The Contribution of the Absorption Processes to the Opacity of DB White Dwarf Atmospheres in UV and VUV Regions

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Abstract. The main aim of this work is to estimate the total contribution to the opacity of DB white dwarf atmosphere of the processes of the He_2^+ molecular ion photo-dissociation and $He + He^+$ collisional absorption charge exchange, and compare it with the contribution of He^-, and other relevant, radiative absorption processes included in standard models.

Keywords: atmospheres, radiative transfer, atomic processes, molecular processes.
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INTRODUCTION

Earlier, for the considered DB white dwarf atmospheres ($T_{eff} = 12000$ K - 14000 K, $\log g = 7 - 8$) as the main source of the continuous absorption was treated the He^- absorption process

$$\varepsilon_\lambda + He + \vec{e} \Rightarrow He + \vec{e}', \tag{1}$$

where ε_λ is the energy of photon with the wavelength λ, and $\vec{e}$ and $\vec{e}'$ denotes the free electron before and after the collision with the He atom. Besides the He^- absorption process, usually included are the bound - free absorption processes, mentioned by [1] including the other relevant reaction channel

$$\varepsilon_\lambda + \begin{cases} He^*(n,L,S) \\ He^+ + \vec{e} \end{cases} \Rightarrow He^+ + \vec{e}', \tag{2}$$

where $He^*(n,L,S)$ is the helium atom in the excited state, n - the corresponding principal quantum number, L and S - quantum numbers of orbital momentum and spin. Continuous absorption opacity due to the processes of He_2^+ molecular ion photo-dissociation

$$\varepsilon_\lambda + He_2^+ \Rightarrow He + He^+, \tag{3}$$

and $He + He^+$ collisional absorption charge exchange

$$\varepsilon_\lambda + He + He^+ \Rightarrow \begin{cases} He^+ + He \\ He + He^+ \end{cases} \tag{4}$$

where $He \equiv He(1s^2)$, $He^+ \equiv He^+(1s)$ and $He_2^+ \equiv He_2^+(X^2\Sigma_u^+)$, were neglected in DB white dwarf atmosphere modeling up to the beginning of nineties. However, in [2] and [3], using DB white dwarf atmosphere models of [4], it was demonstrated that at least for $T_{eff} < 16000$ K, these processes should contribute to the opacity in the optical region. In these papers the absorption coefficients for both (3) and (4) processes have been determined within the semiclassical (quasi-static) method developed by [5].

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The results from [3], obtained for one Koester model (log g =8 and T_{eff} = 12000 K), already enabled a more real picture on the relative importance of He^- and He_2^+ total absorption processes at lest in the region $\lambda \geq 300$ nm. From these results follows the crossing of the curves for He^- and He_2^+ absorption coefficients. In the next paper [6] relative importance of He_2^+ and other relevant absorption processes in the region $\lambda \geq 200$ nm was examined for several Koester's models (T_{eff} = 12000 K, 14000 K, 16000 K, log g =7, 8; see [4]). It was shown that in all considered cases, the contribution to opacity of the processes of He_2^+ molecular ion photo-dissociation and $He + He^+$ collisional absorption charge exchange together, is close or at least comparable with the contribution of the He^- absorption processes (1) and the atomic absorption processes (2).

Here were performed the necessary calculations of absorption coefficients characterizing the processes (3) and (4). The determination of these coefficients was performed by the potential curves of molecular ion He_2^+ in $X^2\Sigma_u^+$- and $A^2\Sigma_g^+$- states, as well as the corresponding dipole matrix element, which were precisely calculated during this research. These characteristics of He_2^+ are here presented.

In order to determine the relative efficiency of the processes (3) and (4) in UV and VUV regions for particular DB white dwarf atmosphere layers, the corresponding absorption coefficients will be compared with the absorption coefficients which characterize the concurrent processes (1) and (2) for $51 \text{ nm} \leq \lambda \leq 400 \text{ nm}$. As the lower boundary of this region was taken $\lambda = 51 \text{ nm}$ which is close to the He atom ionization boundary $\lambda_{He} \cong 50.14$ nm, below which the photo-ionization of the He atom absolutely dominates in comparison with all other absorption processes.

