequence have been considered as suitable objects for systematic studies of the photoionization processes because of their relatively simple divalence structure. In these atomic systems, the photoionization spectrum dominated by the doubly excited states due to the interaction between two valence electrons. Nevertheless, many works have shown relativistic effects play an important role in the photoionization of small atoms, such as Be [1, 2], Ne [3], and Mg [4]. Therefore, it is worthwhile to investigate the interplay between correlation and relativistic effects on the photoionization of atoms or ions with a low nuclear charge.

Applications of the multiconfiguration relativistic random-phase approximation theory (MCRRPA) to the photoionization of Be [5, 6], Mg [7], Sr [8], and Zn [9] have been very successful. In the photon-energy region between \((1s^22s)^2S_{1/2}\) and \((1s^22p)^2P_{1/2}\) ionization thresholds of atomic systems along the Be isoelectronic sequence, double-excitation autoionization resonances are the most prominent feature in its photoionization spectrum. These double-excitation resonances may be classified into five Rydberg series: \((2pns)^1P_0\), \((2pns)^3P^0\), \((2pnd)^1P_0\), \((2pnd)^3P^0\) and \((2pnd)^3P^0\). In this work, photoionization of atomic systems along the Be isoelectronic sequence are studied by using the MCRRPA theory accounting for all relativistic excitation channels.
2. MCRRPA Theory

A detailed formulation of the MCRRPA has been given in a previous paper [10] and only a summary of the essential features will be given here. The N-electron atomic system is described as a superposition of configuration wavefunctions with time-dependent weights. The time-dependent variational principle is employed to determine the response of the atomic system to a time-dependent external field. The resulting terms independent of the external field lead to the usual multiconfiguration Dirac-Fock (MCDF) description of an atomic state. Those terms proportional to the external field lead to the MCRRPA equations describing the linear response of the atomic state to the external field. If we start from a single-configuration reference state, the MCRRPA equations reduce to the RRPA equations. The multiconfiguration reference state is described by a linear combination of three configurations with two valence electrons coupled to zero angular momentum and even parity:

\[ \Psi = C_1(1s^2)S_{1/2} + C_2(1s^2)2s^2 + C_3(1s^2)2p^2, \]

where \( C_1, C_2, \) and \( C_3 \) are configuration-weight coefficients.

We consider seven excitation channels from the valence electrons in the electric-dipole approximation for photon energies between \((1s^22s)^2S_{1/2}\) and \((1s^22p)^2P_{1/2}\) ionization thresholds:

(i) Photoionization channels:
   a. \((2s^2)^1S_0 \rightarrow (2s2p)^1P^0\),
   b. \((2s^2)^1S_0 \rightarrow (2s2p)^3P^0\).

(ii) Photoexcitation channels:
   c. \((2p^2)^1S_0 \rightarrow (2pns)^1P^0, n \geq 3,\)
   d. \((2p^2)^1S_0 \rightarrow (2pns)^3P^0,\)
   e. \((2p^2)^1S_0 \rightarrow (2pnd)^1P^0,\)
   f. \((2p^2)^1S_0 \rightarrow (2pnd)^3P^0,\)
   g. \((2p^2)^1S_0 \rightarrow (2pmd)^3D^0.\)

The couplings between the photoionization and photoexcitation channels generate five autoionization resonance series in the photoionization spectrum.

3. Results and Discussions

We consider the incident photon with energy from the ionization threshold \((1s^22s)^2S_{1/2}\) up to the threshold \((1s^22p)^2P_{1/2}\), where only photoionization channels \(a\) and \(b\) are open. The couplings of the two open channels and remaining five photoexcitation channels producing five Rydberg series of resonances \((2pns)^1P^0, (2pns)^3P^0, (2pnd)^1P^0, (2pmd)^1P^0,\) and \((2pmd)^3D^0\). The calculated cross sections for the Be isoelectronic sequence from Be to F\(^{5+}\) are presented in Figs. 1 and 2. For comparison, we use the dimensionless variable \( \varepsilon \) instead of the photon energy \( h\nu \): \( \varepsilon \equiv (h\nu - I_0)/\Delta I \), where \( \Delta I \equiv I_p - I_s \), and \( I_s \) and \( I_p \) are ionization potentials for \((1s^22s)^2S_{1/2}\) and \((1s^22p)^2P_{1/2}\) respectively. By assuming the form for the ionization potential as \( I_0 = a(Z-b_1+c_1/Z)^2 \), we obtain the fitting formula for the Be isoelectronic sequence as \( \Delta I(Z) = AZ + B + C/Z \), where \( A = 0.0713114, B = -0.1229696, C = -0.0666783, \) and \( Z \) is the nuclear charge.

