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Theoretical X-ray spectra of hot H-rich white dwarfs. Impact of new partition functions of iron, Fe V through Fe VII

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Abstract. In this paper we discuss new method for the atomic partition function (APF) computations, which is then applied to highly ionized iron, Fe V through Fe VII. Subsequently we have computed LTE model atmospheres of two hydrogen-rich white dwarf stars of the effective temperatures $T_{\rm eff} = 8 \times 10^4$ K and 1.2×10^5 K, and $\log g = 8.0$ (cgs units), which included trace abundance of iron. Both models correspond to the hottest DA white dwarfs observed e.g. by ROSAT and EUVE missions in the extreme UV and X-rays, in which stars H-rich atmospheres contain small amount of metals driven outwards by radiation pressure.

Computational results exhibit a significant impact of the new partition functions of Fe V through Fe VII on both the iron ionization stratification in analysed atmospheres, and their theoretical X-ray opacities and spectra. We conclude, that in both stars our improved APF predict increase of their EUV and X-ray luminosities by factors of 3 to 10, as compared with models based on previously published iron partition functions. We demonstrate also the importance of our APF on luminosity ratio $s2/s1$ in both EUV filters of the Wide Field Camera (ROSAT) in case of the hotter, Fe-rich white dwarf of $T_{\rm eff} = 1.2 \times 10^5$ K.

Key words: atomic data – stars: atmospheres – stars: white dwarfs – X-rays: stars

1. Introduction

New advances in space research include many discoveries of hot stellar objects, which radiate most of their thermal energy in the extreme ultraviolet (λ = 912 down to 60 Å) or in soft X-rays (λ = 60 to 12 Å). These sources frequently are hot white dwarf stars, which are remnants of normal stars at the end of their evolution. The other important stellar sources of X-ray or EUV radiation are cool K and M type dwarfs, in which X-rays are emitted by stellar coronae of temperatures reaching few millions K.

Theoretical analysis of a white dwarf atmosphere and its spectrum yields important conclusions concerning the effective temperature, $T_{\rm eff}$, surface gravity, and chemical composition of a star. The accuracy of such an analysis depends very strongly on the accuracy of the assumed physical constants and thermodynamical functions. The former include details of the complex atomic structure of all atoms and ions in the stellar atmosphere, their energy levels and parameters of numerous spectral lines (bound-bound opacities). The latter include the corresponding opacities for radiative photoionization from bound levels (bound-free opacities) as functions of wavelength λ, and the partition functions which determine the ionization state of elements through the well known Saha equation.

Our research is relevant to the recent progress in understanding of H-rich atmospheres of hot white dwarf stars (DA type). Spectral and photometric observations of these stars in the extreme UV and soft X-rays (ROSAT - Wide Field Camera experiments) yielded the conclusion, that DA atmospheres above $T_{\rm eff} \approx 40\,000$ K usually contain some trace amounts of heavy elements. Highly ionized heavy elements are transparent for visual wavelengths, while they are very efficient absorbers for λ below the He I ionization edge at 504 Å. In hot DA atmospheres these ions can be supported against gravity by radiation pressure forces, because they exhibit numerous spectral lines in EUV and X-rays. With $T_{\rm eff}$ decreasing, radiation flux in these regions decreases, and heavy elements sink and disappear in DA spectra, leaving purely hydrogen atmospheres.

The presence of additional absorption in hot DA stars is well illustrated by results of the ROSAT – WFC surveys (Pounds et al. 1993; Pye et al. 1995), in which the number of hot DA white dwarfs is much lower than expected, thus suggesting the existence of additional EUV and X-ray absorption in their atmospheres (Barstow et al. 1993; Marsh et al. 1997, for instance). Moreover, ions of O, Fe, and Ni were also directly detected in the extreme UV spectra in few hot DA white dwarfs, one of them is relatively bright G191-B2B (Vennes et al. 1992; Holberg et al. 1994).

Therefore it is important to examine and improve modeling of physical processes, which influence both theoretical EUV opacity and model atmosphere computations e.g. of DA white dwarfs. We have chosen the problem of partition function computations for elements belonging to the iron group. In this paper we present a new method which allows us to determine atomic partition function (APF) of Fe V – Fe VII, including the contribution from states lying above the ionization limit (autoionizing states), and accounting for those levels below that limit, which

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still are missing in the existing atomic data sets. Note, that partition functions published previously always neglected states of positive energy. Description of the new method and comparison with previous techniques are also given in Halenka & Madej (1999), together with tables of the partition functions for Ni I – Ni III ions.

