Validating a Simple Analysis Model of Spectral Line Profiles Using Solar Reflection Spectra from Jupiter's Moon Europa

K.R. Whight 20/07/2022

Abstract

The solar spectrum reflected from Jupiter's moon Europa has been analysed using a simple model of absorption line profiles developed by the author. The model assumes that the photosphere can be represented as a single layer in thermal equilibrium and the software implementation can simulate the effects of temperature, pressure and rotation on the hydrogen Balmer absorption line profiles. The model can also be used to predict the relative strengths of the absorption lines in the series yielding, in the process, the column density of atoms in the Balmer ground state. In addition it is possible to calculate the thickness and pressure of the photosphere as a function of an atomic impact parameter ρ.

When compared to measured solar spectra the relative amplitudes of the H_α and H_β lines were satisfactorily reproduced. Further, setting the impact parameter $\rho = 4.0e^{-10}$ m, the solar photosphere pressure and thickness were calculated to be 0.135 Bar and 400.4 km respectively in good agreement with published data.

Introduction

Perhaps the first question to be answered is "when studying the solar spectrum, why use reflection spectra from Europa"? The simple answer is that, as an accurate zero intensity level is necessary, a star like target was needed so that measured spectra could have the sky background subtracted. The assumption here is that as Europa is an icy body with no significant atmosphere the solar spectrum is unchanged upon reflection.

Spectra were obtained using a Shelyak HiresIII spectrograph with a 2400 lines per mm grating and processed using Rspec software. The authors own software interfaces with Rspec and writes the numerical results of the various computations into labels that can be displayed on Rspec plots.

Perhaps the next question is "why develop a simple model of spectral line profiles"? To answer this note that a global thermal equilibrium model is a first step toward a local equilibrium model. In addition the author has a background in Physics and computer modelling, specifically in the field of semiconductor devices, and was interested in what information could be extracted from spectra without having to first undertake the equivalent of a PhD in astrophysics. There did not seem to be anything published at

undergraduate level on analysing spectra so such a model would need to be developed. In reality this task proved much more difficult than was anticipated but this paper aims to present and validate the authors completed model.

The basis of the model is the simple assumption that a photosphere can be represented as a single layer in thermal equilibrium. The Sun was chosen as an appropriate validation target because, being our home star, it is close enough that its properties are well studied and therefore known in some detail.

Appendix A gives a detailed account of the spectral analysis model whilst Appendix B details the spectral line synthesis model used for computing emission spectra from photospheres with given properties. The rotation model has not been presented as rotation is not a significant consideration for the Sun.

Spectral Analysis

Figure 1 displays the raw H_a (Hydrogen alpha) spectrum obtained by reflection from Jupiter's moon Europa, the data is not calibrated in terms of wavelength so the x-axis is measured in pixels.

Figure 1: Europa Raw Spectrum

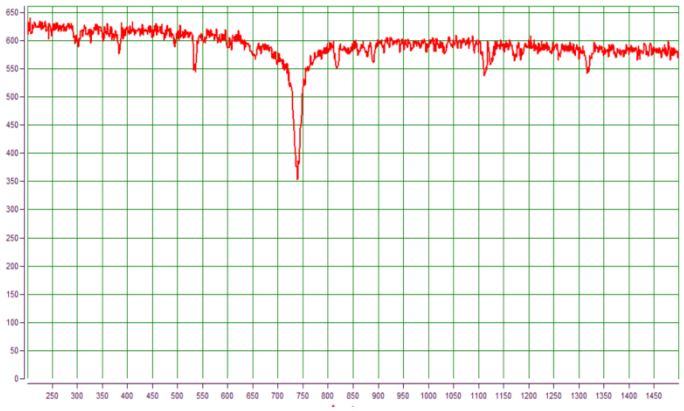
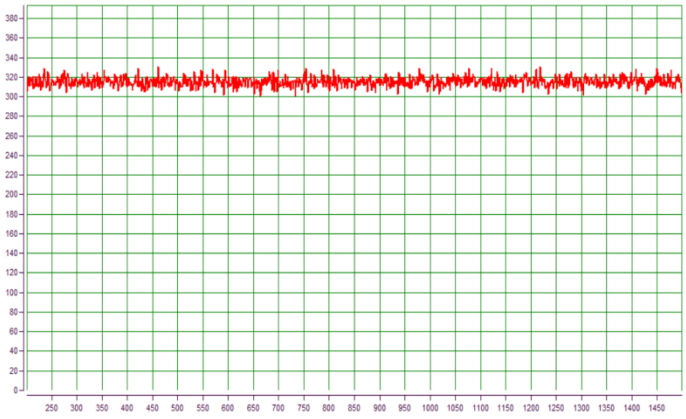


