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New study of the quasi-molecular Lyman α satellites due to H-H and H-H^+ collisions

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Abstract. We present new theoretical calculations of the total profile of the atomic hydrogen Lyman α spectral line perturbed by collisions with neutral hydrogen atoms and protons. The variation of the radiative dipole moment during the collision is taken into account. This leads to an increase in the amplitude of the main spectral line satellites and to a quantitative improvement of the synthetic spectra of λ Bootis stars compared to IUE observations.

Key words: atomic processes – line: profiles – stars: chemically peculiar – white dwarfs

1. Introduction

Structures observed at 1600 Å and 1405 Å in the Lyman α wing due respectively to quasi-molecular absorption of H_2 and H_2^+ molecules have been demonstrated to be very sensitive temperature indicators in DA white dwarfs and have been used in the analysis of UV spectra of variable DA (ZZCeti stars) (Koester et al. 1994, Bergeron et al. 1995, Koester & Vauclair 1997). The λ Bootis stars are population I, type A, stars with normal CNO abundances, but with low atmospheric metal abundances. They also have a large absorption feature centered at 1600 Å discovered by Baschek et al. (1984).

Holweger et al. (1994) have demonstrated quantitatively that this feature is the same Lyman α satellite observed in the spectra of DA white dwarfs and metal-deficient horizontal branch stars of spectral type A. In normal A-type stars, the UV flux is strongly shaped by the continuous opacity. In the range 1300-2000 Å, strong bound-free discontinuities of Si I occur which makes the satellites of Lyman α unobservable in the line wing. These features only can be distinguished in metal-poor A stars. In the range from 1200 to 2000 Å the presence of this 1600 Å satellite as well as the ratio of the intensity of blends dominated by C and Al lines define reliable criteria to detect λ Bootis stars (Faraggiana, et al. 1990; Gerbaldi & Faraggiana, 1993).

In the observed UV spectra of DA white dwarf stars, λ Bootis stars, and laboratory plasmas, the strength of the contributions to the Lyman α wing caused by neutral collisions relative to the contributions caused by charged perturbers depends very strongly on the ionization balance of hydrogen, and thus, through the Saha equation, on the stellar parameters $T_{\rm eff}$ and $\log g$. As a consequence of its dependence on the degree of ionization, the shape of the Lyman α wing is a very sensitive tool for determining these parameters once accurate absorption coefficients for the line wing are known.

The fundamental theory of the Lyman α line described by Allard et al. (1994) is improved considerably when the variation of the electronic transition dipole moment (dipole moment, hereafter) during the collision is included (Allard et al. 1998). The dipole moment taken between the initial and final states of a radiative transition determines the transition probability, but for two atoms in collision, the moment depends on their separation. This modifies relative contributions to the profile along the collision trajectory. In the earlier work it was assumed that the dipole moment was constant during the collision, but with the new theory we can now take into account its dependence on interatomic distance for allowed transitions, and also for transitions which are asymptotically forbidden. These effects are not included when the usual approximations are made in the theory of Anderson & Talman 1956 and Baranger 1958. The resulting profiles show that a large enhancement in the amplitude of a satellite occurs whenever the dipole moment increases through the region of internuclear distance where the satellite is formed.

The new theoretical spectral line profiles have been incorporated into Kurucz' ATLAS12 stellar atmosphere program for the computation of model stellar spectra. A comparison of IUE observations with synthetic spectra of λ Bootis stars shows that the new profiles are essential to determine atmospheric parameters for these stars from a quantitative interpretation of their spectra (Allard et al. 1997).

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2. Theoretical analysis

Close collisions between a radiating atom and a perturber are responsible for transient quasi-molecules which lead to the possible appearance of satellite features in the wing of the line profile. When the difference $\Delta V(R)$ between the upper and lower potentials for a transition presents an extremum $\Delta V_{\rm ext}$, the unified theory (Anderson & Talman 1956; Allard & Kielkopf 1982) predicts that there will be satellites centered periodically at

