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MODEL ATMOSPHERES AND FUNDAMENTAL STELLAR PARAMETERS

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Abstract. I start by illustrating the need for precise and accurate fundamental stellar parameters through there examples: lithium abundances in metal-poor stars, the derivation of stellar ages from isochrones, and the chemical composition of planet-hosting stars. I present widely used methods (infrared flux method, spectroscopy) in the determination of $T_{\rm eff}$, and $\log g$. I comment upon difficulties encountered with the determination of stellar parameters of red supergiant stars, and I discuss the impact of non-LTE and 3D hydrodynamical effects.

Keywords: lithium, red supergiant stars, Betelgeuse, metal-poor stars, NLTE, atomic diffusion, stellar atmospheres, stellar parameters

1 Why do we need accurate and precise stellar parameters

Stellar parameters are the tags with which we identify key properties of the stars we study. Most often stellar parameters we refer to are limited to two: the effective temperature, $T_{\rm eff}$, and the surface gravity, or its logarithm, $\log g$, to which we add the metallicity, or its proxy [Fe/H]. Other parameters include the radius R, and the luminosity L, and of course the detailed element abundance distribution. I will here mostly discuss the primary parameters, linked by the well known relations : $L = 4\pi R^2 \sigma T_{\rm eff}^4$, and $g = GM/R^2$. Before recalling a few commonly used methods to derive stellar parameters, I illustrate the need for accurate and precise stellar parameters through three examples: Li abundances and element diffusion in stellar interiors, stellar ages derived from isochrones, and the possible correlation of the abundance of some elements with the presence of planets.

1.1 Lithium abundances and atomic diffusion

Element diffusion is known to take place in the radiative zones inside stars. Elaborate models have been developed including very detailed physical processes and data, but also an unknown amount of turbulent mixing. This turbulent mixing appears necessary to diminish the predicted effects of combined radiative acceleration and gravitational settling (Richard et al. 2005). The impact of element diffusion is to hide the real stellar chemical composition from our view. The atmospheric abundances we determine differ from the interior and mean abundance of the star. This of course is true only for stars that are not deeply convective. Korn et al. (2007) used the deviation from the internal composition that is largest at the turn-off (TO), diminishes on the lower red giant branch (RGB), and vanishes during the ascension of the RGB to calibrate the amount of turbulent mixing in the models. They observed stars at various evolutionary stages in a cluster (NGC 6397), determining their atmospheric Fe, Ti, Ca, and Mg abundances. A comparison to models allowed them to chose the right turbulent mixing. This model was then applied to correct the abundance of Li measured in the same stars. It turns out that the correction reconciles the Li plateau abundance with the cosmological WMAP calculation (Spergel et al. 2007). This work relies on abundance uncertainties of the order of ± 0.05 dex, in order to secure a detection of the effect at the $3-\sigma$ level. Such a precision in abundances requires a very careful calibration of the $T_{\rm eff}$-scale of TO and RGB stars, as discussed in detail by Korn et al. (2007).

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1.2 Stellar ages from isochrones

Individual stellar ages can be derived from isochrones: knowing the $T_{\rm eff}$, L, and the metallicity of a star, it can be placed on the right set of isochrones computed at the proper metallicity. The isochrone on which it falls will provide a mass, an age and the initial metallicity, as it is affected by diffusion (Korn et al. 2007). This seemingly straightforward method is, however, not always easy to apply, nor giving an unambiguous answer. Isochrones do overlap. Methods can be used that allow a better estimate of stellar age than just by reading out a single isochrone (Jørgensen & Lindegren 2005), but it remains crucial to input precise and accurate stellar parameters.

1.3 Planet-hosting stars

The question whether the chemical composition of stars with and without planets differ is still a matter of debate. One recent development lies in the claim that some planetary systems may have C/O>1 (Delgado Mena et al. 2010; Petigura & Marcy 2011), which would have interesting consequences on the planetary chemistry, including the possibility of "carbon planets". In a follow-up paper, Nissen (2013) notes that the abundances derived in these papers rely on high-excitation carbon lines, and on the zero-excitation forbidden oxygen line. This makes the conclusions very sensitive to the adopted $T_{\rm eff}$, and atmospheric temperature structure. In his detailed study Nissen (2013) shows that systematic effects on the C/O ratio can be important. Using a spectroscopically derived gravity and the forbidden oxygen line leads to C/O ratios higher by about 0.2 compared to using a photometric gravity and the oxygen IR triplet. The different gravities also induce a trend with metallicity. This careful work demonstrates that the discussion of small abundance effects is hampered by uncertainties in fundamental parameters. In this context, better parameters are needed, in particular constrained by distance determinations. Only then can small abundance effects be discussed, with smaller scatter and less systematics.

