Mem. S.A.It. Vol. 81, 921

Memorie della

White dwarf spectra and atmosphere models

D. Koester

Institut für Theoretische Physik und Astrophysik, Universität Kiel, 24098 Kiel, Germany
e-mail: koester@astrophysik.uni-kiel.de

Abstract. We describe the spectral classification of white dwarfs and some of the physical processes important for their understanding. In the major part of this paper we discuss the input physics and computational methods for one of the most widely used stellar atmosphere codes for white dwarfs.

Key words. Stellar spectra, stellar atmospheres

1. Introduction

The classification scheme for white dwarfs (WD) developed at the beginning in analogy to the main sequence spectral types, with a distinguishing letter "D" for degenerate object. DAs thus were stars with very strong Balmer lines, DBs had strong He I lines, DOs He II. Today we know that this classification – in contrast to the main sequence – has not much to do with effective temperature, but is actually an indication of the photospheric composition. The classification used today was developed and described in detail by Sion et al. (1983).

The main characteristic is the division into hydrogen-rich (DA) and helium-rich (DB, DO) atmospheres, but, once again in contrast to normal stars, the most abundant element dominates with very few exceptions by several orders of magnitude. The explanation for this quasi mono-elemental composition is gravitational separation (Schatzman, 1947). In the absence of significant competing macroscopic motions (stellar wind, meridional circulation, convection) the heavier elements diffuse downward, leaving the lightest element present floating on top. The helium-dominated objects in this scenario must have lost their thin outer hydrogen envelope during the formation phase of the white dwarf in the late stages of the asymptotic giant branch or planetary nebular phase.

Besides the major types mentioned above, one distinguishes DC (too cool to show any spectral feature, mostly helium-rich), DQ (atomic or molecular features of carbon), DAZ, DBZ, DZ (objects with traces of metals in hydrogen-rich or helium-rich atmospheres).

The carbon in the DQ is assumed to be dredged up from deeper layers by the growing convection zone in the superficial helium layer (Koester et al., 1982; Pelletier et al., 1986), whereas the other heavy metals must be accreted from an outside source, either the interstellar matter, or some debris from a tidally disrupted asteroid.

A spectral atlas showing many example spectra for all major types has been published by Wesemael et al. (1993).

Send offprint requests to: D. Koester

2. Observational quantities

Stellar parameters (effective temperature $T_{\rm eff}$, surface gravity $\log g$, abundances) are obtained from an analysis of spectroscopic or photometric observations. If the surface of a star could be resolved, as for the sun, and if all relevant properties of our instrument were known, we could in principle determine the energy emitted by a small element of surface area, per unit time, wavelength interval, solid angle, into our line of sight. This quantity is called the (specific) intensity, and in the case of a spherically symmetric star the only geometric variable for the surface value is the angle of emission relative to the normal on the surface element ϑ, that is

$$I = I(\vartheta) \qquad \text{or} \qquad I = I(\mu) \tag{1}$$

with $\mu = \cos\vartheta$. If we cannot resolve the surface we can only measure the average intensity of the stellar disk $\bar{I}$. More specifically, the energy flux f arriving outside the terrestrial atmosphere is related to this average intensity by

$$f = \bar{I}\,\Omega \tag{2}$$

with average intensity

$$\bar{I} = 2\int_0^{\pi/2} I(\vartheta)\cos(\vartheta)\sin(\vartheta)\,d\vartheta = 2\int_0^1 I(\mu)\mu\,d\mu \tag{3}$$

and the solid angle of the star

$$\Omega = \frac{\pi R^2}{D^2} \tag{4}$$

with radius R and distance D.

If we want to determine stellar parameters from a comparison of observed and theoretically calculated spectra, the quantity which has to be calculated is thus the intensity I at the surface of the star. The theory of stellar atmospheres has been developed by many authors over the past century and has reached a very mature state today. Classical works, still worth reading, are e.g. Unsöld (1968) and Mihalas (1978). "Model atmospheres" and "synthetic spectra" as well as computer codes to calculate them are widely available. In the remainder of this paper we will describe in detail the input physics and computational methods used by the author for his model atmospheres, which are used by many groups.

The programming of the code was started by Dr. Thomas Gehren about 1975, with minor contributions by myself. However, since then practically every routine has been completely rewritten several times by the current author, and every remaining programming error is only my fault.

