THE PSEUDOCONTINUUM BOUND-FREE OPACITY OF HYDROGEN AND ITS IMPORTANCE IN COOL WHITE DWARF ATMOSPHERES

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ABSTRACT

We investigate the importance of the pseudocontinuum bound-free opacity from hydrogen atoms in the atmospheres of cool white dwarfs. This source of absorption, when calculated by the occupation probability formalism applied in the modeling of white dwarf atmospheres with $T_{\text{eff}} < 17,000$ K, dominates all other sources of opacity at optical wavelengths. This is unrealistic and not observed. On the other hand, a significant flux suppression in the blue part of the spectra of cool white dwarfs has been reported and mainly interpreted as a result of the pseudocontinuum absorption from atomic hydrogen. We investigate this problem by proposing a new, more realistic approach to calculating this source of opacity. We show that this absorption is orders of magnitude smaller than that predicted by current methods. Therefore, we rule out the pseudocontinuum opacity as a source of the flux deficiency observed in the spectra of cool white dwarfs.

Subject headings: atomic processes — dense matter — stars: atmospheres — white dwarfs

1. INTRODUCTION

Cool white dwarfs are among the oldest objects in the universe. The detection of large populations of these old stars in our Galaxy gives us a unique opportunity to use them as chronometers. To achieve this goal, we need reliable atmosphere models for cool white dwarfs. Such models would allow for a better determination of the atmospheric parameters of observed white dwarf stars, tracking the evolution of their atmospheric composition, and better attainment of boundary conditions for modeling internal structures and the cooling of these stars (Fontaine et al. 2001). One problem in modeling cool white dwarf atmospheres is the implementation of the Däppen-Anderson-Mihalas model (Däppen et al. 1987, hereafter DAM87) in calculating the pseudocontinuum bound-free opacity from the ground state of atomic hydrogen. When this source of opacity is calculated following the DAM87 prescription with the occupation probabilities of Hummer & Mihalas (1988, hereafter HM88) for white dwarfs with $T_{\text{eff}} < 17,000$ K, it dominates all other absorption processes at optical wavelengths. Such strong absorption is completely unrealistic and is not observed (Bergeron 2001; Bergeron et al. 1997). Nonetheless, this process may still be significant in white dwarf atmospheres. In fact, Bergeron et al. (1997) suggested that this absorption mechanism may be responsible for the observed flux suppression in the blue part of the spectra of cool white dwarfs. Following that idea, Bergeron (2001) introduced an arbitrary damping function to the DAM87 pseudocontinuum opacity to obtain good fits of the models to the photometry of selected stars. However, the damping function must be adjusted for each star, indicating how unsuitable the DAM87 model is. As a result, the pseudocontinuum bound-free opacity of hydrogen atoms is ignored in the modeling of cool white dwarf atmospheres. In this paper we readdress this issue by computing this absorption mechanism with a much more realistic physical model to assess its importance in cool white dwarf atmospheres.

The pseudocontinuum bound-free opacity results from the perturbation of hydrogen atoms in their ground state by their interaction with other particles in a dense medium (DAM87). Such perturbations result in a lowering of the ionization barrier of some of the hydrogen atoms and the possibility of a bound-free transition caused by photons with energies that are smaller than the ionization potential of the isolated hydrogen atom. DAM87 considers this process in the framework of the occupation probability formalism proposed by HM88. They constructed a simple model for the optical properties of an interacting hydrogen medium. In the weakly ionized atmospheres of cool white dwarfs, the hydrogen atoms in higher excited states are perturbed mostly by neutral particles (Bergeron et al. 1991) and eventually destroyed (pressure ionized) by excluded volume interactions. The effect is stronger for excited states because the size of a hydrogen atom is a monotonically increasing function of the principal quantum number. This model for the pseudocontinuum opacity is not very precise, as it treats the interparticle interactions and the associated lowering of the ionization potential only in terms of the average sizes of the particles. We show that a quantum mechanical description of the interactions between hydrogen atoms and perturbers, absent in the simple DAM87 model, is necessary to obtain a physically realistic value of the pseudocontinuum opacity of hydrogen atoms in the atmospheres of white dwarf stars.

To accurately account for the effect of lowering the hydrogen ionization barrier in a dense medium, we consider short-range, binary collisions. The ionization energy of the perturbed hydrogen atom is given by the ionization energy of the H-perturber pair. This energy is given by the difference between the exact interaction energy curves calculated quantum mechanically of the neutral and singly ionized dimers (interacting pairs). The probability of having a pair colliding with a given collision distance can be determined from the interaction potential of the neutral dimer. The resulting probabilities of lowered hydrogen ionization potential for the physical conditions of white dwarf atmospheres are orders of magnitude smaller than those obtained from the DAM87 model with the HM88 occupation probabilities.