Besides, here we will consider the hydrogen photo-ionization process

$$\varepsilon_\lambda + H \Rightarrow H^+ + \vec{e}'. \tag{5}$$

Although accordingly to [4] the ratio of hydrogen and helium abundances in the considered DB white dwarf atmospheres is $1:10^5$, our estimations showed that the process (5) could play certain role for $\lambda < \lambda_H$, where $\lambda_H \cong 91.13$ nm is the H atom ionization boundary.

CHARACTERISTICS OF PHOTO-DISSOCIATION AND ION-ATOM ABSORPTION PROCESSES

The photo-dissociation cross-section. The photo-dissociation process (3) is characterized here by the corresponding average cross-section $\sigma_{phd}(\lambda, T)$. This cross-section is defined by

$$\sigma_{phd}(\lambda, T) = \frac{\sum_J \sum_v g_{v,J} \cdot (2J+1) e^{\frac{-E_{v,J}}{kT}} \cdot \sigma_{v,J}(\lambda)}{\sum_J \sum_v g_{v,J} \cdot (2J+1) e^{\frac{-E_{v,J}}{kT}}}, \tag{6}$$

where v and J are the vibrational and rotational quantum numbers of the individual rovibrational states (v, J) of the molecular ion $He_2^+(X^2\Sigma_u^+)$, $\sigma_{v,J}(\lambda)$ - the partial photo-dissociation cross-sections of these states, $E_{v,J}$ and $g_{v,J} \cdot (2J+1)$ - the corresponding energies with respect to the ground rovibrational state and statistical weights, while factor $g_{v,J}$ describes the influence of the nuclear spin. Since for DB white dwarf atmospheres the temperatures $T \geq 8000$ K are relevant, in further considerations we will take that $g_{v,J} = 1$.

Within the dipole approximation the partial cross-sections $\sigma_{v,J}(\lambda)$ are given by the expressions

$$\sigma_{v,J}(\lambda) = \frac{8\pi^3}{3\lambda}\left[\frac{J+1}{2J+1} | D_{E,J+1;v,J} |^2 + \frac{J}{2J+1} | D_{E,J-1;v,J} |^2\right], \tag{7}$$

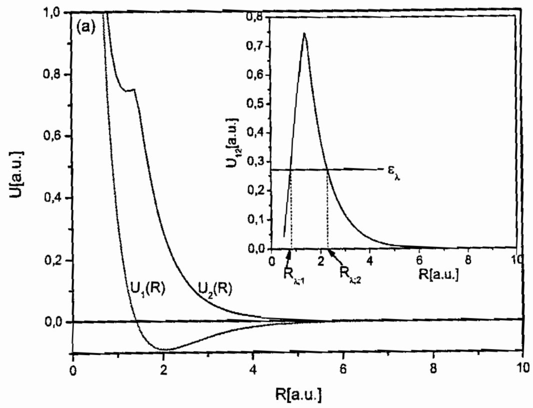
where $D_{E,J+1;v,J}$ and $D_{E,J-1;v,J}$ are the radial matrix elements given by the relations

$$D_{E,J;v,J'} = < \Psi_{2;E,J'}(R) | D_{12}(R) | \Psi_{1;v,J}(R) >, \quad J = J' \pm 1, \tag{8}$$

$$D_{12}(R) = | \mathbf{D}_{12}(R) |, \qquad \mathbf{D}_{12}(R) = < 1 | \mathbf{D}(R) | 2 >, \tag{9}$$

where R is the internuclear distance, $\mathbf{D}(R)$ - the operator of electron dipole momentum, and $|1\rangle \equiv X^2\Sigma_u^+$ and $|2\rangle \equiv A^2\Sigma_g^+$ - the ground and the first excited electronic states of the molecular ion He_2^+ with the potential curves $U_1(R)$ and $U_2(R)$, respectively. With $\Psi_{1;v,J}(R)$ and $\Psi_{2;E,J'}(R)$ are denoted the adiabatic nuclear radial wave functions of the bound state (v,J) in the potential $U_1(R)$ and the continual state (E,J') in the potential $U_2(R)$ respectively, with $E = E_{v,J} + \varepsilon_\lambda$. It is assumed that the wave functions $\Psi_{1;v,J}(R)$ and $\Psi_{2;E,J'}(R)$ satisfy the standard ortho-normalization conditions.

