Emission and recombination coefficients for hydrogen with \( \kappa \)-distributed electron energies

P.J. Storey\(^1\), Taha Sochi\(^1\)*

\(^1\)Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK

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ABSTRACT

We provide a data set of emission and recombination coefficients of hydrogen using a \( \kappa \)-distribution of electron energies rather than the more traditional Maxwell-Boltzmann (MB) distribution. The data are mainly relevant to thin and relatively cold plasma found in planetary nebulae and H \( \text{II} \) regions. The data set extends the previous data sets provided by Storey and Hummer which were computed using a MB distribution. The data set, which is placed in the public domain, is structured as a function of electron number density, temperature and \( \kappa \). Interactive fortran 77 and C++ data servers are also provided as an accessory to probe the data and obtain Lagrange-interpolated values for any choice of all three variables between the explicitly computed values.

Key words: atomic data - atomic processes - radiation mechanisms: general - radiation mechanisms: non-thermal - ISM: abundances - planetary nebulae: general.

1 INTRODUCTION

There are many studies related to the recombination of hydrogen and hydrogenic systems, the most comprehensive being those of Hummer & Storey (1987), Storey & Hummer (1988) and Storey & Hummer (1995). However, all the past work was based on a Maxwell-Boltzmann distribution of electron energies. There has been, and still is a general consensus that this is the appropriate distribution for thin nebular plasmas. However, this was disputed in the past (Hagihara 1944) where considerable deviations from the thermodynamic equilibrium on which the MB relies were claimed although this claim was later discounted (Bohm & Aller 1947).

There has been a recent revival (Nicholls et al 2012) of the proposal of a non-thermal electron energy distribution in planetary nebulae and H \( \text{II} \) regions in the light of the long standing problem in nebular physics of the contradiction between the results for elemental abundance and electron temperature as obtained from the optical recombination lines (ORL) and those obtained from the collisionally excited lines (CEL). According to the recent proposal, the ORL-CEL discrepancy problem can be resolved by assuming a \( \kappa \)-distributed electron energy distribution, specifically the \( \kappa \)-distribution. There have been a few recent attempts to assess the merit of this suggestion (Sochi 2012, Storey & Sochi 2013, 2014, Zhang et al 2014) using spectroscopic means to directly sample the free electron energy distribution. With the exception of Storey & Sochi (2014) they are all inconclusive, in the sense that the data do not differentiate between a single \( \kappa \)-distribution and other models, such as one with two MB components at different temperatures. Storey & Sochi (2014) do, however argue that, with a high degree of certainty, the Balmer line and continuum spectrum of the extreme planetary nebula Hf 2-2 cannot be modeled with a single \( \kappa \)-distributed electron energy distribution, while it can be with a model comprising two MB distributions. It should be noted however that Zhang et al (2014) analyze the same spectra of the same object and conclude that either model can adequately model the spectrum. We return to this apparent contradiction below.

Both Storey & Sochi (2014) and Zhang et al (2014) model the Balmer line and continuum spectrum with MB and \( \kappa \) distributions. Typically the continuum intensity is modeled relative to one of the high Balmer lines, chosen to be close in wavelength to the Balmer edge and apparently unblended. The continuum spectrum is relatively easy to model with an arbitrary electron energy distribution but the modeling of the high Balmer line intensities requires a full treatment of the collisional-radiative recombination process as a function of \( \kappa \) as well as the usual density and temperature variables. Storey & Sochi (2014) made such a calculation in Case B of Baker & Menzel (1938) and presented some results for the line which they used to normalize intensities, H11. Here we publish the full results from those calculations. We note that Zhang et al (2014) also use H11 for normalization but they rely on an approximate treatment taken from Nicholls et al (2012) which applies a \( \kappa \)-dependent scal-

* E-mail: t.sochi@ucl.ac.uk

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ing function to the H11 emission coefficient calculated with a MB distribution. Storey & Sochi (2014) show that this approximation is poor for the very low values of $\kappa$ that are required to model the HF 2-2 spectrum, which may explain why Zhang et al (2014) reach a different conclusion to Storey & Sochi (2014) in the case of HF 2-2.

The results are provided in two text files where the emission and recombination coefficients are given as a function of electron number density $N_e$, electron temperature $T_e$, and $\kappa$. We also provide interactive data servers, in the form of fortran 77 and C++ codes, for mining the data and obtaining interpolated values in the three variables between the explicitly computed values. In section [2], we give a brief theoretical background about the atomic computational model used to generate the data, while in section [3] we explain the structure of the data set and provide general instructions and clarifications about how it should be probed and used. Section [4] contains general conclusions and discussions.