In § 2 we discuss the DAM87 approach to the pseudocontinuum opacity. Our new calculations of this absorption mechanism and its application to the physical conditions found in the atmospheres of cool white dwarfs are presented in §§ 3 and 4, respectively.
2. THE PSEUDOCONTINUUM OPACITY MODEL OF DAPPEN-ANDERSON-MIHALAS

The DAM87 model is based on the occupation probability formalism introduced by HM88 for calculating thermodynamical properties of a nonideal gas. HM88 introduced the nonideal effects on the equation of state by modifying the internal partition functions of bound species. The modified partition function of the hydrogen atom is given by

\[ Z_H = \sum_i g_i \omega_i e^{-\epsilon_i/k_B T} = \sum_i \omega_i \gamma_i, \]

where \( k_B \) is the Boltzmann constant, \( i \) indicates the atomic level, \( g_i \) is the statistical weight, \( \epsilon_i \) is the energy of hydrogen atom counted from the energy of the ground state \((i = 0)\), \( T \) is the temperature, and \( \omega_i \) is the occupation probability. In the HM88 model, \( \omega_i \) represents the strength of nonideal gas perturbations on an atomic level \( i \). Its value for the physical conditions found inside weakly ionized cool white dwarf atmospheres is given by the excluded volume interactions model (Bergeron et al. 1991) and decreases for higher principal quantum number (HM88, eq. [3.4]). The number of hydrogen atoms in the excited state \( i \) is expressed as

\[ \frac{n_i}{n_{\text{tot}}} = \frac{\omega_i \gamma_i}{Z_H}, \]

where \( n_{\text{tot}} \) is the total number density of atomic hydrogen.

DAM87 extended this model for the calculation of the optical properties of hydrogen atoms in the partially ionized plasma. They interpreted the factor \( 1 - \omega_i \) as the fraction of hydrogen atoms with atomic level \( i \) being “dissolved,” i.e., sufficiently perturbed to describe an unbound electron and ion. They assigned this value to the fraction of free electrons state available for a bound-free transition to level \( i \). DAM87 used this interpretation to derive that for the absorption of a photon associated with the transition from level \( i \) to level \( j \), the probability that level \( j \) is bound, and the transition is “bound-bound,” is \( \omega_i / \omega_j < 1 \). Therefore, the probability of having a “bound-free” transition is

\[ P_{\text{bf}} = 1 - \frac{\omega_j}{\omega_i}. \]

To describe the pseudocontinuum absorption to the continuum energy levels localized between two discrete but “dissolved” levels of the hydrogen atom, DAM87 introduced the pseudo-level \( n^* \) with occupation probability \( \omega_{n^*} \). The latter is calculated by the interpolation between the \( \omega_i \) values. Therefore, the probability that during the \( i \) to \( n^* \) transition the absorbing electron goes into the continuum is given by (eq. [32] of DAM87)

\[ P_{\text{bf}} = 1 - \frac{\omega_{n^*}}{\omega_i}. \]

The dominant perturbers in the atmospheres of cool white dwarfs are neutral particles. Therefore, in calculating the DAM87 pseudocontinuum opacity we used the hard sphere model for \( \omega_i \) of HM88 (§ IIIa). In Figure 1 we present the main opacity sources for the photosphere of white dwarf star LP 380-5, considered for the potential presence of pseudocontinuum opacity by Bergeron (2001). The DAM87 pseudocontinuum opacity is much too high and dominates all other opacity sources by orders of magnitude. This is unrealistic and simply not observed. Therefore, the DAM87 model highly overestimates the probabilities of pseudocontinuum bound-free absorption (eq. [4]) in the atmospheres of cool white dwarf stars. In view of the difficulty with this application of the DAM87 model of the pseudocontinuum opacity, we propose a more realistic approach to calculate this source of absorption.

3. A NEW MODEL FOR THE PSEUDOCONTINUUM OPACITY OF HYDROGEN

The bound-free absorption process results in the ionization of a hydrogen atom. The lowering of the hydrogen ionization potential arises from the interaction of the hydrogen atom with neighboring particles (DAM87). However, we are interested in the pseudocontinuum opacity far from the Lyman edge, i.e., \( \lambda \gtrsim 1500 \text{ Å} \). A significant lowering of the hydrogen ionization barrier, by more than \( \sim 5 \text{ eV} \), is required for bound-free absorption at these wavelengths. Such a situation occurs in the case of rare, close collisions for which the interparticle collision distances, \( r_c \), are small enough that the probability, \( P_c \), of finding a colliding pair with an interparticle separation smaller than \( r_c \) is much smaller than unity. In this case, multiparticle collisions are insignificant, as the probability of having a close \( N \)-particle collision is roughly \( \sim P_c^{N-1} \). Therefore, it is sufficient to consider the interaction between a hydrogen atom and its closest neighbor only. Allard et al. (2004) used this approximation to successfully explain the complex shape of the Ly\(\alpha \) line wings detected in the spectra of white dwarfs with \( T_{\text{eff}} \approx 12,000 \text{ K} \).