2 Determination of stellar parameters

Stellar parameters can be derived using various methods, that are more or less dependent on stellar models. Here I only recall two of them used for the determination of $T_{\rm eff}$, and $\log g$.

2.1 The infrared flux method, temperatures, and angular diameters

For the determination of effective temperatures, a direct method was devised by Blackwell & Shallis (1977), who were initially most interested by the measurement of angular diameters of stars. This method, dubbed the Infrared Flux Method (IRFM) has been improved through the years. Casagrande et al. (2010) discuss in detail the various developments and present a comparison of various temperature scales.

The IRFM relies on the comparison of the ratio $\mathcal{R}_{\rm obs} = f_{\rm bol}(earth)/f_\lambda(earth)$, of the bolometric and monochromatic observed fluxes, with the ratio of stellar surface fluxes $F_{\rm bol}(star)/F_\lambda(star) = \sigma T_{\rm eff}^4/F_\lambda(mod) = \mathcal{R}_{\rm calc}$, which can be readily computed using a model atmosphere. The key idea is to choose λ in the IR where the stellar flux is not very temperature sensitive. Starting from a guess temperature, a few iterations until $\mathcal{R}_{\rm calc} = \mathcal{R}_{\rm obs}$ will lead to a value of $T_{\rm eff}$. It will also provide the angular diameter θ of the star given by, e.g., $\theta^2/4 = f_{\rm bol}(earth)/(\sigma T_{\rm eff}^4)$. This implies, however, that the stellar radius can be well defined and that the relation can be written for both the bolometric and the monochromatic flux, i.e., one has also $\theta^2/4 = f_\lambda(earth)/F_\lambda(star)$. Casagrande et al. (2010) compare IRFM derived angular diameters with diameters from interferometry. They find a good agreement, but this comparison is only made for a few stars, and differences amount up to 10 or 20%. This question of the radius is worth discussing further. In stellar atmosphere models the radius can be readily defined at the layer where the Rosseland optical depth $\tau_{\rm Ross} = 1$, or $2/3$. This is a definition that is commonly adopted in 1D hydrostatic models. The effective temperature is thus a measure of the average energy flux at this radius. This can obviously not be done for observations. Interferometric measurements of the radius depend on the center-to-limb intensity variation, and on the wavelength. A discussion of the difficulties faced to properly define the radius and the effective temperature both in models and observations can be found in, e.g., Baschek et al. (1991). I also discuss below a problem recently uncovered with the $T_{\rm eff}$- (and the radius-) scale, of red supergiant (RSG) stars.

2.2 spectroscopic temperatures and gravities

Spectroscopy offers a powerful way of simultaneously deriving $T_{\rm eff}$ and $\log g$ from a set of neutral and ionized lines of the same element, most often iron. The method is based on the idea that if local thermodynamical equilibrium (LTE) prevails, then the fraction Fe II/Fe I is given by the ionization equilibrium (Saha equation), and the Fe I and Fe II energy level populations are given by the Boltzmann equation. Consequently, the abundances derived from a set of lines, by comparing computed line profiles or equivalent widths to observations should not depend on the ionization stage, or the excitation energy. Therefore the $T_{\rm eff}$ of the model is varied until there is no trend in abundance with excitation, and the gravity is adjusted until there is no difference in abundance between the two ionization stages. In hydrostatic 1D models, there is also the need to adjust the micro-turbulent velocity to ensure that the abundance does not depend on the line equivalent width. This is a very widely used method, which is however sensitive to non-LTE effects, and to inhomogeneities due to 3D hydrodynamical effects.

Modern studies, based on very competitive instruments, require a high precision and accuracy of the analysis, as shown above on a few examples. One should therefore not use the assumption of LTE to derive parameters, including the chemical abundances, without circumspection. The paper by Nissen (2013) discussed above offers a good example of how to check the spectroscopic method output. Nissen first combines photometric data, with a bolometric correction, an extinction correction, and a distance to derive the luminosity of each star of his sample. The $T_{\rm eff}$ is computed from photometry or spectroscopy, and finally isochrone fits provide a mass. From these the surface gravity can be calculated for each object. The gravities are also derived using the ionization equilibrium method underlined above. It turns out that there is a trend in $\log g_{\rm phot} - \log g_{\rm spec}$ with $T_{\rm eff}$, from about +0.1 at 5300 K, to about -0.2 at 6400 K. This trend is not understood so far. A similar trend with [Fe/H] exists. We must remain cautious!

3 A number of open problems

3.1 NLTE effects

LTE is an approximation that in principle only holds when collisions are sufficiently numerous to counteract radiative transitions that lead to non-equilibrium populations. It is of course a very convenient approximation allowing quick calculations. We can not, however, be lazy, and we must dare to leave this approximation behind us. We must at least check that NLTE effects are not too strong, and can be safely ignored, or that they can be corrected a posteriori.