Figure 2 similarly displays the sky background obtained by moving the Rspec measure lines just off of the spectral stripe whilst maintaining their separation.

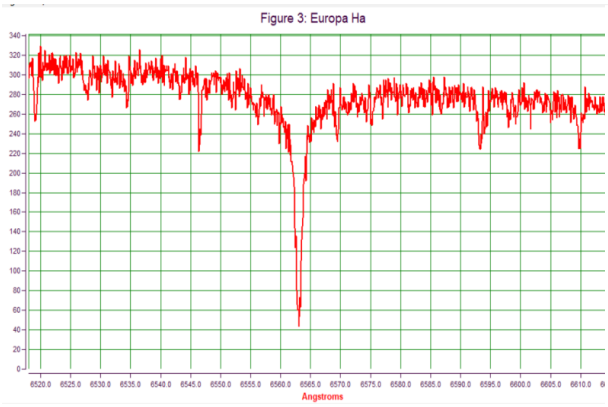
Figure 2: Background

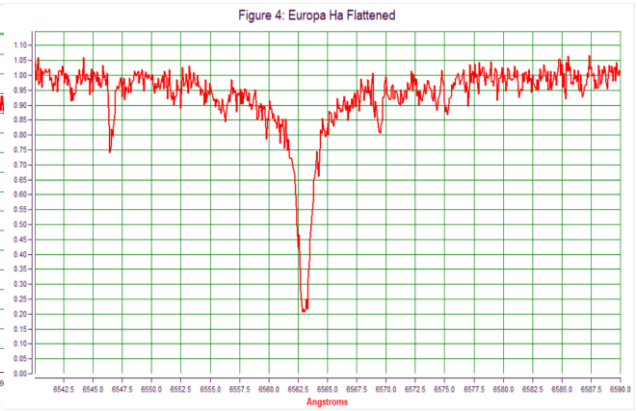


The background signal is then subtracted from the measured spectrum and the result calibrated for wavelength see Figure 3. The data displayed in Figure 3 is input to the authors analysis software which initially re-samples to a uniform wavelength bin width, "flattens" the continuum slope (Figure 4) and finally computes the "effective emission line" corresponding to the measured absorption line (see Appendix A, equation A.2.10). This effective emission line is the "reference profile" or target for the photosphere modeling process and represents the actual "dynamics" occurring within the photosphere.

