Relativistic photoionization cross sections for C II

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The first measurement of highly resolved photoionization cross sections of the ground state of C II was reported recently by Kjeldsen et al. [Astrophys. J. 524, L143 (1999)]. The observed resonance features showed good agreement with the theoretical calculations in the close-coupling approximation [S. Nahar, Astrophys. J. Suppl. Ser. 101, 423 (1995)]. However, there were several observed resonances that were missing in the theoretical predictions. The earlier theoretical calculation was carried out in LS coupling where the relativistic effects were not included. Present paper reports photoionization cross sections including relativistic effects in the Breit-Pauli R-matrix (BPRM) approximation. The configuration interaction eigenfunction expansion for the core C III consists of 20 fine-structure levels dominated by the configurations from 1s2p2 to 1s2p3d. Detailed features in the calculated cross sections exhibit the missing resonances due to fine structure. The results provide a benchmark for the accuracy of BPRM photoionization cross sections, as needed for the recent and ongoing experiments for high-resolution photoionization cross sections at synchrotron-radiation sources.

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I. INTRODUCTION

Although a large number of theoretical calculations for photoionization cross sections have been carried out, the data have not yet been sufficiently calibrated against the new generation of high-resolution experiments. We refer, in particular, to the calculations using the close-coupling R-matrix method extensively utilized in the Opacity Project (OP) [1], the Iron Project (IP) [2] and similar works that accurately consider the numerous autoionizing resonances in cross sections along interacting (overlapping) Rydberg series. Most of the vast amount of photoionization data computed under the OP, IP, and other works, is estimated to be accurate to 10–20%. However, no detailed comparisons with experiments have been possible since photoionization cross sections were not measured with equally detailed features. However, resonances can now be finely resolved in recent experiments being carried out with synchrotron-radiation sources in Refs. [3–5]. Comparing the theoretical calculations with experiments is therefore of considerable current importance. Furthermore, the quality of experimental work is such as to clearly delineate the fine structure, necessitating the inclusion of relativistic effects in an ab initio manner. In this paper we present such a comparison between theory and experiments in detail.

Carbon is one of the most cosmically abundant elements, and C II is an important ion in astrophysical sources, such as the interstellar medium. Study of accurate features of C II is of considerable interest and important for accurate spectral analysis. In their merged ion-photon beam experiment, Kjeldsen et al. [3] measured the first detailed photoionization cross sections ($\sigma_{p\ell}$) of C II with high accuracy. With the synchrotron-radiation from an undulator, their measurements exhibited highly resolved features of autoionizing resonances in cross sections. The features agreed very well with the results from close-coupling approximation using the R-matrix method [6]. However, the theoretical calculations did not include the relativistic effects and therefore did not predict the observed fine structure features.

Extensive earlier works, such as the Opacity Project, were carried out in LS coupling and did not consider the fine structure. The motivation for the present work is to study relativistic effects in relation to the observed features using the Breit-Pauli R-matrix (BPRM) method [7,2,8]. The method has been extended to a self-consistent treatment of photoionization and electron-ion recombination (e.g., [9]). The total recombination cross sections, derived from photoionization cross sections, in an unified treatment have been extensively compared with measured recombination spectra [9,10]. The recombination cross sections require total contributions from photoionization cross sections of all bound levels. The present work, on the other hand, focuses on individual features of photoionization cross sections of the fine-structure levels of the ground configuration $2s^22p$ of C II, in direct comparison with measured cross sections.