Examples of the impact of NLTE effects can be found in numerous papers. Fuhrmann et al. (1997) discuss the case of Procyon, for which they derive an LTE spectroscopic gravity ($\log g = 3.6$), which they compare to an astrometric gravity based on the distance, and the binarity of the star ($\log g = 4.05$). This difference in gravity of a factor of almost 3, stems from a very high sensitivity of Fe II lines to surface gravity, and of Fe I lines to temperature. NLTE effects at work impact severely the ionization balance, leading to this large difference in gravity. Adopting LTE, and setting the gravity to its astrometric value would require an increase of $T_{\rm eff}$ by 300 K, which is unrealistic.

Recently, Ruchti et al. (2013) determined stellar parameters of a large sample of metal-poor stars. The $T_{\rm eff}$ were determined using Balmer line fitting, after checking against interferometric measurements that this method performed better than the IRFM. The analysis was done both in LTE, and including NLTE corrections for Fe. Their conclusion is that large errors are made when using LTE in metal-poor stars. The differences between NLTE and LTE determinations, that are small at near-solar metallicity, increase to more than 400 K at [Fe/H]=-3.0 for $T_{\rm eff}$, while errors in $\log g$ amount to 1.5 dex, and are more than 0.4 dex in [Fe/H]. Differences in the micro-turbulence parameter can be up to -0.6 km/s.

The main difficulty in carrying proper NLTE calculations is the scarcity of physical data for collisions between atoms and electrons, or hydrogen atoms. Quantum computations are difficult, and have only be made for a handful of atoms, e.g. magnesium (Barklem et al. 2012). Therefore, one has relied on the classical Drawin approximation (Drawin 1969; Steenbock & Holweger 1984) to treat inelastic collisions with hydrogen. A empirical factor, $S_{\rm H}$, was introduced to scale this formula. Korn et al. (2003) attempted to calibrate this factor with standard stars with well known parallaxes. This small sample of four nearby stars with well determined luminosities, $T_{\rm eff}$, radii, masses, and gravities was analyzed using NLTE and various values of $S_{\rm H}$. Only a value of $S_{\rm H}$=3 gave a set of spectroscopic parameters consistent with the Hipparcos data. The small size of the sample does not, however, allow any firm conclusion. This kind of work is also sensitive to inadequacies of the model atmospheres, or to the incompleteness of the model atom used in the calculations, as well as to observational errors. Such studies must be expanded to large samples of stars with fundamental parameters well-known from sources independent of spectroscopy, like parallaxes and analyses of astero-seismic data. Such data is becoming available for a large number of stars from Kepler and CoRoT, and parallaxes will soon come from Gaia. Ezzeddine et al. (this volume) are conducting a analysis similar to that of Korn et al. (2003) on a larger sample of red giants of various metallicities. This should at least provide guidelines to future quantum mechanical calculations of hydrogen iron collisions. It seems indeed useless to try to calibrate the S_{H} factor, as was shown by Barklem et al. (2011). They checked the Drawin formula against quantum mechanical calculations for Mg, and concluded that the Drawin formula does not contain the essential physics behind direct excitation by H atom collisions. The Drawin formula compares poorly with the quantum mechanical results, and usually overestimates the collision rates by amounts that depend on the transition.

3.2 *Red supergiant stars parameters*

3.2.1 The example of Betelgeuse

Red supergiant stars parameters are difficult to determine. The example of Betelgeuse illustrates this. Its initial Hipparcos distance of 130 pc was revised to 197 ± 45 pc by Harper et al. (2008), combining Hipparcos and VLA measurements. The angular diameter of Betelgeuse, of about 45 mas (Perrin et al. 2004), is much larger than its parallax (≈ 5 mas). This reflects the fact that RSGs radii are of the order of a few astronomical units (AU). The parallax of these stars is thus determined from the position of the stellar disk photo center, which may wander significantly, and affect the parallax measurement, due to granulation. 3D hydrodynamical simulations of red giant and supergiant atmospheres are now able to make quantitative predictions on the size of granules, their intensity contrast, the shifts and asymmetries affecting spectral line, and their time scales. Chiavassa et al. (2011b) have showed that the fluctuations in the position of the photo center of RSGs are of the order of a fraction of an AU (up to 0.3 AU in the particular simulation shown in their paper). This will result in systematic errors in Gaia's parallax determinations of the order of 5%. In return Gaia measurements will help verify these predictions on a large number of stars, which can not be done with, e.g., interferometers from the ground, as it necessitates repeated observations of a number of stars during a few years.

