

# Solar and stellar photospheric abundances

Carlos Allende Prieto<sup>1</sup>

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**Abstract** The determination of photospheric abundances in late-type stars from spectroscopic observations is a well-established field, built on solid theoretical foundations. Improving those foundations to refine the accuracy of the inferred abundances has proven challenging, but progress has been made. In parallel, developments on instrumentation, chiefly regarding multi-object spectroscopy, have been spectacular, and a number of projects are collecting large numbers of observations for stars across the Milky Way and nearby galaxies, promising important advances in our understanding of galaxy formation and evolution. After providing a brief description of the basic physics and input data involved in the analysis of stellar spectra, a review is made of the analysis steps, and the available tools to cope with large observational efforts. The paper closes with a quick overview of relevant ongoing and planned spectroscopic surveys, and highlights of recent research on photospheric abundances.

**Keywords** Abundances · Stellar atmospheres · Stellar spectra

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✉ Carlos Allende Prieto  
callende@iac.es

<sup>1</sup> Instituto de Astrofísica de Canarias, C/Vía Láctea S/N, 38200 La Laguna, Tenerife, Spain

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## 1 Introduction

Stars drive the chemical evolution of the universe. Starting from hydrogen, stars build up heavier elements, first by nuclear fusion in their cores, and later by neutron bombardment in the final stages of their lives. A fraction of the gas processed in stars makes it back to the interstellar medium, where it can again collapse under gravity and form new stars, repeating the cycle.

This picture is complicated by the fact that the stellar-processed gas mixes with unpolluted (or less polluted) gas, diluting the *metals*<sup>1</sup> available at any given location. Far from being a closed box, the Milky Way strips stars and gas from its immediate neighbors. Depending mainly on their mass, different stars produce (and sometimes destroy) nuclei of different elements, but their nucleosynthetic yields also depend on other parameters such as chemical composition. Most heavy elements are actually produced during the final stages of the lives of stars, in nuclear reactions preceding or driven by supernova explosions. Mixing within stars blurs and modifies the radial stratification predicted by simple, spherically symmetric, models of stars. In addition, close binaries lead to far more complex stellar evolution scenarios where the events expected for an isolated star may happen sooner, or never take place.

The formation and chemical evolution of the Galaxy is therefore closely entangled with the problem of stellar structure and evolution, which includes energy production and nucleosynthesis in stars. Observationally, we see the progressive enrichment in

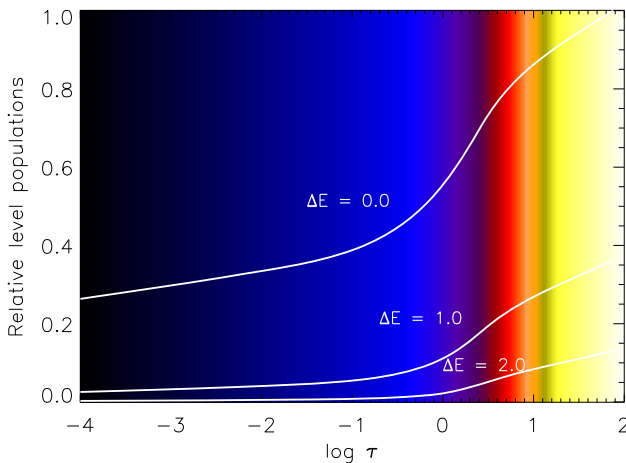
<sup>1</sup> We talk about metals when referring to any element heavier than helium.

metals of the Milky Way in the chemical compositions of intermediate and low-mass stars that were born at different times. The chemical mixtures found in the surfaces of main-sequence stars, essentially undisturbed by the nuclear reactions going on deep in the interior, sample the chemistry of the gas in the interstellar medium from which they formed. Stars preserve those samples for us to study.

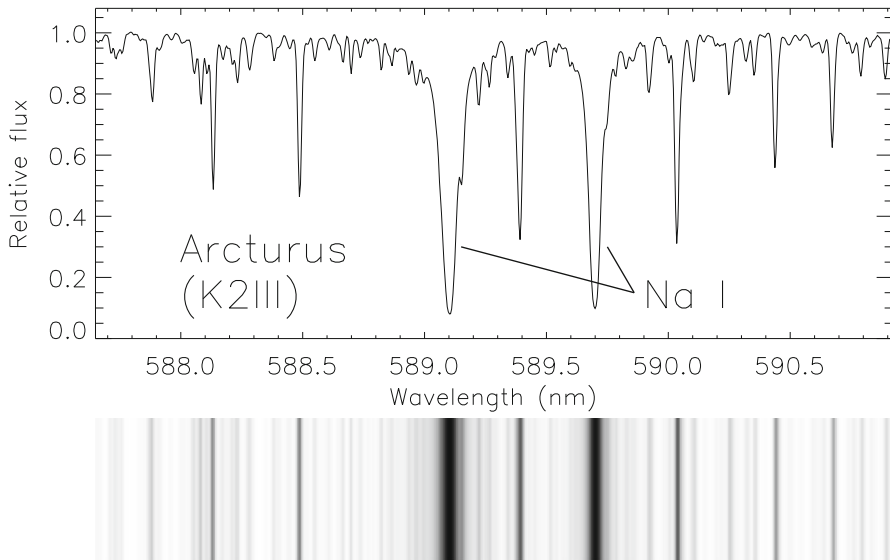
Reading the chemical patterns frozen in the stellar surfaces involves solving a different problem, that of the structure of the outermost layers of a star. Part of the energy initially produced in the nuclear reactions in the interior of a star escapes immediately in the form of neutrinos; this amounts to  $\sim 2\%$  in the solar case. The rest diffuses outwards slowly, finally reaching the surface of the star where photons decouple from matter. The distribution of escaping photons reflects the state of the gas in the stellar atmosphere. Conversely, the radiation field has a profound influence on the physical structure of the atmosphere through its effect on the energy balance.

To model a stellar atmosphere we need to know how much energy flows through it,  $\sigma T_{\text{eff}}^4$ , where  $\sigma$  is the Stefan–Boltzmann constant, the surface gravity of the star,  $g = GM/R^2$ , and its chemical composition. The observed spectrum constrains these parameters, but sometimes there is additional information available. For example, if we know the parallax of a star and its angular diameter, we can readily compute its radius.

Deep enough, the atmosphere is optically thick and Local Thermodynamic Equilibrium (LTE) holds, so that the radiation field is known directly from the gas temperature. As we move upwards in the gravitationally stratified atmosphere, density decreases, photons travel longer distances between their emission and reabsorption or scattering, and begin to escape, cooling the gas (see Fig. 1). Bound–bound transitions within discrete energy levels in atoms and molecules block the light at specific wavelengths, at which the increased opacity shifts the optical depth scale outwards, to cooler



**Fig. 1** Relative LTE populations for three atomic levels of an atom with energies  $\Delta E = 0, 1$  and  $2\text{ eV}$  from the ground state (assuming the same level degeneracy) as a function of Rosseland optical depth ( $\tau$ ) in the solar atmosphere. The populations are arbitrarily normalized to be unity for the ground level in the innermost layer shown. The color in the background indicates temperature, increasing from black (about  $3000\text{ K}$ ) to white (about  $10,000\text{ K}$ ). At the layers relevant for line formation, typically  $-3 < \log \tau < 0$ , the populations of levels separated by  $1\text{ eV}$  differ by a factor of about five



**Fig. 2** A small section of a high resolution spectrum of the red giant Arcturus, the nearest giant at merely 11 pc from us. The strongest transitions in this spectral window are the Na I D doublet

atmospheric layers, imprinting dark stripes, absorption lines, in the spectrum, as illustrated in Fig. 2.

**Absorption lines** are easily seen at high spectral resolution, and constitute the main indicator of the chemical composition of the gas in a stellar atmosphere. Of course, line strengths are **heavily influenced by temperature, which dictates the relative populations of the energy levels**, and somewhat by pressure, which has an impact on ionization and molecular equilibrium, and through collisional broadening. But for any given values of temperature and pressure, the strength of an unsaturated absorption line is proportional to the number of absorbers. This simple fact, allows us to determine the chemical composition of stars.

There is a favorite among the stars: the Sun. This is arguably the best-observed and best-understood star, and constitutes a perfect test bed for spectral analysis techniques. The comparison of the Sun with other stars, and in particular the measurement of accurate absolute fluxes, is complicated by its large angular size, but otherwise the Sun offers multiple advantages. We can resolve its surface, determine the statistical properties of solar granulation, quantify limb darkening, or examine the center-to-limb variation of spectral lines. With the exception of highly volatile elements (hydrogen, carbon, nitrogen, oxygen, and the noble gases), we can compare the derived abundances accessible from the solar spectrum with those in CI carbonaceous chondrites, which are thought to preserve the abundance proportions in the pre-solar nebula.

In the context of the solar system, solar photospheric abundances, having suffered little variation since the formation of the pre-solar nebula,<sup>2</sup> serve as a reference.

<sup>2</sup> Since the solar birth, elements heavier than hydrogen are expected to be reduced at the solar surface by up to 10 % due to diffusion (Turcotte and Wimmer-Schweingruber 2002).

In a stellar context, the Sun is basically a calibrator for our models, both of model atmospheres as explained above, as well as models of stellar structure and evolution, which still have a number of tunable parameters. For example, it is typically imposed that a one-solar mass model has the solar radius and luminosity at 4.5 Gyr, the age of the Sun. In the context of the Galaxy, and galaxy evolution, solar abundances set again a reference to anchor the rest of the abundances—they correspond to the abundances in the interstellar medium 4.5 Gyr ago at a distance from the Galactic center of about 8 kpc.

