Atomic Data for Recombination Calculations

R. Kisielius and P. J. Storey
Department of Physics and Astronomy, University College London,
Gower St., London, WC1E 6BT, UK

A. R. Davey
Mullard Space Science Laboratory, University College London,
Holmbury St Mary, Dorking, Surrey, RH5 6NT, UK

1   Introduction

There exists a significant discrepancy in the abundances of carbon, nitrogen, oxygen, and neon ions that are derived for photoionised nebulae from recombination lines and from collisionally excited forbidden lines. This discrepancy emphasises the need for accurate theoretical work on bound-bound and bound-free radiative data for atomic ions. Such data were generated by the Opacity Project, using the R-matrix formulation of the close-coupling approximation, but are often inadequate for the calculation of recombination coefficients due to the presence of narrow, but important near-threshold resonances which are inadequately resolved and inaccurately positioned. We report on a programme of systematic new calculations of radiative data and line recombination coefficients for singly-ionised atoms of the astronomically most abundant elements (C, N, O, Ne) which uses quantum defect techniques to accurately map resonances.

2   Photoionisation Cross-sections

We treat the $(N+1)$-electron scattering problem in the close-coupling (CC) approximation. Bound states and continuum states of the system are determined using the R-matrix method (see Berrington *et al* [1]) and from the resulting wave functions, radiative data for gf-values (bound-bound transitions) and photoionisation cross-sections (bound-free transitions) are calculated.

Configuration-interaction (CI) wave functions for the N-electron target systems are computed with the SUPERSTRUCTURE code of Nussbaumer and Storey [2]. In the Opacity Project calculations, the CI expansion of the target wave functions consists of $1s$, $2s$, $2p$ spectroscopic orbitals for C, N, O, Ne ions. We expand the configuration basis by adding $\bar{3}s$, $\bar{3}p$, $\bar{3}d$, $\bar{4}f$ pseudo orbitals for C III target and all $\bar{3}l$ and $\bar{4}l$ pseudo orbitals for N III target. In photoionised nebulae, the electron temperature is generally below $20\,000\ K$, so only the near threshold resonances are important in determining recombination coefficients. The non-physical resonances that arise from the use of non-physical correlation orbitals are not a problem at low energies.

The photoionisation cross-sections typically exhibit resonances due to photoexcitation of the core electrons followed by autoionisation. A simple example for C II ions is

$$2s^2nl + h\nu \rightarrow 2s2pnl' \rightarrow 2s^2 + \varepsilon l''. \tag{1}$$

We use quantum defect theory to determine resonance positions and widths. Resonances are due to poles in the scattering matrix $\mathcal{S}$ described by a matrix χ which varies slowly with energy

and contains functions pertaining to both open (o) and closed (c) channels:

$$\mathcal{S} = \chi_{oo} - \chi_{oc}[\chi_{cc} - \exp(-2\pi i\nu]^{-1}\chi_{co}. \tag{2}$$

Diagonalisation of the matrix χ_{cc} yields the effective quantum numbers, ν related to the complex quantum defect μ_c

$$\mu_c = \alpha_c + i\beta_c \tag{3}$$

by $\nu = n - \mu_c$. The energy of the pole $\varepsilon(pole)$ is given by

$$\varepsilon(pole) = \varepsilon_c - (n - \alpha)^{-2} - \frac{i}{2}\gamma \tag{4}$$

where $\gamma = 4\beta(n - \alpha)^{-3}$ is the autoionisation width of resonance and ε_c is the appropriate target energy.

In contrast to the OP data, we use a variable step energy mesh for photoionisation cross-sections that delineates all resonances to a prescribed accuracy. In the first step of the calculation, we determine resonance positions and widths using a coarse energy mesh. In the second step, we determine a new fine energy mesh of variable step length $\Delta\varepsilon$ assuming a Lorentzian profile for the resonance:

$$F(\varepsilon, \gamma) = \frac{(\frac{\gamma}{(2})^2}{(\varepsilon - \varepsilon(pole))^2 + (\frac{\gamma}{2})^2}. \tag{5}$$

To calculate recombination coefficients, we integrate the photoionisation cross-sections using a 3-point Simpson's rule. If we specify a required accuracy as ΔF, we can find the necessary energy interval for a given resonance:

$$\Delta\varepsilon = \frac{90 \times \Delta F}{F^{(4)}(\xi)} \tag{6}$$

where $F^{(4)}(\xi)$ is the 4th derivative of the Lorentzian function. The adopted step length is the smallest value of $\Delta\varepsilon$ obtained for any resonance. In the third step we calculate photoionisation cross-sections using the new variable step mesh.

