Influence of long-lived metastable levels on the electron-impact single ionization of C²⁺

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A joint theoretical and experimental investigation is made of the influence of long-lived metastable levels on the electron-impact single ionization of C^{2+} . It is expected that our electron cyclotron resonance ion source produces a beam with 40% of the C^{2+} ions in the $1s^22s^2$ ${}^{1}S_0$ ground level and 60% in the $1s^22s2p$ ${}^{3}P_{0,2}$ excited levels. The comparison of nonperturbative close-coupling calculations with previous single-pass crossed beams and with our multiple-pass storage-ring measurements for the electron-impact ionization of C^{2+} is consistent with the predicted large metastable fraction. Reasonable agreement is found between the present timedependent close-coupling, *R*-matrix with pseudostates, and converged-close-coupling ionization cross-section calculations for the ground and first excited configuration, and experimental measurement, assuming a 60% metastable fraction in the ion beam. Distorted-wave calculations are found to overestimate the ionization cross section from both the ground and metastable terms, compared with nonperturbative calculations, resulting in an overestimation of the resultant total cross section when compared with experiment. It is clear that collisionalradiative modeling of the evolution of atomic plasmas through the Be-like ionization stage will need to take into account the role of both ground and metastable levels.

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I. INTRODUCTION

The importance of ionization from metastable states has long been recognized in collisional-radiative modeling of finite density plasmas; see, for example, Burgess and Summers [1]. However, the measurement and calculation of accurate ionization cross sections from metastable and excited states has presented significant challenges to the atomic physics community.

On the experimental side, it is often not possible to determine the size of the metastable fraction present in the beam, making isolation of the metastable ionization cross section problematic. In cases where it is known that a significant metastable fraction exists, such as in the 1s2s ³S term of He-like ions, or the 2s2p ³P term of Be-like ions, previous comparisons with theory have often encountered discrepancies. This is true even for comparisons with the most recent nonperturbative ionization calculations. As an example, take the comparisons of ionization cross-section measurements with theory for neutral helium in Colgan *et al.* [2] and in Fursa and Bray [3], where nonperturbative calculations lie significantly below the experimental measurements.

On the theoretical side, for ionized species, distortedwave methods are often employed. Although it is often clear that distorted-wave techniques do well for ionization from the ground states of ionized species (e.g., Li^+ as studied by Colgan *et al.* [4]), recent studies on ionization from the ions of beryllium [5] suggest that the distorted-wave approximation becomes progressively worse as one ionizes from higher *n* shells. It is only recently that nonperturbative calculations for ionization from excited states have become tractable; these include the converged-close-coupling calculations for neutral lithium by Schweinzer *et al.* [6], and the timedependent close-coupling and *R*-matrix with pseudostates calculations for all ion stages of Be by Colgan *et al.* [5].

Ionization from Be-like C^{2+} has presented long-standing discrepancies between theory and experiment. The previous work of Falk *et al.* [7] measured the single-ionization cross section of Be-like B, C, and O ions using the crossed-beams technique. A significant metastable fraction was found for each ion. For C^{2+} , the metastable fraction was estimated as 65% and 90% for their low and high metastable measurements, respectively. The differences between the low and high metastable cross sections were relatively small. Cross sections from the Lotz formula [8] and from distorted-wave calculations by Younger [9] for the ground and metastable states banded the experimental measurements, but were higher than experiment when the estimated metastable fraction was used. Woodruff *et al.* [10] measured the ionization cross section using the crossed-beams technique and the re-

sults were found to be in good agreement with those of Falk *et al.* [7]. Hamdan *et al.* [11] measured the ionization of C²⁺ in a concentric-electron-beam device, with the ions being trapped for about 1 s. The cross-section measurements lay slightly below that of Falk *et al.* [7] and Woodruff *et al.* [10]. A measurement of the metastable fraction in an electron cyclotron resonance (ECR) ion source for different ions was provided by Brazuk *et al.* [12], with measurements being taken for C²⁺, N²⁺, N³⁺, and O⁴⁺. For C²⁺, they measured the metastable fraction to be 0.56 ± 0.11 , and this value appears to be representative of the metastable fraction in most electron cyclotron resonance (ECR) ion sources for C²⁺.