Abundances in the Sun can also be measured from emission lines formed in the upper atmosphere, where the temperature gradient reverses to reach millions of degrees in the solar corona, and from solar energetic particles ejected in flares, or from particles collected from the solar wind. Nevertheless, these measurements are subject to larger uncertainties than those typically involved in the analysis of photospheric absorption lines. The additional sources of error are associated with our limited knowledge about the physical conditions in the upper solar atmosphere, required to interpret measurements, or with distortions introduced before or in the process of performing the measurements. In addition, a poorly-understood fractionation process related to the so-called first ionization potential (FIP) effect leads to elements with ionization energies lower than about 10 eV to appear more abundant in solar energetic particles and in the corona than in the underlying photosphere.

Despite that the Sun's composition sets a reference for chemistry elsewhere in the universe, there are still important gaps in our knowledge of the solar composition. Solar photospheric abundances are usually determined relative to hydrogen, given that the strength of a spectral line is proportional to the ratio of line and continuum opacity, and  $H^-$  is the dominant source of continuum opacity for a solar-like star. Meteoritic abundances, in turn, need to be referred to other elements (usually silicon), as meteorites have little hydrogen left. After rescaling, the agreement between solar photospheric abundances and CI chondrites abundances is better than 10% for most elements, but there are notable exceptions: Sc, Co, Rb, Ag, Hf, W, and Pb show differences in excess of 20%, and beyond the estimated uncertainties. In addition, there are some elements for which the photospheric values have associated significant uncertainties (Cl, Rh, In, Au, and Tl), and the interesting case of Mg, where the estimated error bars appear slightly inconsistent with the observed difference between the Sun and meteorites (Asplund et al. 2009; Lodders 2003).

The biggest headaches are caused by the lack of information from CI chondrites on the abundances of carbon and oxygen in the pre-solar nebula. These elements are quite abundant (oxygen and carbon are the third and fourth most abundant elements in the Sun, respectively, after hydrogen and helium) and therefore have a large weight on the overall *metallicity* of the Sun. A number of studies have recently reduced by 40–50% the photospheric abundances for these elements, and solar models with updated opacities exhibit significant discrepancies with helioseismic determinations of the location of the base of the solar convection zone and the helium mass fraction at the surface (see, e.g., Serenelli et al. 2009, and references therein). There is indication that this problem may find a solution in the opacity calculations used in the interior models (Bailey et al. 2015).

In the century that humankind has been practicing spectroscopy, progress has been spectacular. Detectors have evolved from photographic to photoelectric, expanding to the UV and IR wavelengths. Telescopes and spectrographs that could only observe the Sun have been replaced by ever larger instruments that allow observations of up to thousands of stars simultaneously. Analyses have also evolved from using the simplest two-layer models to sophisticated 3D (magneto) hydrodynamical simulations. Our ability to calculate fundamental atomic and molecular constants has seen dramatic improvements. Together, these advances open up new lines of research, and connect research subjects that were, just a few years earlier, seemingly unrelated.

This paper aims to explain the motivation for our excitement about stellar spectroscopy, and as an overview of the procedures involved in the analysis of stellar spectra, in particular the derivation of chemical compositions of stars. Section 2 describes the basic ingredients needed to model stellar spectra. Section 3 addresses the most important steps that need to be followed to derive abundances, and the software tools available. The paper closes with an overview of ongoing observational projects, selected examples of recent research, and a few reflections on the near- and mid-term future of the field.

Recent or not-so-recent but excellent reviews on closely related subjects have been written by [Gustafsson \(1989\)](#), [Gustafsson and Jorgensen \(1994\)](#), [Asplund \(2005\)](#), [Asplund et al. \(2009\)](#), [Nordlund et al. \(2009\)](#), and [Lodders et al. \(2009\)](#). A clear and concise summary of the theory of stellar atmospheres is given by [Hubeny \(1997\)](#), and more detailed accounts are provided by [Gray \(2008\)](#) and [Hubeny and Mihalas \(2014\)](#).

## 2 Physics

The necessary physical ingredients to quantify chemical abundances in stars can be divided in two main categories: line formation and stellar atmospheres. Both the theory of atmospheres and line formation are nothing but the application of well-known physics, essentially fluid dynamics, statistical mechanics, and thermodynamics. Line formation and stellar atmospheres are tightly coupled, since spectral lines affect the atmospheric structure by blocking and redistributing radiation, and the atmospheric structure will largely control how lines take shape in the spectrum of a star; they are two parts of the same problem that we artificially split for practical purposes.

In addition to the environmental conditions of an atmosphere, namely the stellar surface gravity and the energy per unit area that enters its inner boundary, modeling stellar spectra requires knowledge of the physical constants that define the relationship between atoms, molecules, and the radiation field. These constants are mainly radiative transition probabilities, excitation, ionization and dissociation energies, as well as line broadening constants.

Quantum mechanics is at the source of the microphysics data: distribution functions of the probabilities for atoms and molecules to change from one state to another by collisions with other particles, or the absorption, emission or scattering of light by matter. Depending on the particular process under consideration, these distribution functions and their integrals are labeled collisional or radiative transition probabilities, line absorption profiles, or photoionization and scattering cross-sections, but they are

all either computed from first principles, or determined from laboratory experiments.<sup>3</sup> These input data are further discussed in Sects. 2.2.1 and 2.2.2.

Stellar atmospheres are optically thick in their deepest layers, and optically thin in the outermost regions. Radiative transfer calculations are necessary to evaluate the radiation field, and determine its role in the energy balance, which is critical when computing model atmospheres. At that stage, some approximations can be adopted, and coarse frequency grids are commonly used. However, much more detailed calculations are usually necessary to compute the spectra that will be compared with observations, and this is commonly performed with dedicated codes. We deepen into this subject in Sect. 3.4.

## 2.1 Model atmospheres

In the early days, the excitation of atoms and ions was computed using the Boltzmann equation (5) for a single value of temperature (see, e.g., Russell 1929). Based on theoretical developments by Schwarzschild, Milne, and Eddington, McCrea (1931) started the construction of non-gray model atmospheres, which have grown in sophistication ever since. Line-blanketed models, those taking into account the effect of line opacity on the atmospheric structure, made an appearance in the 1970s (Carbon and Gingerich 1969; Parsons 1969; Alexander and Johnson 1972; Peytremann 1970; Gustafsson et al. 1975; Kurucz 1979) and continued to evolve, hand in hand with more complete sets of opacities and improvements in computational facilities providing a better description of the radiation field (see, e.g., Kurucz 1992; Hauschildt et al. 1999a,b; Castelli and Kurucz 2004; Gustafsson et al. 2008, but we refer to Hubeny and Mihalas' book for a more exhaustive list).

As mentioned in the introduction, the fundamental parameters that define a model atmosphere are the energy flux that traverses it (parameterized as a function of the effective temperature  $T_{\text{eff}}$ ), surface gravity, and chemical composition. Only a few elements in the periodic table are relevant, and therefore this latter parameter is usually simplified to just one quantity, the metallicity<sup>4</sup>:

$$[\text{Fe}/\text{H}] = \log (N_{\text{Fe}}/N_{\text{H}}) - \log (N_{\text{Fe}}/N_{\text{H}})_{\odot}, \quad (1)$$

where  $N_X$  represents number density of nuclei of the elements X. This is practical because reasonably constant ratios are found between the abundances of iron and most other metals, and iron is in general the element easiest to measure with precision due to the large number of iron lines visible in stellar spectra.

Models for hot stars, for which it is quite important to consider departures from LTE, have also made parallel progress since the early developments (see, e.g., Auer and Mihalas 1969), to more recent fully-blanketed calculations (Hubeny and Lanz 1995; Lanz and Hubeny 1995, 2003, 2007; Lanz et al. 1997). At the hot end of the

<sup>3</sup> Hybrid (semi-empirical) techniques are used sometimes.

<sup>4</sup> Occasionally the metal mass fraction is used:  $Z = \sum_i A_i N_i / N_{\text{H}}$ , where  $A$  is the atomic mass in units of the hydrogen mass, with the summation taken over all metals.

spectrum, it becomes necessary to account for stellar winds, and unified models have been presented by, e.g., [Pauldrach et al. \(1986\)](#), [Gabler et al. \(1989\)](#), [Puls et al. \(1996\)](#), or [Hillier \(2012\)](#). LTE models for white dwarfs, where the high density helps to maintain LTE valid, have also been calculated (see [Koester 2010](#), and references therein). A general code, with an emphasis on parallel computations, has been described by [Hauschildt et al. \(1997, 2001\)](#). On the cool end of the mass range, models for low-mass stars, brown dwarfs and planets have seen extraordinary development in the last decade (e.g., [Allard et al. 1997](#); [Marley and Robinson 2014](#)).

In parallel with refinements in 1D models, 2D and 3D models have emerged and started to be applied to stars ([Nordlund and Dravins 1990](#); [Dravins and Nordlund 1990a,b](#); [Stein and Nordlund 1989, 1998](#); [Asplund et al. 2000](#); [Magic et al. 2013](#); [Wedemeyer et al. 2004](#); [Freytag et al. 2012](#); [Tremblay et al. 2013](#)). These models deal with the hydrodynamics of stellar envelopes, and describe convection, which accounts for up to  $\sim 10\%$  of the energy transported outward in the solar photosphere, from first principles. The onset of convection is caused by the recombination of hydrogen at the solar surface. When hydrogen becomes ionized, the number of free electrons increases dramatically, and so does the blocking effect on radiation caused by electron scattering. This takes place when the gas temperature is about 10,000 K, as one would expect from Saha's equation (6), and 100 km above those layers the average temperature in the solar atmosphere drops to nearly 5000 K.

