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Theoretical calculations of the H I, He I and He II free-bound continuous emission spectra

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ABSTRACT

We present coefficients for the calculation of the continuous emission spectra of H I, He I and He II due to electron-ion recombination. Coefficients are given for photon energies from the first ionization threshold for each ion to the $n = 20$ threshold of hydrogen (36.5μ), and for temperatures 100 K $\leq T \leq 10^5$ K. The emission coefficients for He I are derived from accurate *ab initio* photoionization data. The coefficients are scaled in such a way that they may be interpolated by a simple scheme with uncertainties less than 1% in the whole temperature and wavelength domain. The data are suitable for incorporation into photoionisation/plasma codes and should aid with the interpretation of spectra from the very cold ionised gas phase inferred to exist in a number of gaseous clouds.

Key words: atomic data

1 INTRODUCTION

Analyses of optical recombination line (ORL) spectra of photoionised regions have suggested the existence of cold ionised gas (100 K–2000K), mixed within a warmer component at more typical nebular electron temperatures (8000 K–10000 K). The pockets of cold ionised gas of high metal content are invoked as a possible explanation of the long-standing problem of the discrepancy between elemental abundances derived from ORLs and those derived from collisionally excited lines (CELs). In this scenario, ORLs and CELs are preferentially emitted by the cold and warm phases, respectively (for a recent review see Liu, 2002); this problem is closely linked to the observation that Balmer jump temperatures of H II regions and Planetary Nebulae are systematically lower than those derived from the [O III] nebular to Auroral line ratio (Liu & Danziger 1993).

Understanding the complex spectra arising from such regions relies on the construction of detailed photoionisation models able to account for all gas phases that may be present. Currently, one of the major limitations in such modelling is the lack of an accurate atomic data set extending to such low temperatures. The need of low-temperature effective recombination coefficient for the calculation of recombination lines for metals is apparent. However, in addition to the discrete emission line spectrum, a continuous emission is also produced by the ionised gas, mainly due to free-bound recombination processes of hydrogen and helium ions, free-free transitions in the Coulomb fields of H^+, He^+ and He^{2+} and two-photon decay of the $2\ ^2S_{1/2}$ level of H I and He II, and, less importantly of the $2\ ^1S_0$ level of He I. Accurate continuous emission coefficients are essential for the correct prediction of the Balmer jump by photoionisation codes.

The importance of the continuum processes listed above has long been known and emission coefficients have been tabulated (see e.g. Seaton 1955, 1960; Brown & Mathews 1970), for a range of temperatures and wavelengths mainly aimed at the study of optical data for classical H II regions. Ferland (1980) derived H I and He II continuous emission and recombination coefficients for a wider range of temperatures (500 K–$2{\cdot}10^6$ K) and wavelengths to aid the interpretation of ultraviolet (UV) and infrared (IR) as well as optical data from nova ejecta.

In this work we present new calculations of the H I, He I and He II continuous emission coefficients due to free-bound recombination, over temperatures ranging from 100 K to 10^5 K, for the physical conditions thought likely to occur in chemically inhomogeneous regions, which may include pockets of cold ionised material intermixed within typical nebular gas.

2 CALCULATIONS METHOD

Using the Saha-Boltzmann equation and the Milne relation, we may express the continuous emission coefficient $\gamma(\nu)$ corresponding to the recombination process