$$\Delta\omega = k\Delta V_{\rm ext}, k = 1, 2, 3, \ldots$$

(Allard 1978; Royer 1978; Kielkopf & Allard 1979). Here $\Delta\omega$ is the frequency difference between the center of the unperturbed spectral line and the satellite feature, measured for convenience in the same units as the potential energy difference. This series of satellites is due to many-body interactions. The $k^{\rm th}$ satellite corresponds to the simultaneous presence of k perturbers in the collision volume. The number of perturbers in the interaction volume is the determining parameter for the amplitude of the satellites on the spectral line (Allard 1978). In the range of low densities appropriate to white dwarf or λ Bootis stars, the satellite amplitude increases linearly with the average number of perturbers because there is a higher probability of binary collisions than many-body collisions. The amplitude of the first satellite starts to decrease at higher density because the probability of simultaneous collisions with more than two perturbers becomes more important than binary collisions (Allard 1978; Royer 1978; Allard & Kielkopf 1982). The interaction volume depends directly on the potential energy curves which correlate with the atomic levels of the transition (Allard & Kielkopf 1982). The position of the extremum and the functional dependence of the potential difference on internuclear separation determine the amplitude and shape of the satellites. We can see in Figs. 1 and 2 how much the shapes of the difference potential curves differ for the atom-ion and atom-atom interactions that lead respectively to the 1405 Å and 1600 Å satellite features on Lyman α. If the dipole moments were independent of internuclear separation, the 1405 Å satellite would have an amplitude 18 times larger than the amplitude of the 1600 Å satellite for a common perturber density $n_{\rm H} = n_{\rm H^+} = 10^{17}{\rm cm}^{-3}$ (see Table 1). Consequently, accurate theoretical molecular potentials have to be used to describe the interaction between the radiator and the perturber. Approximations for the potentials which are too simple can only lead to qualitative agreement.

The description of the theory with the assumption of constant dipole moment as applied to the shape of the Lyman α line was given by Allard et al. (1994). Calculations based on this theory and accurate *ab initio* potentials have been made by Allard & Kielkopf (1991), Allard & Koester (1992), and Allard et al. (1994). It has been used successfully by Koester & Allard (1993), Koester et al. (1994) and Bergeron et al. (1995) to interpret IUE and HST spectra, and by Kielkopf & Allard (1995) to analyze the vacuum ultraviolet spectra of laser-produced hydrogen plasmas.

As emphasized in Allard et al. (1994), however, the assumption that the dipole moment is constant during the collision may be questionable. Figs. 1 and 2 illustrate that at the distances which lead to the formation of a satellite the relevant probability that a photon will be absorbed during an atom-atom or atom-ion collision can be a factor of 2 larger than it is for a collision-free atom.

Improvements to the theory have been made recently which take into account the dependence of the dipole moment on internuclear distance during the collision (Allard el al. 1998). When

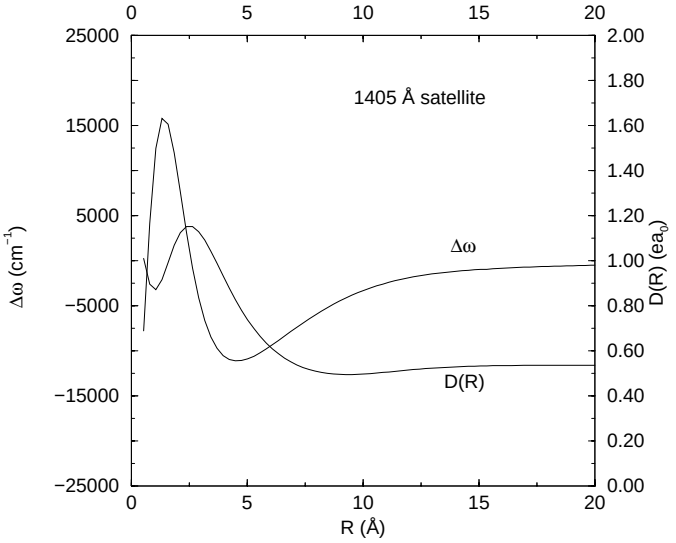

Fig. 1. Difference potential energy $\Delta\omega$ in cm^{-1} for the 1405 Å satellite of Lyman α due to perturbations of the radiating H atom by collisions with H^+. $D(R)$ is the electronic transition dipole moment and is given here in atomic units. The satellite is formed around 4 Å where $\Delta\omega$ is a minimum. The increase in the dipole moment through this region leads to an enhancement of the satellite.