3. Model atmospheres and synthetic spectra

The basic procedure is to specify the element abundances in the atmospheres, and the parameters effective temperature $T_{\rm eff}$ and surface gravity $\log g$, which are used as proxies for the "typical" values of the thermodynamic variables, temperature and pressure. By using a number of simplifying assumptions and basic laws of physics this is sufficient to predict the radiation field (intensity) at the surface of the star. The most important assumptions are

- **homogenous, plane parallel layers:** the depth of the atmosphere is considered to be very small compared to the radius of the star. All matter quantities (density, pressure, temperature) depend only on one geometric variable, the height (in radial direction) z. The intensity depends on z and the angle against the normal ϑ, but not on the azimuthal angle.
- **hydrostatic equilibrium:** at each point within the outer layers, which have a direct influence on the emerging radiation (i.e. the atmosphere or photosphere), the gradient of the gas pressure is in equilibrium with the gravitational attraction (plus possibly the transfer of momentum by photons).
- **radiative and convective equilibrium:** there is no energy generation or loss within the atmosphere, only transport of the energy generated in the deep interior. This transport can occur through radiation, heat

conduction, or convection; the total energy flux as determined by the parameter effective temperature is constant at all depths.

– **Local Thermodynamic Equilibrium:** the matter is in a thermal equilibrium corresponding to the local temperature at each layer, that is, the ionization, excitation, dissociation of molecules etc. are governed by the usual relations of thermal equilibrium (Boltzmann factors, Saha equation, Kirchhoff's law etc.). This is a very important assumption, since it decreases the computational effort by several orders of magnitude. Please note that thermal equilibrium (i.e. the Planck function) is *not* assumed for the radiation field! Except for white dwarfs hotter than about 50000 K this LTE assumption is well justified.

The code is divided into two major parts, which calculate in turn the physical structure of the outer layers (run of temperature, density, pressure, absorption coefficients etc. with depth, this part will be called ATM here), and the surface intensities for many wavelengths (emerging spectrum, called SYN). There are auxiliary programs for additional necessary tasks, e.g. one for calculating the equation of state and absorption coefficients (KAPPA), another one for calculating equivalent widths of spectral lines or theoretical magnitudes in any photometric system (FILT), and so on.

3.1. Equation of State (KAPPA)

If no molecule formation has to be considered (e.g. high temperatures) and no elements besides H and He are present, the thermodynamic calculations are made directly in parallel with the determination of the atmospheric structure in the program ATM. Otherwise, these calculations are made in KAPPA and the results (tables of matter density ρ, electron pressure P_e, entropy, absorption coefficients etc.) are stored in large two-dimensional tables as function of temperature T and gas pressure P_g. The EOS, Saha equation for ionization, and dissociation equilibria for molecules are derived from a model Free Energy, which includes the ideal gas terms, Coulomb corrections and an "Excluded Volume" term for the non-ideal interaction of neutral particles. Electron degeneracy is tested in all layers, but currently not implemented in the EOS, as it has been unimportant in the range of parameters, where I have used my codes.

Partition functions for H, HeI, and HeII are explicitly calculated by using the lowest 100 levels from the TOPBASE database (Cunto & Mendoza, 1992; Cunto et al., 1993) and applying the occupation probability w according to the prescriptions of Hummer & Mihalas (1988); Mihalas et al. (1988). For all other elements, we use tables given by Kurucz (1970) providing the partition function for a nominal cutoff 0.1 eV below the ionization limit. The actual limit is calculated by a hydrogenic fit to the higher levels by using a cutoff determined from the non-ideal terms in the EOS.

Currently dissociation equilibria are implemented for 20 molecules (H_2, CH, NH, OH, MgH, SiH, CaH, C_2, CN, CO, N_2, NO, O_2, TiO, H_2O, HCN, HCO, C_3, CO_2, N_2O) using data from Kurucz (1970) and Tatum (1966).

The non-linear system of Saha and dissociation equations, together with the condition of neutrality and the definition of total gas pressure is solved with a Newton-Raphson iteration.

3.2. Absorption coefficients (KAPPA)

The absorption coefficient κ describes the probability w that a photon will interact (be absorbed or scattered), when traveling a small distance ds in matter of density ρ

$$w = \kappa\rho ds = \sum n_i\, a_i\, ds \qquad (5)$$

For a dimensionless w, κ has to have the dimension of area per mass. It usually is the sum of many different interaction processes, with each contribution determined by the number density of particles in the absorbing atomic state n_i and the area a_i, the cross section for this interaction. The most important processes for white dwarfs and some sources of data or routines are (note that in most cases the data have been transformed by us and/or new routines written for our use):

bound-free and free-free absorption of neutral hydrogen: this can be calculated quasi-classically and corrected to quantum mechanics by the so-called Gaunt factors (Menzel & Pekeris, 1935; Karzas & Latter, 1961; Kurucz, 1970). The free-free coefficient for all other ions (with the exceptions noted below) is calculated hydrogen-like.