The low viscosity of the stellar plasma, and consequently high Reynolds numbers, is responsible for the turbulent behavior of the gas in the solar envelope, including deep photospheric layers. Compared to classical 1D (hydrostatic equilibrium) models, 3D simulations fully account for the effect of velocity fields on the atmospheric structure and spectral lines, which get broadened and (typically) blue-shifted. This is illustrated in Fig. 3, where spectra computed for a solar-like star using a 1D classical model and a CO5BOLD simulation of surface convection are compared. On the other hand, the fact that the model is 3D (spatially) and time-dependent, requires simplifying the calculation of the radiation field to evaluate the energy balance, and the radiative transfer is typically solved for only a few (wisely chosen) frequency bins.

In terms of availability, not all models are made equal. The most complex and costly-to-calculate models tend to be custom-made. On the other hand, large grids of 1D models are publicly available from Kurucz<sup>5</sup> ( $3500 \leq T_{\text{eff}} \leq 50,000$  K), the Uppsala group,<sup>6</sup> and Hubeny and Lanz<sup>7</sup> (NLTE models;  $15,000 \leq T_{\text{eff}} \leq 55,000$  K). Others are available as well, but have been less frequently used, e.g., the PHOENIX models published by [Husser et al. \(2013\)](#) or those at France Allard's web site.<sup>8</sup> Many other families of models, in particular 3D models, are proprietary, but some can be obtained directly from their authors upon request or negotiation. The same is true for

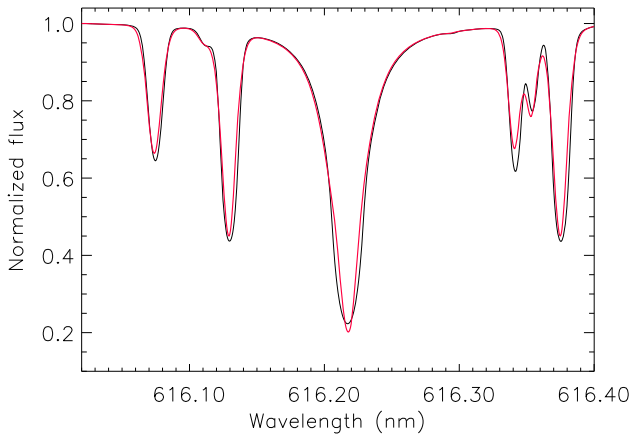
<sup>5</sup> <http://kurucz.harvard.edu> and <http://www.iac.es/proyecto/ATLAS-APOGEE/>, but see also <http://www.univie.ac.at/nemo/>.

<sup>6</sup> <http://marcs.astro.uu.se>.

<sup>7</sup> <http://nova.astro.umd.edu>.

<sup>8</sup> <http://perso.ens-lyon.fr/france.allard/>.





**Fig. 3** Spectra in the vicinity of the Ca I  $\lambda$ 616.2 nm line computed for a solar-like star using a classical hydrostatic model (*black*) and a CO5BOLD hydrodynamical simulation (*red*; see Tremblay et al. 2013)

the model-atmosphere codes. Kurucz's codes and Tlusty are publicly available from the corresponding web sites.<sup>9</sup>

## 2.2 Line formation theory

Radiation plays a key role in determining the atmospheric structure, and therefore has to be described adequately in calculations of model atmospheres. Conversely, once we have a model structure it becomes feasible to perform much more detailed radiation transfer calculations to predict stellar spectra. Armed with an appropriate model atmosphere and the necessary line data, we can proceed to compute spectra that can be compared with observations to infer the chemical makeup of stars.

The detailed shapes and strengths of spectral lines depend on the thermodynamic structure of the atmosphere, which under LTE will dictate the ionization and excitation of atoms and molecules, as well as thermal and collisional broadening. As opposed to the situation with radiative line transition probabilities, laboratory experiments on line broadening by hydrogen atoms, the main perturber in solar-like stars, are extremely hard, and the sensitivity of lines to collisions is usually derived from calculations, as illustrated, e.g., by Barklem et al. (1998) or Barklem and Aspelund-Johansson (2005). As mentioned in Sect. 2.1, convective motions in late-type stars will also directly broaden the line profiles, and the lack of them in 1D models is compensated by introducing two ad hoc parameters: micro- and macro-turbulence.

Depending on the geometry of the model, the radiative transfer equation for quasi-static conditions

$$\frac{\partial I_\nu}{\partial x} = \eta_\nu - \kappa_\nu I_\nu, \quad (2)$$

<sup>9</sup> Note that Kurucz's codes have been ported to Linux, and there is documentation available. See Sect. 3.3.

where  $I_\nu$  is the intensity of the radiation field (energy per unit area, per unit of time, per unit of frequency, per unit of solid angle) at a frequency  $\nu$ ,  $x$  is the spatial coordinate along the ray,  $\kappa_\nu$  is the opacity, and  $\eta_\nu$  the emissivity at that frequency  $\nu$ , will need to be solved somewhere between three (three ray inclination angles for a plane-parallel model neglecting scattering) and millions (3D time-dependent models) of times per frequency. Departures from LTE, considered in Sect. 2.2.2, usually involve many more calculations, as the statistical equilibrium equations are solved iteratively, requiring multiple evaluations of the radiation field at all depths.

A number of LTE codes for solving the radiation transfer equation and computing detailed spectra are available. Typically, there is one such code associated with each of the packages used to compute model atmospheres. For example, there is TURBOSPECTRUM for MARCS (Uppsala) models, SYNTHE for Kurucz models, and SYNSPEC for TLUSTY models.

### 2.2.1 Opacity: lines and continua

Under the assumption of LTE, two thermodynamic variables (e.g., temperature and gas pressure) determine the ionization and excitation fractions, which, together with the line collisional broadening, can be used to calculate how opaque to radiation is matter. Opacity is characterized by the likelihood that a photon is absorbed per flying unit length, which is of course a function of frequency:  $\kappa_\nu$ . Restricting our discussion to LTE, the thermal component of the emissivity,  $\eta_\nu$ , is trivially calculated from the opacity, as the source function,  $S_\nu$ , is equal to the Planck's law, and therefore only depends on temperature

$$S_\nu \equiv \eta_\nu / \kappa_\nu = B_\nu(T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{\frac{h\nu}{kT}} - 1}, \quad (3)$$

where  $T$  is temperature,  $\nu$  is frequency,  $c$  is the speed of light,  $h$  is the Planck constant, and  $k$  is the Boltzmann constant.

All absorption is divided into transitions between bound energy levels (*lines*), or between bound levels and the continuum (*continua*). Transitions between short-lived unbound states, i.e., the absorption of a photon by an atom, ion, or molecule that temporarily forms by the proximity of two particles (e.g., an atom and an electron in the case of  $H^-$ ), cannot only happen, but may contribute significant *free-free* opacity. The strength of a spectral line is critically dependent on the line-to-continuum opacity, and the line opacity can be written as  $l_\nu = N\alpha$ , where  $N$  is the number density of absorbers (i.e., the abundance of ions or molecules with the appropriate excitation ready to absorb the photon), and  $\alpha$  is the absorption coefficient per absorber (i.e., the cross-section)

$$\alpha(\nu) = \frac{\pi e^2}{mc} f \phi(\nu), \quad (4)$$

where  $e$  and  $m$  are the charge and mass of the electron,  $f$  is the oscillator strength or *f*-value (proportional to the radiative transition probability  $A$ ), and  $\phi(\nu)$  is the Voigt function, the result of the convolution of a Gaussian (due to thermal broadening) and a

Lorentzian (due to natural broadening and collisional damping), describing the shape of the absorption probability distribution around the central frequency of the line.

Under LTE, the number density of the absorbers can be split into three factors

$$N = \frac{g}{u_j} N_j e^{-\frac{E}{kT}}, \quad (5)$$

where  $j$  is the charge (in units of the charge of the electron) of the ion (i.e.,  $j = 0$  for neutral atoms),  $N_j$  is the abundance (number density) and  $u_j$  the partition function for the ion  $j$ ,  $E$  is the energy of the state (above the ground level), and  $g$  is its degeneracy. The fraction of nuclei of a given element that are tied in an ion  $j$  is given by Saha's equation (see Fowler 2012)

$$\frac{N_j}{\sum_i N_i} = \frac{\gamma^j u_j}{\sum_i \gamma^i u_i} e^{-\frac{\beta_j}{kT}}, \quad (6)$$

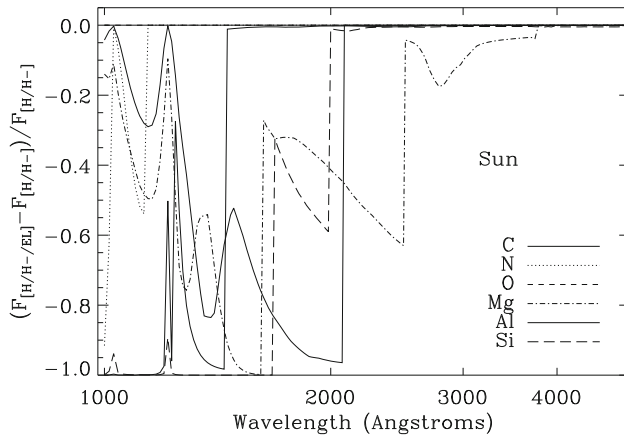
where  $\gamma = 2/(n_e h^3)(2\pi m k)^{\frac{3}{2}} T^{\frac{3}{2}}$ ,  $n_e$  is the number density of electrons, and  $\beta_j = \sum_{i=0}^j \chi_i$ , where  $\chi_i$  is the energy required to rip an electron from the ion  $i - 1$  ( $\chi_0 = 0$ ) in the ground state.

