Resolution and accuracy of resonances in R-matrix cross sections

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Abstract. We investigate the effect of resonances in photoionization and recombination cross sections computed using the R-matrix method. Photoionization and recombination rate coefficients derived from high-resolution cross sections for oxygen ions are compared with earlier works with less resolution and accuracy, such as in the widely used Opacity Project data. We find significant differences in photoionization rates for O II metastable states, averaged over Planck functions corresponding to ionizing radiation fields, with respect to the intrinsic accuracy of the calculations and improved resolution. Furthermore, for highly charged ions other physical effects are also important. Recombination rate coefficients, averaged over a Maxwellian distribution, are extremely sensitive to the position and resolution of near-threshold resonances, and radiation damping, in \((e + O \text{ VII}) \leftrightarrow O \text{ VI} + h\nu\). Surprisingly however, the effect on the monochromatic and the mean Rosseland and Planck bound-free opacities is relatively small, but may be potentially significant.

1. Introduction

A precise treatment of resonances has always been of prime concern in coupled channel calculations for electron impact excitation, photoionization, and recombination. Sophisticated methods have been employed to resolve and/or fit resonances in order that cross sections and averaged rates, the quantities of interest in applications, may be computed accurately. One of the main reasons that the powerful R-matrix method (Burke et al 1971, Hummer et al 1993, Burke and Berrington 1993) has been very successful is because it enables efficient calculations at a large number of energies to affect such a resolution. Following a single diagonalization of the R-matrix for each total electron-ion symmetry LS\(\pi\) or J\(\pi\), cross sections may be obtained at any number of energies. The R-matrix method, and its relativistic variant the Breit-Pauli R-matrix method (BPRM, Berrington et al, 1995), have been employed in large-scale calculations in the Opacity Project (OP, Seaton et al 1994, The Opacity Project Team 1995, 1996),
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and the Iron Project (IP, Hummer et al 1993) for radiative and collisional cross sections for most astrophysically abundant elements, nearly 200 atoms and ions. The OP/IP work involves photoionization and electron scattering cross sections, as well as transition probabilities. The R-matrix method (and BPRM) has been further extended to a unified treatment of electron-ion recombination including radiative and di-electronic recombination (RR and DR) in an ab initio manner, which is also self-consistent with R-matrix photoionization cross sections (Nahar and Pradhan 1992, 1994a; Zhang and Pradhan 1997, Zhang et al 1999, Nahar and Pradhan 2003a). A crucial aspect of the unified method for \((e + \text{ion})\) recombination is the high resolution imperative for the derivation of accurate rate coefficients. However, some physical effects are also very important in determining the accuracy of computed parameters as we demonstrate in this paper. The present work also addresses some of the issues and results described by Ramirez and Bautista (2002).

2. Results

The effect of resolution and accuracy of resonances depends on physical processes. The height of photoionization resonances is theoretically unbounded, unlike electron-ion excitation cross sections where it is limited by the unitarity constraint on the scattering matrix. Therefore resonances in photoionization cross sections may approach unphysical heights if all relevant physical effects are not carefully considered. A complete resolution of resonances in photoionization cross sections, particularly for higher \(n\) and \(\ell\), is difficult to achieve. Neither can the calculated resonances be individually verified by experiments, since the measured cross sections are averages over the beam width and shape. Nevertheless, R-matrix calculations for photoionization cross sections have been experimentally verified, some computed in LS coupling prior to experiments. For example, we note the extremely detailed comparison between R-matrix cross sections and recent experiments on synchrotron based light sources reported by the Reno/Berkeley group for O II (Covington et al, 2001), the Aarhus group for C II (Kjeldsen et al. 1999, Nahar 2002), and the Paris group for O ions (Champeaux et al 2003, Nahar 2004). Near-threshold resonances need to be carefully resolved, often with relativistic fine structure. In the relativistic Fe XVII photorecombination calculations including 359 bound levels with \(n < 10\), Zhang et al (2001) explicitly delineate 2,985 resonances in a very small near-threshold region 0 - 5eV.

2.1. Photoinization cross sections and rates

In Fig. 1 we compare high-resolution R-matrix photoionization cross sections for the ground and two metastable states of O II, \(2s^22p^3(4S^o, 2D^o, 2P^o)\), with the OP data from Topbase (Cunto et al 1993, http://vizier.u-strasbg.fr/OP.html, http://heasarc.gsfc.nasa.gov/topbase/home.html). The OP cross sections were the most accurate attempt at the time of computations to resolve resonances. In general, instead
of a constant energy mesh, a quantum-defect mesh was employed to enable similar
resolution of resonances along a Rydberg series as they get narrower with increasing
n. The quantum-defect mesh ensures a pre-determined number of points (usually 100)
to resolve each range of effective quantum number (ν, ν + 1). Although this does not
guarantee complete resolution, and the OP cross sections may still be under-resolved
for certain applications such as monochromatic spectral modeling, they are considerably
better than those with constant energy mesh.