One misleading aspect of the comparison between theory and experiment arises from the fact that when 100% of the C^{2+} ions are assumed to be in the ground state, numerous theoretical results are in reasonable agreement with experiment, despite evidence for a significant metastable fraction in the beam. Salop [13] used a modified binary-encounter approximation to calculate the ionization cross section for the ground configuration of C^{2+} as part of calculations for C, O, N, Ne, and Ar ions and obtained reasonable agreement with experiment. Moores [14] calculated ionization cross sections from the ground configuration of C^{2+} using a no-exchange Coulomb-Born method. The results do not match the ionization threshold, due to metastable presence in the beam, but there is reasonable agreement from the peak of the cross sections, and above. Jakubowicz and Moores [15] calculated distorted-wave and Coulomb-Born with exchange cross sections for the ground state of C^{2+} ; these were in good agreement with the distorted-wave calculations of Younger [9] at the ionization threshold, but were slightly above the Younger results above the peak of the cross section. Both of these ground-state calculations are in reasonable agreement with experiment. However, when the correct metastable fractions are used for the theoretical calculations, the results are consistently higher than experiment. This is seen in both the distorted-wave calculations of Younger [9] and the planewave Born calculations of McGuire [16]. Because of the persistent discrepancy between theory and experiment, McGuire suggested that the experimental measurements have been consistently underestimated, and need to be rescaled.

In this paper, we present merged-beams measurements for the ionization of C^{2+} performed at the CRYRING storage ring in Stockholm, Sweden. We compare the new experimental measurements with the results of nonperturbative calculations using the time-dependent close-coupling (TDCC), the converged-close-coupling (CCC), and the *R*-matrix with pseudostates (RMPS) methods, as well as with those from perturbative calculations using the distorted-wave (DW) approximation. The rest of this paper is structured as follows. Section II describes the theoretical methods used in the paper. Section III describes the experimental apparatus and technique. Section IV compares our experimental and theoretical results, and in Sec. V we conclude with a brief summary.

II. THEORY

In the calculation of theoretical ionization cross sections, we use one perturbative approach, namely the configurationaverage distorted-wave method, and three nonperturbative approaches, namely the time-dependent close-coupling, the converged-close-coupling, and the *R*-matrix with pseudostates methods.

The theory for the time-independent, configurationaverage, distorted-wave method (CADW) has been described in detail previously by Pindzola et al. [17]. The configuration-average threshold energies and radial wave functions for the bound configurations are evaluated using the Hartree-Fock relativistic atomic structure code of Cowan [18], where the mass-velocity and Darwin terms may be included in the radial Schrödinger equation. The directionization cross-section contributions to the total cross section are calculated in a configuration-average distorted-wave approximation. This method has been very successful in evaluating ionization cross sections, particularly for ionized species [19–21]. However, the method often does not do well for near neutral species, as seen, for example, in the work of Colgan *et al.* [22] on neutral lithium. Also, recent evidence suggests that even for cases where distorted-wave techniques agree with nonperturbative techniques for the ground state of an ion, it may produce marked disagreement for the excited states; this is true, for example, in the ionization calculations for Be^{2+} and Be^{3+} by Colgan *et al.* [5].

Recently, various nonperturbative approaches have been developed which can calculate ionization cross sections. The time-dependent close-coupling (TDCC) method is one such approach, and is described in more detail in Pindzola and Robicheaux [23]. The radial wave function at a time following the collision is obtained by propagating the timedependent close-coupling equations on a two-dimensional finite lattice. The two-electron wave functions fully describe the correlation between the ejected and scattered electrons at all times following the collision. The time-propagated wave functions contain information on all elastic and inelastic processes. The various scattering probabilities are obtained by projecting the two-dimensional radial wave function onto appropriate products of bound and continuum radial orbitals at a suitable time after the collision. The bound and continuum radial orbitals required to describe the initial target state and to calculate projections are obtained by diagonalization of the Hamiltonian on a one-dimensional finite lattice. The direct and local exchange potentials are constructed as pseudopotentials in which the inner nodes of the valence Hartree-Fock orbitals are removed in a smooth manner, to prevent unphysical excitation of filled subshells. This method has been very successful in calculations on H-like [23,24], Lilike [22], Be-like [5], and C-like systems [25]. In the TDCC calculation for C^{2+} , we used a 384×384 grid with a mesh spacing of 0.1 atomic units. We evaluated TDCC partial waves for L=0 through L=7 for the $2s^2 \rightarrow 2s$ ionization, and L=0 through L=8 for the $1s^22s2p \rightarrow 1s^22s$ and $1s^22p$ ionization contributions. To top up the TDCC partial-wave sums, we employed CADW higher partial-wave contributions, which were found to be in good agreement with those from the TDCC calculation for the last few partial waves before the top up started.