bound-free and free-free absorption of the H^- ion: numerical fits from John (1988).

bound-free and free-free transitions of the H_2^+ ion: data and numerical fits from Boggess (1959).

bound-free absorption of neutral helium: cross sections for the 43 lowest levels of HeI are taken from the TOPBASE database.

free-free absorption of He^-: helium does not have a bound state as negative ion, so only the free-free process is needed. Data are from John (1994).

bound-free and free-free absorption of the negative carbon ion C^-: data for the b-f cross sections are from Robinson & Geltman (1967) and Cooper & Martin (1962), for the f-f cross section from John & Williams (1976).

bound-free transitions for elements other than H, He: these cross sections are mostly from the TOPBASE database if they are available there, or hydrogen-like calculations otherwise.

Thomson scattering by free electrons: the constant cross section per electron

$$\sigma = 6.6527 \times 10^{-}25 \quad \mathrm{cm}^2 \tag{6}$$

is used.

Rayleigh scattering by HI, HeI, H_2: cross section fits are from Dalgarno (1962); Dalgarno & Williams (1962); Kurucz (1970).

Molecular absorption: the calculations use the just-overlapping-line or smeared-line approximation in the version developed by Zeidler-K.T. & Koester (1982). This assumes that the density and broadening of rotational lines are so high that they form a quasi-continuum. Currently implemented are molecular data for C_2, C_3, and H_2 molecules.

Spectral line absorption: atomic data (excitation energies, oscillator strengths, line broadening constants) are obtained from a number of atomic databases, predominantly the line lists from Kurucz and collaborators (Kurucz & Bell, 1995), and the VALD (Vienna) database (Kupka et al., 2000, 1999; Ryabchikova et al., 1997; Piskunov et al., 1995).

Satisfactory theories and data for the line profiles do exist for the Stark broadening of neutral hydrogen (Lemke, 1997; Vidal et al., 1973), and for 21 optical lines of neutral helium (Barnard et al., 1969; Beauchamp et al., 1997). These are the so-called “unified theories”, which attempt to describe the total line profile from the core to the far wing. Similarly, the first three Lyman lines of H broadened by ionized and neutral perturbers and including a number of satellite features are well described by the work of Nicole Allard and collaborators (e.g. Allard et al., 2004, and many earlier papers).

For all other processes, the situation is much less satisfactory. Stark broadening parameters for further HeI lines are provided by Dimitrijevic & Sahal-Brechot (1990). In many later papers of the Belgrade group around Dimitrijevic, similar data are provided for other elements.

Below 8000 K for hydrogen-rich and 16000 K for helium-rich atmospheres line broadening by neutral particles becomes important. Since in most objects we have one dominating element, the interaction is usually between H-H or He-He. Resonance broadening is thus important (Ali & Griem, 1965), as well as van der Waals interaction. Only the first three Balmer lines (Barklem et al., 2000) and some He transitions (Leo et al., 1995) have so-called self-broadening theories; in the latter case, however, for very low temperatures (300 K) only. These theories combine the effects of resonance and van der Waals broadening in a more consistent way.

A few experimental measurements of broadening constants do exist, but in the vast majority of metal lines, the Stark and van der Waals broadening constants can only be very roughly estimated by simple approximations (e.g. Unsöld, 1968; Cowley, 1971; Griem, 1966). The line profile in the “impact approximation” is then described by a Lorentz profile with these damping constants, which yields a

Voigt profile after convolution with a Doppler profile for the line-of-sight velocities of the emitting atoms.

3.3. Atmospheric structure

As mentioned above, the basic quantity for the description of the radiation field is the intensity

$$I = I(z, \lambda, \mu) \tag{7}$$

with the geometrical height scale z measured from an arbitrary level outward of the star, wavelength λ, and cosine of the angle against the z-axis $\mu = \cos\vartheta$. Useful quantities derived from this are the mean intensity (averaged over all directions, not to be confused with the disk-averaged intensity $\bar{I}$)

$$J = \frac{1}{4\pi}\oint I\,d\omega = \frac{1}{2}\int_{-1}^{1} I\,d\mu \tag{8}$$

and the energy flux by radiation per unit area

$$F = 2\pi\int_{-1}^{1} I\mu\,d\mu \tag{9}$$

Another useful quantity is

$$K = \frac{1}{2}\int_{-1}^{1} I\mu^2 d\mu. \tag{10}$$

Note that, at the surface of a spherically symmetric star with no radiation from the outside we have

$$F = \pi\bar{I} \tag{11}$$

that is, the energy flux through the surface of a star is the quantity to be calculated for the comparison with non-resolved observations of a white dwarf.