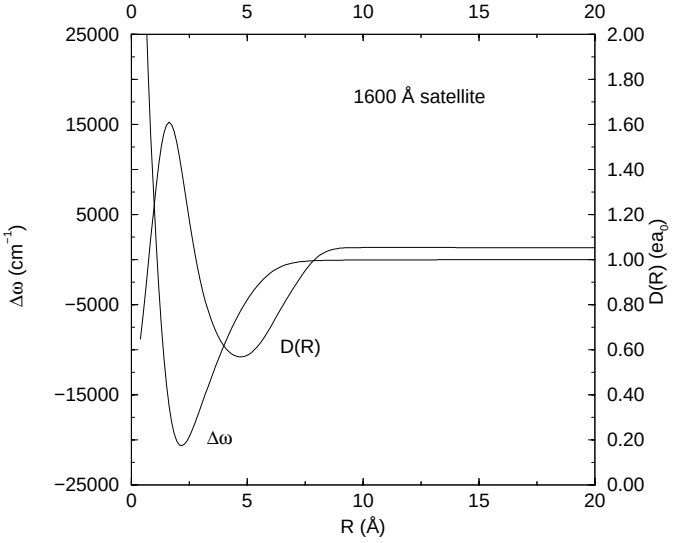

Fig. 2. Difference potential energy $\Delta\omega$ in cm^{-1} for the 1600 Å satellite of Lyman α due to perturbations of the radiating H atom by collisions with other neutral H atoms. $D(R)$ is the electronic transition dipole moment and is given here in atomic units. The satellite is formed around 2.4 Å where $\Delta\omega$ goes through a minimum. In the same region the increase in the dipole moment leads to an enhancement of the satellite.

this theory was applied to the case of Lyman β satellites due to H-H$^+$ collisions, it was shown that large increases (up to 60 %) in the intensity of line wing occur in comparison to the theory based on the assumption of constant dipole moment. As expected, this effect is most important when the dipole moment varies significantly in the range of internuclear distances where the satellite is formed (Allard et al. 1997). In the following we apply the improved theory to the Lyman α line broadened simultaneously by H-H and H-H$^+$ collisions.

2.1. General expression for the spectrum

For an isolated line such as Lyman α we have shown (Allard et al. 1998) that the normalized line shape $J_\alpha(\Delta\omega)$ is given by

$$J_\alpha(\Delta\omega) = \mathbf{FT}[e^{n g_\alpha(s)}] \tag{1}$$

where the frequency

$$\Delta\omega = \omega - \omega_\alpha \tag{2}$$

is measured relative to the unperturbed line. In the classical path approximation, where we assume that the perturber follows a rectilinear trajectory at a single mean velocity $\bar{v}$, we get from Allard et al. (1994,1998):

$$\begin{aligned} g_\alpha(s) \quad &= \frac{1}{\sum_{e,e'}{}^{(\alpha)} |D_{ee'}|^2} \sum_{e,e'}{}^{(\alpha)} \\ &\pi_{ee'} \int_0^{+\infty} 2\pi\rho d\rho \int_{-\infty}^{+\infty} dx \; d_{ee'}(\,R(0)\,) \\ &[\, e^{i\int_0^s dt\, V_{e'e}(\,R(t)\,)}\, d_{e'e}(\,R(s)\,) \;-\; d_{ee'}(\,R(0)\,)\,]\,. \end{aligned} \tag{3}$$

In Eq. (3) e and e' label the energy surfaces which approach the initial and final atomic states of the transition as $R \to \infty$. The atomic states are usually degenerate, and in general there are several different energy surfaces which approach the same asymptotic energy as $R \to \infty$. The weight factor $\pi_{ee'}$ accounts for this degeneracy. If we denote by E_i^∞ and E_f^∞ the asymptotic initial and final state energies, such that $E_e(R) \to E_i^\infty$ as $R \to \infty$ in the presence of perturbers, we have R-dependent frequencies

$$\omega_{if}(R) \equiv (E_f(R) - E_i(R))/\hbar \tag{4}$$

that become the isolated radiator frequency ω_{if} when the perturbers get sufficiently far from the radiator:

$$\omega_{if}(R) \to \omega_{if} \quad \text{as} \quad R \to \infty \tag{5}$$

with

$$\omega_\alpha \equiv \omega_{if} \equiv (E_f^\infty - E_i^\infty)/\hbar\,. \tag{6}$$