With the convergent-close-coupling (CCC) method [26], all target states are determined from an orthogonal Laguerre basis and the close-coupling equations are solved in momen-

tum space. This method associates ionization with excitation of the positive-energy states and has been shown to yield accurate total [27], as well as fully differential [28], electronimpact ionization cross sections of atomic hydrogen. It has been extended to quasi-one-electron targets [29] and applied systematically to the Li-like ionic series [30] and the Na-like series [31]. Here we are concerned with ionization of a quasi-two-electron target. The form of CCC theory employed for C²⁺ is similar to that used for scattering from beryllium [32], and is based on the adaptation of this method to a helium target [33]. We define the C^{2+} two-electron structure by assuming that one of the electrons is fixed to be the 2sorbital of C^{3+} , and the other is allowed to vary freely. In addition, just for the 2s2p ³P and ¹P symmetries, we add the 2p orbital to allow for ionization of the 2s2p configuration leaving the C^{3+} ion in either the 2s or 2p states. This calculation also includes the excitation-autoionization contributions from the terms of the 2pnl configurations that are above the first ionization limit.

The *R* matrix with pseudostates (RMPS) method has been described in detail previously [34–36]. Our implementation of this method employs a set of Laguerre radial wave funtions to represent the high Rydberg states and the target continuum. As with the CCC method, one determines the ionization cross section by summing over the excitation cross sections to the positive-energy pseudostates as well as any doubly excited states with energies above the first ionization limit. This version of the RMPS method has been employed to calculate the ionization cross section for a variety of neutral and ionic species [4,22,31,35]. All radial functions employed in this calculation were generated using the program AUTOSTRUCTURE [37]. Spectroscopic orbitals were employed for all subshells from 1s to 5g, and were determined from a local potential using Slater-type orbitals. A set of nonorthogonal Laguerre pseudo-orbitals was generated for all subshells from 6s to 12g; they were then orthogonalized to the spectroscopic orbitals and to each other. The close-coupling expansion of the target included all terms of the configurations $2s^2$, 2s2p, $2p^2$, 2snl with n=3 to 12 and l=0 to 4, and 2pnl with n=3 to 11 and l=0 to 4. This leads to a total of 316 terms. The RMPS calculation was performed using our recently developed set of parallel *R*-matrix codes [36,38]. This parallel package includes two parts: the first was developed from modified versions of the Breit-Pauli programs with full electron exchange [39], and the second from the no-exchange *R*-matrix programs [40]. An RMPS calculation with exchange was performed for all LS Π partial waves from L=0 to 11. This was then supplemented by a noexchange calculation from L=12 to L=40. The size of the R-matrix box was 34.5 a.u., and we employed 50 basis orbitals to represent the (N+1)-electron continuum for each value of the angular momentum. This was sufficient to carry out the calculation to a maximum energy of about 150 eV. Extending it to higher energies would have required a larger set of basis orbitals, and the present calculation already includes (N+1)-electron Hamiltonian matrices in size up to 48 000.

III. EXPERIMENTAL METHOD

The experiment was performed at the synchrotron storage ring CRYRING in Stockholm, Sweden. The C^{2+} ions were

produced by an electron cyclotron resonance ion source of the hypernanogan type operating with a microwave input of 14.5 GHz at a power of 180 W. The source platform was operated at 36 kV and the extraction system at 10 kV, giving an accelerating potential of 46 kV. Upon injection into CRY-RING, the ions were accelerated by an RF drift tube to a final energy of 2.7 MeV/amu at a current of 77 nA. The ions were cooled by the electron cooler coupled to CRYRING such that the stored ion-beam diameter was approximately 1 mm. The electron cooler also doubles as the electron source for electron-impact ionization measurements. The center-ofmass (c.m.) energies of interest are created by detuning the electron velocity away from the velocity-matched cooling condition. Stored ions which are ionized are separated from the stored beam by the 1.2 T dipole magnet following the electron cooler. The charge-changed ions are then detected by a unity efficiency surface barrier detector.