Radiative transition probabilities, or  $f$ -values, have a direct influence on line strength, just the same as the number density of absorbers. Unfortunately, only for simple (light) elements it is feasible to calculate accurately, using quantum mechanics, radiative transition probabilities. For more complex atoms, most data need to be determined from laboratory experiments, a difficult and time-consuming work. Traditionally, the US National Institute for Standards and Technology (NIST) has done useful compilations, formerly available through a series of books, and now online.<sup>10</sup> Kurucz (and colleagues) have made a tremendous effort to augment significantly the number of lines with available transition probabilities, by performing semi-empirical calculations (see, e.g., Kurucz and Peytremann 1975), even though those are of significantly lower quality than laboratory measurements. Another useful resource for transition probabilities is the Vienna Atomic Line Database (Heiter et al. 2008; Ryabchikova et al. 2011, and references therein), which tries to catch up with the many papers in the literature on line data, whatever its source.

Calculations of bound-free absorption (photoionization) made for light elements ( $Z \leq 26$ ) in the context of the Opacity Project (OP, see Seaton 2005; Badnell et al. 2005, and references provided there), have been available for a long time (Mendoza et al. 2001). This work has been extended more recently by the Iron Project team and Sultana Nahar maintains an online database<sup>11</sup> (Nahar 2011). The accuracy of the energies computed by these ab initio calculations is about 1 %, and therefore it has been recommended that the photoionization cross-section be smoothed accordingly (see, e.g., Bautista et al. 1998). Allende Prieto et al. (2003) have applied this procedure to the OP data, and compiled model ions for use with the codes SYNSPEC and TLUSTY

<sup>10</sup> <http://www.nist.gov>.

<sup>11</sup> [http://www.astronomy.ohio-state.edu/~nahar/nahar\\_radiativeatomicdata/](http://www.astronomy.ohio-state.edu/~nahar/nahar_radiativeatomicdata/).



**Fig. 4** Impact of continuum opacity of different atoms on the shape of the solar flux relative to the dominant source of continuum opacity, bound–free H and H<sup>−</sup> absorption. Image reproduced with permission from Allende Prieto et al. (2003), copyright by AAS

(Hubeny and Lanz 1995). Free–free absorption, as mentioned above, can be important for abundant species, such as H, H<sup>−</sup>, or He<sup>−</sup>. In fact, H<sup>−</sup> bound–free absorption is the dominant source of continuum opacity in the optical for the solar photosphere, followed by atomic H, and free–free opacity from the same ion dominates in the IR. Figure 4 illustrates the estimated impact of bound–free absorption by different atoms relative to the total hydrogen (atomic H and H<sup>−</sup>) continuum opacity on the solar spectrum.

Although we are discussing mainly *upward* transitions because those are directly observed in the photospheric spectrum, the opposite *downward* processes are also taking place—at about the same rate, to have equilibrium. Along with radiative excitation and ionization, we have radiative de-excitation and recombination. Spontaneous (*downward*) radiative transitions also occur. Finally, collisional processes are always competing, though we do not need to take them into account to compute the opacity under LTE, as each process is exactly balanced by the opposite, i.e., *detailed balance* holds (the sum of all radiative transitions between a given energy state and all others must be equal to the sum of radiative transitions from all other states to that one, independently from the collisional transitions).

### 2.2.2 Departures from LTE

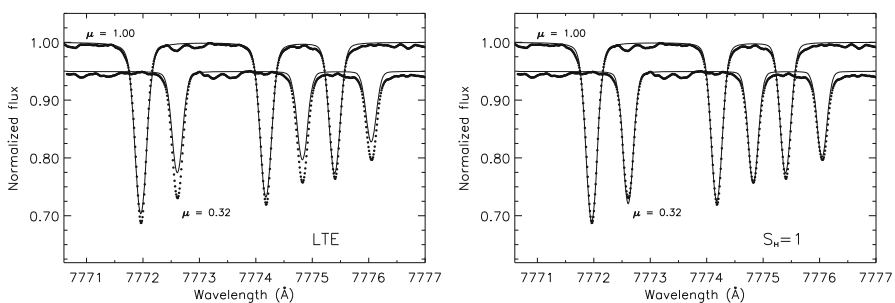
Under the assumption of LTE, radiation and matter are coupled locally, and the source function is equal to the Planck function. But no physical law enforces LTE, in particular when the photon's mean free path is long. From a more general perspective, we can consider a case in which the level populations are time independent, i.e., the sum of all radiative and collisional transitions from an energy level and all others equals the sum of all transitions from all other levels to that one

$$n_i \sum_j (R_{ij} + C_{ij}) = \sum_j n_j (R_{ji} + C_{ji}), \quad (7)$$

where  $R_{ij}$  and  $C_{ij}$  indicate the radiative and collisional rates, respectively, between the states labeled  $i$  and  $j$ . Note that  $R_{ij}$  is closely related to the line absorption coefficient introduced in Eq. (4); it is proportional to the product of  $\alpha$  times the photon density, integrated over the line profile (plus a contribution from spontaneous emission if  $i > j$ ). The system of equations (7) for  $n$  states includes  $n - 1$  linearly dependent equations, and therefore it needs to be closed by adding a total particle number conservation equation.

Solving the statistical equilibrium equations requires many data which are not needed under LTE. To evaluate all possible transition rates across states and ions we need not only radiative cross-sections (i.e., transition probabilities and photoionization cross sections) but also collisional strengths (collisional transition probabilities, if you will). Given their high density, electrons and hydrogen atoms are the main particles responsible for inelastic collisions. As discussed in Sect. 2.2 for line broadening (elastic collisions), laboratory experiments on inelastic collisions with atomic hydrogen are very hard to carry. Approximate formulae exist for electron-impact collisional excitation and ionization (see Allende Prieto et al. 2003), although these are, at best, only good to provide order-of-magnitude estimates. Quantum mechanical calculations of atomic structure can provide much better estimates for collisional strengths for electron impacts (see, e.g., Zatsarinny and Tayal 2003; Barklem 2007a; Belyaev et al. 2014; Osorio et al. 2015), but more involved methods, requiring an adequate knowledge of the relevant molecular potentials, are needed to derive reliable estimates for hydrogen collisions (e.g., Krems et al. 2006; Barklem et al. 2012).

Under solar photospheric conditions, hydrogen atoms dominate by number over free electrons, but inelastic hydrogen collisions tend to have a limited role on line formation (Allende Prieto et al. 2004a; Pereira et al. 2013). Figure 5 illustrates, however, that their effect is visible in the changes of strength experienced by lines such as the O I triplet at 777 nm as a function of heliocentric angle. At lower metallicities, higher pressure and a lower density of free electrons combine to make the role of hydrogen collisions much



**Fig. 5** Observed behavior of the O I triplet at 777 nm in the Sun as a function of the inclination of rays from the solar surface ( $\mu = \cos \theta$ , where  $\theta$  is the angle between the observer and the normal to the solar surface). The filled circles correspond to observations, and the solid lines to models. The observations at disk center ( $\mu = 1$ ) are reproduced in all cases, by changing the oxygen abundance, and the comparison near the limb ( $\mu = 0.32$ ) tests the realism of the calculations. The behavior of the lines can be reproduced considering inelastic collisions with hydrogen atoms in the rate equations. The factor  $S_H$  is introduced to enhance the approximate collisional rates from a Drawing-like formula as proposed by Steenbock and Holweger (1984). Image reproduced with permission from Allende Prieto et al. (2004a), copyright by ESO

more important, as discussed for example by Gratton et al. (1999). Shchukina et al. (2005) predict abundance corrections due to NLTE effects on Fe I in the metal-poor subgiant HD 140283 as large as 0.6 dex for a 1D model atmosphere, and as large as 0.9 dex for a 3D model, in the absence of inelastic hydrogen collisions.

Departures from LTE can be very important in some situations. If they involve important species (say, hydrogen, helium, iron), their impact can be profound and the statistical equilibrium equations may need to be solved together with the model atmosphere problem, as it is usually done for hot stars. In many other cases, the departures affect trace species and particular transitions of interest, which may induce a modest effect on the overall atmospheric structure, but anyway must be considered in order to avoid large systematic errors in the calculated line profiles, and therefore the derived abundances. In this latter case, one can adopt the thermal structure of the atmosphere plus a second thermodynamic variable (usually the electron density) and solve the statistical equilibrium equations (7) for the relevant ions in isolation from the model atmosphere, what is usually referred to as the *restricted* NLTE problem.

There are NLTE codes available for solving the *full* NLTE problem (statistical equilibrium plus atmospheric structure) and some limited to the *restricted* NLTE problem. Among the former, we find the publicly available codes CMFGEN<sup>12</sup> (Hillier 2012), the suite of Munich codes<sup>13</sup> (Pauldrach et al. 1998), and TLUSTY<sup>14</sup> (Hubeny and Lanz 1995), three packages originally developed in the context of hot stars. The code MULTI<sup>15</sup> (Carlsson 1992) deals with the *restricted* NLTE problem, and has been widely used in the context of late-type atmospheres.

### 3 Working procedures

With the basic blocks described above—adequate opacities, and codes to compute model atmospheres and spectra—the only remaining input is an observed spectrum, and a work plan.

The various elements entering in the analysis are tightly coupled. To calculate a model atmosphere, we need to know the basic atmospheric parameters and abundances, precisely the very variables we seek to derive from the spectral analysis. Thus, it is only natural to address the problem iteratively. First, atmospheric parameters are guessed, then a spectrum computed and confronted with the observations to determine the parameters, repeating the cycle as needed. Such process can, in some situations, be simplified, provided we are confident that some parameters are decoupled from others—for example, when we derive the abundance of iron in a solar-like star from lines of neutral Fe, which have only a weak sensitivity to the surface gravity. In some cases, parameters derived from external data, free from systematic errors that model spectra are subject to, are preferred, and that also simplifies the analysis, eliminating the need for iteration.