The sum $\sum_{e,e'}^{(\alpha)}$ in Eq. (3) is over all pairs (e, e') such that

$$\omega_{e',e}(R) \to \omega_\alpha \quad \text{as} \quad R \to \infty \tag{7}$$

where ω_α is the frequency of the transition for an isolated radiator. The total line strength of the transition is $\sum_{e,e'}{}^{(\alpha)} |D_{ee'}|^2$. Here

$$d_{ee'}(R(s)) = D_{ee'}(R(s)) e^{-i\omega_\alpha s} \tag{8}$$

where $D_{ee'}(R(s))$ denotes the R-dependent electronic transition dipole moment.

The difference potential is

$$V_{e'e}(R) = V_{e'}(R) - V_e(R), \tag{9}$$

where the potential energy for the state is

$$V_e(R) = E_e(R) - E_e^\infty\,. \tag{10}$$

The separation of the radiator and perturber is

$$R(t) = [\,\rho^2 + (x + \bar{v}t)^2\,]^{1/2} \tag{11}$$

where ρ is the impact parameter of the perturber trajectory and x is the position of the perturber along its trajectory at time $t = 0$. In the Eq. (3) we neglect the influence of the potentials $V_e(R)$ and $V_{e'}(R)$ on the perturber trajectories, which remain straight lines.

3. Diatomic potentials and electronic transition dipole moments

The adiabatic interaction of the neutral hydrogen atom with a proton or another hydrogen atom is described by potential energies $V_e(R)$ for each electronic state of the H_2^+ or H_2 molecule. Electronic dipole transitions between these states are responsible for the line profile.

The transitions contributing to Lyman α are summarized in the Table 3 and Table 4 of a previous paper (Allard et al. 1994). Eq. (26) of Allard et al. (1994) gives the weight of each of these transitions. Please note that the labels of the a and h triplet states were interchanged in Allard et al. (1994). The present approach now allows us also to take into account the two asymptotically forbidden transitions ($X^1\Sigma_g^+ \to B'^1\Sigma_u^+$ and $b^3\Sigma_u^+ \to h^3\Sigma_g^+$) of quasi-molecular hydrogen which dissociate into $(1s, 2s)$ atoms. Our results show that they give a minor contribution compared to the other transitions.

For H-H$^+$ collisions we have used the potentials of H_2^+ calculated by Madsen & Peek (1971) for the transitions contributing to Lyman α, that is, for those that asymptotically go to the $n = 2$ state of atomic hydrogen and a free proton. Each of the difference potentials for the five allowed transitions has a minimum which leads us to expect the presence of a corresponding satellite feature in the red wing of Lyman α. Dipole moments for H_2^+ have been calculated as a function of internuclear distance by Ramaker & Peek (1972).

For H-H collisions the H_2 potentials contributing to Lyman α are well known and were taken from Sharp (1971) and Wolniewicz & Dressler (1988). The dipole moments of Dressler & Wolniewicz (1985) were used for the transitions between the singlet quasi-molecular states, and preliminary *ab initio* results of Spielfiedel (1994) were used for the transitions between the triplet states. We have also performed new *ab initio* calculations for all the H_2 potentials and dipole moments contributing to Lyman α. The results for the B-X transition of H_2 which gives rise to the 1600 Å satellite are displayed in Fig. 2.

The Gaussian basis sets employed are general contractions based on atomic natural orbitals. The primitive basis set for the

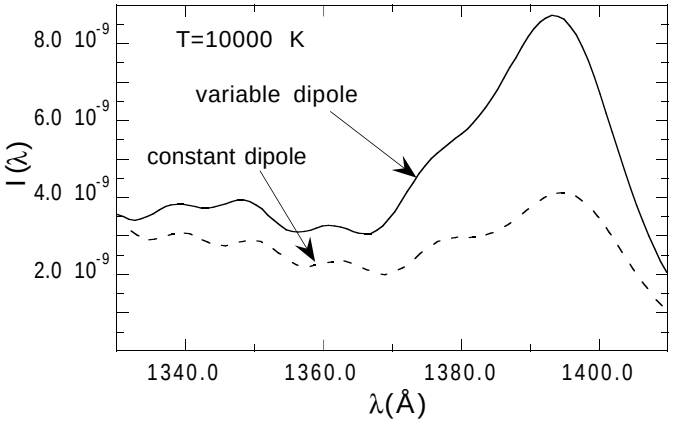

Fig. 3. The 1405 Å satellite of Lyman α due to collisions with H^+ for $n_{H^+} = 10^{17} cm^{-3}$ at 10000 K.