3.3.1. The equation of radiative transfer

The equation of radiative transfer describes the balance between emission and absorption of photons along the path ds, using the geometry described in Fig. 1

$$\begin{aligned} dI &= \rho\varepsilon ds - I\rho\kappa ds \\ \mu\frac{dI}{\rho\kappa dz} &= \frac{\varepsilon}{\kappa} - I \\ \mu\frac{dI}{d\tau} &= I - S. \end{aligned} \tag{12}$$

ε and κ are the emission and absorption coefficients per mass, τ is a new depth variable called optical depth, replacing the geometric variable z, $d\tau = -\rho\kappa ds$. $\tau = 0$ corresponds to the top of the atmosphere. S is the so-called source function, $S = \varepsilon/\kappa$.

For the solution of this differential equation, two boundary conditions have to be specified. For the incoming radiation at the top $I(0, \mu) = 0$ for $\mu < 0$ is usually assumed. At the bottom, at some large value $\tau_B \gg 1$ the incoming intensity from below $I(\tau_B, \mu)$ for $\mu > 0$ must be specified. One possibility is to assume that, at a large depth, the source function is the Planck function B (see below), expand it around the value τ_B and derive from the transfer equation

$$I(\tau, \mu) = B(\tau) + \mu\frac{dB}{d\tau} \tag{13}$$

or higher order approximations.

For the absorption and emission coefficients, we have, even at this phenomenological level of description, to distinguish between two different processes. In the case of absorption, they are called "true absorption" κ_t and "scattering" σ, the corresponding emission processes are "thermal emission" ϵ_t and again scattering ϵ_s. Scattering means that a photon, through interaction with matter, changes its direction, but not the energy, whereas in the case of "true absorption" energy is absorbed by the matter and possibly re-emitted later with a different energy; scattering processes thus do not lead to an energy coupling of the radiation field with matter.

In our case of LTE Kirchhoff's law states

$$\frac{\epsilon_t}{\kappa_t} = B \tag{14}$$

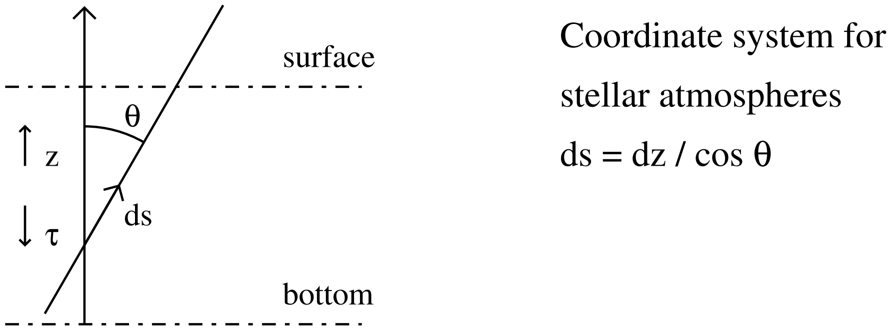

Fig. 1. Geometry for the radiative transfer equation

an extremely powerful result. On the other hand, for isotropically distributed scattering particles we can derive

$$\epsilon_s = \sigma J \tag{15}$$

If both kinds of processes are important, we can write the source function as

$$S = \frac{\varepsilon}{\kappa} = \frac{\epsilon_t + \epsilon_s}{\kappa_t + \sigma} = \frac{\kappa_t}{\kappa_t + \sigma} B + \frac{\sigma}{\kappa_t + \sigma} J \tag{16}$$

Sometimes, only the case with $\sigma = 0$ and therefore $S = B$ is called LTE, or strict LTE. Since the inclusion of scattering in the source function is not very difficult computationally, we do not make this distinction here.