The new results reported in this work are obtained as in the recent calculations for
a number of oxygen ions, O II - O V, using a more extensive eigenfunction expansion
for the target ion than in the OP work; they are in good detailed agreement with
recent experimental measurements (Nahar 2003). Extensive resonances structures are
delineated, especially in the near-threshold region. As Fig. 1 shows, resonances are
more completely resolved in the present calculations, including those along a Rydberg
series converging on to excited thresholds. Moreover, one important point is that the
resonances positions are at somewhat different energies compared to the corresponding
OP data.

Photoionization rates Γ_{PI} are computed using both the present and the OP cross
sections, assuming ionizing radiation fields from a blackbody source (B_{ν}(T)) at radiation
temperatures T represented by a Planck function.

\[
Γ_{PI} = W \int \frac{4πB_{ν}(T)σ_{PI}(ν)}{hν} dν
\]

(1)

\[
B_{ν}(T) = \left( \frac{2hν^3}{c^2} \right) \left[ exp\left( \frac{hν}{k_B T} \right) - 1 \right]^{-1}
\]

(2)

where W is a dilution factor (set to 1 for the present study) and σ_{PI} is the photoionisation
cross section.

We can see in Fig.1, the ground state cross sections agree well. The position of
the resonances are identical. Their heights differ but, as shown below, it should not
affect the rates significantly because the area under these peaks is not significant since
the resonances are narrow. For the two metastable states a shift in the position of the
resonances can be seen. The difference in resolution also modifies the computed shape of
the resonances, especialy for the first ones. These two factors, resolution and accuracy of
the position of the resonances, results in significant deviations in photoionisation rates.

In Fig.2 we present the percentage difference in the rates, obtained using OP cross
sections and the present data, for the three lower states of O II at radiation temperatures
ranging from 10^3 – 10^5 K. While there is little differences for the ground state \(^4S^o\),
because the cross sections agree very well in the position of the resonances as well as
in the resolution between the two set of data, the differences for the two metastable
states are quite significant, up to 30% for \(^2P^o\), and up to 55% for the \(^2D^o\). In order
to ascertain whether the differences are due to resolution, or accuracy as reflected in
the different positions of resonances, another set of rates are obtained on shifting the
resonance positions by a slight amount to match in the two sets of data. This reduces
the differences by 10%, with new maximum differences of 20% and 45%. Resolution
also plays a role in the discrepancy. For the metastable states \(^2P_o\), \(^2D_o\), the first resonance is much broader in the OP data. The areas under this first peak are 1.8 and 1.9 times higher respectively for the OP cross sections compared to the present set. This affects the low temperature regime more severely since the first resonance is crucial in convolving with the Planck function, although less so than with a Maxwellian, considered next.

### 2.2. Recombination rates

A similar situation exists for the highly charged ion Li-like O VI. In previous calculations it was shown that the large KLL resonances were severely under-resolved in previous works, and a very high resolution is required in order to obtain converged values for the resonance oscillator strengths. The peak values of resonances rise more that 4 orders of magnitude above the background cross sections. Moreover, since the core ion is He-like, with a large radiative decay rate for the dominant core \(1s2p(1P_o) \rightarrow 1s^2(1S_0)\) transition, radiation damping is important (Zhang et al 1999). This is particularly so in the calculation of unified photo-recombination rate coefficients for \((e + O \text{ VII}) \leftrightarrow O \text{ VI} + h\nu\) (Nahar and Pradhan 2003b). The unified scheme to obtain total recombination rates, including RR and DR, entails: (A) highly resolved calculations of photoionization cross sections of a large number of bound levels, typically several hundred levels with effective quantum number \(\nu \leq 10\), and (B) DR calculations using an adaptation of the Bell and Seaton theory (1985, Nahar and Pradhan 1994a) for \(10 < \nu \leq \infty\). In addition, for any given ion self-consistency is assured in an ab initio manner between total photoionization and recombination since the same wavefunction expansion is employed for both processes (see Nahar 2003, and references therein).

Another advantage of the method is that level-specific cross sections and rates for all levels with \(\nu \leq 10\) are also obtained.

Total and level-specific rate coefficients for recombination to O VI and O VII have been reported by Nahar and Pradhan (2003b). In a recent work, Ramirez and Bautista (2002) calculated photoionization cross sections for the ground state of highly charged ions such as O VI and Fe XXIV using a method to locate resonances for high resolution (Quigley and Berrington 1996), but neglecting effects such as fine structure and radiation damping. Therefore their photo-recombination rate coefficients are in error by large amounts, as seen in Fig. 3; there is over an order of magnitude discrepancy relative to Nahar and Pradhan (2003b). Thus in this case it is seen that both resolution and accuracy, as reflected in the neglected physical effects, are important. In their work Ramirez and Bautista (2002) discuss the earlier photoionization and \((e + \text{ ion})\) recombination calculations for Fe XVII by Pradhan et al (2001); however their uncertainly estimates of “25-50%” for “integrated resonance contributions” are not derived from direct computations, and are much higher than those computed by Zhang et al (2001).
2.3. Opacity