The calculations of the potential energies $U_1(R)$ and $U_2(R)$ and the matrix element $D_{12}(R)$ were performed under D_{2h} symmetry using the MOLPRO package of programs [7]. They were performed at the multi-reference configuration interaction (MRCI) level using multi-configuration self-consistent field (MCSCF) orbitals with the cc-pv5z basis set of [8] and [9]. We started at the self-consistent field (SCF) level with the ground state electron configuration $a_g^2 b_{1u}^1$. The active space at the MCSCF step contained $3a_g$ and $3b_{1u}$ orbitals without any closed or core orbitals (all three electrons were involved). Obtained potential curves $U_1(R)$ and $U_2(R)$ are presented in Fig. 1a, and dipole matrix element $D_{12}(R)$ - in Fig. 1b.



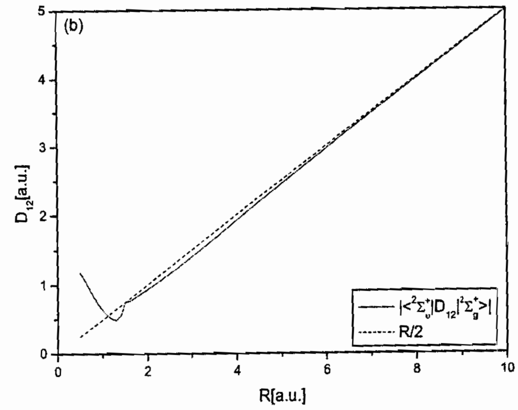


FIGURE 1. (a) The potential curves of the molecular ion He_2^+ : $U_1(R)$ ($X^2\Sigma_u^+$), and $U_2(R)$ ($A^2\Sigma_g^+$); $U_{12}(R) = U_2(R) - U_1(R)$; $R_{\lambda;1}$ and $R_{\lambda;2}$ - two real roots of the equation $U_{12}(R) = \varepsilon_\lambda$; (b) The matrix element $D_{12}(R)$ for the transition between the electronic states $X^2\Sigma_u^+$ and $A^2\Sigma_g^+$ of the ion He_2^+.

The partial absorption coefficients. The efficiencies of the photo-dissociation process (3) and of the charge-exchange absorption process (4) are characterized separately by the partial spectral absorption coefficients $\kappa_{ia}^{(a)}(\lambda) \equiv \kappa_{ia}^{(a)}(\lambda; T, N(He_2^+)) = \sigma_{phd}(\lambda,T)N(He_2^+)$ and $\kappa_{ia}^{(b)}(\lambda) \equiv \kappa_{ia}^{(b)}(\lambda; T, N(He), N(He^+))$ where T, $N(He_2^+)$, $N(He)$ and $N(He^+)$ are the local temperature and the densities of $He_2^+(X^2\Sigma_u^+)$, He and He^+ in the considered layer of the DB white dwarf atmosphere. Following our previous paper [10] and assuming the existence of LTE, we will take the photo-dissociation coefficient $\kappa_{ia}^{(a)}(\lambda)$ in an equivalent form suitable for further considerations, namely

$$\kappa_{ia}^{(a)}(\lambda) = K_{ia}^{(a)}(\lambda, T) N(He) N(He^+), \tag{10}$$

$$K_{ia}^{(a)}(\lambda, T) = \sigma_{phd}(\lambda, T) \cdot \chi_{ia}(T)\,;\ \chi_{ia}(T) = \frac{N(He_2^+)}{N(He)N(He^+)}. \tag{11}$$