Due to its proximity, the interstellar extinction towards Betelgeuse is low. The circumstellar extinction is estimated by Harper et al. (2008) to be at most 0.2 mag in V. The dereddened bolometric flux determinations are in reasonable agreement, i.e., $F_{\mathrm{Bol}} = 1.0 \pm 0.1 \times 10^{-4}\,\mathrm{erg\,cm^{-2}\,s^{-1}}$ (Harper et al. 2001), and $F_{\mathrm{Bol}} = 1.1 \pm 0.1 \times 10^{-4}\,\mathrm{erg\,cm^{-2}\,s^{-1}}$ (Perrin et al. 2004). The bolometric luminosity can then be estimated to $\log L/L_{\odot} = 5.10 \pm 0.22$. Using Meynet & Maeder (2003) evolutionary tracks with rotation and mass-loss gives an initial mass of $20\,\mathrm{M}_{\odot}$ ($18\,\mathrm{M}_{\odot}$ now). The initial mass estimated by Harper et al. (2008) varies from 17 to $24\,\mathrm{M}_{\odot}$, with an age from 13 to 8 Myr, depending on the adopted distance (from 150 to 250 pc).

From the distance and the angular diameter above, the radius of Betelgeuse can be estimated to be $950 \pm 200\,\mathrm{R}_{\odot}$, with the large uncertainty mostly due to the distance error. Levesque et al. (2005) used a fit of the optical spectrum of Betelgeuse to simultaneously derive its $T_{\mathrm{eff}} = 3650$ K, and an extinction $\mathrm{A_V} = 0.62$, which combined give in turn $R = 890\,\mathrm{R}_{\odot}$, consistent with the interferometric value. The extinction is however larger than the estimate of Harper et al. (2008). In conclusion, it is interesting to note that the fundamental parameters of such a bright and nearby star are still a matter of debate.

3.2.2 The RSG T_{eff}-scale

Recent work indicates that there still is an inconsistency in the temperature scale of RSGs. This was found by Davies et al. (2013) using properly calibrated VLT/XSHOOTER (D'Odorico et al. 2006) spectra covering from the B to the K band. When fitting the full spectral energy distribution (SED) with MARCS (Gustafsson et al. 2008) model spectra, they found much hotter effective temperatures than when solely considering the optical part of the spectrum, as done by Levesque et al. (2005). The derived reddening are also larger. The observed SED cannot be reproduced by a single hydrostatic 1D model from the blue to the K band. Davies et al. (2013) suggest that 3D radiative-hydrodynamical model spectra will allow a better fit of the data, based on a single CO5BOLD simulation (Freytag et al. 2012; Chiavassa et al. 2011a). The hint from this simulation is that the fit of observed spectra with 1D hydrostatic model spectra leads to an inconsistent set of parameters (L, Teff, R), i.e. all three must be derived independently. Relying on two of them to compute the third will introduce a systematic error. 3D simulations indeed show that the stellar flux is emitted by only a fraction of the stellar surface, because of the granulation pattern, at least in some spectral region. This might be solved by introducing an effective radius. This stresses the need for the determination of stellar parameters in a redundant way, using independent methods (spectroscopy, interferometry, parallaxes). Further work is in progress, but eventually accurate distances will be needed for a sizable number of RSGs.

4 Conclusions

As observations become more and more precise and detailed, and as models become more and more sophisticated, we find that stellar parameters might not be what we thought they were, and may be tricky to determine. As an illustration, the picture of $T_{\rm eff}$ representing the photospheric temperature at the depth at which the photons we detect are emitted, is much too simple, and should be abandoned. 3D simulations have demonstrated that there are large temperature fluctuations in stellar atmospheres (Ramírez et al. 2009), and that the stellar flux we observe is the addition of contributions from different depths, depending also on the position on the stellar disk, and on time. NLTE is also a factor of complication, that affects spectroscopic methods, and for which we still do not have all the necessary data at hand. Work is in progress on, e.g., inelastic collisions with hydrogen that should lead soon to improved NLTE calculations. These 3D and NLTE effects tend to become stronger in low gravity, and in low metallicity stars.

We must keep on carefully checking stellar parameter determination methods, as new important data become available such as distances from Gaia, and gravities or $T_{\rm eff}$ from Kepler and CoRoT astero-seismic data. Redundancy in the data is useful to cross-check the determinations. It is even necessary in the case of stars like RSGs, where the stellar surface is very affected by granulation, and the stellar diameter is not easily observationally defined.

Finally, beyond the refinements underlined above, that are indispensable for the validation of our stellar evolution and stellar atmosphere models, and further progress in the field, there are parameters which we know very little about. Accurate Gaia distances will allow us to derive, at last, the most commonly missing parameter in Galactic star studies, the luminosity, greatly impacting Galactic and stellar physics studies.

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