Furthermore we prove, that in case of these iron ions such a qualitative improvement can change the APF by many orders of magnitude. Numerical computations of LTE model atmospheres of hot white dwarf stars showed, that our improved APF can increase X-ray luminosity of those objects by factors of 3 to 10, depending on the selected wavelength. Detailed tables of the APF values for Fe V – Fe VII will be presented in the forthcoming paper.

2. Calculation of the atomic partition functions

For plasmas in Local Thermodynamical Equilibrium (LTE) the occupation numbers of energy levels are determined by the Boltzmann law, while the ionization fractions of elements are given by the Saha-Eggert law. Both fundamental equations make use of the partition functions, and the method of APF computation was discussed by Halenka & Madej (1999). This method is briefly described below.

The internal atomic partition function, in energy representation,

$$
\begin{aligned}
U &= \int dV\, W(V)\, Tr\{\exp(-H/kT)\} \\
&= \sum_i \int dV\, W(V)\, \exp(-E_i/kT)\,, \qquad (1)
\end{aligned}
$$

where

$$H = H^{(0)} + V \qquad (2)$$

denotes the interatomic Hamiltonian of an emitter in plasma, and its eigenvalues of the state $|i>$ are denoted by E_i. Function $W(V)$ denotes probability density that the energy of emitter–plasma interaction is included in the range $V, V + dV$. Hamiltonian $H^{(0)}$ corresponds to an isolated emitter. It should be stressed, however, that: (*i*) summation range in Eq. (1) extends over bound states of the Hamiltonian H, and (*ii*) for an ionized emitter the sum defining U diverges for any temperature greater than zero.

Taking into consideration plasma–emitter interaction causes (*i*) lowering of the ionization energy (LIE), consequently the sum in Eq. (3) extends over finite number of terms, and (*ii*) implies small correction of energy levels as compared with those in an isolated atom. The effect (*i*) is very important when computing APF's for an emitter immersed in plasma, whereas the effect (*ii*) is negligibly small. The approximation $E_i^{'} \simeq E_i^0$ is the better justified the higher is the temperature of plasma. An extensive review of models describing plasma–emitter interaction, useful for the computations of APF, can be found in Hummer & Mihalas (1988). However, the authors of this paper express the opinion, that any of the existing models is not satisfactory. Therefore our partition functions were computed on the mesh of arbitrarily chosen values of LIE, in order to avoid any connections with particular models. Strictly speaking, values of U computed in this manner correspond to the particular fractions of emitters, with populations implied by function $W(V)$. (In more distant future when the function $W(V)$ will be known adequately well, our results will be still fully useful). Actually we have assumed, that the given LIE represents that quantity averaged over local microfields in plasma. Assuming the above and moving to the energy scale of excitation, one can compute values of APF in the following way (cf. Halenka & Grabowski 1977, 1984):

$$
\begin{aligned}
U^{(r)}(T, N_e) &= \sum_{p=1}^{p_{max}} \sum_{i=1}^{i(p)_{max}} g_{pi}^{(r)} \exp(-E_{pi}^{(r)}/kT) \\
&= \sum_{p}^{p_{max}} U_p^{(r)}(T, N_e)\,. \qquad (3)
\end{aligned}
$$

Here the set (pi) of the order numbers p and i (numbering the levels from the ground towards the higher ones) describe an eigenstate of the atom in the r-th ionization state: i represents three quantum numbers (nlj) of the optical electron and p the quantum state of the atomic core. $i(p)_{max}$ is the number of all bound energy levels, $g_{pi}^{(r)}$ and $E_{pi}^{(r)}$ being the statistical weight and the excitation energy of the i-th state, in the sequence based on p-th parent level. The numbers $i(p)_{max}$ result from the inequality

$$E_{pi}^{(r)} \le E_{p\infty}^{(r)} - \Delta E^{(r)}, \qquad (4)$$

where $\Delta E^{(r)}$ denotes the lowering of the ionization energy (LIE), and $E_{p\infty}^{(r)}$ (the ionization energy of the p-th level sequence) is equal to the sum

$$E_{p\infty}^{(r)} = E_{1\infty}^{(r)} + E_p^{(r+1)}. \qquad (5)$$

The quantity $E_p^{(r+1)}$ denotes the energy of the atomic core after ionization, $r \rightarrow r+1$. Following Eq. (3) we have computed new values of the APF for highly ionized iron ions, Fe V through Fe VII.

