Contribution to the theoretical investigation of electron and photon interaction with carbon atom and its ions

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Abstract. This work presents results from the theoretical investigation of electron and photon interaction with carbon atoms and its Be-like ion. After an introductory survey on the existing reported theoretical works, we present results from the calculation of energy levels and oscillator strengths for selected transitions in neutral carbon. We also report results from the detailed state selective photo-recombination study in Be-like C\textsuperscript{2+} ions.

1. Introduction
Detailed knowledge of carbon transport properties, and consequently of the accurate cross-section data, is required for the fusion plasma diagnostics. The difficulties in obtaining sufficient quantities of atomic carbon in a well-defined initial state led to a complete absence of experimental cross-section measurements. This absence of experimental data made theoretical investigations a computational grand challenge.

In general, the electron-impact excitation cross sections calculated for neutral carbon with different methods are not in good agreement with each other especially for optically forbidden transitions. Detailed structure calculations have been reported for the astrophysically important transitions \cite{1-4}. More extensive theoretical and experimental reported works exist for the carbon ions. Theoretical works on C\textsuperscript{2+} have been reported by Glass \cite{5}, Berrington \cite{6}, Berrington et al. \cite{7}, and Mitnik et al. \cite{8}. Experimental data have also been published \cite{9}. Results from the electron and photon interactions with C\textsuperscript{1+} have been reported by Wilson and Bell \cite{10}, Wilson et al. \cite{11, 12}, and Nahar \cite{13}. There are a number of publications dealing with the ionization of the C\textsc{i}ii to CV ionization stages. Detailed analysis of the importance of this process in populating the excited levels of ions in plasmas typical for those found in the edge of tokamak for the CIV and CV ionization stages has been recently made by Lawson et al. \cite{14, and references herein}.

We will discuss the existing theoretical models for electron-scattering by neutral carbon atom and will give complementary results for its atomic structure. We report a new set of R-matrix calculation intended specifically to investigate the role of including configuration interaction (CI) wave functions both in the target state expansion and in the (N+1)-electron quadratically integrable function expansion. Target-atom states were computed using the Hartree-Fock ground configuration 2s\textsuperscript{2}2p\textsuperscript{2} plus the near-degenerate configurations 2s2p\textsuperscript{3} and 2p\textsuperscript{4}. In addition, for consistency with the virtual excitation pattern used for scattering wave functions, all virtual excitations of 2s\textsuperscript{2}2p\textsuperscript{2} of the form 2p-np and 2p-nf were included. Results for the energy levels and oscillator strengths for important transitions have been obtained.
The second issue addressed here is the effect of quantum interference between dielectronic (DR) and radiative recombination (RR) on photo-recombination (PR) cross section in Be-like C ion. The calculation was carried out for the excited Rydberg states of type 1s2s2ns(‘S’) which interact with the odd-parity continua up to the C3+ 2p threshold limit. The numerical evaluation has been performed at a fine energy mesh across all the autoionizing Rydberg series of resonances 1s22pns(‘P’) converging to Li-like ion 2p threshold. The method of calculation is based on the on the essential ingredients of the Feshbach projection operator approximation. The photo-ionization cross sections have been evaluated with and without relativistic effects included into the R-matrix numerical procedures, while the allowance for both quantum interference between DR and RR and overlapping resonances has been done using results from the earlier R-matrix Floquet calculation [15]. We present all these results with respect to the effect of quantum interference term on the energy dependence profile of PR cross section.

The paper is structured as follows. Section 2 presents an introductory survey on the existing target model calculation in electron scattering on atomic carbon. The present calculated energy levels are compared with existing experimental data in Atomic Structure Database of the National Institute for Standards and Technology wherever available. Section 3 is focused on photon-interaction with the C2+ ion. The study of resonant single-photon ionization process from the 1s2s2ns(‘S’) states of Be-like Al9+ and C10+, (9 ≤ n ≤ 12, and 5 ≤ n ≤ 12, respectively) has been done [16, 17] in response to the need in the best way of including radiation damping in a non-perturbative treatment of DR of Li-like ion, (9 ≤ n ≤ 12) into Be-like ions. Furthermore, the dominant states in DR of these ions have been investigated [18-21] along with detailed close-coupling calculation of the electron-ion scattering [22-24]. Currently, we employ all these results and carry out a new set of calculation in order to explore the effect of quantum interference between DR and RR on the energy dependence profile of PR cross section in C2+. Section 4 presents our concluding remarks and further direction of research.

2. Structure calculation

In neutral carbon the electron scattering calculation is made difficult by the fact that low-energy electron scattering is dominated by a resonance due to the 1s2s2p33P0 state of the negative ion, C-. The theoretical prediction of the location of this resonance, and of the 1s2s2p14S0 and 2D0 bound states of C-, depends on a balance between short-range correlation and long range polarization effects.