II. THEORY AND CALCULATIONS

The calculations for photoionization cross sections ($\sigma_{p\ell}$) are carried out in the close-coupling approximation using the Breit-Pauli R-matrix method in intermediate coupling. Photoionization is described in terms of an eigenfunction expansion over coupled levels of the residual (“core” or “target”) ion. The total wave function of the $(N+1)$-electron ion is represented by the wave functions of the $N$-electron core, multiplied by the wave function of the outer electron as follows:

$$\Psi_e(e+\text{ion}) = A \sum_i \chi_i(\text{ion}) \theta_i + \sum_j c_j \Phi_j(e+\text{ion}),$$

(2.1)

where $\chi_i$ is the target wave function in a specific state $s_L$, $\pi_i$ or level $J, \pi_i$, and $\theta_i$ is the wave function for the $(N+1)$ th electron in a channel labeled $s_L(J, \pi) \sigma k^2 l, (J, \pi)$; $k^2$ is its incident kinetic energy. $\Phi_j$‘s are the correlation functions of the $(N+1)$-electron system that account for short-range correlation and the orthogonality between the continuum and bound orbitals. The complex resonant structures in photoionization are included through channel couplings.
1.42(1 s term, respectively. The Darwin term, and the spin-orbit interaction and the additional terms represent the one-body mass correction term in the code SUPERSTRUCTURE atomic structure calculations using a scaled Thomas-Fermi approximation in intermediate coupling. The Breit-Pauli Hamiltonian, as adopted in the IP work [2], is

\[ H_{BP}^{N+1} = H_{N+1}^{NR} + H_{mass}^{N+1} + H_{Dar}^{N+1} + H_{SO}^{N+1}, \]

(2.2)

where \( H_{N+1}^{NR} \) is the nonrelativistic Hamiltonian,

\[ H_{N+1}^{NR} = \sum_{i=1}^{N+1} \left\{ -\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j=1}^{N+1} \frac{2}{r_{ij}} \right\}, \]

(2.3)

and the additional terms represent the one-body mass correction term, the Darwin term, and the spin-orbit interaction term, respectively.

Present wave functions for C II are expressed by a 20-level expansion of the core ion C II with 2s^22s2p, 2p^2, 2s^3s, 2s^3p, 2s^3d (the K shell is closed) (Table I). The C III wave functions were obtained from atomic structure calculations using a scaled Thomas-Fermi model in the code SUPERSTRUCTURE [11]. The spectroscopic and correlation configurations, and the scaling parameters in the Thomas-Fermi potential for the orbitals, are given in Table I. The correlation term in Eq. (2.1) considers all possible \((N+1)\)-electron configurations up to \(2p^2, 3s^2, 3p^2, 3d^2, 4s^2, 4p^2\).

The computations of \(\sigma_{pJ}^f\) are carried out using the package of BPRM codes from the Iron Project [8]. The cross sections are computed with a very fine energy mesh in order to delineate the detailed resonance structures as observed in the experiments. It is a computationally demanding procedure because of repeated computations with exceedingly fine energy bins to search and resolve the resonances. Many resonances are sharp and narrow, and cannot be detected individually in the experiment. The resonances are convolved with a Gaussian function of full width at half-maximum (FWHM) equal to the energy bandwidth of the monochromator in the experiment.

### III. Results and Discussions

Photoionization cross sections are obtained for the fine-structure levels of the ground state, \(2s^22p(2P^o)\) in \(LS\) coupling, and of the metastable state, \(2s2p^2(4P_{1/2,3/2,5/2})\) of C II. The fine-structure features are distinct when compared with those in \(LS\) coupling. \(\sigma_{pJ}^f\) for the ground state obtained in nonrelativistic \(LS\) coupling are presented in Fig. 1(a) and in relativistic BPRM approximation in Fig. 1(b), the solid curve for the \(2P_{1/2}^o\) level and the dotted curve for the \(2P_{3/2}^o\) level.

The relativistic \(\sigma_{pJ}^f\) for the levels \(2P_{1/2}^o\) and \(2P_{3/2}^o\) show many overlapping resonances. The number of resonances is considerably larger in the bottom panel than that for the ground \(2P^o\) state in the \(LS\) coupling in the top panel. Inclusion of relativistic effects in the BPRM approximation intro-
duces more Rydberg series of resonances, belonging to the increased number of core ion thresholds through fine-structure splitting, in comparison with nonrelativistic LS coupling calculations. For example, the 12 LS terms of the core ion C III correspond to 20 fine-structure levels. Additional thresholds and associated resonances, allowed in intermediate coupling but not in LS coupling, have resulted in more extensive resonances.