Because of the nature of the boundary conditions, given on both ends of the solution interval, the solution of the first-order equation is numerically difficult. Special precautions have to be taken in order to avoid exponentially increasing parasitic solutions. This is very ingeniously avoided by the method of Feautrier (1964). We introduce new variables by dividing I into a symmetric (u) and an antisymmetric (v) part (we use $\mu > 0$ and write $-\mu$ for the negative angles)

$$u(\tau,\mu) = \frac{1}{2}\left[I(\tau,\mu) + I(\tau,-\mu)\right] \tag{17}$$

$$v(\tau,\mu) = \frac{1}{2}\left[I(\tau,\mu) - I(\tau,-\mu)\right]. \tag{18}$$

It is clear from the definitions that $u(\tau,-\mu) = u(\tau,\mu)$ and $v(\tau,-\mu) = -v(\tau,\mu)$, so we need the solution only for positive μ. Once u and v are known, we can always recover I as well as J and F. Writing the radiative transfer equation separately for positive and negative μ, adding and subtracting the two, we can derive the Feautrier equations

$$\mu^2 \frac{d^2u}{d\tau^2} = u - S \tag{19}$$

$$v = \mu \frac{du}{d\tau} \tag{20}$$

The boundary conditions can easily be transformed into the new variables. The numerical solution of the second order transfer equation above is much easier and stable than for the first-order equation.

3.3.2. Further constraints

The solution of the transfer equation needs the values of B and absorption coefficients at each depth of the atmosphere, and therefore the thermodynamic variables e.g. T and P_g. The additional constraints we have are the constant value of the transported energy flux and the hydrostatic equation

$$F_{tot}(z) = \int_0^\infty F(z,\lambda)\, d\lambda + F_{conv}(z) = \sigma_R T_{\rm eff}^4 \tag{21}$$

Here σ_R is the radiation constant of Stefan's law and F_{conv} the convective energy flux (see below).

The balance between the gradient of the gas pressure, gravitational force and radiative force is

$$\frac{dP_g}{dz} = -\rho g + \frac{1}{c}\int_0^\infty \kappa(\lambda)\, F(\lambda)\, d\lambda \tag{22}$$

where the second term on the right side describes the momentum transferred from the radiation field to the matter. Defining a "standard" absorption coefficient κ_S at a standard wavelength, or as a weighted mean over wavelength (e.g. the Rosseland mean), we can use the associated standard optical depth scale $d\tau_S = -\rho\kappa_S dz$

$$\frac{dP_g}{d\tau_S} = \frac{g}{\kappa_S} - \frac{1}{c\rho\kappa_S}\int_0^\infty \kappa(\lambda)\, F(\lambda)\, d\lambda. \tag{23}$$

The hydrostatic equation thus provides a relation between pressure scale, geometrical, and optical depth. For technical reasons, we use the gas pressure as the independent variable, and the depths z and τ_S at each layer are derived quantities.

Since ρ, F_{conv}, and the absorption coefficients depend also on temperature, the typical method of solution is to assume a temperature stratification $T(P_g)$ and energy fluxes F (e.g. from a previous similar calculation or iteration step) and solve the two constraint equation above together with the radiative transfer. These equations together provide just enough equations for the unknowns, if the temperature structure is known. Since this is in general not the case, an iterative solution is necessary. The temperature dependent quantities are expanded around the current value, e.g.

$$B(z, T, \lambda) = B(z, T_0, \lambda) + \frac{dB}{dT}\Delta T \tag{24}$$

The whole system of equations is then solved at once for the temperature corrections ΔT and iterated with an improved temperature stratification, until the corrections become sufficiently small and all constraints are fulfilled.

As it can be seen from eqs.(21,22) the constraints couple all wavelengths, which is responsible for the huge number of unknowns. If the knowledge of the detailed angle dependence of I or u is not needed the computational burden in some intermediate steps can be considerably reduced by the method of "variable Eddington factors" (Auer & Mihalas, 1970). We start from the Feautrier equation eq.(19) and integrate over μ from 0 to 1

$$\frac{d^2K}{d\tau^2} = J - S \tag{25}$$

Under many conditions, in particular at large optical depths, the ratio K/J tends to a constant value $1/3$. We introduce a "variable Eddington factor" $f = K/J$ to get

$$\frac{d^2 fJ}{d\tau^2} = J - S. \tag{26}$$

Assuming f to be known, the structure of this equation is the same as that of the original Feautrier equation, and can be solved with the same methods. The value of f has of course to be calculated from the original equation, but this can be done for one wavelength at a time and therefore much faster.

3.3.3. Convection

Convection under the conditions of white dwarfs is highly turbulent. There is as yet no satisfactory theory describing the energy transport from first principles, nor any realistic numerical simulation, which could be implemented in routine calculations of atmospheric models. One has therefore to resort to the very crude mixing-length approximation, originally by Prandtl (1925), and adapted to stellar conditions by Böhm-Vitense (1958).