Here the photo-dissociation cross-section $\sigma_{phd}(\lambda,T)$ is given by Eqs. (6)-(7), and the quantity χ_{ia}, which contains the density $N(He_2^+)$, is determined from the law of mass action

$$\chi^{-1}(T) = \left(\frac{\mu k T}{2\pi\hbar^2}\right)^{\frac{3}{2}} \cdot \frac{g(He)g(H^+)}{\sum_J \sum_v g_{v,J} \cdot (2J+1) e^{\frac{-E_{v,J}}{kT}}} \cdot \exp\left(-\frac{D}{kT}\right), \tag{12}$$

where μ and D are the reduced mass and the dissociation energy of the molecular ion He_2^+, and $g(He) = 1$ and $g(He^+) = 2$ - the statistical weights of the atom He and ion He^+. The charge-exchange absorption coefficient $\kappa_{ia}^{(b)}(\lambda)$ is defined by

$$\kappa_{ia}^{(b)}(\lambda) = K_{ia}^{(b)}(\lambda, T)N(He)N(He^+), \tag{13}$$

where the coefficient $K_{ia}^{(b)}(\lambda, T)$ is determined here by the semi-classical method developed in [5] on the basis of the quasi-static approximation [3,6,10]. Within this method, only the λ region where the equation

$$U_{12}(R) \equiv U_2(R) - U_1(R) = \varepsilon_\lambda \tag{14}$$

has real roots is considered. Consequently, in the helium case the quasi-static method is applicable in the region $\lambda \geq 62$ nm where this equation has two real roots (see Fig. 1a), $R_{\lambda;1}$ and $R_{\lambda;2} > R_{\lambda;1}$. In [6], where optical region of λ was treated, only the larger of these roots has been taken into account. However, in far UV and VUV regions both roots should be taken into account. Consequently, we will take here $K_{ia}^{(b)}(\lambda, T)$ in the form

$$K_{ia}^{(b)}(\lambda,T) = 0.62\cdot 10^{-42}\sum_{i=1}^{2}\frac{\left[\frac{2D_{12}(R_{\lambda;i})}{eR_{\lambda;i}}\right]^2}{\gamma(R_{\lambda;i})}\left(\frac{R_{\lambda;i}}{a_0}\right)^4 \exp\left[-\frac{U_1(R_{\lambda;i})}{kT}\right]\cdot\xi(R_{\lambda;i}) \tag{15}$$

$$\gamma(R_{\lambda;i}) = \left|\frac{d\ln\left[\frac{U_{12}(R)}{2Ry}\right]}{d(R/a_0)}\right|_{R=R_{\lambda;i}}, \quad \xi(R_{\lambda;i}) = \begin{cases} 1, & U_1(R_{\lambda;i}) \geq 0, \\ \dfrac{\Gamma\left(\frac{3}{2}; -\frac{U_1(R_{\lambda;i})}{kT}\right)}{\Gamma\left(\frac{3}{2}\right)}, & U_1(R_{\lambda;i}) < 0, \end{cases} \tag{16}$$

where e and a_0 are the electron charge and the atomic unit of length, and $K_{ia}^{(b)}(\lambda, T)$ is expressed in [cm^5].

The total absorption coefficient. The efficiency of absorption processes (3) and (4) together is characterized by the total spectral absorption coefficient $\kappa_{ia}(\lambda) \equiv \kappa_{ia}(\lambda; T, N(He), N(He^+))$ given by: $\kappa_{ia}(\lambda) = \kappa_{ia}^{(a)}(\lambda) + \kappa_{ia}^{(b)}(\lambda)$. Using Eqs. (10) and (13) for $\kappa_{ia}^{(a)}(\lambda)$ and $\kappa_{ia}^{(b)}(\lambda)$ we will take $\kappa_{ia}(\lambda)$ in the form

$$\kappa_{ia}(\lambda) = K_{ia}(\lambda, T)N(He)N(He^+), \quad K_{ia}(\lambda, T) = K_{ia}^{(a)}(\lambda, T) + K_{ia}^{(b)}(\lambda, T), \tag{17}$$

where $K_{ia}^{(a)}(\lambda, T)$ is given by Eq. (11), and $K_{ia}^{(b)}(\lambda, T)$ - by Eq. (15). For the comparison of the efficiency of processes (3) and (4) with the efficiencies of the concurrent processes (1), (2) and (5) just the total absorption coefficients $\kappa_{ia}(\lambda)$ and $K_{ia}(\lambda, T)$ are needed.