The ground-state configuration of carbon in the independent-particle model is (1s)2(2s)2(2p)2, which leads to the ground-state terms 1P, 1D, 1S. In order to get reliable data, the wave functions of the N-electron target state and of the negative ionic states that have N+1electrons should be calculated with the same degree of accuracy. In the calculation of low-energy electron scattering by neutral carbon atoms, one must take into account long-range polarization effects and short-range correlation between the incident electron and the electron attachment effects that lead to scattering resonances. The early theoretical models and methods applied to low-electron energy scattering from atomic carbon could be summarized as follows: a) the polarized-orbital method [25-27]. This is single configuration-based method which treats the target-atom dipole polarizability and the resulting long-range polarization potential accurately, but involves approximations to the short-range interaction that are difficult to evaluate. The polarized-orbital method cannot describe resonances; b) the close-coupling method [28, 29] which is capable, in principle, of representing the full structure of the electronic continuum wave functions through a series of expansion in the stationary sates of the target atom. Elaborate calculation including some target correlation effects and a limited pseudostate representation of target polarizability has been reported by Saraph [30], Rountree, Smith and Henry [31], Le Dourneuf [32], Le Dourneuf et al. [33]; c) the matrix variational method including configuration interaction approximation (CI) that takes into account the effect of near-degenerate configuration interaction [34-36]. The major innovation in this method is that LS eigenfunctions are used through the calculations, but does not describe resonances. All these calculations were limited in elastic scattering from ground states and transitions amongst the n=2 states at low collision energies.
In the last two decades, the most detailed works have been reported by Dunseath et al. [37], Zatsarinny et al. [38] and Liu, Wang and Zhou [39]. In the work by Dunseath et al. [37], two independent standard R-matrix calculations were performed. In the first, all levels of carbon with \( n \leq 3 \) have been included in the expansion of the total wave function. In the second calculation, all levels with \( n \leq 4 \) have been considered in the target model calculation. Extensive calculation of cross sections and collision strengths for important transitions to the \( n = 3 \) and \( n = 4 \) levels of carbon has been performed using the asymptotic distorted wave method available in the FARM package [40] after which the top-up procedure was used. These authors reported some resonance structures in the low-energy region, and pointed out the importance of the target-model in scattering calculation. The correlation effects were only included in the first model-calculation.

In their work, Zatsarinny et al. [38] presented theoretical results based on the extended version of the R-matrix method, where a B-spline basis is employed for the representation of the continuum functions. These authors revealed a prominent resonance structure for the most electron-induced transitions in atomic carbon at low energies. The close-coupling expansion has included the bound and autoionizing states derived from the 1s\(^2\)2s\(^2\)2p\(^3\) \((l=0, 1, 2)\), 1s\(^2\)2s\(^2\)2p4s, 2s\(^2\)2s2p\(^3\), and 1s\(^2\)2p\(^3\) configurations, plus eight pseudo-states to account for the target continuum. The calculated cross sections and effective collision strengths for important transitions from the ground state 2p\(^2\)3P, and the metastable 2p\(^2\)1D and 3S states show significant discrepancies with those reported by Dunseath et al. [37] in a similar scattering model. This work also provides a detailed analysis of the resonance structure in the low-energy near-threshold regions.

In the third and most recent theoretical calculation by Liu et al. [39], the authors use the momentum space coupled-channels optical (CCO) method to solve coupled-integral equations for a finite set of discrete physical states of target to convergence. The continuum is treated via an ‘ab initio’ complex equivalent-local potential. The model-calculation includes 12 states in the coupled-channels. They were described by single configuration Hartree-Fock approximation.

We conclude this introductory survey by mentioning that in these works the cross sections agree well in shape, but large discrepancies in magnitude exist, namely the Dunseath’s excitation cross sections are 32% higher than those obtained from the calculation of B-spline R-matrix method, and the results of CCO method are 18% lower than the calculation of B-spline R-matrix method. A database has been constructed [41] consisting of the recommended cross sections for electron-impact excitation and ionization of carbon atoms and ions, as well as for charge exchange processes between carbon ions and hydrogen atoms.

In the present work, we report results concerning the non-relativistic and relativistic atomic structure calculation in neutral carbon. An initial LS coupling- standard R-matrix atomic structure calculation has been performed in order to investigate the role of including configuration interaction wave functions both in the target state expansion and in the (N+1)-electron quadratically integrable function expansion. The electron correlation effects have been explored by carrying out separate calculations with and without the configurations: 2s2p\(^3\), 2s2p\(^5\)nl \((n =3, 4)\), 2p\(^3\) in the target state expansion, and 2s\(^2\)p\(^3\), 2s2p\(^4\), 2s2p\(^3\)nl \((n =3, 4)\) in the (N+1)-electron wave function. In table 1, results for selected state energies, in eV units, are compared with existing reported experimental data in Atomic Structure Database of the National Institute for Standards and Technology [42] wherever available. Comparison with the earlier published theoretical works is also provided in this table.

In our target model calculation, the \((N+1)\)-electron configurations data have been obtained by adding one electron to the \( N \)-electron configurations in all possible ways. This wave function was augmented by including all configurations arising from virtual excitation of a 2p orbital. Exploratory calculations indicated that further 2s virtual excitations could be neglected.

As a further check on reported structure calculation, table 2 shows the calculated oscillator strengths and comparison with previously reported theoretical and experimental values.
Table 1. Excitation energies (in eV) for the spectroscopic target states.