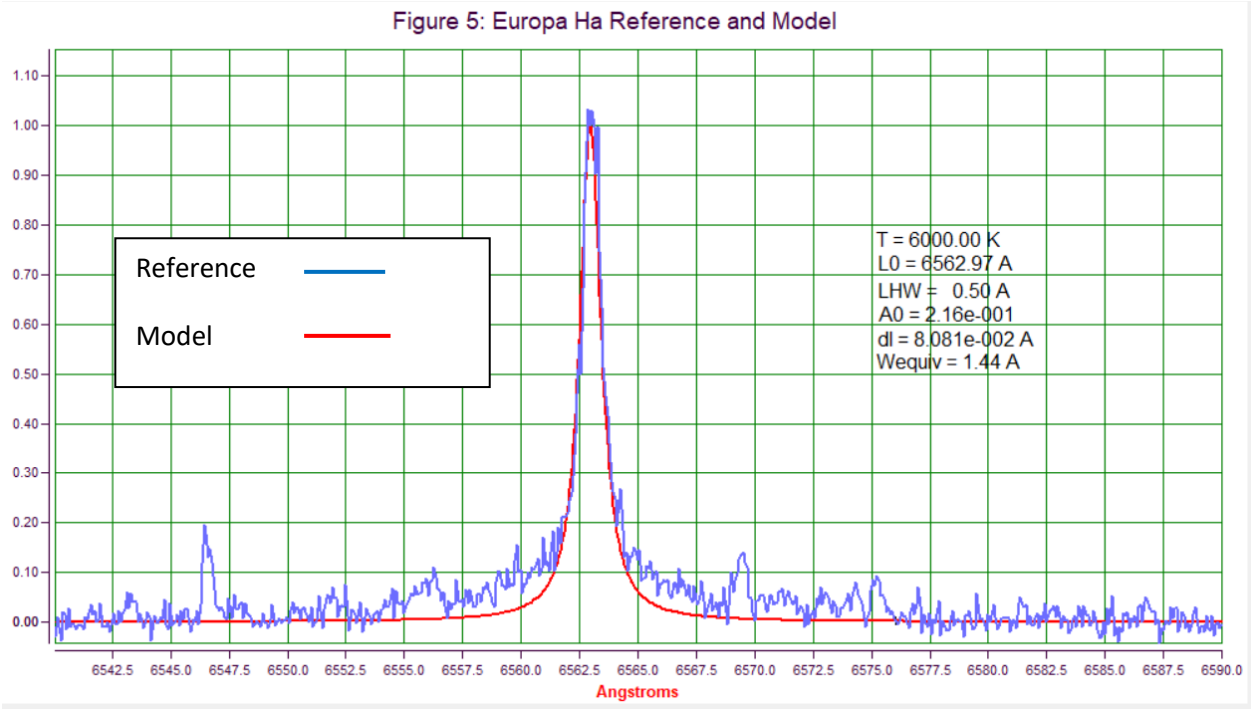
When the simulation software is run, with the reference profile as input, various photosphere properties can be set e.g. Temperature (T), the half-width of the Lorentzian or "pressure profile" (LHW) and finally if necessary rotation effects can be modelled. All these effects are convolved together to produce a

"model" profile that can be compared to the reference profile. The input parameters are adjusted to give a good fit between the reference and model profiles.





In practice the Temperature would be obtained by fitting a Planck continuum function to a low resolution spectrum spanning the whole visual range of wavelengths so the only free parameters are