$$X^+ + \mathrm{e}^-(\epsilon) \rightarrow X^* + h\nu$$

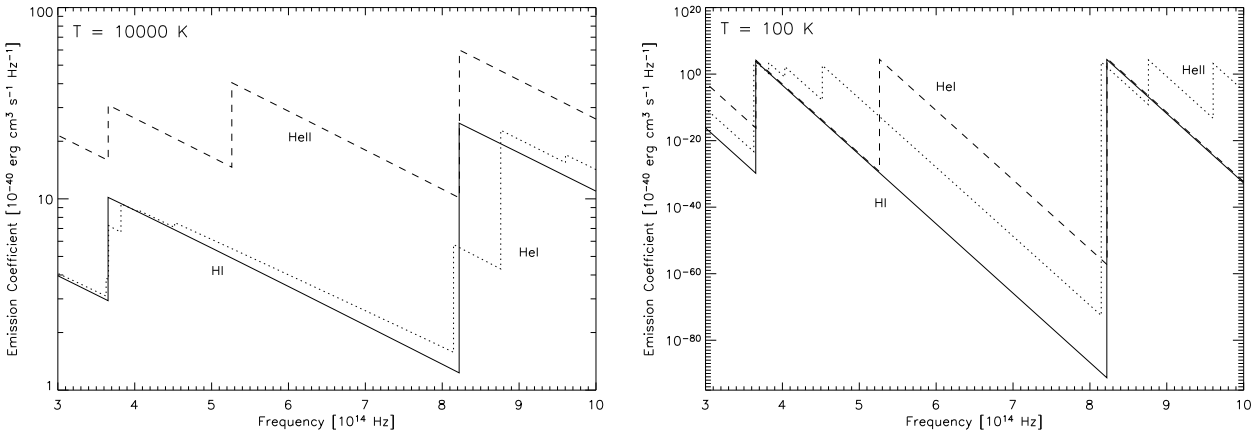

Figure 1. Frequency-dependent continuum emission coefficients $\gamma(\nu)$ for H I (*solid line*), $\gamma(\nu)$ for He I (*dotted line*) and $\gamma(\nu)$ for He II (*dashed line*), calculated at T = 10000 K (left panel, to be compared with Figure 1 from Brown & Matthews, 1970) and T = 100 K (right panel).

in terms of the photoionization cross-section $\sigma_\nu(X^*)$

$$\gamma(\nu) = \frac{4\pi h}{c^2}(\frac{h^2}{2\pi mkT})^{3/2}\mathrm{e}^{-\epsilon/kT}\frac{\omega^*}{\omega^+}\nu^3\sigma_\nu(X^*)$$

where ω^+ and ω^* are the statistical weights of the recombining ion initial state and final state respectively, and ϵ is the free electron energy. In terms of $\gamma(\nu)$, the energy emitted per unit volume per unit time in frequency interval ν to $\nu + \mathrm{d}\nu$ is $N_e N(X^+)\gamma(\nu)\mathrm{d}\nu$.

For the contribution $\gamma_n(\nu)$ at frequency ν from recombinations to states of principal quantum number n of H^0 and He^+ we compute the necessary energy-dependent photoionization cross-sections using the hydrogenic codes described by Storey & Hummer (1991). The total emission coefficient $\gamma(\nu)$ is then

$$\gamma(\nu) = \sum_{n_0}^{\infty}\gamma_n(\nu)$$

where in practice we truncate the sum at $n = 200$ for H I and $n = 350$ for He II, which is sufficient to ensure convergence to all figures given in the Tables.

For recombination to atomic helium we use the *ab initio* calculated photoionization cross-sections described by Hummer & Storey (1998). Cross-section data are available for n^1S, n^3S, n^1P^o, n^3P^o, n^1D, n^3D, n^1F^o and n^3F^{o}states with $l + 1 \leq n \leq 20$. For higher values of n and for $l > 3$ we use hydrogenic data. Thus for $n \geq 5$ the emission coefficient has nine distinct thresholds for each n corresponding to the eight separate terms plus a threshold at the hydrogenic energy. Hummer & Storey (1998) showed that the results of their *ab initio* calculation of the photoionization cross-sections are in better agreement at threshold with the highly accurate bound-bound calculations of Drake (1996) than any of the other methods used to compute helium recombination processes.

Contributions due to bremsstrahlung emission of a Maxwellian distribution of electrons in the Coulomb fields of hydrogen and helium ions are not included in our results, but can be obtained readily using (e.g.) equation 2 of Brown & Mathews (1970) or the free-free computer code published by Storey & Hummer (1991).

Contributions to the continuum emission from two-photon emission are also not included but can be computed using the formulae of Nussbaumer & Schmutz (1984).

3 RESULTS

The full tables of continuous emission coefficients, Tables 3, 4 and 5 for H I, He II and He I respectively are available in electronic form only. In Table 1 we show an extract from the table for H I. Coefficients are tabulated for log T[K] = 2.0(0.1)5.0 and for photon energies (in Rydbergs) from just less than the ground state threshold energy to just above the energy of the threshold at $n = 20$. Values are tabulated on either side of each threshold and at some additional nodal points inserted to make interpolation sufficiently accurate. At low temperatures the coefficients fall rapidly and exponentially at energies above each threshold making interpolation difficult so rather than $\gamma(\nu)$ we tabulate $\gamma^\dagger(\nu)$ defined by

$$\gamma^\dagger(\nu) = \gamma(\nu)\ 10^{34}\ T^{3/2}\mathrm{e}^{\Delta E/kT} \quad (1)$$

$$= \gamma(\nu)\ 10^{40}\ t^{3/2}\mathrm{e}^{15.7887\Delta E_R/t} \quad (2)$$

where $t = T[K]/10^4$, ΔE is the difference between the photon energy, hν, and the energy of the nearest threshold of lower energy and ΔE_R is the same energy in Rydberg units. Thresholds are indicated by index 1 and additional nodal points by index 0.