| State       | Term | Present | Ref. [37] | Ref. [38] | NIST [42] |
|-------------|------|---------|-----------|-----------|-----------|
| 1           | 2s^2p^2 | 3P     | 0.00      | 0.00      | 0.00      |
| 2           | 2s^2p^2 | 1D     | 1.557     | 1.545     | 1.353     | 1.260     |
| 3           | 2s^2p^2 | 1S     | 2.602     | 2.545     | 2.833     | 2.680     |
| 4           | 2s^2p^3 | 1S     | 3.092     | 3.133     | 4.069     | 4.179     |
| 5           | 2s^2p^3 | 1P     | 7.401     | 8.488     | 7.488     | 7.481     |
| 6           | 2s^2p^3 | 1P     | 7.740     | 8.936     | 7.727     | 7.680     |
| 7           | 2s^2p^3 | 3D     | 8.340     | 8.412     | 8.082     | 7.942     |
| 8           | 2s^2p^3 | 1P     | 8.451     | 9.456     | 8.528     | 8.534     |
| 9           | 2s^2p^3 | 3P     | 9.309     | 10.390    | 8.822     | 8.845     |
| 10          | 2s^2p^3 | 1D     | 9.443     | 10.757    | 9.012     | 8.998     |
| 11          | 2s^2p^3 | 1S     | 10.424    | 11.370    | 9.256     | 9.168     |
| 12          | 2s^2p^3 | 3P     | 9.517     | 9.981     | 9.504     | 9.326     |
| 13          | 2s^2p^3 | 1P     | 9.772     | 10.719    | 9.647     | 9.627     |
| 14          | 2s^2p^3 | 3P     | 10.142    | 10.810    | 9.708     | 9.683     |
| 15          | 2s^2p^3 | 1D     | 10.549    | 10.834    | 9.708     | 9.709     |
| 16          | 2s^2p^3 | 3P     | 9.517     | 10.809    | 9.729     | 9.695     |
| 17          | 2s^2p^3 | 1D     | 9.607     | 10.888    | 9.731     | 9.705     |
| 18          | 2s^2p^3 | 1P     | 9.607     | 10.947    | 9.759     | 9.732     |
| 19          | 2s^2p^3 | 1P     | 9.653     | 10.970    | 9.782     | 9.758     |
| 20          | 2s^2p^3 | 1D     | 13.407    | 11.018    | 9.983     | 9.830     |
| 21          | 2s^2p^3 | 1P     | 14.470    | 14.645    | 12.984    | 12.132    |
| 22          | 2s^2p^3 | 1P     | 13.407    | 15.366    | 13.273    | 13.114    |
| 23          | 2s^2p^3 | 1P     | 15.927    | 16.182    | 14.949    | 14.860    |
| 24          | 2s^2p^3 | 1P     | 19.361    | 21.149    | 19.986    |
| 25          | 2s^2p^3 | 1P     | 19.621    | 22.677    | 20.877    |
| 26          | 2s^2p^3 | 1S     | 20.479    | 26.227    | 24.389    |
Table 2. Oscillator strengths in C.

| Lower level | Upper level | Present  | Ref. [37] | Ref. [38] | NIST [42] |
|-------------|-------------|----------|-----------|-----------|-----------|
| $2s^2p^2 \frac{3}{3}P^0$ | $2s^2p3s \frac{3}{3}P^0$ | 0.124    | 0.154     | 0.133     | 0.140     |
|             | $2s^2p^3 \frac{3}{3}D^0$ | 0.098    | 0.152     | 0.107     | 0.072     |
|             | $2s^2p^3 \frac{1}{3}P^0$ | 0.028    | 0.117     | 0.055     | 0.063     |
|             | $2s^2p4s \frac{3}{3}P^0$ | 0.023    | 0.010     | 0.009     | 0.021     |
|             | $2s^2p3d \frac{3}{3}D^0$ | 0.112    | 0.132     | 0.107     | 0.094     |
|             | $2s^2p3d \frac{1}{3}P^0$ | 0.340    | 0.069     | 0.098     | 0.040     |
|             | $2s^2p3d \frac{3}{3}S^0$ | 0.171    | 0.269     | 0.134     | 0.152     |
| $2s^2p^2 \frac{1}{2}D$ | $2s^2p3s \frac{1}{2}P^0$ | 0.128    | 0.103     | 0.118     | 0.118     |
|             | $2s^2p3d \frac{1}{2}D^0$ | 0.009    | 0.007     | 0.013     | 0.013     |
|             | $2s^2p4s \frac{1}{2}P^0$ | 0.004    | 0.010     | 0.004     | 0.011     |
|             | $2s^2p3d \frac{1}{2}F^0$ | 0.061    | 0.099     | 0.118     | 0.085     |
|             | $2s^2p3d \frac{1}{2}P^0$ | 0.018    | 0.014     | 0.011     | 0.009     |
|             | $2s^2p3d \frac{1}{2}D^0$ | 0.344    | 0.529     | 0.396     |           |
|             | $2s^2p^3 \frac{3}{3}P^0$ | 0.351    | 0.333     | 0.257     |           |
| $2s^2p^2 \frac{1}{2}S$ | $2s^2p3s \frac{1}{2}P^0$ | 0.021    | 0.076     | 0.098     | 0.094     |
|             | $2s^2p4s \frac{1}{2}P^0$ | 0.007    | 0.001     | 0.004     | 0.005     |
|             | $2s^2p3d \frac{1}{2}P^0$ | 0.050    | 0.142     | 0.196     | 0.125     |
|             | $2s^2p^3 \frac{1}{2}P^0$ | 0.122    | 0.633     | 0.458     |           |

Next, we initiated fine-structure splitting calculation employing the full relativistic GRASP (General-purpose Relativistic Atomic Structure Package) code [43], subsequently revised by several workers under the names GRASP, GRASP92 and GRASP2K. In our work we used GRASP0 code [44]. The code is fully relativistic and it is based on the jj coupling scheme. Further relativistic corrections arising from the Breit interaction and QED effects (vacuum polarization and Lamb shift) have also been included. Additionally, we have used the option of extended average level, in which a weighted (proportional to $2j+1$) trace Hamiltonian matrix is minimized. This produces a compromise set of orbitals describing closely lying states with moderate accuracy. For comparison purposes, we have performed parallel calculations with the Flexible Atomic Code (FAC) [45]. This is also a fully relativistic code, which provides a variety of atomic parameters, and (generally) yields results for energy levels and radiative rates comparable to GRASP. Results from FAC are helpful in assessing the accuracy of our energy levels and radiative rates, and in estimating the contribution of resonances to effective collision strengths.