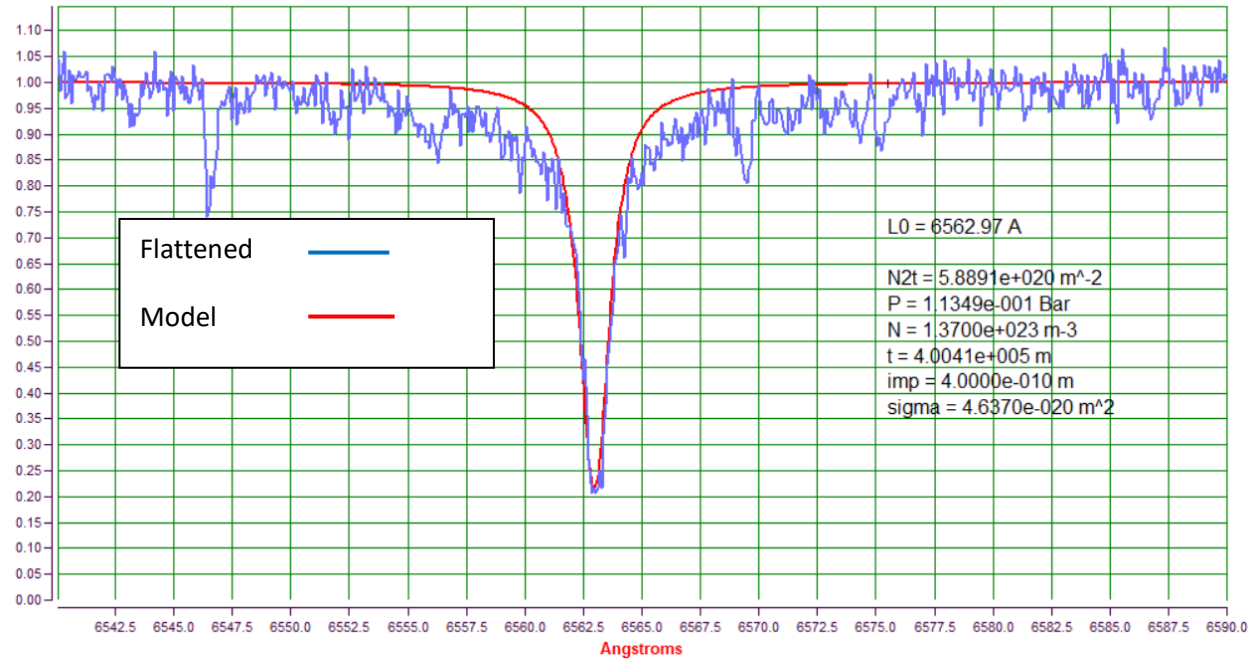
those that represent pressure and rotation effects. Figure 5 shows the result of this modelling process, where key parameters are displayed as labels. In this case we have:-

- T: the temperature of the photosphere
- L0: the central wavelength of the spectral line
- LHW: the Lorentzian half-width
- A0: the amplitude of the absorption line at the central wavelength
- dl: the wavelength bin width
- Wequiv: the emission line "equivalent width", effectively the model emission line area

These values are important for predicting the amount of absorption at other wavelengths in the Balmer series (see Appendix A).

Finally the modelled effective emission line can be converted back (Appendix A equation A.2.11) by the software into a corresponding absorption line, see Figure 6. The agreement between the two profiles is good especially in the core of the line.

Figure 6: Europa Ha Absorption



In this conversion process additional parameters are computed and are displayed in Figure 6 i.e.:-

- N2t: the column density of atoms in the Balmer ground state with principle quantum number 2
- P: the pressure of the photosphere
- N: the number density of neutral atoms
- T: the thickness of the photosphere
- Imp: an impact parameter, input by the user, that was used to split N2t into the previous 3 parameters which are functions of the impact parameter.
- Sigma: the H_a photon capture cross-section.

This final stage of the modeling process can be repeated many times with different impact parmeters to obtain the data displayed in Figure 7 where we plot the solar photosphere pressure and thickness as a function of the impact parameter value.

Computation of an impact parameter from fundamental principles has not been attempted but if a relatively simple model to achieve this exists the author would like to be informed (via the RSpec user group). The impact parameter therefore is regarded as an adjustable parameter that will be obtained experimentally by comparison to known Solar properties. When extrapolating to the properties of other stars some additional physical considerations would need to be included in the model.

With an impact parameter value of 4.0 A i.e. approximately eight Bohr radii, the pressure and thickness are calculated to be 1.135 e-1 Bar and 400.41 km respectively as displayed in Figure 6. This is a good prediction for the average pressure and thickness of the Solar photosphere as can be seen from published details as displayed in Figure 8. It is also a strong validation of the model as that particular value of the impact parameter splits the calculated column density of atoms in principle quantum state n = 2 into two correct properties of the photosphere.

We can now use the model of the photosphere to predict the equivalent emission line for any line of the Balmer series then, equation A.3.5 (see Appendix A) can be used to determine the depth of the absorption line at its corresponding central wavelength. This process has been performed for the H_b (Hydrogen Beta) line and the results plotted in Figure 9.