The efficiency of processes (3) and (4) within DB white dwarf atmosphere is compared here with the efficiency of the concurrent absorption processes (1) and (2), which are characterized by the spectral absorption coefficients $\kappa_{ea}(\lambda)$ and $\kappa_{ei}(\lambda)$, namely

$$\kappa_{ea}(\lambda) = K_{ea}(\lambda, T)\cdot Ne\cdot N(He), \qquad \kappa_{ei}(\lambda) = K_{a;ei}(\lambda, T)\cdot Ne\cdot N(He^+), \tag{18}$$

$$K_{a;ei}(\lambda, T) = \sum_{n\geq 2, L, S}\sigma_{nLS}(\lambda)\cdot\chi_{nLS}(T) + K_{ei}(\lambda, T), \qquad \chi_{nLS}(T) = \frac{N(He^*(n, L, S))}{N_e N(He^+)}. \tag{19}$$

where $K_{ea}(\lambda, T)$ and $K_{ei}(\lambda, T)$ are the rate coefficients which describe absorption by $(e + He)$- and $(e + He^+)$-collision systems. With N_e and $N(He^*(n, L, S))$ are denoted the densities of the free electrons and the excited atoms $He^*(n, L, S)$, and with $\sigma_{nLS}(\lambda)$ - corresponding excited atom photo-ionization cross-section. It was found that in all considered cases the absorption processes (2) play a minor role in comparison with the electron-atom process (1). This is a consequence of the fact that helium plasma in considered layers of DB white dwarf atmosphere is weakly ionized. The relative efficiency of the processes (3) and (4) with respect to processes (1) and (2) together is characterized by the parameter $F_{He}(\lambda)$ defined by

$$F_{He}(\lambda) = \frac{\kappa_{ia}(\lambda)}{\kappa_{ea}(\lambda) + \kappa_{ei}(\lambda)} = \frac{K_{ia}(\lambda, T)\left[N(He^+)/N_e\right]}{K_{ea}(\lambda, T) + K_{ei}(\lambda, T)\left[N(He^+)/N(He)\right]}. \tag{20}$$

In calculations of $F_{He}(\lambda)$ the coefficient $K_{ea}(\lambda, T)$ was determined by means of the data from [11], and $K_{a;ei}(\lambda, T)$ - by means of expressions from [12] for the partial photo-ionization cross-section $\sigma_{nLS}(\lambda)$ and the free-free electron-ion absorption coefficient $K_{ei}(\lambda, T)$.

As in [3,6] the parameter $F_{He}(\lambda)$ is treated as a function of $\log\tau$, where τ is Rosseland optical depth of the considered atmosphere layer [13]. The values of $\log\tau$ are taken from [4]. The behavior of $F_{He}(\lambda;\log\tau)$ is illustrated in Fig. 2, for atmosphere of DB white dwarfs with $T_{eff} = 12000$ K and $\log\tau = 8$. According to the expectations, the relative efficiency of absorption processes (3) and (4) in far UV and VUV regions was increased several times with respect to the optical region. The result is that the processes (3) and (4) in the region $80 \text{ nm} \leq \lambda \leq 200 \text{ nm}$ dominate in comparison with the concurrent processes (1) and (2) in significant parts of DB white dwarf atmospheres (maximal values of $F_{He} \approx 2.5$).