The recommended procedure for deriving the emission coefficient at a given temperature and photon energy is to interpolate linearly in the appropriate table in the variables log T and photon energy to obtain the scaled coefficient $\gamma^\dagger(\nu)$. Equation 1 can then be applied to obtain $\gamma(\nu)$. Table 2 gives exact values of $\gamma(\nu)$ and values derived from the recommended interpolation scheme for each ion at a range of photon energies.

Comparison of the tabulated values with calculations performed on a finer frequency grid and temperature grid show that linear interpolation in log T and photon energy yields accurate results with maximum deviations of 1% and average deviations much smaller than this.

Figure 1 shows the non-scaled continuum emission coefficients, $\gamma(\nu)$ for H I, He I and He II in the optical wavelength range for a temperature of 10000 K (left panel) and 100 K (right panel). The left panel of figure 1 is directly comparable to figure 1 of Brown & Mathews (1970). We can only compare the magnitude of the discontinuity at each threshold directly with the results of Brown & Matthews (1970), since their results incorporate all continuum processes while ours only deal with free-bound processes. Comparing results for H I and He II we find a maximum difference

Table 1. [Abridged] Scaled H I free-bound continuum recombination coefficients, $\gamma^{\dagger}(\nu)$ for H I [erg cm^{-3} sec^{-1} Hz^{-1}].