In the calculation of stellar evolution, or even stellar atmospheres for "normal stars", our colleagues are generally content with one free parameter to describe the energy flux by convection in the mixing-length approximation. This parameter is the ratio of the mixing length to the pressure scale height $\alpha = l/H_P$. In the case of white dwarfs, we have gone further and use three numbers a, b, c, which appear in the heuristic derivation of the theory, as additional free parameters. Different versions of the MLT are then denoted as e.g. ML1/α = 1, or ML2/α = 0.6, where ML1, ML2 describe the choice of a, b, c, and α the mixing-length (Fontaine et al., 1981; Tassoul et al., 1990; Jordan et al., 1998). Comparison of UV with optical spectra of ZZ Ceti DA white dwarfs around $T_{\rm eff}$ = 11000 - 12000 K has shown that a consistent description is possible with ML1/2.0 (Koester et al., 1994) or ML2/0.6 (Bergeron et al., 1995), both of which describe what is called "intermediate efficiency" convection. The latter choice is at present used as quasi standard for DAs, also by this author. It is, however, quite clear that MLT in general is a very poor approximation and WD parameters are therefore still uncertain, when convection is important.

3.3.4. Numerical solution

The solution is obtained by a discretization of the depth scale P_g, the wavelengths λ, and angles μ. Typical numbers for the grid points are 4 values for μ between 0 and 1, 100 depth points, and 1000 to 100000 wavelength points. Derivatives are approximated by difference quotients, and integrals by sums. For the integration over angles (to obtain J, F) Gaussian quadratures are used for higher accuracy with few points. For the integration over wavelength, simple trapezoidal rule or Simpson's rule are used. We then obtain a huge system of linear equations for the variables I at each depth, wavelength, and angle, and the ΔT at all depths.

Fortunately, the matrix of this system is very sparse – a tridiagonal band structure of sub-matrixes and some extra lines and columns from the constraint equations. Rybicki (1971) has demonstrated a very efficient elimination scheme, which results in a final linear system of rank equal to the number of depth points (e.g. typically 100), which is full and has to be solved by standard methods to determine the temperature corrections. When these corrections are deemed small enough (the relative temperature corrections are smaller than 0.001 and the total flux at each depth is correct to 0.1 percent), the atmosphere structure is determined and all important quantities (temperature, gas pressure, electron pressure, density, specific heat, adiabatic gradient, number densities of molecules, absorption coefficients) as function of depths are saved in a file for further use.

3.4. Synthetic spectra (SYN)

The calculation of the atmospheric structure with ATM needs of course also the radiation field, including the spectrum emerging from the surface. The reasons why we use a separate program SYN to calculate this again are the following:

For the calculation of the atmospheric structure all wavelengths are coupled through the constraint equations, thus limiting the number to typically a few 1000. On the other hand, because of the necessity to calculate the total energy flux, the wavelength grid has to cover a large range, from X-ray to far infrared. For the comparison with observations, we typically need only a smaller range, but with a much higher wavelength resolution. As the structure is now known, we do not need to consider the wavelength coupling again, but can calculate the radiation field for each wavelength independently.

Because of this reduced burden, we are free to use many more (even weak) spectral lines, or more sophisticated line broadening theories. We can also include much more detailed calculations of molecular absorption bands.

3.4.1. Numerical method

The emerging spectral energy distribution $F(0, \lambda)$ could be calculated using the Feautrier equations. However, for technical reasons, we use a different method here. Integrating the original transfer equation over angle μ, we can derive an integral equation for the flux

$$F(\tau) = 2\pi \int_{\tau}^{\infty} S(\tau')\, E_2(\tau' - \tau)\, d\tau'$$

$$- \; 2\pi \int_0^{\tau} S(\tau')\, E_2(\tau - \tau')\, d\tau'. \tag{27}$$

with the exponential integral function E_2. In abbreviated form we write this as the flux integral operator Φ

$$F(\tau) = \Phi\,[S(\tau)]\,. \tag{28}$$

A special case is the flux emerging from the surface of the star, which as we know is equal to the observational quantity disk-averaged intensity $F(0) = \pi \bar{I}$

$$F(0) = 2\pi \int_0^{\infty} S(\tau')\, E_2(\tau')\, d\tau'. \tag{29}$$

In strict LTE $S(\tau) = B(T(\tau))$, which is known from the atmospheric structure, and the calculation would be reduced to a simple integration. In general, however, the source function may include a scattering term, and we need the mean intensity J. Formally, this can be derived directly from the transfer equation in a similar way as for F, with the result

$$J(\tau) = \frac{1}{2} \int_0^{\infty} S(\tau')\, E_1(|\tau - \tau'|)\, d\tau' \tag{30}$$

with the exponential integral E_1. The integral operator in this equation is called the Λ operator

$$J(\tau) = \Lambda\,[S(\tau)] = \Lambda\,[\alpha B + (1 - \alpha) J]\,. \tag{31}$$

We call this a formal solution, since S on the right hand side also contains the unknown J, which makes this an integral equation.