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<sup>12</sup> <http://kookaburra.phyast.pitt.edu/hillier/web/CMFGEN.htm>.

<sup>13</sup> <http://www.usm.uni-muenchen.de/people/adi/Programs/Programs.html>.

<sup>14</sup> <http://nova.astro.umd.edu/>.

<sup>15</sup> <http://folk.uio.no/matsc/mul22/>.

The amount of information available directly from a spectrum will be limited by its spectral coverage, signal-to-noise, and resolution.<sup>16</sup> In addition, spectra show a strong response to some parameters (e.g., the effective temperature), and a much weaker or null reaction to others (e.g., the abundance of ytterbium). Tracking correlations is extremely important to arrive at reliable uncertainty estimates for the inferred abundances.

Because of the shallow temperature structure in the outer layers of the photosphere, lines with fairly opaque cores saturate, i.e., their strength does not grow linearly with the abundance of the absorbers, and therefore relatively weak lines are preferred. Weak lines demand high spectral dispersion, which usually implies narrow spectrograph slits and high frequency variations in the instrument's throughput (i.e., poor accuracy in flux calibration), and more limited spectral windows. For this reason, the analysis of high-resolution spectra is usually supplemented with lower-dispersion spectrophotometry or photometry.

In what follows, we will briefly split the abundance determination process into three steps: gathering data, choosing atmospheric parameters, and deriving abundances.

### 3.1 Obtaining stellar spectra and reference data

Because the atmospheric parameters are related to the fundamental stellar parameters, and these can be constrained from many other data independent from spectra, we should compile all the relevant information available from the literature. If we aspire to provide a physically consistent picture of the observed objects, the atmospheric parameters used in the spectroscopic analysis need to be consistent both with the spectrum and with the available external data, whenever possible.

Examples of useful data are: trigonometric parallaxes from astrometric measurements, angular diameters from interferometry, or mean densities from asteroseismology (see, e.g., [Bruntt et al. 2010a](#); [Pinsonneault et al. 2014](#); [Coelho et al. 2015](#); [Silva Aguirre et al. 2015](#)). However, be aware that in most cases deriving fundamental quantities such as radii, masses, or distances from these observations involves to some extent the use of models of stellar structure and evolution, subject to their own issues and systematic errors. If the stars of interest are members of binary systems, there may be very useful constraints on the stellar masses from the system dynamics, and if we are lucky enough to have an eclipsing system, then masses and radii may be constrained with exquisite accuracy ([Popper 1980](#); [Andersen 1991](#); [Torres et al. 2010](#)), but the likelihood for such alignment is very low.

Digital data can be handled and stored with ease, and as instruments become more efficient and observations more homogeneous, there are more and more data archives that offer collections of stellar photometry and spectra of different kinds. In Sect. 4.1 we provide a list of some of the most popular collections of spectra for nearby and bright stars.

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<sup>16</sup> One may define a *power-to-resolve*  $P$  that combines these three parameters to quantify approximately the information content in a spectrum ([Allende Prieto 2016](#)).

Photometric information, and most of all, spectrophotometric information, is of high value when it comes to constraining atmospheric parameters, in particular effective temperature, although the interstellar extinction complicates the analysis. There are large libraries with spectrophotometry for stars, some of which are mentioned in Sect. 4.1.

A word should be said here about photometric calibrations for deriving stellar effective temperatures. Direct calibrations are rarely used, due to the high sensitivity of the model atmospheres and irradiance calculations to the input physics, and in particular the equation of state. The most widely-used calibrations are based on the so-called infrared flux method (Blackwell et al. 1980; Alonso et al. 1999; Ramírez and Meléndez 2005; González Hernández and Bonifacio 2009; Casagrande et al. 2010), which exploits a more robust prediction from the models, the ratio of the monochromatic flux at a given infrared wavelength to the bolometric flux of a star.

In many cases, spectra for the stars of interest are not available from existing data bases, and we will need to obtain new observations. Observing facilities are continuously progressing. However, spectral resolution is not increasing as spectrographs become larger to mate with larger telescopes. For a given grating, the product of the resolving power and the slit width is proportional to the ratio of the collimator and telescope diameters, making it difficult to reach high dispersion without using narrow slits and losing light. In addition, there has only been modest progress in feeding multiple objects to high-resolution spectrographs, at least in comparison with the massive multiplexing capabilities now available and planned for lower dispersion instruments.<sup>17</sup> Many observatories offer high-resolution spectrographs, but reviewing the existing choices is out of the scope of this paper. We will go back to discussing some of the largest projects, ongoing and planned, in Sect. 4.

### 3.2 Atmospheric parameters

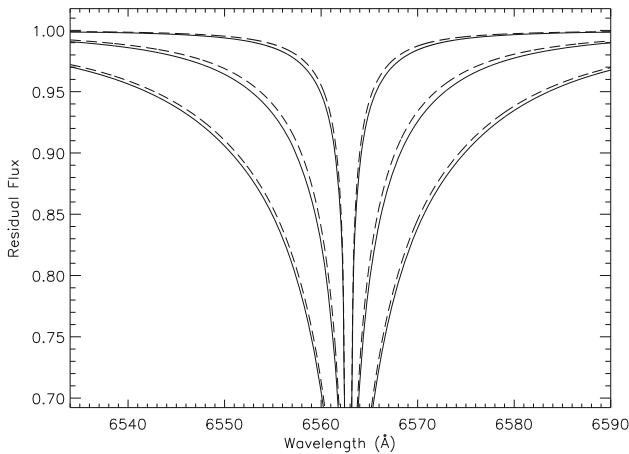
Provided with a wide spectral range, it may be feasible and convenient to derive all the relevant atmospheric parameters needed to calculate a model atmosphere from the very same high-resolution spectra that will be later used to derive abundances. Nevertheless, alternative paths are useful for two reasons: as a sanity check (remember that the analysis of the high-resolution spectra will have associated caveats, as it involves many approximations), or simply because a high-resolution spectrum will have a limited sensitivity to some parameters, with surface gravity being the most typical case. We mentioned in the previous section several possibilities to constrain the atmospheric parameters from measurements other than high-resolution spectra. Here we will highlight the most useful features available in spectra when lines are resolved.

The effective temperature is usually derived from the excitation balance of atomic iron, calcium, silicon or titanium, i.e., by requiring that lines with different excitation

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<sup>17</sup> MUSE for the VLT employs image slicers to feed 24 spectrographs at once (Bacon et al. 2012), and VIRUS for the Hobby–Eberly telescope has some 30,000 fibers feeding 75 spectrographs simultaneously (Hill et al. 2012).



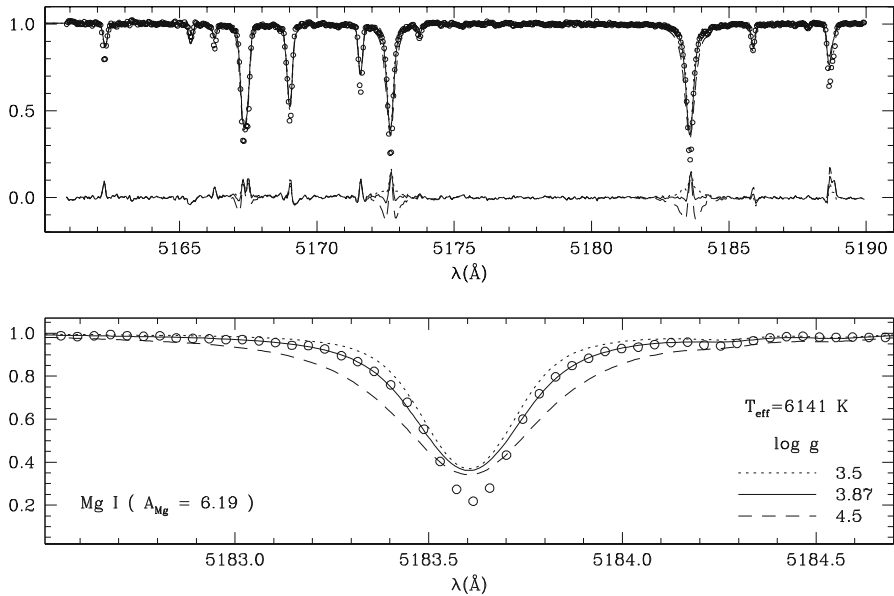


**Fig. 6** Sensitivity of computed profiles for  $H\alpha$  with the stellar effective temperature ( $T_{\text{eff}} = 5000, 6000, 7000 \text{ K}$ ), for an atmosphere with solar surface gravity and composition. *Stronger lines* correspond to warmer atmospheres. The differences between *solid* and *dashed profiles* illustrate variations between two theoretical calculations of the contribution of H–H collisions. Image reproduced with permission from [Barklem et al. \(2000\)](#), copyright by ESO

energy give the same abundance. This technique simply takes advantage of the Boltzmann equation [see Eq. (5)], where  $T$  is the temperature in the relevant atmospheric layers for the lines, which is of course tightly coupled to the effective temperature of the star  $T_{\text{eff}}$ . Unfortunately, the de-saturation of strong lines induced by small-scale motions of the iron atoms (micro-turbulence), complicates somewhat the performance of this method, which is sensitive to this parameter, as well as to departures from LTE.