The $2s^2p^2$, $2s^2p3l$, $2s^2p4l$, $2s^2p5s$, $2p^3$ and $2p^4$ configurations of carbon give rise to 88 fine structure levels, $J = 0 – 5$, odd and even parity. In table 3 we compare level energies obtained with GRASP (without and with the inclusion of Breit and QED effects) with the critically evaluated data compiled by NIST for the lowest 51 levels. Also included in this table are results obtained from the FAC code (FAC) including the same CI (configuration interaction) as in GRASP. The level energies obtained without the Breit and QED effects (GRASP1) are consistently higher than the NIST values up to ~ 0.03Ryd. However, the orderings are nearly the same as those of NIST. The inclusion of Breit and QED effects (GRASP2) lowers the energies by a maximum of ~ 0.0001 Ryd. The FAC level energies are consistently lower by up to 0.003 Ryd than GRASP results, and hence they are comparatively in better agreement with the NIST listings. The level ordering from FAC are also in
A further inclusion of the $2p^5 l, l = 2 - 4$, configurations, labeled FAC2 calculation in table 3 makes no appreciable difference either in the magnitude or ordering of the levels.

Table 3. Fine-structure splitting calculation in C. NIST: \url{http://www.nist.gov}; GRASP1: energies from the GRASP code with 88 level calculations without Breit and QED effects included; GRASP2: energies from the GRASP code with 88 level calculations with Breit and QED effects; FAC1: energies from the FAC code with 88 level calculations; FAC2: energies from the FAC code with 134 level calculations.

| Index | Configuration/Term | NIST | GRASP1 (Ryd) | GRASP2 (Ryd) | FAC1 (Ryd) | FAC2 (Ryd) |
|-------|-------------------|------|--------------|--------------|------------|------------|
| 1     | $2s^22p^3 \, ^3P_0$ | 0.000 | 0.000        | 0.00000      | 0.00000    | 0.00000    |
| 2     | $2s^22p^3 \, ^3P_1$ | 0.0001494 | 0.0001873 | 0.0001570    | 0.000064   | 0.000064   |
| 3     | $2s^22p^3 \, ^3P_2$ | 0.0003955 | 0.0005584 | 0.0004093    | 0.00015105 | 0.000150   |
| 4     | $2s^22p^3 \, ^1D_2$ | 0.09288208 | 0.1164040 | 0.1162848    | 0.11214485 | 0.112139   |
| 5     | $2s^22p^3 \, ^1S_0$ | 0.1972712 | 0.1862982 | 0.1862062    | 0.18620175 | 0.185830   |
| 6     | $2s^22p^3 \, ^3S_2^0$ | 0.3074178 | 0.2209301 | 0.2207590    | 0.24013273 | 0.240146   |
| 7     | $2s^22p3s \, ^3P_0^0$ | 0.5497987 | 0.5672529 | 0.5670994    | 0.5637540  | 0.563779   |
| 8     | $2s^22p3s \, ^3P_1^0$ | 0.5499736 | 0.56743662 | 0.56723954  | 0.5638635  | 0.563888   |
| 9     | $2s^22p3s \, ^3P_2^0$ | 0.5503428 | 0.56781234 | 0.5673131    | 0.5640918  | 0.564117   |
| 10    | $2s^22p3s \, ^1P_0^0$ | 0.5648199 | 0.5915391 | 0.5912947    | 0.5898824  | 0.589799   |
| 11    | $2s^22p^3 \, ^3D_3^0$ | 0.5840030 | 0.6287575 | 0.62851954   | 0.6215855  | 0.620708   |
| 12    | $2s^22p^3 \, ^3D_4^0$ | 0.5840297 | 0.62877758 | 0.6286506   | 0.6216502  | 0.620772   |
| 13    | $2s^22p^3 \, ^3D_2^0$ | 0.5840397 | 0.6287918 | 0.6286165    | 0.6216703  | 0.620793   |
| 14    | $2s^22p3p \, ^1P_1$ | 0.6274650 | 0.6419229 | 0.6416769    | 0.6335048  | 0.632521   |
| 15    | $2s^22p3p \, ^3D_1^0$ | 0.6350573 | 0.6500307 | 0.6498481    | 0.6404025  | 0.639685   |
| 16    | $2s^22p3p \, ^3D_2^0$ | 0.6352503 | 0.65024712 | 0.6500201   | 0.6408055  | 0.640223   |
| 17    | $2s^22p3p \, ^3D_3^0$ | 0.6355544 | 0.6505814 | 0.65028541   | 0.6409477  | 0.640081   |
| 18    | $2s^22p3p \, ^3P_1^0$ | 0.6446663 | 0.66232293 | 0.6620727    | 0.6515510  | 0.651184   |
| 19    | $2s^22p3p \, ^3P_0^0$ | 0.6502119 | 0.68021956 | 0.6800215    | 0.6806422  | 0.680232   |
| 20    | $2s^22p3p \, ^3P_1^0$ | 0.6503248 | 0.68032504 | 0.6801031    | 0.6811181  | 0.680783   |
| 21    | $2s^22p3p \, ^3P_2^0$ | 0.6505114 | 0.68052371 | 0.6802520    | 0.6811958  | 0.680232   |
| 22    | $2s^22p3p \, ^1D_2^0$ | 0.6616776 | 0.6933946 | 0.6931423    | 0.6938854  | 0.680783   |
| 23    | $2s^22p3p \, ^1S_0^0$ | 0.6741181 | 0.70517591 | 0.7049219    | 0.6933448  | 0.692573   |
| 24    | $2s^22p^3 \, ^3P_1^0$ | 0.6857646 | 0.714868994 | 0.7147168   | -          | -          |
| 25    | $2s^22p^3 \, ^3P_2^0$ | 0.6857765 | 0.71493401 | 0.71481283   | -          | -          |
| 26    | $2s^22p^3 \, ^3P_0^0$ | 0.6857842 | 0.71506221 | 0.714676964  | -          | -          |
| 27    | $2s^22p3d \, ^1D_2^0$ | 0.7078706 | 0.72124488 | 0.72098426   | 0.6971971  | 0.696376   |
| 28    | $2s^22p4s \, ^3P_0^0$ | 0.7117449 | 0.727291515 | 0.72739911   | 0.6963345  | 0.696337   |
Detailed PR and radiative damping calculations have been carried out using the collision strengths, and from the photo-absorption and photo-ionization (PI) cross sections calculation, Zabaydullin and Dubau [50]. These authors have reported results on the effects of radiative decay on Bell and Seaton [48]. The method has been applied by Pradhan and Seaton [49] and more recently by Robicheaux et al. [51]. They proposed treating the electron scattering process using a coupled channel method of procedure has been suggested by Davies and Seaton [47], a general theory of DR, based on the quantum defect and including radiative damping in the close-coupling equations, was developed by Bell and Seaton [48]. The method has been applied by Pradhan and Seaton [49] and more recently by Zabayedullin and Dubau [50]. These authors have reported results on the effects of radiative decay on collision strengths, and from the photo-absorption and photo-ionization (PI) cross sections calculation, respectively. Detailed PR and radiative damping calculations have been carried out using the R-matrix code which includes relativistic Breit-Pauli effects. The method of procedure has been suggested by Robicheaux et al. [51]. They proposed treating the electron scattering process using a coupled channel method which includes relativistic Breit-Pauli effects.