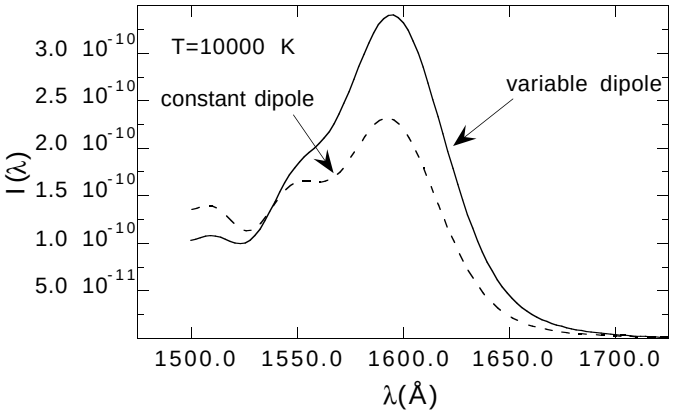

Fig. 4. The 1600 Å satellite of Lyman α due to collisions with other neutral H atoms for $n_H = 10^{17} cm^{-3}$ at 10000 K.

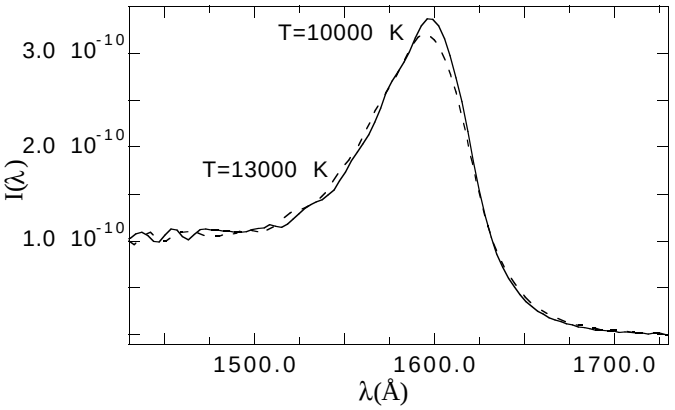

Fig. 5. The 1600 Å satellite of Lyman α at temperatures of 10000 K (—) and 13000 K (- - -).

H atom comprises the [6s] set of van Duijneveldt (1971) contracted to [4s] and the [3p, 2d,1f] polarization set of Dunning (1989). This set was augmented by diffuse functions with exponents $.00945, .00378, .0015$ (s), $.0339, .0136, .0054$ (p) and $.076$ (d). Orbitals ($1\sigma - 8\sigma$, $1\pi - 3\pi$) in u and g symmetries were included in the calculations. Multireference configuration interaction (MRCI) wave functions using a multiconfiguration

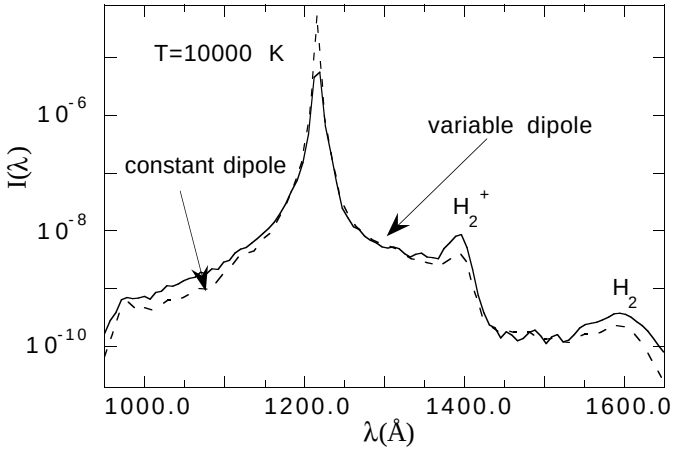

Fig. 6. A comparison of the Lyman α profile calculated with an R-dependent electronic transition dipole moment (—) to a calculation with a constant dipole moment (- - -).

self-consistent field (MCSCF) as a reference were built in order to obtain the best accuracy for both the potential energy and dipole moment functions (Werner & Knowles 1985; Knowles & Werner 1985, 1988). The calculations were performed with the MOLPRO code (Werner & Knowles 1998).

