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The modelling of the spectra and atmospheres of evolved stars

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Abstract.
The method and results of the computation of the model atmospheres and spectral energy distributions of chemically peculiar stars, are discussed. The models are computed with a special consideration of the particular problems encountered when computing model atmospheres for M and C-giants, and of hydrogen deficient stars. We present some computed model atmospheres for Sakurai's object, giants of globular clusters, and C-giants.

Key words. Stars: abundances – Stars: atmospheres – Galaxy: globular clusters – stars: carbon isotopic ratios

1. Introduction

The computations of model atmospheres of and theoretical spectra of stars is an essential part of many modern astrophysical projects. An extended grid of model atmospheres and spectra were computed recently using the most complete sets of opacities (see Kurucz (1993, 1999), Hauschildt et al. (1999). In most of the computations the solar abundances (Anders & Grevesse 1989) or solar abundances scaled by the metallicity factor [Fe/H] are used. However, the metal abundances in the atmospheres of evolved stars can significantly differ from the solar abundance ratios. The reason for this is because convection and other mixing processes dredge up the products of the nucleosynthesis from the stellar interior.

The atmospheres of the most evolved stars (R CrB, Sakurai's object, etc) present another interesting problem. They are helium and carbon rich, therefore the opacity due to H^- absorption is not as important. The temperature structure of the model atmospheres of these stars is the different from the case of the "normall" abundances due to the changes of opacity.

2. Model atmospheres and synthetic spectra

We computed plane-parallel model atmospheres of the evolved stars in LTE, with no energy divergence by SAM12 program (Pavlenko 2003). The program is a modification of ATLAS12 (Kurucz 1999).

Chemical equilibrium is computed for the molecular species, by assuming LTE. The nomenclatures of molecules accounted for are different in atmospheres of hydrogen rich and hydrogen poor, carbon-rich and carbon poor stars. We account mainly for the molecules which are the most abundant or most important sources of opacities.

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SAM12 uses the standard set of continuum opacities from ATLAS12. The adopted opacity sources account for changes in the opacity as a function of temperature and element abundance. We add some opacities sources which are of importance in the atmospheres of carbon-rich, hydrogen-deficient stars:

– The opacities due to C I, N I, O I bound-free absorption over a wide (0.1–8 μm) wavelength region were computed using the OPACITY PROJECT (Seaton et al.1992) cross sections database (Pavlenko & Zhukovska 2004).

– The opacity of C^- (Myerscough & McDowell 1996) also is taken into account (see Pavlenko 1999 for more details).

The opacity sampling approach (Sneden et al. 1976) is used to account for atomic and molecular line absorption. The atomic line data are taken from the VALD database (Kupka et al. 1999). Lists of diatomic molecular lines of ^{12}CN, ^{13}CN, $^{12}C_2$, $^{13}C_2$, $^{12}C^{13}C$, ^{12}CO, ^{13}CO, SiH, and MgH are taken from Kurucz (1993). We account for TiO and VO opacities in the atmospheres of oxygen-rich stars in the framework of JOLA (just-overlapping-line) approximation. In the atmospheres of the carbon-rich stars the absorption by CS lines (Chandra et al. 1994) was accounted for.

Bands of polyatomic molecules appear in the spectra of the coolest evolved stars:

a) Water vapour band form strong features in the infrared spectra of cool stars with oxygen-rich atmospheres. We computed H_2O opacities using AMES line lists (Partrige & Schwenke 1998).

b) In the cool atmospheres of C-stars HCN/HNC bands dominate in the infra-red region of the spectrum. We computed the HCN/HNC opacity using detailed line line list (Harris et al. 2002, 2003, 2006).

The shape of each molecular or atomic line was determined using the Voigt function $H(a, v)$. Damping constants were taken from line databases or computed using Unsold's (1955) approach.

The following molecular electronic bands were accounted for: CaO ($C^1\Sigma$ - $X^1\Sigma$), CS($A^1\Sigma$ - $X^1\Sigma$), SO ($A^3\Pi$ - $X^3\Sigma$), SiO ($E^1\Sigma$-$X^1\Sigma$), SiO($A^1\Pi$ - $X^1\Sigma^+$, NO ($C_2\Pi_r$- $X_2\Pi_r$), NO($B_2\Pi_r$ -$X_2\Pi_r$), NO($A^2\Sigma^+$ - $X_2\Pi_r$), MgO($B^1\Sigma^+$ - $X^1\Sigma^+$), AlO($C^2\Pi$ -$X^2\Sigma$), AlO($B^2\Sigma^+$ - $X^2\Sigma^+$), in the framework of the JOLA approach.

Convection plays an important role in these atmospheres. We use the mixing length theory of 1D convection modified by Kurucz(1999) in ATLAS12.