Computations of our partition functions were performed in the following way. The basic data, i.e. the values of energy of known bound levels and their statistical weights, were taken from Sugar & Corliss (1985), and Kurucz (1994). However, many levels predicted by quantum mechanics are actually lacking in both the above catalogues, which contain mostly the "observed" levels. We have appended the contribution from levels missed in the above data sets to our values of APF, including all autoionizing levels, following the method outlined in papers by Halenka & Grabowski (1977, 1984). Both papers give also very detailed description of the APF computations.

3. Model atmosphere calculations

Exact computations of stellar theoretical spectra always require simultaneous computation of the corresponding model atmospheres. The structure of a stellar atmosphere is determined by the run of temperature T, gas pressure P_{gas}, density ρ and opacity distributions, the latter given over both geometrical depth z and photon frequency ν (we assume that the star has spherical symmetry). Model atmosphere of a hot, stationary star is subject to the condition of radiative equilibrium

$$\frac{dF_{bol}}{dz} = 0 \,, \tag{6}$$

which states that the integrated (bolometric) flux of radiative energy is constant with the geometrical depth. The effective temperature of a stellar atmosphere is directly related to the flux by the relation $F_{bol} = \sigma_* T_{\rm eff}^4$, where σ_* denotes the Stefan–Boltzmann radiation constant. Eq. (6) is valid in all atmospheres, where the transport of energy by convection is inefficient and can be neglected. This occurs in atmospheres of main sequence (MS) stars and of white dwarfs with $T_{\rm eff} \geq 9000$ K.

The second constraint, on which model atmospheres are frequently based, is the condition of hydrostatic equilibrium of the form

$$\frac{dP_{gas}}{dz} + \frac{dP_{rad}}{dz} = -\rho g \,, \tag{7}$$

where g denotes gravitational acceleration in the atmosphere. Eq. (7) with constant value of g is valid in most layers of hot main sequence stellar atmospheres and in atmospheres of hot white dwarfs, where the total thickness of the atmosphere is small as compared with the radius of a star.

The distribution of radiative energy in the outgoing spectrum is given by solution of the transport equation for photons being absorbed, scattered, and emitted by a hot plasma in the atmosphere (the equation of radiative transfer). Both the structure of an atmosphere and the spectrum of radiation critically depend on the assumption of the local thermodynamical equilibrium (LTE), and the assumed sources of frequency–dependent opacity.

The useful review of numerical techniques for the model atmosphere and theoretical spectrum computations can be found in Mihalas (1978). Computational results of this paper were obtained from the Compton scattering code described in Madej (1994, cf. also 1998). The code includes opacities of neutral H, He and He^+, and noncoherent Compton scattering opacity. Since we require in this paper model atmosphere computations with the standard (coherent) Thomson scattering, we have simply set the Planck constant h in the code to zero. We appended to the code a very extensive set of LTE bound-free opacities from over 1000 levels of Fe V through Fe VII, with their treshold energies taken from the Opacity Project database (cf. Seaton 1987; K. Butler – data for Fe V; C. Mendoza – Fe VI; H.E. Saraph and P.J. Storey – Fe VII, respectively). Bound-free opacities from levels with non-equivalent electrons were computed following the hydrogenic approximation (Eq. 4–114 of Mihalas 1978). In case of levels with equivalent electrons the principal quantum number n cannot be defined, and therefore the strict hydrogenic approximation cannot be applied. For each such level we still estimated its b-f opacity from the hydrogenic expression, assuming arbitrarily that n equals to the average principal quantum number of a few levels with similar energies of excitation.

Table 1. Wide Field Camera colors

$T_{\rm eff} = 8.0 \times 10^4$	$\log g = 8.0$	$s2/s1 = 0.2130$	HAL
		$s2/s1 = 0.2271$	SUG
$T_{\rm eff} = 1.2 \times 10^5$	$\log g = 8.0$	$s2/s1 = 0.04647$	HAL
		$s2/s1 = 0.05727$	SUG

We assumed also the following expression for the lowering of ionization energy (LIE)

$$\Delta\chi = Ze^2/D = 3 \times 10^{-8} Z N_e^{1/2} T^{-1/2} \qquad \text{[eV]} \tag{8}$$

(Eq. 9–106 of Mihalas, 1978), where $D = 4.8\,(T/N_e)^{1/2}$ [cm] is the Debye length in hydrogen dominated plasma, and N_e denotes electron concentration. On each level of a model atmosphere, values of $\Delta\chi$ and temperature T were used to interpolate our tables of Fe V – Fe VII partition functions and to determine iron ionization fractions and iron b-f opacities.