The first two resonances in \( \sigma_{P1} \) in LS coupling [Fig. 1(a)] belong to the Rydberg series of autoionizing states \( 2s2p(3P^o)n(2D) \) and \( 2s2p(3P^o)n(2S) \), respectively, where \( n=4 \). A Rydberg series may be identified by the quantum defects. The effective quantum number \( n \) of an autoionizing state can be obtained from the quantum-defect formula, \( \nu=\sqrt{E-E_T} \), where \( \nu \) is the ion charge, \( E \) is the resonance energy, and \( E_T \) is the threshold energy in Rydbergs. Given that \( n=\nu+\mu \), the quantum defect \( \mu \) is \( \sim 0.6 \) for an \( s \) electron, \( \sim 0.4 \) for a \( p \) electron, \( \sim 0.1 \) for a \( d \) electron, and so on. The above-mentioned two series of resonances are allowed in LS coupling and are common in both panels of Fig. 1, denoted as R2 and R3 series in the BPRM \( \sigma_{P1} \) [Fig. 1(b)]. Photoionization of the ground state \( 2s^22p(2P^o) \) is allowed to the even parity \( 2S \) and \( 2D \) continua, but not to \( 2P \), in LS coupling. The autoionizing states \( 2s2p(3P^o)n(2P) \) cannot decay via a radiationless transition to the \( 2s^2(1S)\ell \) continuum with the same symmetry \( 2P \). However, all three Rydberg series of resonances, \( 2s2p(3P^o)n(2S,2P,2D) \), converging on to the thresholds of \( 2s2p(3P^o) \) are allowed in relativistic intermediate coupling (IC). The sharp, narrow R1 series of resonances in the BPRM crossing sections in Fig. 1(b) correspond to \( 2s2p(3P^o)n(2P) \) states. The channel couplings for the \( J=1/2 \) level mixes \( 2S_{1/2} \) with a component of \( 2P_{1/2} \), and for the \( J=3/2 \) level mixes \( 2D_{3/2} \) with \( 2P_{3/2} \) through IC, and thus enable the symmetry \( 2P \) to autoionize. Indirect decay to \( 2P \) continuum via radiative decay first to, for example, \( 2s2p(3P^o)3d(2P) \) state followed by autoionization is possible, but not likely to be significant [3].

The R4 series of resonances in Fig. 1(b), which could be identified as the combination of states \( 2s2p(1P^o)n(2D,2P,2S) \), are also common (except for the \( 2P \) component) to both panels in Fig. 1. These resonances are weak, especially in LS coupling calculations, partially due to coarser energy mesh in the previous work. Our identification of this series differs from that of Kjeldsen et al. [3]. This series was not observed in the experiment. Additional series of resonances are introduced starting from the fourth complex, which overlap with other complexes. Small shifts in the energies of resonances seen in the upper and lower panels of Fig. 1 are due to statistical averaging of LS term energies over their fine-structure components.

The BPRM photoionization cross sections are compared with the measured cross sections by Kjeldsen et al. after convolution of the calculated resonances with a Gaussian distribution function of FWHM of 35 meV, the monochrometer bandwidth of the experiment. The calculated ionization energy for the \( 2P_{1/2} \) ground level is 1.7885 eV, compared to the measured energy of 1.7921 eV; for the \( 2P_{3/2} \) level it is

1.78 793 eV compared to the measured value 1.7916 eV. Calculated cross sections have been slightly shifted to the measured ionization thresholds to compare with the experimentally measured \( \sigma_{P1} \), as shown in Fig. 2.