2 ATOMIC MODEL

The fundamental quantity required for the calculation of the hydrogen recombination line intensities is the coefficient for recombination to a state $n\ell$ of H. For a free electron energy distribution $f(E)$, this is given by (e.g. Storey & Sochi 2014)

$$\alpha(n\ell) = \frac{R^3}{\sqrt{2\pi} e m_e^3} \omega(n\ell) \omega^+ \int_0^\infty \left(\frac{h\nu}{E}\right)^{\frac{1}{2}} \sigma(\nu, n\ell) f(E) \frac{dE}{E}$$

(1)

where $R$ is the Rydberg energy constant, $\omega^+$ and $\omega(n\ell)$ are the statistical weights of the initial and final states respectively. $\nu$ is the frequency of the emitted photon, $E$ is the energy of the free electron, $\sigma(\nu, n\ell)$ is the cross-section for photoionization which is the inverse process to recombination, and the other symbols have their standard meanings.

The calculation of the recombination line emission coefficients in a full collisional-radiative treatment has been described by Hummer & Storey (1987) and Storey & Hummer (1995) and we use the same methods here.

Traditionally, $f(E)$ is the Maxwell-Boltzmann distribution function. Here we use instead the $\kappa$ distribution which is given by Vasyliunas (1968) and Summers & Thorne (1991).

$$f_\kappa(E, T_e) = \frac{2\sqrt{\pi}}{\sqrt{\pi kT_e}^{\frac{3}{2}}} \frac{\Gamma(k + 1)}{(k - \frac{3}{2}) \Gamma(k - \frac{1}{2})} \left(1 + \frac{E}{(k - \frac{3}{2}) kT_e}\right)^{-(k+1)}$$

(2)

where $\kappa$ is a parameter defining the distribution, $\Gamma$ is the gamma function of the given arguments, and $T_e$ is a temperature characteristic to the particular distribution. For sufficiently large $\kappa$, $f_\kappa(E, T_e)$ tends to the Maxwell-Boltzmann distribution.

For energetically low-lying states of H the dominant processes are recombination and radiative decay. For higher states, collisional processes become important, with $l$-changing collisions being the most frequent. In our calculations the $n\ell$ states of hydrogen are assumed degenerate with respect to $l$ and in this case the dominant processes that change $l$ are collisions not with electrons but with H$^+$, He$^+$ and He$^{++}$ ions. In the results described here we retain a Maxwell-Boltzmann distribution for these heavier particles. We also retain a Maxwell-Boltzmann distribution for the processes that change energy and $n$, which are dominated by collisions with electrons. Consequently the emissivities that we calculate should be treated with caution for the high-$n$ states for which $l$- and $n$-changing collisional processes become important. The boundary of this region is primarily a function of the electron density, being at approximately $n = 100, 75, 50, 30$ and 20 for densities of $10^2, 10^3, 10^4, 10^5$ and $10^6$ cm$^{-3}$ respectively.

The rate coefficients for $l$-changing collisions used to obtain the above boundary $n$ values were calculated using the theory described by Pengelly & Seaton (1964). Vrinceanu and co-workers have published a series of papers (Vrinceanu 2005, Vrinceanu et al 2012, 2014) on electron and proton induced collisions with Rydberg states of hydrogen. In Vrinceanu et al (2012) they state that the rate coefficients for proton induced $\Delta l = 1$ transitions are overestimated by the theory of Pengelly & Seaton (1964) by about an order of magnitude. The calculation of the rate coefficient depends upon an integration of the probability for an $l$-changing transition over the impact parameter of the incident particle, assumed to travel on a straight-line trajectory. It is well known that this integral is divergent for $\Delta l = 1$ transitions in a quantum mechanical treatment. The approximate treatment of the transition probability by Pengelly & Seaton (1964) converges on the quantum mechanical result at large impact parameter as illustrated in Figure 1 of Vrinceanu et al (2012). Pengelly & Seaton (1964) introduce a cut-off at large impact parameter to remove the divergence based on collective effects in the plasma or the finite lifetime of the Rydberg state. The semi-classical approach of Vrinceanu et al (2012) does not correctly replicate the quantum behavior at large impact parameter with the probability instead falling discontinuously to zero at a finite and relatively small value of the impact parameter. The missing contribution from large impact parameter is the origin of the order of magnitude difference they report between their results and those of Pengelly & Seaton (1964). We see no reason to prefer their semi-classical result over the quantum treatment at large impact parameters and therefore consider the Pengelly & Seaton (1964) results to be more reliable.

3 DATA

The $\kappa$-dependent emission coefficients, $\epsilon(N_e, T_e, \kappa)$ are provided in a single text file called ‘elbk.d’. The energy emitted per unit volume per unit time is then $N_e \epsilon(N_e, T_e, \kappa)$ where $N_e$ is the H$^+$ number density and where all quantities are in cgs units. The structure of this file is explained in the following bullet points:

- The first row of this file contains (in the following order) the number of $N_e$ values, the number of $T_e$ values and the number of $\kappa$ values for which data are provided.
- The 9 values of $N_e$ are specified by $\log_{10} N_e = 2.0 (0.5) 6.0$.
- The 16 values of $T_e$ are specified by $\log_{10} T_e = 2.0 (0.2) 3.8, 3.9 (0.1) 4.4$. 