For the numerical solution, the depth scale is discretisized again, thus transforming the continuous variables J, B into vectors and the Λ operator into a matrix. We use an 18-point Gaussian integration formula; the emerging flux $F(0, \lambda) = \pi \bar{I}$ as well as the intensity $I(0, \lambda, \mu)$ can finally be calculated from the source function S by a simple integration (summation).

3.5. Theoretical photometry and equivalent widths

The final results of SYN are stored in a binary disk file. This file contains a table of fluxes (or intensities) as a function of vacuum wavelengths, the "synthetic spectrum" at the stellar surface, and, in addition, the basic parameters and structure data of the atmosphere model. These data are in a format, which can be used as input for the ATM program to start the iteration for a similar model.

Auxiliary programs are available to transform these data, e.g. to air wavelengths, or into an ASCII file for use by other authors. These "export" files contain the flux table and a header similar to the FITS headers with all important parameters of the calculation. I strongly encourage my users to never separate this header from the table.

A program FILT calculates equivalent widths of spectral lines from the flux table. It can also calculate theoretical photometry in arbitrary filter systems as e.g.

$$V = -2.5 \log \int_0^{\infty} \bar{I}(\lambda)\, S_V(\lambda)\, d\lambda + C_V \tag{32}$$

with the total transmission S_V of the filter plus optics, terrestrial atmosphere, etc. The constant C_V has to be determined from standard stars with known absolutely calibrated spectrum and measured magnitude in the corresponding system. Very often Vega is used for this purpose.

4. Some very technical remarks and outlook

The code is currently written in the programming language FORTRAN77, but slowly – as time permits – transformed to FORTRAN95, which is much less prone to programming errors and much easier to maintain. Although considered a very old-fashioned programming language by many (who most likely never used it), I have been able to use my code over more than 30 years on dozens of computers and operating systems, in most cases without ever changing a single line of code. I am very grateful for that and do not plan to ever change to another language.

For more than twenty years, and through very fundamental changes, the complete code has been under control of a version control system, starting with SCCS, RCS, and about two years ago changed to MERCURIAL. This means that I can recall the complete programs for any date or any version back to about 1985, IF I know the relevant data (version, compilation date, calculation date, etc.). These identifiers are written into every output file, including the ASCII format of the synthetic spectra, which are so widely distributed.

These files also contain the information for some free parameters, like the mixing-length version used, or changes to the Hummer-Mihalas occupation probabilities. For this reason I urge users, to always keep the header with the spectrum table, so that the code version used can be identified in case of problems or questions. Unfortunately, the system is not perfect, since it does not keep track of a few data files, which have to be changed for different calculations, the most important being the file with the spectral line data. Different databases provide quite often different data for oscillator strengths or broadening constants. Depending on what I believe at the time of calculation to be the most reliable values, these change from time to time, and I cannot always reconstruct what has been used after some years. I am thinking how to solve this problem, but so far without result.

From the programming aspect, as mentioned above the code is slowly moved to FORTRAN95. It is already very modular, with many modules free of any side effects and being reused unchanged in different programs. Programming the way I now know it should be, has been a hard learning experience over decades, and I am glad that FORTRAN95 supports almost all my ideas and preferences much better than the older versions. The current aim is to make the whole program system very user-friendly, so as to be able to put it in the public domain under a GPL or similar license in a few years.

Acknowledgements. I want to thank the organizers of the School of Astrophysics "F. Lucchin" in Tarquinia (Italy) in June 2008 for inviting me to this very pleasant experience. I am also grateful to get the chance to describe my white dwarf atmosphere model calculations in a widely available journal, for the information of the users.

I am grateful to Dr. Thomas Gehren, who got me interested in stellar atmospheres (though not for white dwarfs), and to the large number of colleagues, who have used my calculations and contributed to many improvements through their demands.