4. Numerical results and conclusions

We have computed a pair of LTE model atmospheres corresponding to hot white dwarf stars, with $T_{\rm eff} = 8 \times 10^4$ and $T_{\rm eff} = 1.2 \times 10^5$, and the gravity $\log g = 8.0$ (cgs units). Such a value of surface gravity is typical for white dwarfs, whereas the assumed values of $T_{\rm eff}$ are very high as compared both with white dwarfs and main sequence stars. The above effective temperatures correspond to the hottest known X-ray white dwarfs, which were recently discovered by the satellite X-ray experiments (e.g. by German–US ROSAT experiment or US Extreme Ultraviolet Explorer).

We have assumed hydrogen-rich chemical composition with traces of helium and iron, in which the number abundances relative to hydrogen, $N_{He}/N_H = 1 \times 10^{-4}$ and $N_{Fe}/N_H = 3.7 \times 10^{-4}$ (solar-like iron abundance).

The results of model atmosphere computations are presented in Figs. 1–2. We have computed two pairs of models, in which the distributions of iron ionization states vs. standard optical depth were computed from the Saha–Eggert equation either with our iron partition functions (APF), or with those obtained by direct summation over energy levels given in Sugar & Corliss (1985). Theoretical energy fluxes in both pairs of models differ by factors 3–10 for wavelengths between 100–180 Å (extreme UV - soft X-rays), while our APF yield higher luminosity (solid lines in Figs. 1–2). Therefore we conclude, that our iron partition functions can serve as a very important tool for interpretation of the observed X-ray spectra, at least as long as the helium abundance in a hot white dwarf atmosphere is very small.

It is interesting to investigate the significance of our partition functions on photometric colors of both pairs of model atmospheres in the extreme UV. Table 1 presents the predicted luminosity ratios $s2/s1$, where $s1$ and $s2$ are luminosities seen in both EUV filters of the Wide Field Camera. Peak transparency of $s1$ filter is at $\lambda \approx 135$ Å and peak of $s2$ at $\lambda \approx 110$ Å. Exact transparency profiles of both filters were taken from Pounds et al. (1993). We compare EUV luminosities for models computed

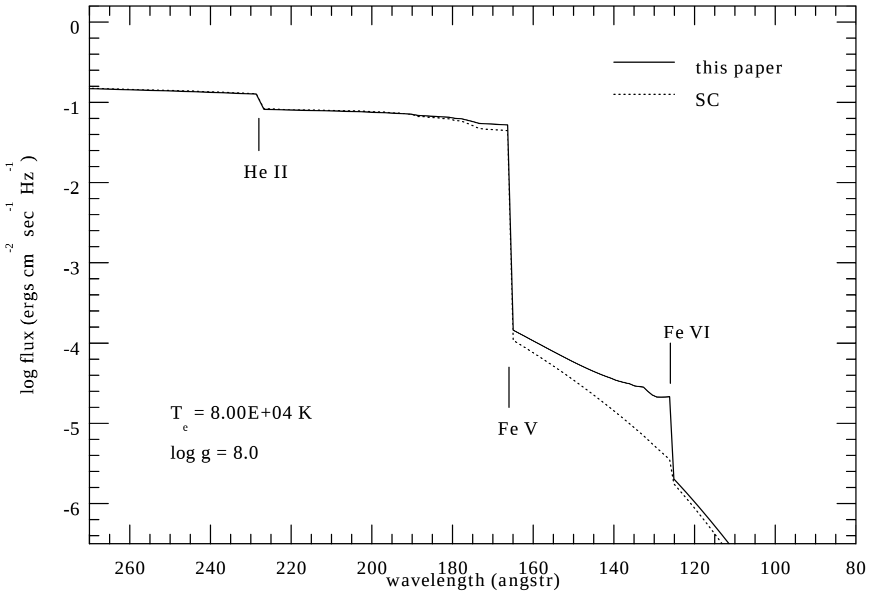

Fig. 1. Continuum spectra of a hot DA white dwarf star, with the effective temperature 8×10^4 K and $\log g = 8.0$ (cgs units). The atmosphere consists of hydrogen with small amounts of helium and iron. Two different model atmospheres correspond to partition functions of iron computed according to energy levels by Sugar and Corliss, 1985 (short dashed line), and to our method (solid line). Bound-free opacity jumps from ground levels of He II, Fe V, and Fe VI are indicated. Our partition functions significantly change ionization of iron there and increase luminosity of the star by factors of 3 to 5 in far UV and soft X-rays.