The damping wings of hydrogen lines, largely controlled by Stark broadening induced by elastic collisions with free electrons but also affected by collisions with the surrounding hydrogen atoms, are also highly dependent on the thermal structure in layers close to Rosseland optical depth  $\tau \sim 1$ , which provides an excellent thermometer (see [Fuhrmann et al. 1993, 1994](#); [Barklem et al. 2000, 2002](#); [Stehle et al. 1983](#); [Stehle 1994](#), and references therein). This is illustrated in Fig. 6. Here a difficulty for one-dimensional models, in addition to getting right the microphysics for Stark broadening, is to account properly for the effect of convective motions on the thermal structure of deep photospheric layers. Three-dimensional models based on hydrodynamics get rid of this problem. Investigations of departures from LTE on the wings of Balmer lines have also shown that these effects need to be considered if high accuracy is sought (see [Przybilla and Butler 2004](#); [Barklem 2007b](#)). In any case, [Cayrel et al. \(2011\)](#) have demonstrated that the scale can be calibrated using external data. Most sensitive, but hard to calibrate in absolute terms, is perhaps the technique based on line-depth ratios (see, e.g., [Gray and Brown 2001](#)).

The surface gravity of a star is the parameter that has the smallest effect on the spectrum. This is unfortunate to constrain it from the spectrum itself, but at the same time it means that this parameter will have a limited impact on the derived abundances. As mentioned earlier, there are cases in which we can use external data to constrain



**Fig. 7** The *top panel* shows part of the spectrum of the metal-poor star BD+17 4708, while the *bottom panel* provides a close view of one of the Mg I b lines in the spectrum of the star compared with calculations for models with a range in surface gravity. The analysis focuses on the wings, since the line core is not matched due to departures from LTE. Image reproduced with permission from [Ramírez et al. \(2006\)](#), copyright by ESO

surface gravity, but until the Gaia catalog is available this will not apply to many stars.

Using the spectrum, gravity can be constrained taking advantage of the way the electron pressure enters in Saha's equation (Eq. 6): at a given temperature, the lower the electron density, the higher the ionization. Such effect is readily noticeable in cool stars on the H bound–free ionization edges, e.g., in the Balmer jump in the optical. The wings of strong metal lines are also very useful to constrain gravity. As surface gravity increases, so does the effect of broadening by collisions between the absorber and H (and partly He) atoms, enhancing the wings of metal lines, as illustrated in Fig. 7 for one of the lines of the Mg I b triplet in the spectrum of the metal-poor star BD+174708.

The overall metallicity, usually approximated by the iron abundance, is derived, like any other abundance, from lines of weak-to-moderate strength. This is either done from equivalent widths or line profiles, but this choice will be further discussed in the next section.

### 3.3 Determining abundances from spectra

Once we have decided on the best set of atmospheric parameters for a star which, we recall, are likely to be revised during the analysis, we can proceed calculating, or obtaining from a data base, an appropriate model atmosphere. Of course, if some or all

of the atmospheric parameters are constrained from observed line strengths, as opposed to other external information such as photometry, spectrophotometry, or astrometry, we will need the model atmospheres earlier in the process. Any theoretical fluxes to be compared to observations, i.e., photometry or spectrophotometry, also require model atmospheres, but unlike high-resolution spectra, these fluxes are usually available together with the libraries of model atmospheres, and one does not need to calculate them in most instances.

Depending on the type of star, the accuracy being sought, more mundane factors such as access to computing resources and human collaborators, we should decide on the type of model atmosphere to adopt, and how to secure it. We have already mentioned the most widely used possibilities in Sect. 2.1.

The Kurucz codes have been used in modern operating systems, and are publicly available (e.g., from Castelli's site<sup>18</sup>). The MARCS code is not, although custom-made models are kindly provided by the core MARCS community—mostly residents or former residents of the Swedish town of Uppsala. There are many different interpolation tools that have been used in the literature, although few are publicly available and documented. An interpolation code for MARCS models is available from the MARCS site, and others for Kurucz's models are available from A. McWilliam and from me.<sup>19</sup>

As mentioned earlier, in addition to a model atmosphere, deriving abundances requires basic data associated with the atomic or molecular transitions we plan on using as diagnostics: wavelengths, transition probabilities, the energy of the lower level connected by the transition, and damping constants. With these inputs, we have all we need to calculate a model spectrum, since other auxiliary data are typically included in radiative transfer codes. Once we are able to compute model spectra, we can iteratively compare those with observations to infer the chemical compositions of stars. Section 3.4 is devoted to tools commonly used for these tasks.

### 3.4 Tools for abundance determination

As outlined above, the process of abundance determination requires a certain degree of iteration. At the very least, when the atmospheric parameters are well constrained, and the overall metal content of the star is known in advance, we need to iterate the last step of calculating a synthetic spectra to arrive at the chemical composition that best matches the observations.

Traditionally, for the analysis of a small number of spectra, iterations are performed under the careful control of a person. The basic workhorse software is a radiative transfer code, that predicts what the observed spectrum would look like for a given model atmosphere and chemical composition. We mention the most popular choices (there are many more!) in Sect. 3.4.1. When the number of spectra to analyze is very large, a manual analysis using interactive software is no longer possible, and more powerful tools become necessary. These are the subject of Sect. 3.4.2.

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<sup>18</sup> <http://wwwuser.oats.inaf.it/castelli>.

<sup>19</sup> See KMOD.PRO at <http://www.as.utexas.edu/~hebe/stools/>.

### 3.4.1 Interactive tools

The fundamental tool for chemical analysis is a spectral synthesis code. For a given set of input data: model atmosphere, and atomic and molecular line and continuum opacities, the code can be used to predict spectra for different abundances to identify the value that matches observations—one or an array of absorption lines. Some of the most commonly used spectral synthesis codes publicly available have already been mentioned in Sect. 2.2: these are MOOG<sup>20</sup> (Sneden 1974), SYNSPEC<sup>21</sup> by Hubeny and Lanz, TURBOSPECTRUM<sup>22</sup> by Plez (2012) (see also Alvarez and Plez 1998). Many more codes are available but less frequently used, for example MISS (Allende Prieto et al. 1998; see also Ruiz Cobo and Toro Iniesta 1992), RH by Uitenbroek,<sup>23</sup> ASSET by Koesterke 2009, or SPECTRUM<sup>24</sup> by R. O. Gray.

Using line equivalent widths (the total absorption associated with a spectral line) is operationally convenient (one number per transition instead of an array of fluxes) and makes the results independent from macro-turbulence and rotational broadening. For those reasons, despite it represents a loss of information, equivalent widths are still used in many studies. This requires measuring line equivalent widths in both observed and model spectra. One of the software packages commonly used to measure manually equivalent widths is the *plot* package within IRAF.<sup>25</sup> Codes such as MOOG can be used to provide abundances directly from equivalent widths (see Sect. 3.4.2). This modus operandi is highly effective for processing large numbers of transitions for many stars, and it has been used with success in numerous projects (see, e.g., Reddy et al. 2003; Bensby et al. 2003; Santos et al. 2004; Fulbright et al. 2010; Nissen 2015, to mention a few examples).

### 3.4.2 Automated tools

There are several codes that automate the measurement of equivalent widths. The most used ones are ARES (Sousa et al. 2007) and DAOSPEC (Stetson and Pancino 2008; Cantat-Gaudin et al. 2014). As already mentioned, the derivation of abundances from observed equivalent widths has been automated for a long time in codes such as MOOG or those in the Uppsala package. The automation of the task of directly fitting spectra with models has a more recent history.

SPECTROSCOPY MADE EASY<sup>26</sup> by Valenti and Piskunov (1996) is a package for fitting spectra by wrapping an optimization algorithm around a spectral synthesis

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<sup>20</sup> <http://www.as.utexas.edu/~chris/moog.html>.

<sup>21</sup> <http://nova.astro.umd.edu/Synspec49/synspec.html>.

<sup>22</sup> <http://www.pages-perso-bertrand-plez.univ-montp2.fr/>.

<sup>23</sup> <http://www4.nso.edu/staff/uitenbr/rh.html>.

<sup>24</sup> <http://www.appstate.edu/~grayro/spectrum/spectrum.html>.

<sup>25</sup> IRAF (Image Reduction and Analysis Facility) is distributed by the National Optical Astronomy Observatory, which is operated by the Association of Universities for Research in Astronomy (AURA) under cooperative agreement with the US National Science Foundation.

<sup>26</sup> <http://www.stsci.edu/~valenti/sme.html>.

code. ULYSS<sup>27</sup> by Koleva et al. (2009) is also spreading in use. FERRE<sup>28</sup> by Allende Prieto et al. (2006) includes several algorithms and is optimized for dealing with large samples. Two more options are VWA<sup>29</sup> by Bruntt et al. (2010b) and Starfish<sup>30</sup> by Czekala et al. (2015). Many more packages of general application have been employed in the literature, but they are not publicly available, e.g., MATISSE by Recio-Blanco et al. (2006), TGMET<sup>31</sup> by Katz et al. (1998), or MYGISFOS by Sbordone et al. (2013). Some packages have been developed for particular instruments or projects, such as various parts of the SEGUE Stellar Parameter Pipeline (Lee et al. 2008a, b, 2011a; Allende Prieto et al. 2008), or the original RAVE analysis pipeline (e.g., Boeche et al. 2011; Siebert et al. 2011).

Although these tools are very useful to deal with large samples, one should avoid using them blindly. There is no substitute for understanding which spectral features can be modeled accurately and which ones cannot, and the information they convey. The importance of checking thoroughly, using well-studied stars, the performance of an automated tool on a particular data set, cannot be overemphasized.

## 4 Observations

There is a wide variety of collections of spectra readily available on the internet. This includes libraries with typically high-quality data for specific sets of stars, and data repositories for large surveys. We describe the most significant ones below, as well as the most exciting instruments now in operation or being planned for the future.