The Opacity Project photoionisation data were generated using a relatively coarse energy mesh. These data sometimes have poor resolution in resonance areas. In Fig.1, we show the photoionisation cross-sections for the $2s2p^2$ ^{2}D state of the C II ion. One can notice a difference in the number of energy points and in the resonance resolution. As a result, the area under the cross-section for the $2s2p^2$ ^{2}D state (Fig.1) is 1.585 Mb·Ry from the Opacity Project data and 4.573 Mb·Ry from our data. These differences are reflected directly in the recombination coefficients.

All *ab initio* calculations of the photoionisation cross-sections position the resonances incorrectly. An error of a few thousand inverse centimetres in a resonance position is typical and may significantly affect the resulting recombination coefficients, particularly at low temperatures (10 000 K or less). It is worth noting that earlier work on low-temperature dielectronic recombination (e.g. Storey, [3]), which treats the resonances as bound states, uses the experimental resonance positions and is not vulnerable to this uncertainty, although the quality of the wave functions and hence the radiative data, was certainly inferior. Therefore for C II ions, where near-threshold resonances $2s2p(^3P^o)3d$ ^{2}F^o and ^{2}P^o make important contributions to the recombination coefficient, and the resonance positions are experimentally known, we adjust the resonance positions to their experimental values: 3301 cm^{-1} and 5523 cm^{-1} above the $2s^2$ ^{1}S threshold instead of theoretical values of 3778 cm^{-1} and 6127 cm^{-1}. This is done by calculating the resonance contribution to the recombination coefficient from a Fano profile fit to the cross-section near the resonances rather than from the calculated cross-sections themselves. The resonance positions can then be adjusted within the fit. These adjustments bring about an increase of 20% in the total recombination coefficient for the $2s2p^2$ ^{2}D state at temperatures below 5000 K.
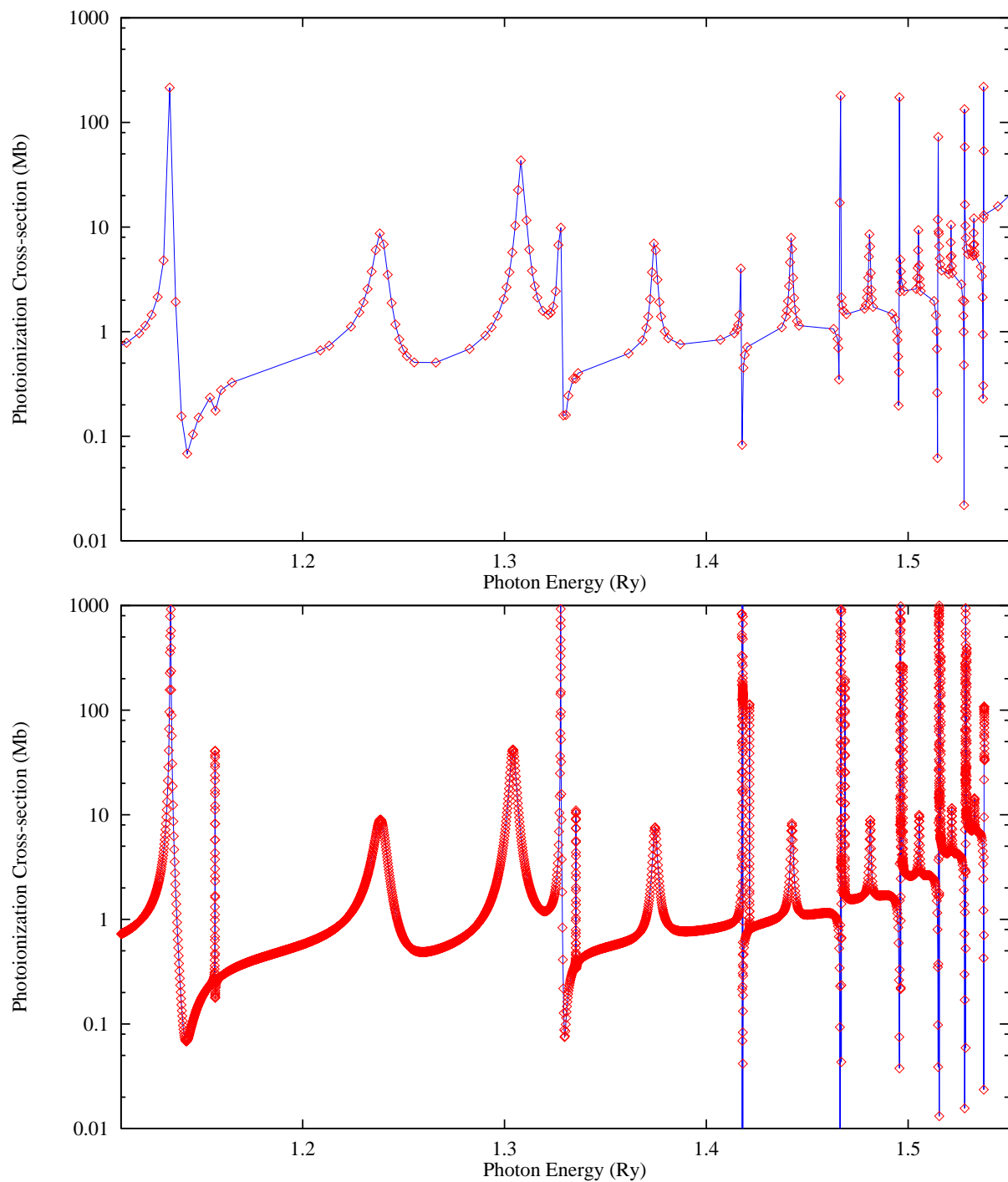
Figure 1: Comparison of the C II photoionisation cross-section for 2s2p² ²D calculated by the Opacity Project (top) and this work. The OP cross-section consists of 199 points, based on a quantum defect mesh, whilst the latter is based on an energy mesh of 3281 points.