In the Fig. 1 we show the computed SEDS for two model atmospheres of the same effective temperature, surface gravity and metallicity, i.e 3000/0.0/0, but with a different C to O ratios. The differences in the opacity nomenclatures are clearly seen.

The temperature structure of model atmospheres of the evolved giants show very strong dependence on the adopted abundances and other parameters (Fig. 2).

Synthetic spectra are calculated with the WITA6 program (Pavlenko 2000), using the same approximations and opacities as SAM12. In the computations we use TiO line list (Plez 1998) instead of JOLA, and the CO (Goorvitch 1994) line list instead of the Kurucz(1993) line list. Naturally, much smaller wavelength steps in the synthetic spectra are adopted ($\Delta\lambda = 0.02$ and 0.1 in the blue and IR spectral regions, respectively.

3. Fits to observed spectra

3.1. Veiling-free case

To determine the best fit parameters, we compare the observed fluxes F_ν with the computed fluxes following the scheme of Jones et al (2002) and Pavlenko & Jones (2003). We let

$$F_\nu^x = \int F_\nu^y \times G(x-y) * dy,$$

where r_ν^y and $G(x-y)$ are respectively the fluxes computed by WITA6 and the broadening profile. We adopt a gaussian + rotation and/or extension profile for the latter. We then find the minima of the 3D function

$$S(f_s, f_h, f_g) = \sum (F_{obs} - F^x)^2 ,$$

where f_s, f_g, f_g are the wavelength shift, the normalisation factor, and the profile broadening parameter, respectively. The parameters

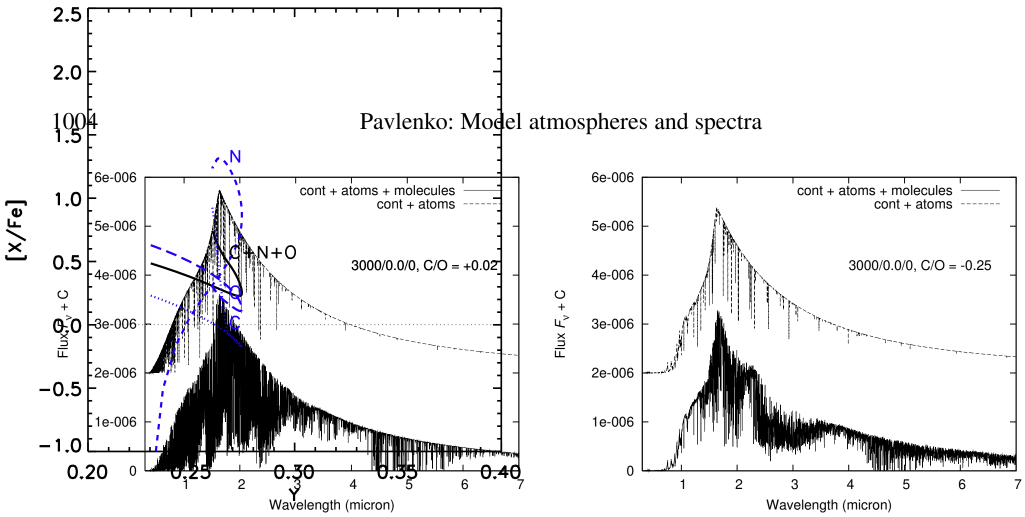

Fig. 1. Spectral energy distributions computed for two giants with T_{eff}/log g/[Fe/H] = 3000 K/0.0/0 and different C/0 = -0.25 (left) and (+0.02) (right).

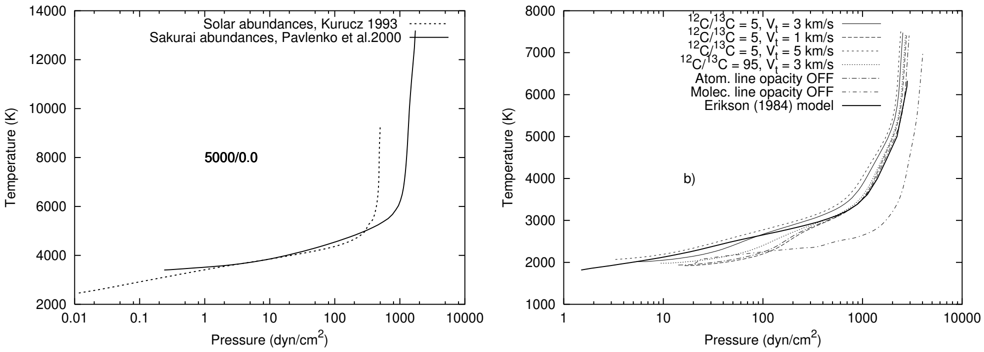

Fig. 2. Left: temperature structure of the model atmosphere of giant 5000/0.0 computed with a normal abundance and with a hydrogen deficient abundance, i.e. [H]=0, -2.4 (see section 4.3). Right: the response of the atmosphere temperature of a C-giant 3000/0.0/0 to the variation of some input parameters.

f_s, f_h and f_g are determined by the minimisation procedure for every computed spectrum. Then, ¿From the grid of the better solutions for the given abundances and/or other parameters (microrurbulent velocity, effective temperature, isotopic ratios, etc), we choose the best-fitting solution.