### Table 3 - continued

| Index | Configuration/Term | NIST | GRASP1 (Ryd) | GRASP2 (Ryd) | FAC1 (Ryd) | FAC2 (Ryd) |
|-------|-------------------|------|--------------|--------------|------------|------------|
| 29    | 2s2p4s 3P1/2      | 0.7118521 | 0.727461988 | 0.72741456 | 0.6964099 | 0.696260  |
| 30    | 2s2p4s 3P1/2      | 0.721378  | 0.727641373 | 0.72708323 | 0.6964513 |           |
| 31    | 2s2p3d 3F1/2      | 0.7126024 | 0.72773354  | 0.7274672 | 0.70124003 | 0.697085  |
| 32    | 2s2p3d 3F1/2      | 0.7127522 | 0.727461988 | 0.72721555 | 0.70194265 | 0.701930  |
| 33    | 2s2p3d 3F1/2      | 0.7130659 | 0.727715995 | 0.72740876 | 0.7016843 | 0.701672  |
| 34    | 2s2p3d 3D1/2      | 0.7134628 | 0.73556129  | 0.73533694 | 0.7062923 | 0.706266  |
| 35    | 2s2p3d 3D1/2      | 0.7135916 | 0.73563534  | 0.73538238 | 0.7065979 | 0.701226  |
| 36    | 2s2p3d 3D1/2      | 0.7136884 | 0.735720808 | 0.734715436 | 0.70641018 | 0.706377  |
| 37    | 2s2p4s 1P1/2      | 0.7138892 | 0.73662305  | 0.7363463 | 0.70456333 | 0.704580  |
| 38    | 2s2p3d 1F1/2      | 0.7156146 | 0.734973379 | 0.73471543 | 0.7078843 | 0.707857  |
| 39    | 2s2p3d 1P1/2      | 0.7174521 | 0.736623055 | 0.7363463 | 0.71068036 | 0.710583  |
| 40    | 2s2p3d 3P1/2      | 0.7227336 | 0.72771599  | 0.72740876 | -           |           |
| 41    | 2s2p3d 3P1/2      | 0.7228059 | 0.72766176  | 0.72741456 | -           |           |
| 42    | 2s2p3d 3P0/2      | 0.7228458 | 0.72764137  | 0.72739912 | 0.70470595 | 0.704203  |
| 43    | 2s2p4p 1P1/2      | 0.7341427 | 0.7470183265 | 0.74676676 | 0.7327676 | 0.732111  |
| 44    | 2s2p4p 3D1/2      | 0.7361444 | 0.75000403  | 0.74980834 | 0.7338335 | 0.733358  |
| 45    | 2s2p4p 3D2/2      | 0.7362153 | 0.75021145  | 0.74997625 | 0.73421335 | 0.733736  |
| 46    | 2s2p4p 3D3/2      | 0.7366192 | 0.75054157  | 0.75024022 | 0.73423192 | 0.737361  |
| 47    | 2s2p4p 3S1/2      | 0.7390834 | 0.75599413  | 0.75573827 | 0.7362784 | 0.736073  |
| 48    | 2s2p4p 3P0/2      | 0.7409604 | 0.77657497  | 0.7763905 | 0.74538969 | 0.744327  |
| 49    | 2s2p4p 3P1/2      | 0.7410949 | 0.77672703  | 0.77651882 | 0.7458102 | 0.744682  |
| 50    | 2s2p4p 3P2/2      | 0.7412610 | 0.777024551 | 0.77675744 | 0.74578021 | 0.744703  |
| 51    | 2s2p4p 1D2/2      | 0.7451412 | 0.776778183 | 0.77651438 | 0.75620790 | 0.745683  |

3. **State-selective photo-recombination cross sections in C^{2+}**

In competition with the electron-ion scattering occurs the photo-recombination process (PR). PR is an important cooling mechanism in the hot plasmas and is also used as a plasma diagnostics [46]. It can proceed non-resonantly, through the electron-ion continuum (radiative recombination (RR)). It can also proceed resonantly, through intermediate doubly excited states (dielectronic recombination (DR)). In addition, the emitted photon can be recaptured by the ion, giving rise to a modification of the electron-ion collision cross section, called radiative damping.