	E [Ryd]	log T [^{o}K]											
		2.0	2.1	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0	.....
.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....
1	0.00999455	1.764E-01	1.891E-01	2.069E-01	2.309E-01	2.622E-01	3.015E-01	3.485E-01	4.021E-01	4.603E-01	5.205E-01	5.800E-01	.....
1	0.00999457	2.188E-01	2.289E-01	2.441E-01	2.659E-01	2.954E-01	3.340E-01	3.822E-01	4.398E-01	5.052E-01	5.756E-01	6.479E-01	.....
1	0.01233896	2.216E-01	2.318E-01	2.472E-01	2.691E-01	2.989E-01	3.378E-01	3.865E-01	4.445E-01	5.103E-01	5.812E-01	6.540E-01	.....
1	0.01233898	2.891E-01	2.959E-01	3.075E-01	3.257E-01	3.520E-01	3.882E-01	4.359E-01	4.956E-01	5.669E-01	6.477E-01	7.346E-01	.....
1	0.01561650	2.935E-01	3.004E-01	3.122E-01	3.306E-01	3.572E-01	3.938E-01	4.419E-01	5.022E-01	5.742E-01	6.557E-01	7.433E-01	.....
1	0.01561652	4.040E-01	4.072E-01	4.142E-01	4.270E-01	4.478E-01	4.788E-01	5.225E-01	5.808E-01	6.546E-01	7.434E-01	8.444E-01	.....
1	0.02039707	4.115E-01	4.148E-01	4.219E-01	4.349E-01	4.560E-01	4.875E-01	5.317E-01	5.907E-01	6.653E-01	7.551E-01	8.572E-01	.....
1	0.02039709	5.979E-01	5.987E-01	6.013E-01	6.076E-01	6.203E-01	6.424E-01	6.774E-01	7.284E-01	7.983E-01	8.889E-01	9.997E-01	.....
1	0.02776269	6.119E-01	6.128E-01	6.154E-01	6.218E-01	6.347E-01	6.572E-01	6.928E-01	7.446E-01	8.156E-01	9.075E-01	1.020E+00	.....
1	0.02776271	9.433E-01	9.433E-01	9.437E-01	9.451E-01	9.495E-01	9.599E-01	9.805E-01	1.016E+00	1.072E+00	1.153E+00	1.261E+00	.....
1	0.03997831	9.720E-01	9.720E-01	9.724E-01	9.738E-01	9.783E-01	9.890E-01	1.010E+00	1.047E+00	1.103E+00	1.186E+00	1.296E+00	.....
1	0.03997833	1.617E+00	1.617E+00	1.617E+00	1.617E+00	1.617E+00	1.619E+00	1.624E+00	1.639E+00	1.668E+00	1.721E+00	1.804E+00	.....
0	0.05000000	1.652E+00	1.652E+00	1.652E+00	1.652E+00	1.652E+00	1.654E+00	1.660E+00	1.675E+00	1.705E+00	1.758E+00	1.842E+00	.....
1	0.06246618	1.683E+00	1.683E+00	1.683E+00	1.683E+00	1.684E+00	1.686E+00	1.692E+00	1.706E+00	1.737E+00	1.791E+00	1.876E+00	.....
1	0.06246620	3.120E+00	3.120E+00	3.120E+00	3.120E+00	3.120E+00	3.120E+00	3.120E+00	3.121E+00	3.126E+00	3.140E+00	3.174E+00	.....
0	0.07000000	3.162E+00	3.162E+00	3.162E+00	3.162E+00	3.162E+00	3.162E+00	3.162E+00	3.163E+00	3.168E+00	3.183E+00	3.216E+00	.....
0	0.09000000	3.246E+00	3.246E+00	3.246E+00	3.246E+00	3.246E+00	3.246E+00	3.246E+00	3.247E+00	3.252E+00	3.267E+00	3.301E+00	.....
1	0.11105122	3.308E+00	3.308E+00	3.308E+00	3.308E+00	3.308E+00	3.308E+00	3.308E+00	3.309E+00	3.314E+00	3.329E+00	3.364E+00	.....
1	0.11105124	7.258E+00	7.258E+00	7.258E+00	7.258E+00	7.258E+00	7.258E+00	7.258E+00	7.258E+00	7.258E+00	7.258E+00	7.259E+00	.....
0	0.12000000	7.340E+00	7.340E+00	7.340E+00	7.340E+00	7.340E+00	7.340E+00	7.340E+00	7.340E+00	7.340E+00	7.340E+00	7.341E+00	.....
0	0.14000000	7.493E+00	7.493E+00	7.493E+00	7.493E+00	7.493E+00	7.493E+00	7.493E+00	7.493E+00	7.493E+00	7.493E+00	7.495E+00	.....
0	0.18000000	7.716E+00	7.716E+00	7.716E+00	7.716E+00	7.716E+00	7.716E+00	7.716E+00	7.716E+00	7.716E+00	7.717E+00	7.718E+00	.....
1	0.24986635	7.964E+00	7.964E+00	7.964E+00	7.964E+00	7.964E+00	7.964E+00	7.964E+00	7.964E+00	7.964E+00	7.964E+00	7.966E+00	.....
1	0.24986637	2.365E+01	2.365E+01	2.365E+01	2.365E+01	2.365E+01	2.365E+01	2.365E+01	2.365E+01	2.365E+01	2.365E+01	2.365E+01	.....
0	0.26000000	2.384E+01	2.384E+01	2.384E+01	2.384E+01	2.384E+01	2.384E+01	2.384E+01	2.384E+01	2.384E+01	2.384E+01	2.384E+01	.....
0	0.28000000	2.417E+01	2.417E+01	2.417E+01	2.417E+01	2.417E+01	2.417E+01	2.417E+01	2.417E+01	2.417E+01	2.417E+01	2.417E+01	.....
0	0.32000000	2.474E+01	2.474E+01	2.474E+01	2.474E+01	2.474E+01	2.474E+01	2.474E+01	2.474E+01	2.474E+01	2.474E+01	2.474E+01	.....
0	0.40000000	2.559E+01	2.559E+01	2.559E+01	2.559E+01	2.559E+01	2.559E+01	2.559E+01	2.559E+01	2.559E+01	2.559E+01	2.559E+01	.....
0	0.56000000	2.667E+01	2.667E+01	2.667E+01	2.667E+01	2.667E+01	2.667E+01	2.667E+01	2.667E+01	2.667E+01	2.667E+01	2.667E+01	.....
0	0.88000000	2.775E+01	2.775E+01	2.775E+01	2.775E+01	2.775E+01	2.775E+01	2.775E+01	2.775E+01	2.775E+01	2.775E+01	2.775E+01	.....
1	0.99946710	2.798E+01	2.798E+01	2.798E+01	2.798E+01	2.798E+01	2.798E+01	2.798E+01	2.798E+01	2.798E+01	2.798E+01	2.798E+01	.....