For a given colliding pair the change in the ionization energy results from the formation of a temporary dimer, whose ionization energy differs from that of the isolated hydrogen atom, \( I_0 = 13.598 \text{ eV} \). This modified ionization barrier, \( I_p \), is given by the ionization energy of a dimer calculated at a fixed interparticle separation \( r_c \),

\[ I_p(r_c) = V_{H^+ - \text{pert}}(r_c) - V_{H^+ - \text{pert}}(r_c). \]
where $V_{\text{H-per}}(r_c)$ and $V_{\text{H}^+\text{-per}}(r_c)$ are the energies of the neutral and singly ionized dimers, respectively. This picture is in the spirit of the Franck-Condon principle, which states that as a result of large differences between the mass of the absorbing electron and the nuclear mass, the nuclei remain fixed during the absorption/emission of a photon (Davydov 1965, § 123). The differential probability of finding such a dimer with an interparticle separation between $r_c$ and $r_c + dr_c$ in the low-density medium ($\rho \leq 0.1 \text{ g cm}^{-3}$) is given by (Martynov 1992).

$$dP(r_c) = n_{\text{pert}} \left( \int_{\theta, \phi} e^{-V_{\text{H-per}}(r_c, \theta, \phi)/k_B T} \sin \theta \, d\theta \, d\phi \right) r_c^2 \, dr_c,$$

$$\text{(6)}$$

**Fig. 2.** Interaction energy curves as a function of the interparticle collision distance for neutral dimers (bottom curves) and the corresponding single-ionized dimers (top curves). The different curves for the H-H interaction are for the bound (solid line) and antibound (dotted line) interaction potentials for H-H and H$_2^+$. The different energy curves for the H-H$_2$ interaction represent the potentials for different orientation of the molecule, with the angle defined between the line connecting the perturber to the center of H$_2$ and the molecular axis. Interaction for the following angles are shown: 90° (solid line), 45° (dotted line), and 0° (dashed line).

**Fig. 3.** Same as Fig. 2, but for the ionization energy of dimers.
where \( n_{\text{pert}} \) is a number density of perturbers, and \( V_{\text{H-pert}} \) is the interaction energy between a hydrogen atom and the perturber localized at the position \((r_c, \theta, \phi)\) in relation to the hydrogen atom, which is assumed to be at the origin of the coordinate system. The dominant species, and therefore the main perturbers, in the atmospheres of cool white dwarfs are H, H\(_2\), and He. The sources for the potentials for the interaction of hydrogen atom with perturbers are chosen to be H-H (Kolos & Wolniewicz 1965), H-H\(_2\) (Broothroyd et al. 1991), and H-He (Shalabi et al. 1998). The corresponding potential curves for the singly ionized dimers are chosen to be H\(_2^+\) (Bates & Reid 1968), H\(_3^+\) (Prosmitt et al. 1997), and HeH\(^+\) (Green et al. 1974). These potentials are plotted in Figure 2. As a result of the gerade/ungerade symmetry in the H-H interaction, we have to consider both the “bound” and the “antibound” H-H potential energy curves. For the singly ionized dimers we choose the ground state potential energy curves because the upper energy curves (like the antibound state for H\(_2^+\); Fig. 2) would result in a much smaller decrease in the ionization energy for a given \( r_c \). This decrease occurs with much smaller probability than the same change in the ionization potential that results from the ionic ground states at a much larger \( r_c \), and therefore can be neglected. The resulting ionization energy \( I_p(r_c) \) for a given dimer as a function of the collision distance is plotted in Figure 3. The ionization energy can decrease to \( \approx 5 \) eV, which occurs at very small \( r_c \). Because of the strong repulsion in the neutral dimer at short separation (Fig. 2), such a lowering of the ionization energy occurs with very small probability, as for small \( r_c \), the Boltzmann factor \( e^{-\Delta E_{\text{emp}}/k T} \ll 1 \) in equation (6). Moreover, in the case of the H-H interaction, only the antibound potential leads to a significant decrease of the ionization barrier (Fig. 2).
The probability of a hydrogen atom having an ionization energy $I_p$ sufficiently small for photoionization to be caused by a photon of frequency $C_2^3$ is

$$P = \frac{I_p(r_c)}{hC_2^3} \quad \text{with} \quad r_c < hC_2^3$$

where the integration is performed over the range of separations $r_c$ such that $I_p(r_c) < hC_2^3$. The resulting probabilities, as a function of photon wavelength $k$, of having a bound-free transition for hydrogen for two temperatures and three different compositions are shown in Figure 4. The corresponding probabilities from the DAM87 model (also shown in Fig. 4) are a few orders of magnitude larger. We find that for a given density, collisions with H$_2$ are most effective at lowering the ionization energy of hydrogen, because for a given value of $I_p(r_c)$, the interaction potential $V_{H-H^2}(r_c)$ computed for the orientation angle $\theta = 90$° (see caption of Fig. 2 for definition) is much less repulsive than $V_{H-H}(r_c)$ and $V_{H-He}(r_c)$.