Following the pioneering work by Davies and Seaton [47], a general theory of DR, based on the quantum defect and including radiative damping in the close-coupling equations, was developed by Bell and Seaton [48]. The method has been applied by Pradhan and Seaton [49] and more recently by Zabaydullin and Dubau [50]. These authors have reported results on the effects of radiative decay on collision strengths, and from the photo-absorption and photo-ionization (PI) cross sections calculation, respectively. Detailed PR and radiative damping calculations have been carried out using the R-matrix code which includes relativistic Breit-Pauli effects. The method of procedure has been suggested by Robicheaux et al. [51]. They proposed treating the electron scattering process using a coupled channel method which includes relativistic Breit-Pauli effects.
method (e.g. an R-matrix method) but adding an imaginary part, to the energy of the closed channels
to take account of the radiative decay. Then the execution of the substantive calculations has been
promoted as international collaboration [52]. The allowance for both interference and overlapping
resonances in a practical calculation usually has been done using the Feshbach projection operator
methods by LaGattuta [53], Haan and Jacobs [54] and Jacobs and Behar [55]. The theoretical works
by Badnell and Pindzola [56], and more recently by Behar et al. [57] have reported results for highly
charged uranium ions, and for the He-like Ar and Fe ions, respectively.

Employing projection-operator techniques, the energy-averaged unified PR cross section is a sum
over three terms:

\[ \sigma_{PR} = \sigma_{RR} + \sigma_{DR} + \sigma_{int} \]  

where \( \sigma_{RR} \), \( \sigma_{DR} \) and \( \sigma_{int} \) represent the RR cross section, the DR cross section and the interference
(denoted by int ) between the RR and DR transition amplitude, respectively.

To begin with, one class of configurations which creates channels for DR are analyzed in this work,
namely L shell channel 1s22pnl - 1s22ns n', with \( \Delta n = 0, \Delta l = 0 \). The first 2s + e→ 2pnl levels to lie
in the continuum for C\textsuperscript{3+} ions belong to \( n = 5 \). Doubly excited levels in the \( \Delta n = 0 \) channel are
sometimes below the continuum for low enough values of \( n \); in this case the level cannot be formed by
capture plus excitation as serves in the present work as a final level for the recombined ion. A similar
situation occurs in C\textsuperscript{3+} for the 1s22p4s level of Be-like C\textsuperscript{2+} which is below the continuum, whereas the
1s22p5s level is in the continuum and contributes to DR through:

\[ 1s^22s + e^- \leftrightarrow 1s^22p5s \rightarrow 1s^22s5s + h\nu \]  

In order to understand the method of calculation, we recall here the principal idea of the working
DR model. An initial calculation based on the standard R-matrix program [58] has been done to obtain
the field-free atomic states of type 1s2s2ns, 1s2p2ns and 1s2p2nd in Be-like ions, relative to (\( ^2S_e \)) and
(\( ^2P_0 \)) ionization threshold respectively, including a full description of the electron-electron correlation.

Figure 1. R-Matrix Edlén plot for 1s22pns (\( ^1P_0 \)) (solid) and 1s2p2nd(\( ^2P_0 \))(dotted) Rydberg serie of
resonances in C III, as function of the resonance position (in atomic units, au) below the \( ^2P_0 \) threshold.
The \( n \) values are the principle quantum numbers for the associated data point.
The series of resonances, of type $^1P^0$, are allowed in $LS$ coupling. They have been identified by the quantum defect theory (QDT) and method. The effective quantum number $\nu$ of the autoionizing state has been obtained from the quantum-defect formula, $\nu = z / \sqrt{(E - E_T)}$ where $z$ is the ion charge, $E$ is the resonance energy, and $E_T$ is the threshold energy in Rydbergs.

**Plot in the complex plane for freqs. 0.3085 and 0.3087 au**

![Plot](image)

Figure 2. Trajectories of the complex energies of $1s^2 2s 5s(^1S^e)$ and $1s^2 2p 7s(^1P^0)$ states as function of field intensity and frequency. For each frequency, there are two curves, one connected adiabatically to the ‘bound’ and the other to the autoionizing state. The intensity is varied from 0 to $5 \times 10^{13}$ W cm$^{-2}$. The small dots give intensity in steps of $5 \times 10^{11}$ W cm$^{-2}$. The atomic units are used and the energy scale is chosen such that ground states energy is set to zero.

The DR cross section has been calculated utilizing the Feshbach projection operator approximation [57] where the physical quantities correspond to our model as follows:

$$
\sigma_{df}^{DR} (\varepsilon) = \frac{(2\pi \hbar)^3}{8me^2} \frac{(2J_d + 1)}{2(2J_f + 1)} \Gamma_{df} L_d (\varepsilon) B_{df}^D
$$

(4)

with

$$
L_d (\varepsilon) = \frac{\Gamma (d) / 2\pi}{(\varepsilon - \omega_{\text{line}})^2 + \left( \frac{\Gamma (d)}{2} \right)^2}
$$

and

$$
B_{df}^D = \frac{\hbar \Gamma_{df}}{\Gamma (d)}
$$

In the above equations, $\varepsilon$ and $\omega_{\text{line}}$ are the electron collision and the photon frequency, respectively, and $B_{df}^D$ is the branching ratio.