References

Ali, A. W. & Griem, H. R. 1965, Phys. Rev., 140, A1044
Allard, N. F., Kielkopf, J. F., & Loeillet, B. 2004, A&A, 424, 347
Auer, L. H. & Mihalas, D. 1970, MNRAS, 149, 65
Barklem, P. S., Piskunov, N., & O'Mara, B. J. 2000, A&A, 363, 1091
Barnard, A. J., Cooper, J., & Shamey, L. J. 1969, A&A, 1, 28
Beauchamp, A., Wesemael, F., & Bergeron, P. 1997, ApJS, 108, 559
Bergeron, P., Wesemael, F., Lamontagne, R., et al. 1995, ApJ, 449, 258
Boggess, A. I. 1959, ApJ, 129, 432
Böhm-Vitense, E. 1958, Zeitschrift fur Astrophysik, 46, 108
Cooper, E. D. & Martin, R. W. 1962, Phys. Rev., 126, 1482
Cowley, C. R. 1971, Observatory, 91, 139
Cunto, W. & Mendoza, C. 1992, Revista Mexicana de Astronomia y Astrofisica, vol. 23, 23, 107
Cunto, W., Mendoza, C., Ochsenbein, F., & Zeippen, C. J. 1993, A&A, 275, L5
Dalgarno, A. 1962, , Tech. rep., Geophys. Corp. of America
Dalgarno, A. & Williams, D. A. 1962, ApJ, 136, 690
Dimitrijevic, M. S. & Sahal-Brechot, S. 1990, A&AS, 82, 519
Feautrier, P. 1964, C.R. Acad. Sci. Paris, 258, 3189
Fontaine, G., Villeneuve, B., & Wilson, J. 1981, ApJ, 243, 550
Griem, H. R. 1966, Phys. Rev., 165, 258

Hummer, D. G. & Mihalas, D. 1988, ApJ, 331, 794
John, T. L. 1988, A&A, 193, 189
John, T. L. 1994, MNRAS, 269, 871
John, T. L. & Williams, R. J. 1976, MNRAS, 174, 253
Jordan, S., Koester, D., Vauclair, G., et al. 1998, A&A, 330, 277
Karzas, W. J. & Latter, R. 1961, ApJS, 6, 167
Koester, D., Allard, N. F., & Vauclair, G. 1994, A&A, 291, L9
Koester, D., Weidemann, V., & Zeidler, E. . 1982, A&A, 116, 147
Kupka, F., Piskunov, N., Ryabchikova, T. A., Stempels, H. C., & Weiss, W. W. 1999, A&AS, 138, 119
Kupka, F. G., Ryabchikova, T. A., Piskunov, N. E., Stempels, H. C., & Weiss, W. W. 2000, Baltic Astronomy, 9, 590
Kurucz, R. 1970, Smithson. Astrophys. Obs. Spec. Rep., 309
Kurucz, R. L. & Bell, B. 1995, Atomic Line Data, Tech. rep., Cambridge, Mass.
Lemke, M. 1997, A&AS, 122, 285
Leo, P. J., Peach, G., & Whittingham, I. B. 1995, J. Phys. B: At. Mol. Opt. Phys., 28, 591
Menzel, D. H. & Pekeris, C. L. 1935, MNRAS, 96, 77
Mihalas, D. 1978, Stellar atmospheres /2nd edition/ (San Francisco, W. H. Freeman and Co., 1978. 650 p.)
Mihalas, D., Dappen, W., & Hummer, D. G. 1988, ApJ, 331, 815
Pelletier, C., Fontaine, G., Wesemael, F., Michaud, G., & Wegner, G. 1986, ApJ, 307, 242
Piskunov, N. E., Kupka, F., Ryabchikova, T. A., Weiss, W. W., & Jeffery, C. S. 1995, A&AS, 112, 525
Prandtl, L. 1925, Z. angew. Math. Mech., 5, 136
Robinson, E. J. & Geltman, S. 1967, Phys. Rev., 153, 4
Ryabchikova, T. A., Piskunov, N. E., Kupka, F., & Weiss, W. W. 1997, Baltic Astronomy, 6, 244
Rybicki, G. B. 1971, Journal of Quantitative Spectroscopy and Radiative Transfer, 11, 589
Schatzman, E. 1947, Annales d'Astrophysique, 10, 341
Sion, E. M., Greenstein, J. L., Landstreet, J. D., et al. 1983, ApJ, 269, 253
Tassoul, M., Fontaine, G., & Winget, D. E. 1990, ApJS, 72, 335
Tatum, J. B. 1966, Publ. Domin. Astr. Obs. Victoria, 13, 1
Unsöld, A. 1968, Physik der Sternatmosphären (Berlin: Springer-Verlag)
Vidal, C. R., Cooper, J., & Smith, E. W. 1973, ApJS, 25, 37
Wesemael, F., Greenstein, J. L., Liebert, J., et al. 1993, PASP, 105, 761
Zeidler-K.T., E.-M. & Koester, D. 1982, A&A, 113, 173