### 4.1 Libraries

If you are interested in a bright star, its high-resolution optical spectrum may be available in the Elodie archive<sup>32</sup> (Moultaka et al. 2004), S<sup>4</sup>N<sup>33</sup> (Allende Prieto et al. 2004b), the UVES-Paranal library<sup>34</sup> (Jehin et al. 2005), or the Nearby Stars Project<sup>35</sup> (Luck and Heiter 2005). If the spectrum has been ever obtained with HST, you will find it in MAST,<sup>36</sup> and if it has been secured in recent times with ESO instruments, there is a good chance it is publicly available in the ESO archive,<sup>37</sup> although you may need to reduce the data yourself. Other observatories have their own archives, and very many are now becoming publicly available, but they are too many to list here,

<sup>27</sup> <http://ulyss.univ-lyon1.fr/>.

<sup>28</sup> <http://hebe.as.utexas.edu/ferre>.

<sup>29</sup> <https://sites.google.com/site/vikingpowersoftware/>.

<sup>30</sup> <http://iancze.github.io/Starfish>.

<sup>31</sup> <http://www.obs-hp.fr/guide/elodie/tgmet-doc/TGMET1.HTML>.

<sup>32</sup> <http://atlas.obs-hp.fr/elodie/>.

<sup>33</sup> <http://hebe.as.utexas.edu/s4n/>.

<sup>34</sup> <https://www.eso.org/sci/observing/tools/uvespop/interface.html>.

<sup>35</sup> <http://bifrost.cwru.edu/NStars/>.

<sup>36</sup> <https://archive.stsci.edu/>.

<sup>37</sup> <http://archive.eso.org/cms.html>.

and their reservoir of public high-dispersion spectra is anyway limited. A new library under development at Leiden is based on observations with X-Shooter, offering a wide spectral coverage at medium-high resolving power (Chen et al. 2012).

Regarding spectrophotometry, it is worthwhile to highlight the Indo-US library<sup>38</sup> by Valdes et al. (2004), and MILES<sup>39</sup> by Falcón-Barroso et al. (2011), and references therein from the ground, and the STIS Next Generation Spectral Library<sup>40</sup> by Gregg et al. (2006) and Heap and Lindler (2007) from space. The ESA mission Gaia should bring accurate parallaxes and spectrophotometry (with very low resolution though) for  $10^9$  stars before the end of the decade (Lindegren et al. 2008), but we will come back to this important observatory in Sect. 4.3.

## 4.2 Ongoing projects

We live in a time when instruments with high multiplexing capabilities are revolutionizing the study of the chemical compositions of stars in the Milky Way and other nearby galaxies. For the most part, the distinction between instruments and surveys is blurred, since these instruments serve mainly a single or a small number of projects.

For the sake of limiting the size of this article, we will concentrate on the largest projects and the instruments with the largest multiplexing capabilities currently in operation, and which are being massively used for the acquisition of stellar spectra that have become or will soon become public, at the expense of leaving out excellent instruments that do not meet those conditions.

The Sloan Digital Sky Survey (SDSS; York et al. 2000) is the most dramatic example of a modern survey making efficient use of a suite of instruments. In addition to five-band photoelectric photometry of a third of the sky, the SDSS has obtained  $R = 2000$  spectra for several million galaxies and about a million stars since it started operations in 2000. The project uses a dedicated 2.5-m telescope (Gunn et al. 2006) with a field-of-view of 7 square degrees. Originally equipped with two double-arm spectrographs (Smee et al. 2013), fed by 640 fibers, and subsequently upgraded to 1000, providing a wide spectral coverage (360–1000 nm approximately) the project concentrates on stars in the magnitude range  $14 < V < 21$ . These data have been used for studying the structure of the Milky Way disk and halo in a series of papers (see, e.g., Allende Prieto et al. 2006; Schlafman et al. 2009, 2011, 2012; Bond et al. 2010; Lee et al. 2011b; Cheng et al. 2012; Schlesinger et al. 2012; Fernández-Alvar et al. 2015; López-Corredoira and Molgó 2014), but many more studies are to be expected as observations continue (at least to 2020). SDSS releases their data publicly every one or two years, a move that has been decisive in making it one of the most scientifically productive observatories in the world.

A few years ago, SDSS added a new instrument optimized for the observation of stars in the  $H$ -band (1.5–1.7  $\mu\text{m}$ ) at high  $R = 22,500$ . The Apache Point Galactic Evolution Experiment (APOGEE) has collected so far nearly half a million spectra

<sup>38</sup> <http://www.noao.edu/cfib/>.

<sup>39</sup> <http://www.iac.es/proyecto/miles/pages/stellar-libraries/miles-library.php>.

<sup>40</sup> <https://archive.stsci.edu/prepds/stisngsl/>.

for some 100,000 stars in the Milky Way (see [Holtzman et al. 2015](#); [Majewski et al. 2015](#)) and results are already appearing on various subjects (see, e.g., [Deshpande et al. 2013](#); [Majewski et al. 2013](#); [Frinchaboy et al. 2013](#); [Mészáros et al. 2013](#); [Zasowski et al. 2013](#); [García Pérez et al. 2013](#); [Bovy et al. 2012](#); [Nidever et al. 2014](#); [Hayden et al. 2015](#)). The project is expanding this collection of spectra by a factor of several between 2014 and 2020, including observations from Las Campanas, accessing the Magellanic clouds, parts of the disk not available from the North, and getting a better perspective of the central parts of the Milky Way. In the SDSS tradition, APOGEE's spectra and derived data products are made public on a regular basis.

The Radial Velocity Experiment (RAVE) (see, e.g., [Kordopatis et al. 2013a](#), and references therein), already done with the data taking, has targeted stars with brighter magnitudes ( $5 < V < 14$ ) and therefore located at closer distances, with higher resolution  $R = 8500$  and a narrower spectral range (837–874 nm) than SDSS. Many results from the survey are already out (see, e.g. [Kordopatis et al. 2013a,b](#); [Piffl et al. 2014](#); [Conrad et al. 2014](#); [Kos et al. 2013](#); [Williams et al. 2013](#)), and the associated spectra for about half a million stars will probably become public sometime in the future.

The Large Area Multi Object fiber Spectroscopic Telescope (LAMOST) resembles in many respects SDSS but with 4000 fibers, an original telescope with an effective aperture between 3.6 and 5.9 m, and a robotic fiber positioner. After some difficulties the project is now showing results (see, e.g., [Yi et al. 2014](#); [Yang et al. 2014](#); [Ren et al. 2013](#); [Zhang et al. 2013](#); [Zhao et al. 2013](#); [Liu et al. 2015](#)), and a lot more is envisioned to come out in coming years.

The Gaia-ESO Survey (GES) is a massive ESO public survey that is using 300 nights on the Very-Large Telescope to obtain high-resolution spectra for about 100,000 stars ([Gilmore et al. 2012](#)), thought out to complement the observations from Gaia (see Sect. 4.3). About 90 % of the observations are made at a resolving power of about 15,000 with the GIRAFFE spectrograph ([Hammer et al. 1999](#); [Blecha et al. 2000](#)), and the remainder at higher resolution with the cross-dispersed UVES spectrograph ([Dekker et al. 1992](#); [Hammer et al. 1999](#)). It involves a large European collaboration, and has two distinct parts, one focusing on field stars and a second one devoted to clusters. The observations started at the end of 2012, the raw spectra are quickly made public on the ESO archive, and the advanced data products (fully reduced spectra, radial velocities and stellar parameters including abundances) are following on a fast-paced schedule. There are plenty of examples of science results from this project (e.g., [Magrini et al. 2015](#); [Lind et al. 2015](#); [Sacco et al. 2015](#)).

The GALactic Archaeology with HERMES project (GALAH) (see [Zucker et al. 2013](#)) expands on the idea of chemical tagging and producing a chemical map of stars in the Galaxy to provide optical high-resolution spectroscopy ( $R = 28,000$ ) for over a million stars using the 4-m AAT telescope in Australia. The HERMES instrument was commissioned at the end of 2013, and the first results are eagerly expected.

The Hobby–Eberly Telescope Dark Energy Experiment (HETDEX; [Hill et al. 2012](#)), although conceived mainly as a cosmology project, leaves no star behind, at least of those that fall on their Integral-Field Units during the course of the experiment, which will last five years. These spectra will be deep ( $V < 22$ ) and reach into the UV (350–550 nm), although of low resolution ( $R = 700$ ), with the particular plus



of having no selection biases (like Gaia). As of this writing the observations are a few months from starting.

### 4.3 In the future

If current and ongoing surveys are tremendously exciting, there are instruments in the design and construction phase that will make the future even more thrilling. Having in mind that this is a live review, and accepting the task of coming back to complete information as time progresses, the following paragraphs will only mention projects that are subjectively perceived by this writer as the most promising ones.

Gaia has long been declared as the ultimate survey of the Milky Way. There is no doubt that Gaia's capabilities are impressive. The satellite was launched in December 2013, and the first catalog is expected in 2016. This ESA cornerstone mission is building a full-sky catalog of the stars in the Milky Way with a unique suite of instruments that provide exquisite astrometry, and (spectro-)photometry for about  $10^9$  stars, and high-resolution spectroscopy (847–874 nm) for about  $10^8$  stars. Rather than providing all the details on Gaia, I will simply refer the reader to [Lindegren et al. \(2008\)](#) and the updates on the ESA pages<sup>41</sup>, but not without noting that all other spectroscopic efforts are largely complementary to Gaia, since its high-resolution spectrograph is only effective to provide radial velocities for a small fraction of the astrometric sample, due to the short integration times and the implied low signal-to-noise ratio of the spectra.