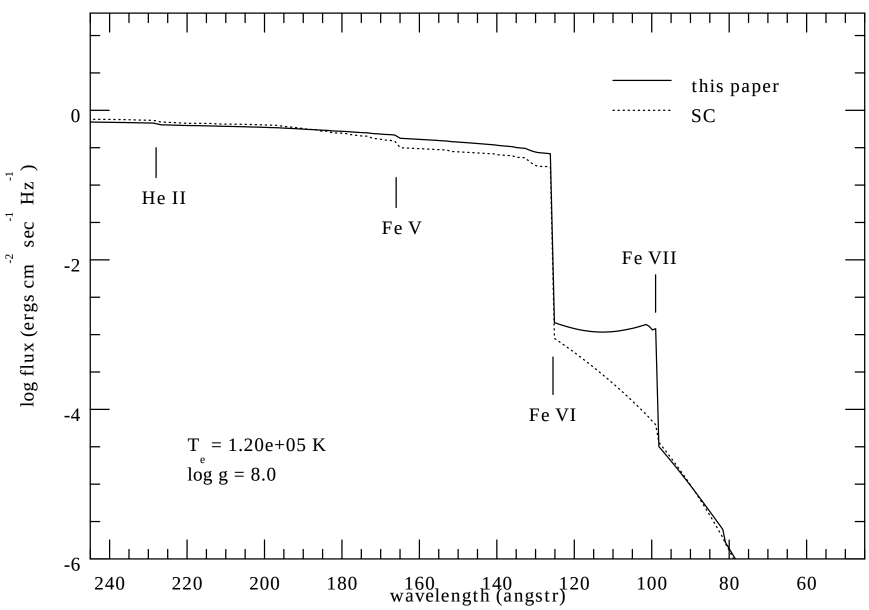

Fig. 2. The same for hotter model of $T_{\rm eff} = 1.2 \times 10^5$ K and $\log g = 8.0$. Both spectra exhibit distinct bound-free jumps from the ground levels of Fe VI and Fe VII. Our improved iron partition functions increase X-ray flux by a factor 10 at $\lambda > 140$ Å.

with old iron partition functions (SUG; cf. Sugar & Corliss, 1985) with those for models computed with ours (HAL, cf. also Halenka & Madej, 1999).

Numbers $s1$ and $s2$ in Table 1 were obtained by direct integration

$$s_{1,2} = \int_0^\infty F_\lambda \, p_{1,2}(\lambda) \, d\lambda \,, \tag{9}$$

where $p_{1,2}$ denote dimensionless transparency profiles of both EUV filters, and F_λ denotes flux rescaled to counts sec^{-1} cm^{-2} Å^{-1}.

Table 1 shows, that in the case of the hotter model our improved iron partition functions (APF) change its color, $s2/s1$, by about 20%. Therefore our APF can contribute to correct interpretation of EUV colors, at least for hot white dwarfs of the extreme $T_{\rm eff}$, which are rich of iron (or perhaps nickel).

One should note, that partition functions of iron discussed in this paper are strictly valid only in conditions satisfying the Local Thermodynamic Equilibrium. We would like to note, that plasma in very hot white dwarf atmospheres fulfils the LTE criteria (Griem 1974, 1997; cf. also Napiwotzki 1997), perhaps except the uppermost layers of very low density. Therefore we believe, that the fluxes of LTE iron continua in our model atmospheres can be used to test the new iron partition functions.

On the other hand, the presence of numerous lines of iron (which are formed in the highest layers) can drive level populations of iron ions far from LTE values e.g. in hot atmospheres of white dwarfs. We believe, that our APF values can easily be adapted to NLTE plasmas, since NLTE effects influence mostly low-lying levels. We note also, that the advantage of our APF's is due to inclusion of numerous levels of high excitation energy and autoionizing levels, for which populations always converge to LTE values (Mihalas 1978).

Our partition functions for Fe V – Fe VII will be implemented soon into a few widely used computer codes for NLTE model atmosphere calculations, for instance the Tlusty 195 code (cf. Hubeny 1988; Hubeny & Lanz 1992, 1995).

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