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The data therefore consist of 6336 blocks (= 9 × 16 × 44).

The first row of each block contains information about the block which consists of the following:

\[ Z \log_{10} N_e \log_{10} T_e \log_{10} \kappa \times \]

where \( Z = 1 \) is the atomic number of hydrogen, ‘B’ refers to Case B and \( n_{min} \) and \( n_{max} \) are the minimum and maximum upper state principal quantum numbers for which emission coefficients are tabulated. Each block therefore contains 4850 (= \( \frac{1}{2} n_m (n_m - 1) - 1 \)) entries. These 4850 entries are arranged in 607 rows and hence the total number of rows in each block is 608.

Of the three variables, \( N_e, T_e \) and \( \kappa \), the fastest varying is \( N_e \) followed by \( T_e \) followed by \( \kappa \), and hence the ordinal number of a block is given by:

\[
O_B = O_N + (O_T - 1)9 + (O_\kappa - 1)144
\]

where \( O_B, O_N, O_T \) and \( O_\kappa \) are the ordinal numbers of block, \( N_e \) value, \( T_e \) value and \( \kappa \) value respectively. For example the ordinal number of the block for \( \log_{10} N_e = 4 \) (\( O_N = 5 \)), \( \log_{10} T_e = 2.6 \) (\( O_T = 4 \)) and \( \log_{10} \kappa = 0.27 \) (\( O_\kappa = 8 \)) is:

\[
O_B = 5 + (4 - 1)9 + (8 - 1)144 = 1040
\]

and hence it starts on row 631714 (= 608\( O_B - 1 \) + 2) and ends on row 632321 (= 608\( O_B \) + 1).

The 4850 values of emission coefficients in each block are arranged for transitions from upper levels \( n_u \) to lower levels \( n_l \) with \( n_u \) in descending order from \( n_{max} \), and \( n_l \) in ascending order from 1 to \( (n_u - 1) \), and hence the ordinal number for a transition \( tr(n_u, n_l) \) is given by

\[
O_{tr} = n_l + \frac{1}{2} (n_m - n_u) (n_m + n_u - 1)
\]

Emission coefficients to \( \alpha = 1 \) are not calculated for Case B and hence are set to zero.

A second file named ‘t1bk.d’ contains the hydrogen total recombination coefficients in Case B, \( \alpha(N_e, T_e, \kappa) \), and the total recombination coefficients to the 2s state of hydrogen, \( \alpha_{2s}(N_e, T_e, \kappa) \), such that the number of recombinations per unit volume per unit time is \( N_e N_s \alpha \) in cgs units. This file contains 12672 entries arranged in 1584 rows. The first half (6336) of these entries are the total recombination coefficients of hydrogen while the second half are the total recombination coefficients to the 2s state. The entries in each one of these two blocks correspond to the 6336 values of physical conditions (i.e. various combinations of \( N_e, T_e \) and \( \kappa \)) positioned according to equation (4).

4 CONCLUSIONS AND DISCUSSIONS

In this paper we computed atomic emission and recombination coefficient data for hydrogen with electron energies described by a \( \kappa \)-distribution. The atomic model used in the computation of these data uses the techniques described by [Hummer & Storey (1987)] and [Storey & Hummer (1995)]. The data, which are placed in the public domain, span ranges of electron number density, temperature and \( \kappa \) useful for modeling and analyzing plasmas such as those found in planetary nebulae and H II regions. Interactive data servers provide easy access to the data with Lagrange-interpolated values in all three variables.

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REFERENCES

Baker J.G., Menzel D.H., 1938, ApJ, 88, 52
Bohm D., Aller L.H., 1947, ApJ, 105, 131
Hugihara Y., 1944, Proceedings of the Japan Academy, 20, 493
Hummer D.G., Storey, P.J., 1987, MNRAS 224, 801
Nicholls D.C., Dopita M.A., Sutherland R.S., 2012, ApJ, 752, 148
Pengelly R.M., Seaton M.J., 1964, MNRAS, 127, 165
Sochi T., 2012, PhD thesis, University College London
Storey P.J., Hummer, D.G., 1988, MNRAS 231, 1139
Storey P.J., Hummer D.G., 1995, MNRAS 272, 41
Storey P.J., Sochi T., 2013, MNRAS, 430, 599
Storey P.J., Sochi T., 2014, MNRAS, 440, 2581
Summers D., Thorne R.M. 1991, Phys. Fluids B, 3, 1835
Vasyliunas V.M., 1968, JGR, 73, 2839
Vinceeanu D., 2005, Phys. Rev. A, 72, 022722
Vinceeanu D., Onofrio R., Sadeghpour H.R., 2012, ApJ, 747, 56
Vinceeanu D., Onofrio R., Sadeghpour H.R., 2014, ApJ, 780, 2
Zhang Y., Liu X-W., Zhang B., 2014, ApJ, 780, 93