Finally, we investigate these effects on a larger scale, in the total opacity of O II. Fig. 4 shows the monochromatic bound-free (bf) opacity due to O II (in atomic units) at a representative stellar temperature of $2 \times 10^4$ K and electron density of $10^{17}$ cm$^{-3}$, computed as described in Seaton et al (1994).

$$
\kappa_{bf}(\nu) = \sum_i N_i \sigma_{i}^{bf}(\nu)[1 - e^{-\frac{h\nu}{k_BT}}]
$$  \hspace{1cm} (3)

The top panel shows results using the present high-resolution photoionization data for 329 bound states of O II, compared with results from OP data. At this temperature and density, 197 bound states of O II contribute to the bf-opacity in the present calculations, and 169 in the OP data. The difference in number of bound states is inconsequential; the additional states in the present work are mostly highly excited ones. The monochromatic opacity is sampled at $10^5$ points in both calculations. As Fig. 4 shows, there is overall very good agreement between the two sets, despite significantly better resolution and accuracy of the present calculations. This is expected since strong features dominate the opacity spectrum, and are found in both sets of calculations. The present Rosseland and Planck mean bf-opacities

$$
\frac{1}{\kappa_{bf}^R} = \int \frac{1}{\kappa_{bf}^P} F_R(\nu) d\nu
$$  \hspace{1cm} (4)

$$
\kappa_{bf}^P = \int \kappa_{bf}^P F_P(\nu) d\nu
$$  \hspace{1cm} (5)

where

$$
F_R(\nu) = \frac{15}{4\pi^4} \left(\frac{h\nu}{k_BT}\right)^4 \frac{e^{-\frac{h\nu}{k_BT}}}{(1 - e^{-\frac{h\nu}{k_BT}})^2}
$$  \hspace{1cm} (6)

$$
F_P(\nu) = \frac{15}{4\pi^5} \left(\frac{h\nu}{k_BT}\right)^3 \frac{e^{-\frac{h\nu}{k_BT}}}{(1 - e^{-\frac{h\nu}{k_BT}})}
$$  \hspace{1cm} (7)

are 0.159 and 2.12 respectively, compared to 0.146 and 2.42 from the OP data, i.e. the Rosseland means are 8% higher, and the Planck means are 14% lower than OP (electron scattering opacity is included to provide a background, and is the same in both calculations). In the present opacity calculations the resonances are better resolved, and in many cases narrower compared to the OP data, which results in a smaller Planck mean; conversely, since the minima in resonances are better sampled, the Rosseland mean is slightly higher. However, the total Rosseland mean opacities differ only by 2.6%, if we include the same (much larger) bound-bound contribution from lines in the two calculations — 0.345 from the present vs. 0.336 from the OP data.
3. Conclusion

In conclusion we note that:

1. For photoionization and NLTE modeling applications, it may be necessary to compute photoionization cross sections with higher accuracy and resolution than in the Opacity Project data. Accuracy of resonance positions is crucial in the determination of \((e + \text{ion})\) and photoionization rates. A number of self-consistent computations are in progress as part of a program to calculate photoionization and unified \((e + \text{ion})\) recombination (RR plus DR) cross sections and rates (Nahar and Pradhan 2003a).

2. Although the monochromatic and mean opacities are not measurably different using the high-resolution data for oxygen ions, as opposed to the Opacity Project data, these quantities may differ considerably for more complex atomic systems such as the low ionization stages of iron. In a previous work (Nahar and Pradhan 1994b), we showed that the Rosseland mean opacities using new improved data for Fe II differed by up to 50% from OP values. There is increasing evidence that there is "missing UV opacity", possibly due to Fe I, that is critical to the determination of abundances in the Sun and other objects (e.g. Asplund 2003). New atomic and opacities calculations for iron ions are needed with higher accuracy and resolution.

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Figure 1. Photo-ionization cross sections of the ground state $1s^22s^22p^3\,(^4S^o)$ and two meta-stable states $1s^22s^22p^3\,(^2P^o,\,^2D^o)$ of O II (from top to bottom). The present high-resolution data are on the left and the Opacity Project data from Topbase are on the right. The insets show the shift in resonance positions and the effect of resolution in the near threshold region.
Figure 2. Percentage differences in photoionization rates for the ground state $1s^22s^22p^3(4S^o)$ and metastable states $1s^22s^22p^3(2P^o, 2D^o)$ of O II, at radiation temperatures $T_{rad}$. 
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Figure 3. Photo-recombination rate coefficient for the ground state of O VI (1s²2s²S₁/₂): solid line - using cross sections from Nahar and Pradhan (2003), dashed line - Ramirez and Bautista (2002); the differences are due to neglect of radiation damping in the latter calculations.
Figure 4. Monochromatic bound-free opacity of O II using the present high-resolution atomic data for photoionisation cross sections of 329 bound states (upper panel), and using the Opacity Project data for the same states (lower panel).