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How to SYN in Seven Easy Steps

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The calculation of expected spectral line strengths and profiles is a powerful tool for the analysis of the solar atmosphere, and other stellar atmospheres. We present here a recipe in seven easy steps for the development of such spectral synthesis software.

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1. Introduction

The solar spectrum can be calculated by (numerically) solving the radiative transfer equation:

$$\mu \frac{dI_\lambda}{d\tau_\lambda} = I_\lambda - S_\lambda \tag{1}$$

If we know the source function S_λ, then finding the emergent spectrum is straightforward. With a model solar atmosphere, we have the LTE source function, $S_\lambda(z) = B_\lambda(z)$, the Planck radiation function, as a function of physical depth. Unfortunately, it is not sufficient to know S_λ as a function of physical depth z; we must convert the physical depth scale to an optical depth scale:

$$\tau_\lambda(z) = \int_z^\infty \rho(z')\kappa_\lambda(z')dz' \tag{2}$$

This requires calculation of the opacity κ_λ; this is the core task of a spectral synthesis program. The opacity can be considered to consist of a continuous opacity, and opacity due to atomic line transitions. The main contribution to the continuous opacity is due to bound-free and free-free H^- transitions; other major sources (H_2^+ molecule, photoionisation of metals) also need to be considered. The line opacity can be found from the line strength and line profile for each line in the spectral region of interest.

2. Model atmospheres

The solar atmosphere is highly stratified; its physical properties vary strongly with height within the photosphere. Thus, the photosphere can be well represented by a plane-parallel *model atmosphere*. Many model atmospheres are available, with those by Holweger and Müller [1] and Kurucz [2] being commonly used.

A model atmosphere tabulates temperature, pressure, electron pressure, density, and opacity at 5000 Å.

With this data, and assuming LTE conditions, then the source function is simply equal to the Planck radiation function:

$$
\begin{aligned}
S_\nu(z) &= B_\nu(T(z)) \\
&= \frac{2h\nu^3}{c^2}(\exp(-h\nu/kT) - 1)^{-1} \tag{3}
\end{aligned}
$$

3. The continuous opacity

The continuous opacity (maximum at 8200 Å) is dominated by the H^- ion, due to its large interaction cross-section. We can also consider other abundant absorbers. If we are only considering a small spectral region, we can assume that the continuous opacity is uniform. In general, we use approximation formulae and table lookup [3].

The H^- opacity is due to both bound-free (H^- + photon $\leftrightarrow$ H + e^-) and free-free (H + e^- + photon $\leftrightarrow$ H + e^-) processes. Approximation formulae for both processes are given by Gingerich [4]

Due to its high abundance, we should also consider bound-free and free-free absorption due to neutral hydrogen, which depend on the Gaunt factors g_{II} and g_{III}. Approximation formulae for

1. Calculate $S_\lambda(z)$

2. Calculate continuous opacity

3. Calculate line opacities.
   This requires:
   - line strengths
   - damping
   - thermal and mass motion

4. Calculate optical depth scale

5. Effect of intermediate scale mass motion

6. Numerical integration of radiative transfer equation (1)

7. Non-plane parallel corrections – large scale mass motion

Figure 1. Recipe for spectral synthesis

g_{II} and g_{III} are given by Mihalas [5].

Other sources of opacity which can be considered include the H_2^+ molecule, for which cross-sections have been calculated; a convenient tabulation for interpolation is available in [4]. The abundances of heavier elements much lower than that of hydrogen, and they contribute far less to the opacity. Only the most abundant species need be considered, Mg and Si being the most important. Calculations by Peach [6] can be used for interpolation.

4. Line opacities

The opacity due to a spectral line depends strongly on the wavelength – which is why it's a line – which makes it necessary to calculate the line opacity on a sufficiently dense grid of wavelength points. For a single (not too strong) line, a total wavelength range of ≈ 1 Å is enough; a few hundred wavelength points will be sufficient. The use of a non-uniform grid of wavelength points can greatly speed up line opacity calculation, at the cost of a greater effort to implement. Note that it is largely unimportant as to whether the calculation is performed over a grid of wavelength points or frequency points, since conversion from one to the other is simple.

The opacity of a single line depends on

1. population of the absorber,

2. intrinsic strength of the transition,

3. and the line profile.

The populations of absorbers depend on the atomic abundances and the equilibrium between the atomic species, the rest of the atmosphere, and the radiation field. We can simplify this greatly by assuming LTE.

The strength of the transition – the oscillator strength, or f-value can be obtained from a suitable source of data such as the NIST Atomic Spectra Database at `http://physics.nist.gov/cgi-bin/AtData/main_asd` or the Vienna Atomic Line Database (VALD) at `http://www.astro.univie.ac.at/~vald/`.

4.1. The line profile

The line profile function of a stationary atom is the Lorentz profile:

$$\phi(\nu) = \frac{\Gamma/4\pi^2}{(\nu-\nu_0)^2 + (\Gamma/4\pi)^2} \tag{4}$$

Thermal motions will produce a profile that is the convolution of the Lorentz profile and the Maxwellian Doppler shift profile, giving the Voigt profile:

$$\begin{aligned}\phi(\nu) &= \frac{a}{\pi^{3/2}} \int_{-\infty}^{\infty} \frac{\exp(-x^2)}{(v-x)^2 + a^2} dx \\ &= \frac{1}{\sqrt{\pi}} H(a,v)\end{aligned} \tag{5}$$

where $a = \Gamma/4\pi\Delta\nu_D$ and $v = (\nu-\nu_0)/\Delta\nu_D$, where Γ is the natural (Lorentzian) line width, and $\Delta\nu_D$ is the Doppler shift due to the most probable speed.