The pseudocontinuum opacity is then obtained with

$$\kappa_{bf}(\nu) = n_{H}P(\nu)\sigma_{bf}^{0}(\nu), \quad h\nu < 13.598 \text{ eV},$$

where $\sigma_{bf}^{0}(\nu)$ is the bound-free cross section of the isolated hydrogen atom extrapolated beyond the Lyman edge (DAM87), $n_{H}$ is the number density of hydrogen atoms, and $\rho$ is the mass density. A proper calculation would consider the bound-free cross section of the dimer as a function of interparticle separation. To our knowledge this information is not available. However, as the photoionization cross sections for H (Palenius et al. 1976) and H$_2$ (Ford et al. 1975) differ by less than a factor of 3, and the cross section is the effective size of the absorbing system as seen by the photon, we estimate that the extrapolation of the bound-free cross section of the isolated hydrogen atom beyond the Lyman edge introduces an uncertainty no larger than an order of magnitude on $\kappa_{bf}(\nu)$ calculated by equation (8). In helium-rich atmospheres, where the density can be as high as $2 \times 10^{13}$ cm$^{-3}$, equation (6) should be corrected when $\rho > 0.1$ g cm$^{-3}$, by a factor $e^{3}\omega_{H-pert}$ (Martynov 1992), where $\omega_{H-pert}$ is a thermal potential that arises from the correlations in the dense fluid. Solving the Ornstein-Zernike equation in the Percus-Yevick approximation (Martynov 1992) for fluid helium, we have verified that in the helium-rich atmospheres of cool white dwarfs, $e^{3}\omega_{H-pert} < 100$. Therefore, because of correlations in the most extreme case, equation (8) leads to an underestimate of $\kappa_{bf}$ of no more than 2 orders of magnitude. We see below that this does not affect our conclusions.

4. IMPORTANCE OF THE PSEUDOCONTINUUM OPACITY IN COOL WHITE DWARF ATMOSPHERES

Our goal is to investigate the suggestion of Bergeron et al. (1997) and Bergeron (2001) that the pseudocontinuum bound-free
absorption by atomic hydrogen beyond the Lyman edge may be the missing source of opacity in the atmosphere models of cool white dwarfs ($T_{\text{eff}} \lesssim 6000$ K). For this purpose, we have computed opacities for temperatures, densities, and He/H compositions that are representative of the photospheres of these stars. The pseudocontinuum opacity calculated with our model dominates all other sources of opacity at wavelengths shorter than $\sim 2000$ Å (Fig. 5). For these cool stars the flux at these wavelengths is extremely small and completely negligible (see Bergeron 2001, Fig. 5). We also note that the uncertainty in the photoionization cross section and our neglect of the correlations in dense helium-rich atmospheres do not alter the pseudocontinuum opacity enough to make it important at $\lambda > 2000$ Å.

Figure 1 reproduces the opacity plot of Bergeron (2001, Fig. 4). This figure represents the main sources of opacity for the physical conditions found at the photosphere of the white dwarf star LP 380-5. Our pseudocontinuum opacity is several orders of magnitude smaller than that necessary to fit the blue spectrum (3000–4000 Å) of this star (Bergeron 2001) and is completely insignificant at $\lambda > 2000$ Å.

5. CONCLUSIONS

The possible presence of an unknown absorption mechanism in the atmospheres of cool white dwarfs has been reported by Bergeron (2001) and Bergeron et al. (1997). This opacity source has been attributed to the pseudocontinuum bound-free opacity from hydrogen atoms in their ground state that results from a lowering of the ionization potential because of interparticle interactions in the gas. Opacity models based on the occupation probability formalism highly overestimate this source of absorption in the atmospheres of cool white dwarfs. For this reason, it is usually omitted in models. In this paper we presented a realistic model for this absorption mechanism based on binary collisions, exact pair interaction potentials, and the ionization energy of the colliding pair. We find that the pseudocontinuum bound-free opacity decreases very rapidly with wavelength beyond the Lyman edge and becomes completely negligible beyond $\lambda \sim 2000$ Å over the entire range of temperature, density, and H/He composition relevant to cool white dwarf atmospheres. Therefore, another absorption mechanism must be invoked to explain the flux excess of the models in the blue part of the spectrum of these stars.

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