The Dark Energy Spectral Instrument (DESI; [Levi et al. 2013](#)) is an ambitious project conceived as a natural follow-up of the Baryon Oscillations Spectroscopic Survey (BOSS; [Schlegel et al. 2007](#); [Eisenstein et al. 2011](#)), part of the SDSS. Improving on telescope area (from the 2.5-m SDSS telescope to the 4-m Mayall telescope at Kitt Peak), doubling spectral resolution, enhancing multiplexing capabilities (from 1000 to 5000 fibers, from plug-plates to a robotic positioner), all without losing field of view and synoptic operations. Like BOSS and the follow-up eBOSS project, DESI will mainly measure redshifts to identify the imprint left by primordial baryonic acoustic oscillations on large scale structure, but there is no doubt that this instrument will also make an important contribution for Galactic studies of stars.

In addition to DESI, there are other instruments planned for 4-m-class telescopes. These instruments have somewhat more modest multiplexing capabilities but differ from DESI in that they provide various spectral settings, allowing higher resolution observations, and therefore will enable stellar science that DESI cannot do, and smaller, more targeted projects. These are WEAVE for the 4.2-m WHT in La Palma ([Dalton et al. 2014](#)), or 4MOST for the 4-m VISTA at Paranal ([de Jong et al. 2014](#)). Yet another high-multiplexing spectrograph with the ability of reaching a resolving power of  $R = 20,000$  in the infrared for up to  $\sim 1000$  targets simultaneously, MOONS, is projected for the 8-m ESO VLT ([Cirasuolo et al. 2014](#); [Oliva et al. 2014](#)).

One can imagine the ultimate spectroscopic experiment, let's call it the Final Uniform Spectroscopic Survey, using a Field Ultra-dense Survey Spectrograph (FUSS), a natural endpoint of all the surveys described above, providing radial velocities and

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<sup>41</sup> <http://www.cosmos.esa.int/web/gaia>.



chemistry to complement Gaia's astrometry and photometry. This would consist of a pair of large-field large-aperture telescopes (one per hemisphere), perhaps 6 to 8-m-class, resembling the LSST, with massive integral field units (IFU) covering their entire field of view à la VIRUS (the HETDEX spectrograph), surrounded by a farm with tens of thousands of compact fiber-fed spectrographs. Over the course of the project, probably about a decade, these telescopes would scan the entire sky once, getting spectra of everything down to  $V = 20$  mag. This project has not yet been seriously proposed, but I would be surprised if it is not started by 2025!

#### 4.4 Examples of recent applications

The analysis of stellar spectra to derive chemical compositions of stars has led, in the last decade, to vast progress across fields in astrophysics. With the aim of highlighting practical applications of stellar photospheric abundances, a series of topics that are the subject of active research are briefly presented below. These are only a few examples, and other writers would surely choose other topics.

##### 4.4.1 *The Galactic disk*

Stars in the Galactic disk were found to split nicely into two components with densities falling exponentially from the plane and scale heights of about 0.3 (thin disk) and 1 kpc (thick disk; [Gilmore and Reid 1983](#)). The spectroscopic studies of these populations carried out in the last decade have also shown a split in their  $\alpha$ -element (O, Mg, Si, Ca, Ti) to iron abundance ratios, as well as in age, with stars in the thick disk being fairly old ( $>8$  Gyr) and those in the thin disk younger, between 1 and 8 Gyr (see, e.g., [Fuhrmann 1998](#); [Bensby et al. 2003](#); [Reddy et al. 2006](#); [Allende Prieto et al. 2006](#); [Adibekyan et al. 2013](#); [Nidever et al. 2014](#); [Anders et al. 2014](#); [Ruchti et al. 2015](#)).

Despite the rich information available from spectroscopic data, it is yet unclear how this two-component structure came together, and even whether the two disks are intimately linked or not. It is recognized that gas accretion from early galactic neighbors and radial migration of stars in the disk must have played a role, but the sequence of events that gave rise to the present-day Galactic disk has so far evaded our understanding. This is an area where the data flow from Gaia and the spectroscopic surveys mentioned above, hand by hand with models and simulations, will likely be of great help in the following years.

##### 4.4.2 *Globular clusters*

For the most part of the twentieth century, globular clusters were considered groups of stars sharing age and chemical composition. Unlike Galactic (open) clusters, globulars are old and metal-poor, associated with the Milky Way halo (or thick disk), and as such are excellent probes to study the early evolution of the Galaxy. Then we came to realize that was not true. Star to star variations in some elements became apparent. Sodium to oxygen or magnesium to aluminum correlations. Even worse, space-based photometric studies revealed multiple sequences, suggestive of different helium fractions, in the most massive clusters (see, e.g., [Norris 2004](#)).

The details of how globular clusters formed remain elusive, but it seems clear that some of the stars in the clusters formed from gas that has been polluted by previous cluster stars (Gratton et al. 2004). Furthermore, at least some of the most massive globular clusters in the Milky Way appear to be the remnants of small galaxies that were torn apart in the Galactic potential (Bellazzini et al. 2003).

#### 4.4.3 *The most metal-poor stars*

Since the chemical composition of the Universe after the primordial nucleosynthesis following the Big Bang was basically hydrogen and helium, the overall lack of heavier elements in a star can be interpreted as a sign of a primitive composition and a very old age. Observational cosmology has traditionally targeted galaxies at high redshift, but the objects with the most primitive compositions have been found right here in the Milky Way. These are extremely metal-poor stars with iron-to-hydrogen ratios orders of magnitude lower than the Sun: up to 7 orders of magnitude in the case of the star recently discovered by Keller et al. (2014).

The relative numbers of stars with different metallicities in the halo constrain the star formation history and initial mass function in the early Milky Way. Furthermore, the oldest stars in the Galaxy can inform us about what happened in the early Universe.

For stars to form, the gas in the interstellar medium needs to cool down for gravity to win over pressure. At very low metallicity, the lack of lines from metals makes it very difficult for gas to radiate and cool down. As a result, massive stars form, but no low-mass stars, producing a mass distribution shifted to higher masses than what we observe today in the disk of the Milky Way (Bromm and Larson 2004). The discovery a few years ago by Caffau et al. (2012) of a dwarf star in the halo with an overall metallicity of  $[\text{Fe}/\text{H}] \simeq -4$  sets an upper limit to where that threshold can be, constraining theories of star formation.

#### 4.4.4 *Solar analogs*

Uncertainties in atomic and molecular data, especially oscillator strengths, directly propagate into the derived abundances from stellar spectra. That applies to absolute abundances. However, in a differential analysis between two stars that are very similar, systematic errors cancel out.

Differential studies between the Sun and similar stars can render a precision in the derivation of atmospheric parameters at the level of a few K in  $T_{\text{eff}}$  and 0.01 dex in  $\log g$ , which are also accurate to that level, since the absolute surface temperature and gravity of the Sun are known even better. In this fashion, relative abundances can be derived to better than 0.01 dex in  $[\text{Fe}/\text{H}]$  (Nissen 2015), or more than 10 times better than absolute abundances.

This level of precision opens new opportunities for discovery in astrophysics. Detailed studies of nearby stars with parameters very close to solar have shown that there are subtle differences in composition between most of them and the Sun (Meléndez et al. 2009; Ramírez et al. 2009), which may be related to the sequestration in rocks or rocky planets of refractory elements that do not make it into the star. Needless to say, we look forward to future applications of this technique to other types of stars.

## 5 Reflections and summary

The analysis of the chemical compositions of stars evolved from early experiments by Bunsen, Kirchhoff and Fraunhofer in the nineteenth century into a quantitative field through the theoretical foundations provided by Schwarzschild, Eddington, Milne, and others. The LTE numerical codes for computing model atmospheres developed in the 1970s and 80s, mainly by Gustafsson and Kurucz, set the standard for modern analyses of AFGKM-type stars, while NLTE codes were developed for warmer ones. Atomic and molecular data, at a modest pace, has been perhaps the most significant improvement in modeling late-type stellar spectra over the last two decades, with the exception of the development of hydrodynamical models, which represent a dramatic advancement in our ability to match in close detail spectral line shapes, even though their overall impact on the inferred abundances is limited.

The rate at which spectroscopic observations are gathered has been revolutionized, and a few individual projects have obtained more spectra in the last few years than the accumulated data from previous history. These projects are providing vast and homogeneous data sets, which have not been fully explored, while new and larger projects are appearing in the scene. In response, spectral analysis software is being transformed from interactive tools to industrial chain processing.

The extraordinary new observations soon to become available from the Gaia mission, and the constraints on atmospheric parameters for individual stars that they will provide, will help enormously to uncover the deficiencies of standard analyses, driving improvements in modeling spectra. The new spectroscopic data from large ongoing and upcoming ground-based surveys will slowly but surely enlighten our understanding of the formation and evolution of the Milky Way, and as result, of galaxy formation and evolution in general.

These large spectroscopic efforts are producing large data bases of atmospheric parameters and chemical abundances, which in order to materialize into knowledge will need to be confronted with models of galaxies and their chemical evolution. At the same time, the making of such models is informed by the results of observational efforts. Hopefully, the process will, over the next decade, converge to provide us with some clear quantitative statements on many of the pending questions. Among the highest priority issues, we need to find out how many of the Milky Way stars were formed in situ and how many come from smaller galaxies that merged, what are the time scales and formation processes for each of the main stellar populations in the Galaxy, and how they relate.

Massive observational projects are providing us with a detailed census of a significant fraction of the Milky Way stars and their fundamental parameters. This information will allow progress on many other fields aside from galaxy evolution. To cite a few examples, the information will shed light on stellar evolution, extrasolar planetary systems and their relation to the chemistry of their hosting stars, the structure of the interstellar medium, or star formation and stellar dynamics.

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tions on a draft of this article. I would like to request readers that find mistakes or omissions to please send those to me and they will be fixed!

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