3.2. A case with the dust veiling

For the case of the most evolved stars, some of the flux originates in the optically thin envelope around the star. Third provides a source of veiling the observed spectra: $F_{total} = F_{atmos} + F_{envelope}$. In this case we should minimise $F_{total} - F_{obs}$, whilst considering $F_{envelope}$ as an additional parameter (see section 4.3 and Pavlenko et al. 2004 for more details).

4. Results

4.1. C-giants

The *ab initio* HCN linelist (Harris et al. 2002, 2003) was used to compute new model atmospheres and synthetic spectra for the carbon stars (Pavlenko 2003). Recently the accuracy of the first *ab initio* line list was improved by by using an accurate database of 5200 HCN and HNC rotation-vibration energy levels, determined from existing laboratory data.

Model atmospheres and synthetic spectra computed with this new linelist provide better fit to the spectrum of WZ Cas in which the absorption feature at 3.56 μm is reproduced to a higher degree of accuracy than has previously been possible (see Harris et al, 2006 for more details).

Using the new HCN line list, we computed a new grid of carbon rich model atmospheres for a wide range of [Fe/H], C/O, $T_{\rm eff}$, log g. They can be used for the express analysis of the new data obtained for C-giants in our Galaxy (Yakovina et al. 2003) and/or other galaxies (Dominguez et al. 2005).

4.2. $^{12}C/^{13}C$ in giants of globular clusters

Pavlenko, Jones & Longmore (2003b) investigated changes in the ^{12}C/^{13}C isotopic ratio and the carbon abundances in atmospheres of red giants of in the galactic globular clusters M71, M5, M3 and M13 covering the metallicity range from –0.7 to –1.6 and $T_{\rm eff}$= 3500–4900 K. Observational data were obtained with the UKIRT telescope in 1993. Model atmospheres and synthetic spectra of the $\Delta\nu$=2 CO bands around 2.3 μm were computed for a fixed $T_{\rm eff}$and log g, but with different V_t, C/O, ^{12}C/^{13}C . We then apply the minimisation procedure (see sect. 3.1) to obtain the best solution. An example of the best fit to an observed spectrum of II-46 giant of globular cluster M3 is shown in Fig. 3. We find:
– lower ^{12}C/^{13}C for more luminous hotter objects.
– relatively low carbon abundances which are not affected by the value of oxygen abundance.
– For most giants the determined ^{12}C/^{13}C ratios are consistent with the equilibrium value for the CN cycle.
– a larger dispersion of ^{12}C/^{13}C in giants of M71 of metallicity [M/H] = -0.7 in comparison with other giants of M3, M5, M13 which are more metal deficient (Fig. 3).

Our results suggest a complete mixing on the ascent of the stars up the red giant branch. This is in contrast to the substantially higher values suggested across this range of parameters by the current generation of theoretical models of stellar evolution (see Pavlenko et al. 2003b for more details).

4.3. R CrB and V4334 Sgr

It has been firmly established that the two most abundant elements in the atmospheres of the evolved R CrB-like stars are helium and carbon (see Asplund et al 1997). A hydrogen deficient model atmosphere for R CrB was computed by Pavlenko (1999), see www.mao.kiev.ua/staff-/yp/Results/Mod.rcrb1999.tar.gz.

Sakurai's object (V4334 Sgr) provides another extreme case of stellar evolution. The "novalike object in Sagittarius", was discovered by Y. Sakurai on February 20, 1996 (Nakano et al. 1996). Soon after discovery, it was found to be a final He flash object, a rare type of star on the evolutionary track that leads from the central star of a planetary nebulae back to the red giant region. These objects are often referred to as "born-again giants". Its progenitor was a faint blue star ($\sim 21^{\rm m}$) in the centre of a low surface brightness planetary nebula (Duerbeck & Benetti 1996).