All the new calculated potentials agree very well with the most recent published results (Wolniewicz (1975), Wolniewicz & Dressler (1988), Kolos & Rychlewski (1990,1995)) and the dipole moments of the singlet states are very similar to those of Dressler & Wolniewicz (1985) and Wolniewicz (1975). This lends confidence to the good quality of our values for the dipole moments between the triplet states.

4. Study of the 1405 and 1600 Å satellite features

The line profile calculations of Figs. 3 and 4 have been done at a temperature of 10000 K for a perturber density of 10^{17} cm^{-3}. In Figs. 1 and 2 we have displayed $D(R)$ together with the corresponding $\Delta\omega(R)$ for two transitions which produce satellites on Lyman α in order to point out the importance of variation of dipole moments on the formation of these satellites. An examination of these figures leads us to expect a significant increase in the amplitude of the 1405 Å and 1600 Å satellites, because their dipole moments have maximum values which differ notably from the asymptotic values used in the constant transition dipole moment approximation. Although the position of this maximum in $D(R)$ is at smaller R than the minimum of the difference potential $\Delta\omega(R)$, the corresponding dipole moment increases through the well region of the potential responsible of each satellite.

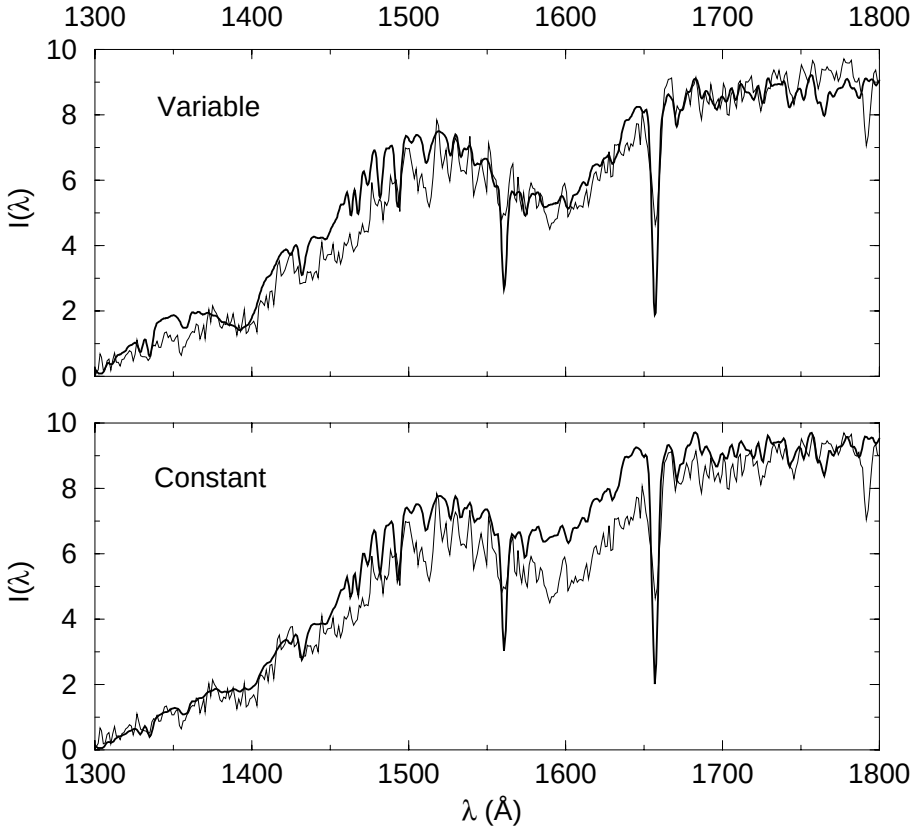

Fig. 7. A comparison of synthetic spectra (—) including Lyman α profiles with and without R-dependence of the electronic transition dipole moment and an IUE spectrum of the star λ Boo (—).