We denoted with $i$, $d$, $f$ the initial, the doubly excited (continuum), and the excited (bound) state, respectively. The transition probabilities for autoionization process are denoted by $\Gamma_{di}^a$ and the
radiative process from the same $d$ state is represented by $\Gamma_{dj}$. The total (natural) width of the doubly-excited levels ($d$) in Eq. 4 is defined as follows:

$$\Gamma(d) = \hbar \left( \sum_f \Gamma_{dj} + \sum_i \Gamma_{di} \right)$$

(5)

where $\Gamma_{dj}$ is the spontaneous radiative decay from the doubly excited $d$ state to final $f$ state and $\Gamma_{di}^a$ is the rate for autoionization from the resonance $d$ state to the non-resonant electron-continuum $i$ state. According to our model calculation [16, 17], $\Gamma(d)$ corresponds to the LIDS width. If the autoionization is affected by the radiative rates, the interaction with the radiative field has to be comparable in strength with the electron-electron interaction. In other words, for each photon energy, i.e. one-photon channel, the imaginary part of the quasi-energy corresponding to autoionizing states, $\Gamma_{di}^a$, includes $\Gamma_{df}^{field}$ signifying the correction due to the interaction with the ion field. Finally, the quantity $\Gamma_{di}^a/(\Gamma_{dj} + \Gamma_{di}^a + \Gamma_{df}^{field})$ arises directly from the calculation. Moreover, the problem of overlapping resonances is solved exactly. Table 4 presents the results for the position and width of the autoionization states of type $1s^22pns$, and the total natural width of doubly excited states of type $1s^22pns$, with $n = 5 – 11$.

Table 4. The total natural width, $\Gamma(d)$, of doubly excited states, the autoionization probability, $\Gamma^\alpha$, and the position, $(E_a)$, of states of type $1s^22pns$ belonging to the C III ions, $n = 5 – 12$. Atomic units (au) are used.

| Ion Li-like | Initial states | Intermediate states L shell channel $1s^22pns$ | $\Gamma(d)$ \/ au | $\Gamma^\alpha$ \/ au | $E_a$ \/ au |
|------------|----------------|-----------------------------------------------|-------------------|-------------------|---------|
| C$^{3+}$   | $1s^22s$       | $n = 5$                                       | $0.272 \times 10^{-02}$ | $0.5518 \times 10^{-02}$ | $0.09496$ |
|            |                | $n = 6$                                       | $0.143 \times 10^{-02}$ | $0.298 \times 10^{-02}$ | $0.15984$ |
|            |                | $n = 7$                                       | $0.900 \times 10^{-03}$ | $0.17948 \times 10^{-02}$ | $0.19794$ |
|            |                | $n = 8$                                       | $0.598 \times 10^{-03}$ | $0.11658 \times 10^{-02}$ | $0.22221$ |
|            |                | $n = 9$                                       | $0.420 \times 10^{-03}$ | $0.8004 \times 10^{-03}$ | $0.23861$ |
|            |                | $n = 10$                                      | $0.290 \times 10^{-03}$ | $0.5736 \times 10^{-03}$ | $0.25021$ |
|            |                | $n = 11$                                      | $0.181 \times 10^{-03}$ | $0.4252 \times 10^{-03}$ | $0.26514$ |

The DR cross sections for each channel were obtained from Eq.4. Figure 3 illustrates the plot of DR cross section (in Megabarn, 1 Mb = $10^{-18}$ cm$^2$) versus electron collision energy (in Ryd.) for the DR process: $e^+ + 1s^22s \rightarrow 1s^22p7s – 1s^22s7s + h\nu$ in CIV.

In the absence of radiation damping, the cross section for photo-recombination $\sigma_{pr}$ is related to the cross section forphoto-ionization $\sigma_{pi}$ through detailed balance given by the Milne relation:

$$\sigma_{pr} = \sigma_{fi} \frac{g_i}{g_f} \frac{\alpha^2 E_{ph}^2}{4(E_{ph} - I)}$$

(5)

in atomic units. In this equation, $g_i$ and $g_f$ are the statistical weights of the initial and residual ions respectively, $E_{ph}$ and $I$ are the photon energy and ionization potential of the final ionic state, respectively, and $\alpha$ is the fine-structure constant. We have carried out successive non-relativistic and relativistic calculation of the PI cross sections. In the first calculation, the PI calculation from the 1S state of the Be-like systems:

$$1s^22sns(^1S_0^0) + h\nu \rightarrow [1s^2nl + e^-(kl')](^3\Pi_{1/2})$$

(6)
is performed employing the computational package RMATXI [58]. At this level of accuracy we have obtained the total PI cross section from the ($^1S$) to all Li-like states converging to ($^1P^0$) ionization threshold in the vicinity of 2pnl ($^1P^0$) and 2pnd ($^1P^0$) resonances. In order to depict the individual PR cross sections of narrow resonances, we have performed a new set of calculation in vicinity of the only 1s$^2$2pns resonance complexes. The relativistic resonance energies and orbitals were obtained by using the multiconfigurational Dirac-Fock atomic structure code [59].

![Figure 3. Dielectronic recombination (DR) cross section (Mb) versus collision energy (Ryd)](image)

for $e^- + 1s^22s \rightarrow 1s^22p7s - 1s^22s7s + h\nu$ in the C IV ion.