3   The Level Population Problem

We calculate recombination coefficients for C II, N II, O II and Ne II ions. We determine both the total recombination coefficients and the effective recombination coefficients for particular spectral lines as functions of electron temperature T_e and electron density N_e. In our model, recombination rates are determined using the LS-coupling scheme for ion states and, therefore, assuming no radiative transitions between states of different multiplicity.

Because of the very large number of levels included into the model, we have to partition the calculation of level populations according to the principal quantum number n. We define a principal quantum number $n = n_d$, such that for $n < n_d$, the population structure is determined solely by radiative processes. Collisionally induced transitions for these levels can be neglected. The value of n_d depends on plasma density and temperature.

For $n > n_d$, the population depends on n and l-changing collisions and populations are taken from purely hydrogenic calculation of departure coefficients, b_{nl} by Hummer and Storey [4]. For $10 < n \leq n_d$, populations are still determined only by radiative transitions but no accurate atomic data are available. Various approximate methods (quantum defect method, Coulomb approximation, hydrogenic approximation (when $l > 3$)) are used to obtain the necessary rate coefficients. For $n < 10$, all atomic terms are included in the calculation of populations, irrespective of their parentage. It is assumed that the population is determined solely by recombination and radiative cascading from higher states.

4   Theoretical Emission Spectra and Ion Abundances

The calculated level populations together with gf-values are used to calculate theoretical emission spectra. Lines arising from $3d - 3p$ and $4f - 3d$ transitions in O II ions are prominent in observed spectra of some astrophysical objects. Comparing the measured intensities of these lines with those for hydrogen lines, we are able to determine abundances of O^{2+} ions in observed objects.

Theoretical spectra were determined using intermediate coupling (IC) and LSJ-coupling schemes. For intermediate coupling (IC) spectra, we use level populations determined in LS-coupling and gf-values calculated using the Breit-Pauli Hamiltonian with spin-orbit interaction included. Alternatively, LSJ-coupling spectra are computed using the same LS-coupling level populations and splitting multiplet intensities using angular algebra only.

Relative intensities of various multiplets are used to determine the O^{2+} ion abundances in the planetary nebulae NGC 7009 and NGC 3242. The need for IC calculations was demonstrated by the comparison of the theoretical spectra with observed data by Liu *et al* [5]. Use of IC reduced significantly the scatter of the derived abundances demonstrating a breakdown of LSJ-coupling. Using IC yields considerable improvement in the consistency of the derived abundances.

References

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