4.1. Calculations of the satellite features with an average velocity

As with our previous work on the Lyman α profile, we have first assumed rectilinear trajectories for the atoms moving with a common relative uniform velocity

$$\bar{v} = (8kT/\pi\mu)^{1/2} , \tag{12}$$

where μ is the reduced mass of the atoms. These results are shown in Figs. 3 and 4.

As expected, the effect of variable $D(R)$ is notable in the line shape of both satellites. The dipole moment variation increases the amplitude by a factor 2 for the 1405 Å satellite and by 1.5 for the 1600 Å satellite. Because of a larger increase of the dipole moment during the collision which gives rise to the 1405 Å satellite, the effect on it is more important and leads to an increase in the ratio of the amplitude of the 1405 Å satellite to that at 1600 Å for equal ion and neutral perturber densities. As noted in Table 1, the ratio changes from 17.9 to 25.7 when the variation in $D(R)$ is included in the model.

4.2. Average over velocity

We also investigated the effect of averaging over the velocity and of the dependence of the satellites on temperature. Profiles of Lyman α leading to the 1405 and 1600 Å satellites were calculated with an average over velocity using 24 point Gauss-Laguerre integration. There is no significant effect, compared to a calculation without the average, except that the oscillations are somewhat smeared out by averaging, as predicted in Allard & Koester (1992). This justifies our use of the average velocity given by Eq. 12 in evaluating Eq. 3, rather than averaging g over velocity.

The calculations presented Fig. 5 have been done with average over velocity at temperatures of 10000 K and 13000 K. We see that there is not much change with temperature in either the shape or amplitude of the satellite. This result justifies our use of theoretical profile calculations at 10000 K in a simulation of the spectrum of λ Boo with a temperature of 8600 K-8650 K, as discussed below.

Table 1. Comparison of the 1405 and 1600 satellite amplitudes for $n_H = n_{H^+} = 10^{17}\mathrm{cm}^{-3}$ at 10000 K.

dipole	1405 satellite	1600 satellite	1405/1600 ratio
constant	4.12 10^{-9}	2.3 10^{-10}	17.9
variable	8.73 10^{-9}	3.4 10^{-10}	25.7
variable/constant	2.11	1.48	

5. Theoretical profiles of Lyman α and application to synthetic spectra of λ Bootis stars

In Fig. 6 the complete profile obtained in the approximation of constant dipole moment is compared to the present calculations. It is interesting to see how much the amplitude for the two calculations differs according to the satellite. In the new results the variation of the dipole moment with R significantly changes only the satellites at 1405 Å and 1600 Å. The effect is minor on the other transitions which contribute to the line profile.

In Fig. 7 we display a comparison between synthetic spectra computed with constant and variable dipole moments and the spectrum of the star λ Boo observed at low spectral resolution with the IUE satellite (SWP17872l). The synthetic spectra have been calculated by Kurucz (Allard et al. 1997) from a model atmosphere computed with the Atlas 12 program. The atmospheric parameters of the synthetic spectra are: $T_{\rm eff} = 8650$ K, $\log {\rm g} = 4.0$; O and N have a solar abundance; $[{\rm C/H}] = -0.37$ (Venn & Lambert 1990) and all the other elements are depleted by a factor of 100 compared to the solar abundance.

The synthetic spectra in Fig. 7 have been multiplied by an arbitrary factor to match the observed one in the range 1700-1800 Å. The synthetic spectrum based on a Lyman α profile with an R-dependent dipole moment agrees best with the observed spectrum. The improvement in the model compared to one with a constant dipole moment is particularly notable in the regions of the quasi-molecular satellite features.

6. Conclusion

Satellites in the wings of atomic lines which arise during collisions between the radiating atom and perturbers can be used as diagnostics of the stellar temperature and gravity. The entire line wing and the characteristic wavelength, strength, and shape of these features depend directly on the potential energy curves for the electronic states of transient quasi-molecule correlated to the atomic levels of the transition (Allard & Kielkopf 1982). Usually, the profiles are calculated assuming that the dipole moment is constant during a collision of the radiator with a perturber. It is well known, however, from examples in other radiative processes such as bound-free transitions leading to spontaneous radiative dissociation (Stephens & Dalgarno 1972), that the dependence of dipole moment on the separation of the radiator and the perturber has to be taken into account to obtain reliable results. In this work we have seen that it is also necessary to include this effect in order to model accurately the far wing of Lyman α in stellar spectra.

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