The PI cross sections have been calculated for all the 1s$^2$2sns(1S) states, with $5 \leq n \leq 12$ belonging to Be-like C ion. For a given $n$, the only ten non-relativistic configuration state functions such that 1s$^2$2s, 1s$^2$2p, 1s$^2$2sns, 1s$^2$2snd, 1s$^2$2snf, 1s$^2$2snf, 1s$^2$2pnp, 1s$^2$2pnp, and 1s$^2$2png have been included in the average level (EAL) calculation, while 1s$^2$, 2s$^2$ and 2p$^2$ shells were kept full. These $jj$-coupled configuration state functions (CSF’s) result in a set of 74 levels that are limited to the following symmetry-parity combinations $J\pi = 0^\pm, 1^\pm, 2^\pm, 3^\pm, 4^\pm, 5^\pm$. To stabilize the order of the levels (odd or even), an initial analysis on each parity has been done. The method of procedure is well described in Ref. [20].

Radiative rates were obtained for the decay of even-parity resonance levels to the configurations: 1s$^2$2snp and 1s$^2$2snf, while the autoionization rates were determined for the decay of the even-parity resonance levels to the single configuration levels involving the even-parity configurations 1s$^2$2s$\alpha$, 1s$^2$2s$\sigma$ and 1s$^2$2s$\omega$, $\varepsilon \leq n$. For the decay of odd-parity resonance levels, the radiative rates were determined to the multiconfiguration levels involving the even-parity configurations 1s$^2$2p$^2$, 1s$^2$2sns and 1s$^2$2snd, while the autoionizing rates were determined for the decay of the odd-parity resonance levels to the single configuration levels involving the odd-parity configurations: 1s$^2$2snp, 1s$^2$2sns and 1s$^2$2snf levels. To check the accuracy of the resonance positions, we have compared our calculated energies with those reported by the opacity team [60]. Figure 4 presents on logarithmic scale results
for the PI and RR cross sections involving the only 1s\(^2\)2s7s(^1S) state in Be-like C ion. In this case, relativistic effects are included into the calculation. The photon energy ranges from 0.295 au to 0.3004 au.

![Figure 4](image1.png)

**Figure 4.** Plot on logarithmic scale of the cross sections (in Mb units) for the photoionization, \(\sigma_{\mathrm{PI}}\), and the radiative recombination, \(\sigma_{\mathrm{RR}}\), for state 1s\(^2\)2s7s(^1S) state to 1s\(^2\)2p7s(^1P_0) state in C\(^{2+}\), versus electron collision energy (in Ryd).

The final term in Eq. (2) has been determined using the Fano parameter evaluated directly from the 2-state model of Latinne et al. [61] Figure 5 shows the energy dependence quantum interference cross section (\(\sigma_{\mathrm{int}}\), Mb) contributing to the PR cross section in 1s\(^2\)2s7s-1s\(^2\)2p7s transition calculated in the vicinity of 1s\(^2\)2p7s autoionizing state, in C\(^{2+}\) ion.

![Figure 5](image2.png)

**Figure 5.** Quantum interference cross section (Mb) versus collision energy (Ryd) for 1s\(^2\)2p7s – 1s\(^2\)2s7s transition in C IV.
The state selective photo-recombination cross section have been evaluated for all $\Delta n = 0$ channels in C$^{3+}$ ion at incident electron energies in the vicinity of the $1s^22pns$ autoionizing-configuration complexes. Results are shown in Figure 6.

![Figure 6](image)

Figure 6. The energy dependence profile of photorecombination(PR) cross section (Mb) in the vicinity of $1s^22pns(5 \leq n \leq 10)$ ($^1P^0$) autoionizing states in CIV ion. Damping radiative effect in dielectronic recombination and quantum interference between dielectronic and radiative recombination processes are included into the calculation.

As a result of our analysis[61], we find that for the majority of dielectronic recombination—resonance transitions considered in the present investigation, only a weak degree of asymmetry was found. This is due to the absence of configuration mixing involving $1s^22pnd(^1P^0)$ autoionizing states, which could alter our $\Delta n = 0$ transition rates. In order to obtain more detailed representation for significant and experimentally observable interference effects, the configuration mixing including $1s^22pnd(^3P^0)$ autoionizing states should be considered in a further investigation. This investigation could facilitate the scaling analysis for this isoelectronic sequence. Additionally, the plasma environmental conditions are expected to be important and will be considered in our further theoretical work.

4. Concluding remarks
The present theoretical work reports some results from extensive non-relativistic and relativistic calculation of energy levels and oscillator strengths in the neutral carbon atom. In addition, results from detailed five-state close coupling calculation for photo-recombination cross sections in the Li-like C ions have also been reported.

We have attempted to obtain an accurate description of electron correlations both in the initial and final states of electron scattering on carbon atom. The target model considered here has included the configuration interaction allowing for distortion of the initial-state and excited-state orbitals due to electron correlation effects. Furthermore, based on a variety of comparisons among various calculations with GRASP and FAC codes, our fine structure splitting data are in good agreement with
the experimental values. Based on these various relativistic calculations more detailed investigations are needed for the radiative rates, oscillator strengths, line strengths and lifetimes.

Photo-recombination cross-sections are important to analyze spectra emitted by fusion plasmas. The present theoretical work extends our previous R-matrix Floquet calculation exploring the role of the quantum interference term on the energy dependence profile of photo-recombination cross section. We have presented results for all the set of photo-recombination transitions involving the 1s2pns doubly excited autoionizing states of Be-like C ions. Only a weak degree of asymmetry was found. In order to obtain more detailed representation for significant and experimentally observable interference effects, the configuration mixing including 1s2pnd(P0) autoionizing states should be considered in a further investigation.

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