A description of the data analysis technique used in this work has been previously reported in several articles on electron-ion recombination at CRYRING, in which the same analysis procedure is used to derive c.m. energies and rate coefficients [41,42]. The rate coefficient is related to the cross section by the expression

$$\alpha(E) = \langle v \, \sigma(E) \rangle, \tag{1}$$

where v is the mean electron velocity and $\sigma(E)$ is the cross section. To obtain the ionization cross section, we simply divide the rate coefficient by the mean velocity at each respective data point in the spectrum. The results represent a 100-point averaging of the final experimental data with the total error shown by error bars. The c.m. energy resolution is mainly determined by the longitudinal electron temperature (kT_{long}) in the electron cooler and is given by

$$\Delta E = 4\sqrt{E_d k T_{\text{long}} \ln 2},\tag{2}$$

where E_d is the c.m. detuning energy (eV) and kT_{long} is 0.1 meV. This yields a ΔE ranging from 0.1 to 0.5 eV over the energy range investigated. The error in the cross section is primarily due to a determination of the number of ions stored in the ring, from ion current measurements, and the uncertainty in the effective electron cooler interaction length, estimated at 80 cm. Together these yield an error of 15%, which includes a statistical error of 3%.

Previous studies on ECR ion sources by Brazuk *et al.* [12] found that for C²⁺, the metastable fraction is expected to be 0.56 ± 0.11 . We expect our current ECR ion source to produce a similar metastable fraction. This is consistent with atomic structure calculations of lifetimes for Be-like C²⁺ ions. Of the levels in the 2s2p ³P term, only ³P₁ has a significant decay rate to the ground $2s^2$ ¹S₀ level, via an intercombination transition that is possible through weak spinorbit mixing of the ³P₁ level with the ¹P₁ level. Nussbaumer and Storey [43] calculated an A value of 95.92 s⁻¹ for the 2s2p ³P₁ $\rightarrow 2s^2$ ¹S₀ transition, and Doerfert *et al.* [44] measured a value of (102.94 ± 0.14) s⁻¹. The resultant lifetime of \sim 9.7 ms is significantly shorter than the 15–20 s for which ions circulate in our storage ring experiments. For the 2s2p ³P₂ $\rightarrow 2s^2$ ¹S₀ magnetic quadrupole transition, Nuss-



FIG. 1. Ionization cross sections for the $2s^2$ configuration. The squares show the TDCC results for the $2s^2$ configuration, the dotdashed line shows the CCC results for the $2s^2$ ¹S term, the dashed line shows the RMPS results for the $2s^2$ ¹S term, and the solid line gives the CADW results for the $2s^2$ configuration. (1.0 Mb=1.0 $\times 10^{-18}$ cm².)

baumer and Storey [43] calculated a lifetime of 192.75 s and Glass [45] calculated a lifetime of 192.6 s, suggesting that a significant fraction should still be present in the storage-ring experiment. The $2s2p^{3}P_{0}$ level can decay to the ground only via a hyperfine-induced transition, for which very few lifetime calculations exist. Doerfert et al. [44] calculated a lifetime of 2×10^{10} s, while Brage [46] calculated a much lower lifetime of 1106 s. In either case, there is likely to be a significant 2s2p ${}^{3}P_{0}$ metastable fraction present. Note that a recent measurement of this transition in Be-like N [47] yields a lifetime of 2.5 s, indicating that Z scaling of these transitions may lead to a much smaller metastable fraction present in higher members of the Be isoelectronic sequence. This is consistent with recent dielectronic recombination studies on Cl^{13+} [48], which saw no metastable fraction in the ion beam. However, from the lifetime data for C^{2+} , we see that if the ion source populates all the states of the $2s^{2}$ ¹S and 2s2p ³P terms equally, on statistical grounds, one would expect the 2s2p ³P term to contain 60% of the beam population.