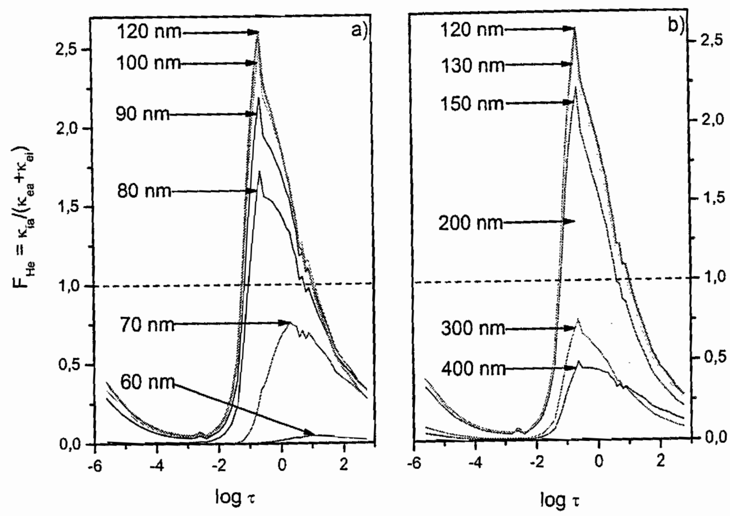


FIGURE 2. The quantity $F_{He} = \kappa_{ia}/(\kappa_{ea} + \kappa_{ei})$ for DB white dwarf in the case $\log g = 8$ and $T_{eff} = 12000$ K.

Apart of that, the efficiency of the absorption processes (3) and (4) in the region $\lambda_{He} < \lambda \leq \lambda_H$ is compared with the efficiency of the hydrogen photo-ionization process (1), which is characterized by the spectral absorption coefficient $\kappa_H(\lambda) \equiv \kappa_H(\lambda; N(H))$ defined by $\kappa_H(\lambda) = \sigma_{phi}(\lambda)N(H)$, where $N(H)$ is the local density of atom H, and $\sigma_{phi}(\lambda)$ - the corresponding photo-ionization cross-section. Consequently, the relative efficiency of the processes (3) and (4) and (5) for $\lambda \leq \lambda_H$ can be characterized by the parameter $F_H(\lambda)$ defined by

$$F_H(\lambda) = \frac{\kappa_{ia}(\lambda)}{\kappa_H(\lambda)} = \frac{K_{ia}(\lambda, T)N(He^+)N(He)}{\sigma_{phi}(\lambda)N(H)}, \tag{21}$$

where the cross-section $\sigma_{phi}(\lambda)$ is taken from [14]. It was found that the behavior of $F_H(\lambda)$ in DB white dwarf atmospheres considered in [6] is qualitatively similar. Consequently, the behavior of $F_H(\lambda)$ is illustrated only by Fig. 3 for the case $T_{eff} = 12000$ K and $\log g = 8$. Namely, for each λ from this region there is a significant part of DB white dwarf atmosphere where the process (5) dominates comparing to the other absorption processes.

* * *

Obtained results give possibility to estimate which absorption processes give the main contribution to the opacity in DB white dwarf atmospheres, in different spectral regions. So, from these results follows that the helium absorption processes (3) and (4) are dominant in the region $70 \text{ nm} \leq \lambda \leq 200 \text{ nm}$, while in the region $\lambda > 200$ nm, the principal role have the He^- absorption processes (1). However, the absorption processes (3) and (4) deserve to be included not only in codes developed by e.g. [15], but also in other used for DB white dwarf research. Finally, it was shown that in the region $\lambda_{He} < \lambda < 70$ nm, the hydrogen photo-ionization processes (5) take the dominant role in spite of the fact that the ratio of hydrogen and helium abundances in the considered DB white dwarf atmosphere is $1 : 10^5$.

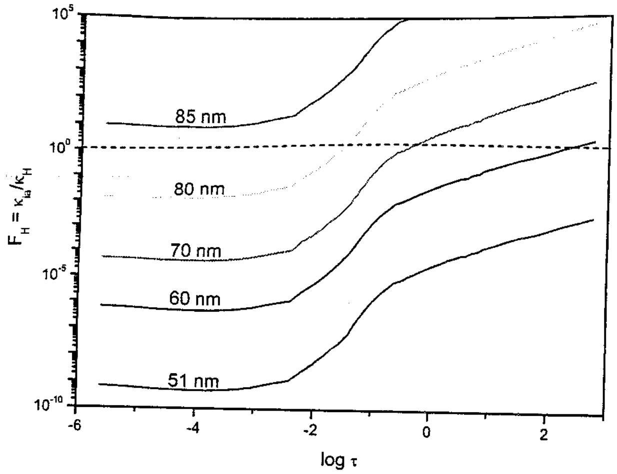


FIGURE 3. The quantity $F_H = \kappa_{ia}/\kappa_H$ for DB white dwarf in the case $\log g = 8$ and $T_{eff} = 12000$ K.

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