We can expect a spectral synthesis code to spend a major part of the execution time repeatedly calculating the Voigt function. Various

methods are available [7]. Fast methods usually use asymptotic methods where possible (since the Voigt profile approaches the Lorentz and Maxwell profiles in the limit), and other approximate (eg power series) methods elsewhere. Alternately, the Voigt profile can be calculated by convolution of the Lorentz and Maxwell Doppler profiles, using Fourier transformation methods for speed.

4.2. Damping

The most important contribution to damping is collisions with neutral hydrogen (almost all of which is in the ground state). Damping due to electrons is 50 times smaller, or even less, and damping due to helium about 30 times smaller. Other sources can be neglected.

The line broadening theory developed by Anstee and O'Mara [8] has been shown to be accurate. Collisions with hydrogen atoms in the photosphere are fast; the impact approximation can be used. The line width (HWHM) is

$$\Delta \nu_{\text{coll}} = N \int_0^\infty v f(v) \sigma(v) dv \qquad (6)$$

where σ is the line broadening cross section, and $f(v)$ is the normalised Maxwellian velocity distribution.

Data calculated using this theory is available [9], and code to calculate broadening has been developed [10] (available at `http://www. astro.uu.se/~barklem`) which can be used either for stand-alone calculation, or can be incorporated into a spectral synthesis program. This code calculates the linewidth per unit hydrogen atom density for a given temperature.

The total Lorentzian width is the sum of the collisional damping width, the natural line width, and the stimulated absorption/emission width. Only the collisional damping width will be important in the photosphere.

4.3. Small-scale mass motion

We can expect small-scale turbulent motion to have a Gaussian velocity distribution (Kolmogorov turbulence). The effect will be the same as that of thermal motion, and the two can be combined. The average photospheric microturbulence is 0.845 km/s. We can simply use this average value as a uniform microturbulence, or a depth-dependent value can be used.

5. Integrating the radiative transfer equation

All of the processes that affect the opacity have been considered. The radiative transfer equation (1) can be integrated. The radiative transfer equation (1) is well behaved, provided we solve it in a reasonable manner. In order to avoid the growth of errors, we integrate

$$I_\lambda(\tau = 0) = \int_0^\infty S_\lambda(\tau_\lambda) \exp(-\tau_\lambda/\mu) \frac{1}{\mu} d\tau_\lambda. \qquad (7)$$

In practice, we step through the layers of our model atmosphere, from the top to the bottom, with the step size for the numerical integration being determined by the spacing in the model atmosphere. By the time the bottom of the model atmosphere is reached, the contributions to the emergent intensity are negligible.

6. Large-scale mass motion – beyond the plane-parallel approximation

Large-scale flows prevent the photosphere from being strictly plane-parallel. The main motion at this scale is that due to the granulation. A granular cell is typically about 1000km across, consisting of a hot, slowly rising, central region, and a cooler, more rapidly falling outer region.

Even a simple model of granulation can greatly improve the results of spectral synthesis, compared with assuming a Gaussian distribution of large-scale motion (macroturbulence). The granule can be divided into three purely plane-parallel regions: the rising core, the falling outer region, and a transition region between the two. We can assume that the flow velocity in each region varies with height h as

$$V = V_0 \exp(-h/V_s), \qquad (8)$$

where V_s is the velocity scale height. We can expect the microturbulence, since it is driven by the large scale flow, to have the same depth dependence. A Gaussian macroturbulent velocity can also be associated with each region to model

inter-granular variation. The emergent spectra from each region are calculated separately, and then combined to give the total spectrum.

A suitable granular model is shown in table 1. Using this granular model, calculated spectral lines closely match observed spectral lines in width and asymmetry. The given granular model improves the fit between observed and calculated spectra by a factor of 2.5, as measured by the squared deviation between the spectra, with the improvement mostly due to matching the observed asymmetry [3].

Parameter	Upflow	Transition	Downflow
Area	0.45	0.40	0.15
Brightness	1.07	0.97	0.87
Weighting	0.48	0.39	0.13
V_0	0.577	0	-1.072
V_s	368	368	368
micro	1.58	3.67	3.67
macro	1.6	1.6	3.5

Table 1
Granular model. All velocities are in km/s, and heights in km

7. Spectral synthesis

The presented recipe allows the rapid development of simple, modular, customisable spectral synthesis software for the accurate calculation of small regions of the solar spectrum, suitable for the study of spectral line shapes and strengths, and the photospheric processes affecting them – abundance, damping, granulation, etc.

In particular, the granular model presented here provides a convenient compromise between computational speed and ease of implementation on one hand, and accurate modelling of photospheric motion on the other. It provides a suitable starting point for further investigation of processes affecting line profiles.

Such codes can be readily implemented on a typical PC. A number of spectral synthesis codes are available [11,12].

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