IV. RESULTS

In Figs. 1 and 2, we show a comparison of the cross sections from the various theoretical methods employed in this paper for ionization of the $2s^2$ ground configuration and the 2s2p excited configuration. Since there is only one term in the ground configuration, in Fig. 1 the term-resolved RMPS (dashed line) and CCC (dot-dashed line) calculations will be equivalent to the configuration-average CADW (solid line) and TDCC (squares) results. The TDCC and CCC results are seen to be in very good agreement, while the RMPS results agree near the threshold, but are lower than the TDCC and CCC results at higher energies. The CADW results are slightly higher than those from all of the nonperturbative methods, though the differences between the various theoretical cross sections for the $2s^2$ configuration are all relatively small.



FIG. 2. Ionization cross sections for the 2s2p configuration. The open squares show the TDCC results for the direct ionization of the 2s2p configuration; the closed squares are the TDCC results with excitation-autoionization included. The dot-dashed line shows the configuration-average CCC results for the 2s2p configuration; the dashed line shows the configuration-average RMPS results for the 2s2p configuration. The dotted line shows the CADW results for the direct ionization of the 2s2p configuration, and the solid line shows the CADW results with excitation-autoionization included. (1.0 Mb= 1.0×10^{-18} cm².)

In Fig. 2, for the ionization cross section from the 2s2p excited configuration, the RMPS and CCC cross sections agree well up to about 75 eV and the DW cross section is only slightly larger. Above this energy, there are some differences in the results of all the various calculations which must be considered. The TDCC (open squares) and CADW (dotted line) represent the configuration-average direct-ionization cross section from the 2s2p configuration. Both the RMPS and CCC calculations are term-resolved; however, for the purpose of comparing the different theoretical results, we have determined configuration-average (CA) cross sections from the 2s2p ¹P and ³P results. These are shown by a dotdashed line for the CCC results and by a dashed line for the RMPS results. In both cases, the CA cross sections are about 2 Mb above the ³P cross sections.

As noted in Sec. II, both the RMPS and CCC cross sections include the effects of excitation-autoionization. For this reason, we have added excitation-autoionization contributions to both the CADW and TDCC ionization results by using a CADW excitation program and data from the TDCC calculation to determine the cross sections for the transitions from the 2s2p configuration to the 2pnl doubly excited autoionizing configurations. From NIST energies [50], the levels of the 2p4d configuration straddle the ionization threshold, and all 2pnl configurations above it are autoionizing. In our CADW and TDCC excitation calculations, we did not include contributions from the 2p4d configuration, but we did include the contributions for excitation from the 2s2pconfiguration to all configurations from 2p4f to 2p6f.

The CADW ionization results, corrected in this way for the contributions from excitation-autoionization, are shown by the solid line, and the corrected TDCC results are shown by the solid squares. In both the TDCC and CADW cases,



FIG. 3. Theoretical ionization cross sections for C²⁺, assuming 40–60 % mixture of the ground and excited configurations, compared with the experimental results from the CRYRING experiment (diamonds). The theoretical results consist of CCC results (dot-dashed line), TDCC results (open squares for the direct ionization, solid squares for the results with excitation-autoionization), RMPS results (dashed line), and CADW results, including excitation-autoionization (solid line). (1.0 Mb= 1.0×10^{-18} cm².)

excitation-autoionization adds about 10% to the cross section. However, in comparing the corrected CADW and TDCC results with the RMPS and CCC cross sections, some of the differences may still be due to the excitationautoionization contributions. First, in both the CCC and RMPS calculations, some levels of the configuration 2p4dare autoionizing and are included as part of the total ionization cross section; this would tend to increase the contribution from excitation followed by autoionization. On the other hand, the effects of coupling on the excitation cross sections to these doubly excited states that are included in both of the CCC and RMPS calculations will tend to reduce the excitation-autoionization contributions. As we see, the CADW results, corrected for excitation-autoionization, are above the various nonperturbative results and the RMPS results peak before the CCC and corrected TDCC results. Furthermore, above 100 eV, the difference between the CCC and corrected TDCC cross sections is about the same as the difference between the corrected TDCC and RMPS cross sections, with the CCC results higher than the other two.