Figure 2(a) presents the total detailed calculated cross sections of the levels \( 2P_{1/2}, 2P_{3/2} \) (solid and dotted curves, respectively), while Fig. 2(b) presents the convolved \( \sigma_{P1} \) on the eV scale. Fig. 2(c) presents the measured cross sections [3]. Very good agreement is seen, in general, in resonance features between the calculations [Fig. 2(b)] and the measurements [Fig. 2(c)]. The resonance peaks are also in good agreement in the first three resonance complexes. However, some differences are noted for the higher complexes. Peaks of some calculated resonances at higher energies are higher than the measured ones. The peaks may be reduced by radiative decays or the process of dielectronic recombination. The peak values were checked by including the radiation damping effect, with no significant reduction. This is expected for a low-charge carbon ion since the radiative decay rates of the excited core thresholds (\( \approx 10^8, 10^9 \) sec\(^{-1}\)) are several orders of magnitude lower than typical autoionization rate (\( \approx 10^{13-14} \) sec\(^{-1}\)), thus causing very little damping. How-
However, some explanation can be given for the differences. Although Gaussian averaging of resonances has shown good agreement with the measured cross sections, as carried out in the present case and shown by the experimental group [3], the distribution may not be adequate throughout the energy range. The same FWHM may not remain constant with energies. A convolved peak can be flattened with a larger bandwidth. Also, resonances become narrower and denser as the energy approaches the convergent threshold, requiring a narrower bandwidth monochrometer for finer resolution. To see the structures at higher energies near the highest CIII states, J = 3/2 and J = 5/2 in BPRM approximation. The arrow points to the ionization threshold for the fine-structure levels.

Convolution of detailed resonances may result in some variations of peaks depending on the monochrometer bandwidth, choice of energy distribution function, and resolution of the resonances to belong mainly to nd series, i.e., to 2s2pnd (n = 7, 8, . . .) rather than to ns series, since the transition rates to the higher l are usually more dominant. However, transitions to 2s2pns states are also possible. These observed resonances are seen in the BPRM σPI. However the convolved resonance peaks are relatively lower, except for the first one, compared to observations. Resonances in this energy region are extremely narrow; further resolution could conceivably have improved agreement with the measured ones.

Photoionization cross sections of 4P state in LS coupling are presented in Fig. 3(a) (top panel) for comparison. No cross sections can be seen below the threshold at 1.872 Ry, photoionizing to 2s2p(3Po) state of C III. However, in the σPI for the fine-structure levels 4P1/2,3/2,5/2, shown separately as solid, dotted, and dashed curves in Fig. 3, extensive narrow resonances are seen below this threshold with almost no background. The ionization thresholds for these levels lie at about 1.4 Ry (pointed by arrow in the figure), and each level exhibits presence of a near threshold resonance. As explained above, these resonances are allowed by relativistic mixing of states through IC. For example, IC allows J = 1/2 and 3/2 levels of autoionizing states 2s2p(3Po)nd(4Do) to decay to J = 1/2 and 3/2 of continuum 2s2(1S)ep(2Pvo) via radiationless transitions. As we are mainly interested in the energy region corresponding to photoionization of the ground state of C II, resonances in photoionization of the levels J = 1/2,3/2,5/2 are resolved with a much finer energy mesh from ∼1.75 Ry to about 1.87 Ry, and are convolved with the same monochrometer bandwidth of 35 meV and are presented in Fig. 2(d) for comparison with the measured cross sections.

IV. CONCLUSION

We have demonstrated that the theoretical fine structure photoionization cross sections account for nearly all experimentally observed features that may not be obtained in the nonrelativistic LS coupling calculations. The relativistic BPRM σPI of the ground 2s2p(2Pvo) state and the first excited 2p2p21P0 state of C II reveal the fine structure observed in the experiment [3] and are in very good agreement. Convolution of detailed resonances may result in some variations of peaks depending on the monochrometer bandwidth, choice of energy distribution function, and resolution of resonances.

Similar to the experimental work by Kjeldsen et al. [3], Phaneuf et al. [12] plan collaborative measurements on C II with the Aarhus group at higher resolutions using a different setup at the ALS (Advance Light Source). Cross-section values from the present work are available electronically for comparison with other experiments.

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