Model atmosphere and spectra of Sakurai's object on later stages of evolution were investigated by Pavlenko et al. (2000), Pavlenko & Duerbeck (2002). We show the effective temperature of the pseudo-photosphere of Sakurais object drops monotonically from 5500 in July, 1997 down to 5250 K in August, 1998. In March 1997 the first evidence of dust formation was seen (Kimeswenger et al. 1997, Kamath & Ashok 1999, Kerber et al. 2000). Pavlenko & Geballe (2002) *spectroscopically* showed the presence of the dust veiling of the infrared part of the Sakurai's spectrum (see Fig. 4). Later, Pavlenko et al. (2004) using the procedure decsribed in section 3.2 determined ^{12}C/^{13}C = 4 ± 1 in atmosphere of Sakyrai's object from the fit to 2.3 μm CO bands observed by UKIRT in July, 1997 (see Fig. 4) which is consistent with VLTP (the star on very late thermal pulse) interpretation of V 4334 Sgr (Herwig 2001).

5. Conclusions

Due to the high sensitivity of computed model atmospheres and synthetic spectra of evolved stars on the adopted input data, the analysis of their spectra should be done in the frame-

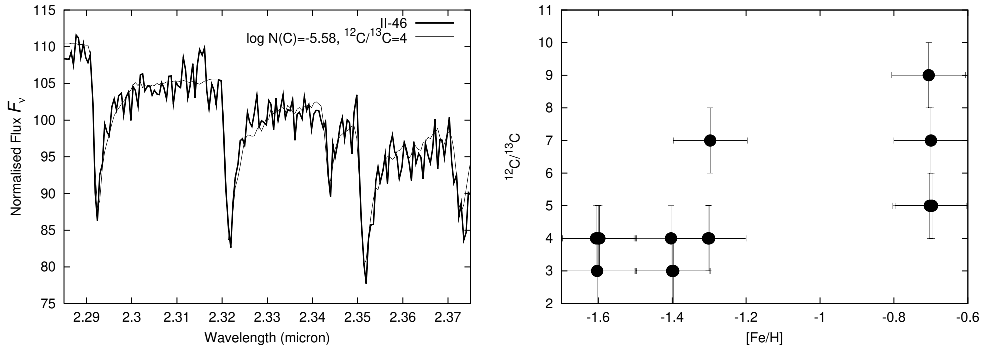

Fig. 3. Left: fits to observed spectrum of II-46 giant in the globular cluster M3. Right: the found $^{12}C/^{13}C$ for giants of globular clusters of different metallicities (Pavlenko et al. 2003b).

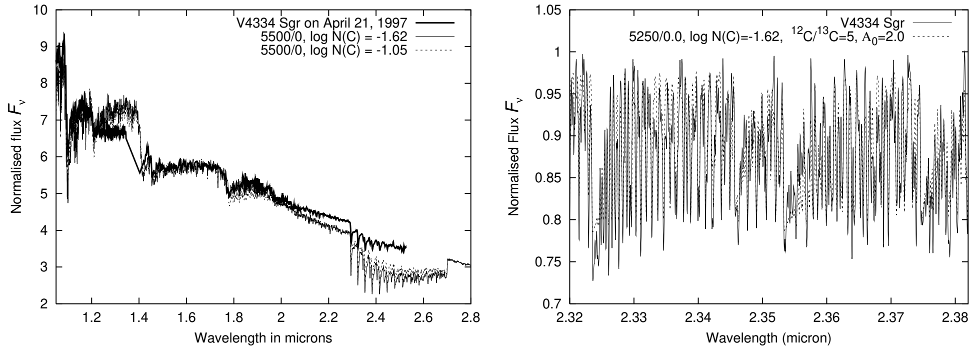

Fig. 4. Left: fits to observed spectrum of of Sakurai's Object on 1997 July 13. Right: the fit to ^{12}CO and ^{13}CO bands. Synthetic spectra were computed for a microturbulent velocity of 6 km/s.

work of the self-consisted approach. Model atmospheres should correspond with the obtained abundances and other physical parameters. Even in the case of the "normal" red giants the temperature structure should be computed with the correct abundances. Otherwise, the abundance determination results might be affected by significant errors (> 0.2-0.3 dex, see Pavlenko & Yakovina 1994 for more details). Generally speaking, existed grids of the model atmospheres can be used as zero-approach tool to be refined in the process of analysis.

Despite a substantial efforts to develop more sophisticated model atmosphere, a few problems provide the real challenge for the modern theory of stellar astrophysics:

– atmospheres of the most evolved stars do not exist in hydrostatic equilibrium. In some cases effects of sphericity can be essential.

– Convection in the extended photospheres can be properly described only in the 3D approach.

– The further computation of line lists and other physical parameters (dissociation energies, partition functions, etc) of polyatomic molecules is absolutely essential for cool stellar atmosphere modelling to progress. In particular little, no or only poor data exists for species such as C_3, CH_4 and C_2H_2. These species provide substantial opacity in the coolest atmospheres. Even the existing line lists of diatomic molecules, such as CN, C_2, CH, are not accurate enough to be used for the high resolution analysis of observed spectra.

Naturally, these problems can be solved one at a time. However, it is only possible when paying special attention to theoretical support of current observations.

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