Interpreting the Hydrogen IR Lines
– Impact of Improved Electron Collision Data

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Abstract. We evaluate the effect of variations in the electron-impact excitation cross sections on the non-LTE line formation for hydrogen in early-type stars. While the Balmer lines are basically unaffected by the choice of atomic data, the Brackett and Pfund series members allow us to discriminate between the different models. Non-LTE calculations based on the widely-used approximations of Mihalas, Heasley & Auer and of Johnson fail to simultaneously reproduce the observed optical and IR spectra over the entire parameter range. Instead, we recommend a reference model using data from \textit{ab-initio} calculations up to principal quantum number $n \leq 7$ for quantitative work. This model is of general interest due to the ubiquity of the hydrogen spectrum.

1 Introduction

The quantitative interpretation of the hydrogen line spectrum is one of the foundations of modern astrophysics. Being the most abundant and most basic element in the universe hydrogen imprints its signature on the spectra of stars, nebulae and accretion phenomena. For decades the focus laid in the modelling of the first members of the Balmer series for deriving the physical properties of astronomical objects. In the meantime developments in instrumentation have opened the IR window to routine observation, which will even gain in importance in the future, with \textit{Crires} and \textit{Visir} on the VLT being important cornerstone projects. The next generation of ground-based large telescopes and the next large space telescope will focus on this wavelength range, primarily to study the high-z universe. But it will also allow to investigate local objects in otherwise inaccessible environments, e.g. ultra-compact H\textsc{ii} regions, the Galactic centre and dust-enshrouded nearby starburst galaxies. The Brackett and Pfund lines are among the key diagnostics at these wavelengths. Here we report on the findings of our reinvestigation of the non-LTE line-formation problem for hydrogen [1]. We confront H\textsc{i} model atoms of different degree of sophistication with observations of early-type stars in order to derive a set of reference data which is, of course, of much broader interest than for stellar analyses alone.

2 Model calculations

The line-formation computations are carried out using two methods. For main sequence stars of spectral types later than O and BA-type supergiants a hybrid approach is chosen. Based on hydrostatic, plane-parallel, line-blanketed
Fig. 1. Comparison of effective collision strengths for transitions $n-n'$, as indicated. The curves are: B04 (solid), J72 (dotted), MHA (dashed), PR (dash-dotted).

LTE models calculated with the ATLAS9 code [2] the non-LTE computations are performed using updated versions of DETAIL and SURFACE [3,4]. For the modelling of early B and O-type stars we use the non-LTE model-atmosphere/line-formation code FASTWIND [5] which accounts for spherical extension and hydrodynamic mass-outflow. It has been recently updated to include an approximate treatment of non-LTE line-blocking/blanketing [6].

Several model atoms for H\textsc{i} have been implemented. The two-body nature of the hydrogen atom allows the radiative data to be obtained analytically. On the other hand, excitation (and ionization) processes involving a colliding particle require a numerical solution of the resulting three-body Coulomb problem. Non-LTE computations had to rely on approximation formulae [7,8] (MHA, J72) for determining collisional excitation rates until recently, as only few measured cross-sections are available. Using data from extensive *ab-initio* calculations up to $n \leq 7$ [9] (B04) we realise a third model atom, further improved by application of the approximation formula of [10] (PR) for determining electron-collision excitation rates for the remaining transitions with $n,n' \geq 5$. A comparison of electron collision strengths in Fig. 1 shows good agreement of the MHA and J72 approximations with the results of the detailed computation for the 1–2 transition. However, for transitions among levels with higher $n$, like 5–6, large differences can occur, which ultimately will manifest themselves in model spectra via their impact on the rate equations and thus the level populations. Line broadening is accounted for by using the tables of [11]. In the case of the Brackett and Pfund lines we apply the theory of [12].

The mechanisms driving departures of H\textsc{i} from detailed balance in stellar atmospheres have been well understood since the seminal work of [13,14] (for early-type stars), and numerous subsequent contributions – for line formation in the IR e.g. by [15]. The issue here is to study the impact of the local processes that affect the radiatively induced departures from LTE, namely collisional interactions, which are assumed to be of secondary importance. Indeed, the actual choice of such data produces no significant differences in the stellar continuum.
Fig. 2. Comparison of model profiles for Brα and Pfα in Vega: non-LTE computations using our recommended model atom (electron collision data of B04+PR+MHA, solid), models using MHA (dashed) and J72 data (dash-dotted) and LTE profiles (dotted).

Fig. 3. Run of departure coefficients $b_i$ (left) and ratio of line source function $S_L$ to Planck function $B_\nu$ (right) in β Ori as a function of Rosseland optical depth $\tau_{\text{Ross}}$. The curves are encoded as in Fig. 2. Individual sets of graphs are labelled by the level’s principal quantum number. Line formation depths for several transitions are indicated.

or the Balmer line profiles. However, consider Fig. 2 where the results from our model calculations for prominent IR lines in Vega are shown. Apparently, the choice of collisional data is not a second-order effect, but a dominant factor for line-formation computations in the IR. In the following we want to discuss the theoretical background of this behaviour.