Figure 7: Solar Photosphere Thickness and Pressure vs Impact Parameter

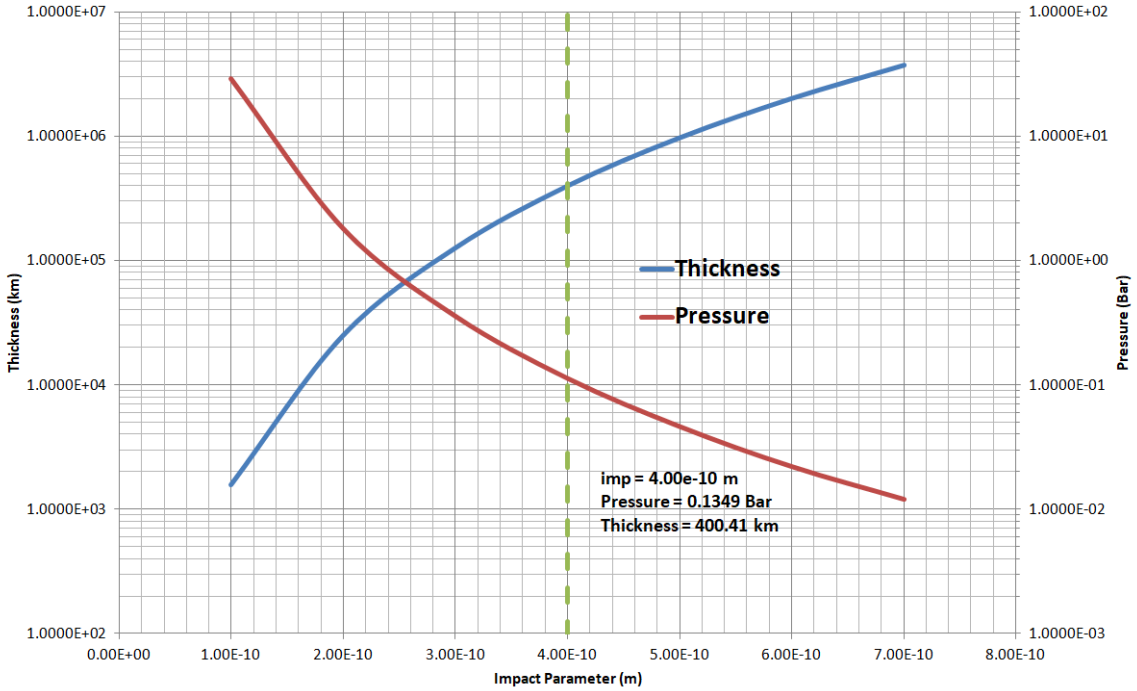


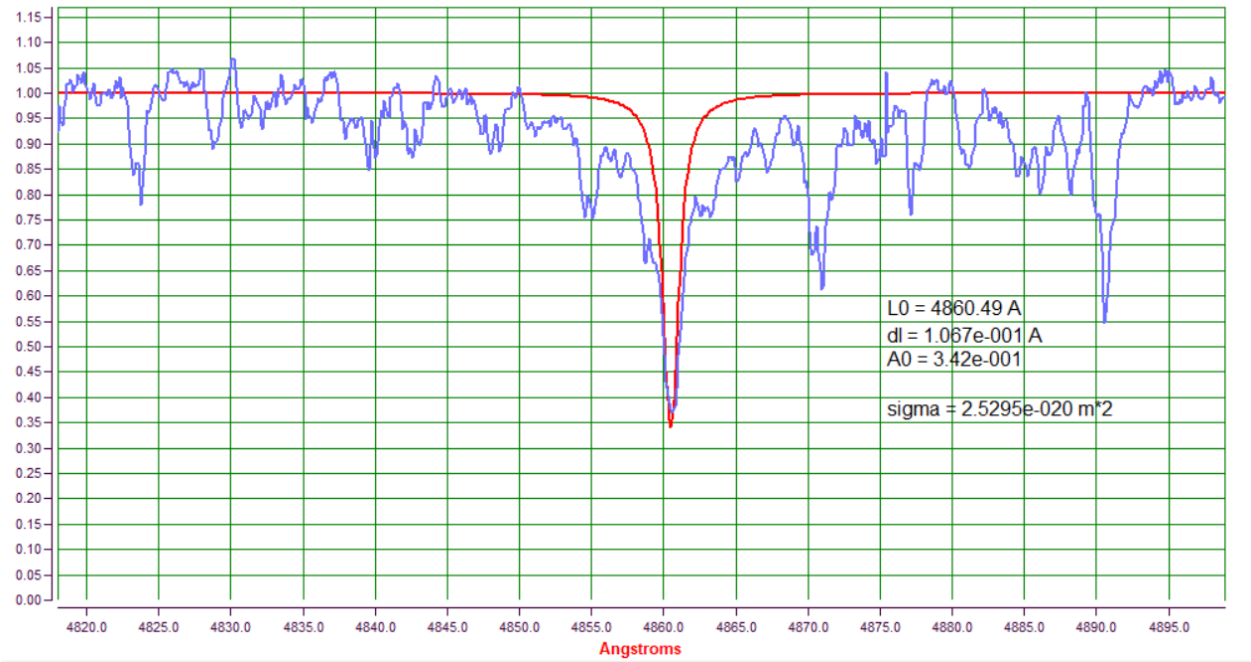
Figure 8: Published Solar Data

Solar Photosphere as a Function of Depth

Depth (km)	% Light from this Depth	Temperature (K)	Pressure (bars)
0	99.5	4465	6.8×10^{-3}
100	97	4780	1.7×10^{-2}
200	89	5180	3.9×10^{-2}
250	80	5455	5.8×10^{-2}
300	64	5840	8.3×10^{-2}
350	37	6420	1.2×10^{-1}
375	18	6910	1.4×10^{-1}
400	4	7610	1.6×10^{-1}

Source: Fraknoi, Morrison, and Wolf, *Voyages through the Universe*

Figure 9: Europa Hb Absorption



Again It can be seen that the result is quite good in the core of the line though the wings are less well reproduced than at the H_a wavelength, possibly because of more photons arriving from the deeper higher pressure regions of the solar photosphere or the presence of other elemental lines.

Discussion

The model presented here is not the author's first attempt at analysing spectra. This analysis differs from previous attempts in that, apart from yielding reasonable predictions for multiple stars (more papers will follow this) the use of the photon number flux form of the Planck function as the starting point made the derivation of capture cross-sections much more straight forward.

The conventional approach to spectral analysis focuses on the absorption profile equivalent widths, oscillator strengths etc. In the approach presented here the focus is on the "equivalent emission" line profile which is a direct representation of the dynamics of a particular star's photosphere i.e. temperature, atomic collision rates and state of rotation. This seemed a more natural starting point for computing line profiles.

It was found that the Einstein B coefficients in themselves were not directly useful for computing relative line strengths, for whilst the B coefficients are a (temperature independent) function of equilibrium level populations and the Planck photon field, capture cross-sections are a different (temperature dependent) function of those same variables. As functions of the same variables however a relation between them can be derived if desired.

A dimensional argument was used to move from equation A.4.10 to equation A.4.11, as a dimension of time had to be removed. The obvious choice was multiplication by a function of the Einstein A coefficients and that function had to be common to all lines in the series.

A further encouraging feature of the model is that the internal parameters i.e. capture cross-sections and impact parameter, have believable values when computed or in the case of the impact parameter, adjusted to fit experimental data. Capture cross-sections are found to be of the order of a Bohr radius circle and the impact parameter is of the order of approximately 8 Bohr radii. Had these properties been on any other scale the model would have been much less believable.

Conclusions

The aim of this work was to produce a simple model of stellar photospheres, based on a single layer in thermal equilibrium, that could be used to calculate the relative depths of hydrogen Balmer series absorption lines and yield reasonable estimates of the pressure and thickness of the Solar photosphere.