Figure 3 shows the new experimental measurements for the ionization cross section of C^{2+} . The new experimental data presented here can be downloaded from [49]. The present CRYRING results are in close agreement with the data of Falk *et al.* [7], though they trend slightly below those results above about 170 eV. The current measurements are also in good agreement with the previous measurements of Woodruff *et al.* [10] and lie slightly higher than the results of Hamdan *et al.* [11].

In Figs. 3 and 4, we show the various theoretical results, compared with the current (Fig. 3) and the older (Fig. 4) experimental results, assuming a 40–60 % fraction of the beam in the ground and metastable terms. Both the CCC and RMPS cross sections are within the error bars of the present CRYRING measurements, although the CCC cross sections



FIG. 4. Theoretical ionization cross sections for C²⁺, assuming 40–60 % mixture of the ground and excited configurations, compared to the low metastable experimental results from Falk *et al.* [7] (triangles) and the measurements of Woodruff *et al.* [10] (open circles). The theoretical results consist of CCC results (dot-dashed line), TDCC results (open squares for the direct ionization, solid squares for the results with excitation-autoionization), RMPS results (dashed line), and CADW results, including excitation-autoionization (solid line). (1.0 Mb= 1.0×10^{-18} cm².)

are about 10% above the RMPS results and the experimental point at about 120 eV. The CADW results are higher than experiment, and the TDCC results are within the experimental error bars, but higher than the other nonperturbative results. The TDCC and CADW metastable calculations are of the 2s2p configuration-average cross section, rather than the 2s2p ³P cross section, and thus are both about 2 Mb too high, due to term-dependent effects. This would bring the TDCC results into much better agreement with the other nonperturbative calculations. The CADW results would still be higher than the experimental error bars, the remaining difference being due to the fact that the CADW calculations overestimate both the $2s^2$ and $2s^2p$ cross sections. We note in Fig. 4 that the TDCC, CCC, and RMPS results are in similar agreement with the previous experimental measurements of Falk et al. [7] and Woodruff et al. [10].

As a further check on the metastable fraction, dielectronic recombination measurements were taken simultaneously with the present CRYRING ionization cross-section measurements. From theoretical calculation of the peak heights of resonances attached to both the $2s^{2} {}^{1}S_{0}+e^{-} \rightarrow 2s2pnl$ series, and those attached to $2s2p {}^{3}P_{0,2}+e^{-} \rightarrow 2p^{2}nl$ series, it was estimated that a metastable fraction of 60% was present in the experimental beam, in good agreement with our conclusions from estimations from lifetime calculations, and from our ionization cross-section calculations. The results of this dielectronic recombination study are to be published in a separate paper [51].

V. SUMMARY

In this paper, we have compared experimental measurements for the electron-impact single-ionization cross section of C²⁺ with calculations using the time-dependent closecoupling, converged-close-coupling, R-matrix with pseudostates, and distorted-wave techniques. We estimate the 2s2p ³P metastable fraction present in our ECR ion source to be 60%, which is consistent with atomic structure calculations of radiative rates. There is reasonable agreement between the TDCC, CCC, and RMPS ionization cross sections for both the $2s^2$ and the $2s^2p$ configurations. It was found that the 2s2p ³P cross section lies about 2 Mb below the configuration-average result, due to term-dependent effects. Also, excitation-autoionization is likely to add about 10% to the direct-ionization cross section. The converged-closecoupling and *R*-matrix with pseudostates calculations for the ionization cross section, assuming a 40-60 % ground and metastable mixture, are in reasonable agreement with experiment. The TDCC results are within the experimental error bars, but higher than the other nonperturbative results. This difference is largely due to term-dependent effects not accounted for in the configuration-average TDCC calculation. The CADW results are higher than experiment. Term dependence effects would bring the CADW results closer to experiment, though it would remain above the experimental error bars. The remaining discrepancy is due to the distortedwave calculations from the $2s^2$ ground configuration and the 2s2p excited configuration both being slightly too high. To our knowledge, this is the first time, for a light species, that agreement between theory and experiment has been achieved for the ionization cross section of species with a significant metastable fraction in the beam. In the future, we plan to extend our nonperturbative calculations from excited configurations to look at ionization of all ion stages of carbon, and ionization from highly excited states of helium, with a view to improving the atomic data for elements of fundamental importance to fusion modeling.

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