Departure coefficients $b_i$ for selected levels from computations using the different model atoms are displayed exemplarily for β Ori in Fig. 3. The overall behaviour, i.e. the over- and underpopulation of the levels of H1 and of H11, is governed by the radiative processes, while the differences in the collisional data lead to modulations. These are small for the ground state and become only slightly more pronounced for the $n = 2$ level, as these are separated by compar-
Table 1. Stellar parameters

| Object | $T_{\text{eff}}$ (K) | $\log g$ | $y$ | $R/R_\odot$ | $v_{\text{turb}}$ (km s$^{-1}$) | $M$ (M$_\odot$ yr$^{-1}$) | $v_\infty$ (km s$^{-1}$) | $\beta$ |
|--------|-----------------|---------|----|-------------|-----------------|-----------------|-----------------|-------|
| Vega   | 9550            | 3.95    | 0.09 | 2.8         | 2               | ...             | ...             | ...   |
| $\beta$ Ori | 12000       | 1.75    | 0.135 | 104         | 7               | ...             | ...             | ...   |
| $\tau$ Sco | 31400       | 4.24    | 0.09 | 5.1         | 3               | $9.00 \cdot 10^{-9}$ | 2000          | 2.4/2.5 |
| HD 93250 | 46000          | 3.95    | 0.09 | 15.9        | 0               | $3.45 \cdot 10^{-6}$ | 3250          | 0.9   |

Attractively large energy gaps from the remainder of the term structure. Only colliding particles in the high-velocity tail of the Maxwellian velocity-distribution are able to overcome these energy differences at the temperatures encountered in the star’s atmosphere. However, line-formation computations in the IR will be affected, as maximum effects from variations of the collisional data are found for the levels with intermediate $n$ at line-formation depth. The line source function $S_L$ is particularly sensitive to variations of the ratio of departure coefficients

$$|\Delta S_L| = \left| \frac{S_L}{b_i/b_j - \exp(-h\nu/kT)} \Delta(b_i/b_j) \right| \approx \left| \frac{S_L}{(b_i/b_j - 1) + h\nu/kT} \Delta(b_i/b_j) \right|$$

when $h\nu/kT$ is small. This makes these lines very susceptible to small changes in the atomic data and details of the calculation.

3 Confrontation with observation

In order to determine which model atom is suited best for quantitative studies we compare model predictions for IR lines with observations for a few objects sampling the parameter space, see Figs. 4–6. This has to rely on a variety of sources for the observations, see [1] for details. The stellar parameters adopted for the model calculations are summarised in Table 1 ($y$ is He abundance by number and $\beta$ the wind velocity parameter).

We conclude from this comparison that model atoms using the MHA approximation overestimate the thermalising effects of electron collisions, thus dampening the non-LTE effects (as determined in the high density environment of the main sequence star Vega). On the other hand, use of the J72 approximation leads to an unrealistic non-LTE strengthening in supergiants, like in the case of $\beta$ Ori. In both cases good agreement between theory and observation is obtained using the superior atomic data from ab-initio computations (Fig. 4). The IR lines of the early B-type star $\tau$ Sco turn out to react highly sensitive to the atmospheric conditions (Fig. 5), as they are subject to considerable non-LTE amplification (Eqn. 1). Finally, HD 93250 may act as a benchmark for the study of objects at the earliest phases of stellar evolution of massive stars. Here, the differences in the predicted equivalent widths from the different model atoms may reach a factor $\sim 2$ (Fig. 6). The Balmer lines remain basically unaffected by the choice of the atomic data in all the cases studied.
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Fig. 4. Comparison of selected synthetic spectra (encoded as in Fig. 2) with observed IR hydrogen lines (thick solid). LTE modelling fails to reproduce the observations. Model atoms relying on the MHA approximation underestimate the NLTE strengthening of the Brγ line core in the main sequence star (left). Those using the J72 approximation predict too strong features in BA-type supergiants (right). Our recommended model provides good fits consistently throughout the high and low density regimes.

Fig. 5. Spectrum synthesis for hydrogen lines in τ Sco (encoded as in Fig. 2). Left: hydrostatic computations; using the MHA approximation we reproduce the findings of [15], i.e. obtain a fair fit of the IR core-emission peaks. However, the other model implementations indicate no emission cores. Right: hydrodynamic approach; slight differences in the atmospheric structure at line-formation depths suffice to improve the quality of the line fits. Notable residuals are still present for Brα, a consequence of the sensitivity of the calculation to the non-LTE amplification close to population inversion.
Fig. 6. Spectrum synthesis for an early O-type star (encoded as in Fig. 2). Accurate electron collision data are mandatory for consistent modelling of the Brackett and Balmer lines. H\(\alpha\) shows some residual nebular emission.

4 Recommendations

Use of electron collision data from \textit{ab-initio} computations is \textit{mandatory} in order to derive consistent results from the diagnostic lines in the visual and IR. We recommend the data of [9] for the evaluation of collision rates of H\(1\), supplemented by the approximation formulae by [10] and of [7] for those transitions not covered by the \textit{ab-initio} computations. This applies not only to the modelling of early-type stars as we have done but to all hydrogen plasmas.

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