The results presented show that the model produced does indeed yield reasonable results for the relative depth of absorption at H_a and H_b wavelengths for the Sun. In addition the model yields reasonable estimates of the average solar photosphere pressure and total thickness i.e. 1.1349 e-1 Bar and 400.41 km respectively when a single adjustable impact parameter takes the value 4.0 A.

The scale of the calculated capture cross-sections and the magnitude of the impact parameter necessary to obtain correct solar properties are consistent with expected values.

The applicability of the model to other stars will be investigated if future work.

A global thermal equilibrium model is a first step toward a more realistic multi-layer local thermal equilibrium model.

Appendix A: Spectral Analysis Model

In this section we will first justify and describe the linear absorption model that we shall use assuming a single layer photosphere in thermal equilibrium. Next we will relate the absorption line profile to the dynamics of the absorbing atoms in the photosphere and finally obtain a relationship between the amount of absorption occurring between different lines of a series.

A.1 Thermal Equilibrium

The principles behind this model can best be understood if we imagine isolating a section of a stellar photosphere in an insulating box with perfectly reflecting walls - as far as the photosphere's Planckian photon field is concerned. The walls are however perfectly transparent to all photons from an external Planckian source of the same temperature. If the external source is viewed through the box then we assume only those photons that suffer no absorption emerge from the front face of the box. Any absorbed photons from the external source are scattered and emerge from other faces of the box. Thus from the side of the box we would see an emission spectrum whilst the front face would present an absorption spectrum. This configuration may seem somewhat contrived but such is the power of assuming thermal equilibrium that, as the configuration could occur and everything "adds up", then it must be indistinguishable from other possible configurations. The downside is of course that in reality not all, and possibly few, photospheres will be well modelled by a single layer in thermal equilibrium. However by comparing real spectra to this simple model it should be possible to speculate on the reasons for any deviation.

In Thermodynamic equilibrium the perfect gas law states that:-

$$PV = nRT \qquad \text{(A.1.1)}$$

where *P* is pressure, *V* is volume, *T* is absolute temperature, n is the number of moles of the particles, *R* (= 8.31441) is the molar gas constant therefore:-

$$P = \frac{n}{V}RT \equiv n_v RT \qquad \text{(A.1.2)}$$

where n_v is the number of moles of the particles per unit volume, defining *N* as the number of particles per unit volume we have:-

$$P = \frac{N}{N_A}RT \qquad \text{(A.1.3)}$$

where N_A is Avogadro's number (= 6.022045e23). An alternative way of writing the same equation is:-

$$P = NkT \qquad \text{(A.1.4)}$$

Where *k* is Boltzmann's constant (=1.380662e-23).

Another important thermal equilibrium equation is Saha's equation which relates the number of neutral atoms N_I and ionised atoms N_{II} . Saha's equation states:-

$$N_{II}^2 = \frac{N_I}{\Lambda^3}\exp\left(-\frac{E_{ion}}{kT}\right) \qquad \text{(A.1.5)}$$

where E_{ion} is the ionisation energy of, in this case, Hydrogen (13.6eV), Λ is the electron thermal de Broglie wavelength $\left(\Lambda = \sqrt{\frac{h^2}{2\pi m_e kT}}\right)$ and m_e is the electron rest mass. Note that $N_I = N - N_{II}$ therefore A.1.5 can be solved as a quadratic in N_{II} given N.

A.2 Linear Absorption Model

The *i* to *j* principle quantum level transition absorption line profile (*j*>*i*) at a given temperature *T*, expressed as a photon number flux per unit wavelength, will be represented by the function $P_{ij}(\lambda, x)$. The change in $P_{ij}(\lambda, x)$ when passing through a unit area slab of thickness *dx* at position *x* is given by:-

$$dP_{ij}(\lambda, x) = -\sigma_{ij}P_{ij}(\lambda, x)N_i(\lambda)d\lambda dx \qquad \text{(A.2.1)}$$

P_{ij} is a function of wavelength λ by virtue of the dynamics of the stellar photosphere (pressure, rotation and thermal motion). This dynamics is represented by the function $N_i(\lambda)$ which is the number of absorbing atoms per cubic metre per unit wavelength in the *i*th principle quantum state and able to transition to the *j*th state by absorbing a photon of wavelength λ. The final factor σ_{ij} is a "capture cross-section" and represents the probability of absorbing a photon to transition from the *i*th to *j*th state and is defined in the rest-frame of an atom where we always have $\lambda = \lambda_{ij}$.