Table 2. Representative values of the exact and interpolated coefficients, $\gamma(\nu)$

ν [Hz]	E [Ryd]	$\lambda_{\rm vac}$[Å]	$\gamma(\nu)[10^{-40}$erg cm^3 s^{-1} Hz^{-1}]					
			H I(exact)	H I(interp)	He I(exact)	He I(interp)	He II(exact)	He II(interp)
1.000(+14)	0.030397	29979.246	2.415(+01)	2.418(+01)	2.408(+01)	2.408(+01)	7.393(+01)	7.412(+01)
2.000(+14)	0.060793	14989.623	2.852(+00)	2.858(+00)	3.026(+00)	3.028(+00)	3.222(+01)	3.233(+01)
3.000(+14)	0.091190	9993.082	1.653(+00)	1.655(+00)	2.067(+00)	2.068(+00)	7.034(+01)	7.047(+01)
4.000(+14)	0.121586	7494.811	4.442(+01)	4.442(+01)	5.948(+01)	5.947(+01)	9.356(+01)	9.366(+01)
5.000(+14)	0.151983	5995.849	6.996(−01)	6.988(−01)	2.848(+00)	2.856(+00)	1.457(+00)	1.458(+00)
6.000(+14)	0.182380	4996.541	1.093(−02)	1.092(−02)	5.478(−02)	5.495(−02)	3.098(+01)	3.098(+01)
7.000(+14)	0.212776	4282.749	1.698(−04)	1.694(−04)	1.015(−03)	1.017(−03)	4.807(−01)	4.805(−01)
8.000(+14)	0.243173	3747.406	2.629(−06)	2.628(−06)	1.828(−05)	1.831(−05)	7.437(−03)	7.438(−03)
9.000(+14)	0.273569	3331.027	2.376(+01)	2.376(+00)	1.795(+02)	1.795(+02)	5.054(+01)	5.054(+01)
1.000(+15)	0.303966	2997.925	3.704(−01)	3.702(−01)	1.097(+01)	1.100(+01	7.823(−01)	7.821(−01)

of 1% for H I at the Balmer threshold and at the lowest temperature tabulated by them of 4000K. The difference is attributable to Brown & Matthews using an approximate expression for the hydrogenic threshold photoionization cross-sections while we use the exact expressions incorporated in the codes of Storey & Hummer (1991). A similar comparison for He I shows that for all thresholds except that corresponding to the 3 ^{3}P$^{\rm o}$ state at an air wavelength of 7849Å, our results differ by no more than 2.1% from those of Brown & Matthews (1970). The differences that do exist are due to the approximate method used by Brown & Matthews to calculate the helium photoionization cross-sections. In the case of the 3 ^{3}P$^{\rm o}$ threshold, we find much larger differences reaching 21% at 4000K. This is almost certainly due to a numerical error in the work of Brown & Matthews, since the magnitude of the discontinuity at the 3 ^{3}P$^{\rm o}$ threshold does not obey the correct scaling with temperature in their work.

We also compared our values of $\gamma(\nu)$ for H I and He II with those published by Ferland (1980) and found, in general, good agreement, with typical deviations of the order of 2-5% in the overlapping temperature range.

The electronic tables are structured as follows: node/threshold (0/1) indices are given in column 1, the photon energies in Ryd are given in column 2, the scaled free-bound emission coefficients for temperatures in the 100 K-100000 K range are given in the remaining columns. For He I and He II coefficients are tabulated for log T[K] = 2.0(0.1)5.0 while for He I, log T[K] = 2.0(0.04)5.0. The maximum photon energy is slightly less than the ground state ionization energy for each ion and the minimum photon energy corresponds to the $n = 20$ threshold in H I.

4 CONCLUSIONS

We have presented new calculations of the free-bound continuous emission coefficients for the hydrogen and helium ions. The results for He I are derived from accurate *ab initio* photoionization cross-section data. The coefficients are given for a wide range of temperatures and frequencies, extending to the previously unexplored very low-temperatures regime. This is needed for the interpretation of spectra from very cold ionised gas, which has been inferred to exist, possibly in the form of density/chemical inhomogeneities, from observations of ORLs in H II regions and planetary nebulae. The data are presented under an interpolation scheme that allows estimates to be obtained over the entire temperature and energy range presented with less than 1% uncertainty.

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