In Fig. 1, two Rydberg series of double-excitation resonances, a broad series \((2pns)^1P^0\) and a narrow series \((2pnd)^1P^0\), can be clearly identified in the photoionization profiles of the Be atom. Because the photoionization continuum \((2s2p)^1P^0\) and the double-excitation series \((2pns)^1P^0\) and \((2pnd)^1P^0\) all arise from the \( n = 2 \) atomic complex and with the same total spin and orbital angular-momenta, the couplings between them are very strong such that only these two Rydberg series are prominent in the spectra. The broad \((2pns)^1P^0\) and narrow \((2pmd)^1P^0\) resonance profiles reveal the shorter and longer lifetimes of the respective doubly excited states.
Figure 1. Photoionization cross sections for Be, B⁺, and C²⁺ between the ionization thresholds \((1s^22s)^2S_{1/2}\) and \((1s^22p)^2P_{1/2}\). The broad-hump series \((2pns)^1P_0^o\) and the narrow-spike series \((2pnd)^1P_0^o\) sandwiched amid the series \((2pns)^1P_0^o\) for Be are shown in the upper panel. For B⁺ in the middle panel and C²⁺ in the lower panel, the \((2pnd)^1P_0^o\) series consists of sharp peaks, while the \((2pns)^1P_0^o\) series appears as broad dips. Extremely sharp resonance structures are triplet resonances \((2pns)^3P_0^o\), \((2pnd)^3P_0^o\), and \((2pnd)^3D_0^o\).

As shown in Figs. 1 and 2, the characteristics of the photoionization profiles are however very similar among the Be-like ions. The \((2pnd)^1P_0^o\) series consists of sharp peaks, while the \((2pns)^1P_0^o\) series appears as broad dips. The photoionization cross section of each ion shows an average background with resonance structures, where the background decreases from roughly 2 Mb for the Be atom to about 0.5 Mb for the F⁵⁺ ion with increasing nuclear charge.

Because of low nuclear charge for Be, B⁺, and C²⁺, they behave rather nonrelativistically, and only two of five Rydberg series of resonances show up distinctly in the photoionization cross section. Experimental results [11, 12, 13] or the cross sections in nonrelativistic calculations [14, 15, 16] should be similar to the MCRRPA result but without the extremely sharp resonance structures of triplet resonances \((2pns)^3P_0^o\), \((2pnd)^3P_0^o\), and \((2pmd)^3P_0^o\). However, the gradual onset of relativistic effects with increasing nuclear charge, additional Rydberg series of resonances show up in the photoionization spectra of higher members of the Be isoelectronic sequence N³⁺, O⁴⁺, and F⁵⁺.

Physically, the coupling strength between the bound and continuum components of the wave function of a doubly-excited state is measured by the resonance width, which also determines the nonradiative decay rate of an autoionization state. Because the orbital symmetries of the photoionization channels \((2sep)^3P_0^o\) and \((2sep)^1P_0^o\) are of P-type, the coupling of resonances \((2pnd)^3D_0^o\) with these photoionization channels are weaker such that their widths are much narrower. Our MCRRPA calculation includes relativistic and correlation effects in an \textit{ab initio}
Figure 2. Photoionization cross sections for N$^{3+}$, O$^{4+}$, and F$^{5+}$ between the ionization thresholds $(1s^22s)^2S_{1/2}$ and $(1s^22p)^2P^o_{1/2}$. The $(2pnd)^1P^o_1$ series consists of sharp peaks, while the $(2pns)^1P^o_1$ series appears as broad dips. Extremely sharp resonance structures are triplet resonances $(2pns)^3P^o_1$, $(2pnd)^3P^o_1$ and $(2pnd)^3D^o_1$.

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