Equation (A.2.1) can be integrated to yield:-

$$\hat{P}_{ij}(\lambda, t) \equiv \frac{P_{ij}(\lambda,t)}{P_{ij}(\lambda,0)} = e^{-\sigma_{ij}tN_i(\lambda)d\lambda} \qquad \text{(A.2.2)}$$

Where *t* is the thickness of the photosphere and we have normalised the photon number to a continuum of 1.0. The photon number at *x = 0* is given by the Planck function in the form of a number flux i.e:-

$$P_{ij}(\lambda, 0) = \mu(\lambda, T)d\lambda = \frac{2\pi c}{\lambda^4}\frac{d\lambda}{e^{\frac{hc}{kT\lambda}}-1} \qquad \text{m}^{-2}\,\text{s}^{-1} \qquad \text{(A.2.3)}$$

$\hat{P}_{ij}(\lambda, t)$ in fact represents the measured normalised absorption profile, in the remainder of this section we will not indicate the photosphere thickness explicitly and just refer to the normalised photon *i* to *j* absorption profile as $P_{ij}(\lambda)$.

Note that:-

$$\int N_{ij}(\lambda)d\lambda = N_i \qquad \text{(A.2.4)}$$

Where N_i is the total number of atoms m^{-3} in state *i*. Now defining a scale factor s_j using:-

$$s_j \int \widehat{N}_{ij}(\lambda)d\lambda = N_i \qquad \text{(A.2.5)}$$

Where $\widehat{N}_{ij}(\lambda_{ij}) = 1$, we can write (A.2.2) as:-

$$P_{ij}(\lambda) = e^{-\sigma_{ij} t s_j \tilde{N}_{ij}(\lambda) d\lambda} \quad \text{(A.2.6)}$$

Next we shall modify the notation further by defining an "equivalent emission line" via:-

$$E_{ji}(\lambda) \equiv \widehat{N}_{ij}(\lambda) \quad \text{(A.2.7)}$$

$E_{ji}(\lambda)$ is the normalised emission line profile that would be seen if we could selectively observe the *j* to *i* emission process within the star's photosphere.

So we can write:-

$$P_{ij}(\lambda) = e^{-\sigma_{ij} t s_j E_{ji}(\lambda) d\lambda} \quad \text{(A.2.8)}$$

And as $E_{ji}(\lambda_{ij}) = 1$ it follows that:-

$$P_{ij}(\lambda_{ij}) = e^{-\sigma_{ij} s_j t d\lambda} \quad \text{(A.2.9)}$$

Taking natural logarithms of (A.2.8) and (A.2.9) we can deduce:-

$$E_{ji}(\lambda) = \frac{Ln\left(P_{ij}(\lambda)\right)}{Ln\left(P_{ij}(\lambda_{ij})\right)} \quad \text{(A.2.10)}$$

and therefore:-

$$P_{ij}(\lambda) = P_{ij}(\lambda_{ij}) e^{E_{ji}(\lambda)} \quad \text{(A.2.11)}$$

We can use (A.2.10) to generate an equivalent emission line corresponding to a particular measured absorption line. This emission line can then be analysed to produce a model of the photosphere dynamics (Temperature, Pressure and Rotation). The resulting model can then be used to generate the equivalent emission line for a second line in the spectral series. To complete the process (A.2.11) can be used to predict the expected absorption line. The following subsections will fill in the details of this analysis method.

A.3 Relation between two lines of a series

For a second line of a spectral series we can write (A.2.8) as:-

$$P_{ik}(\lambda) = e^{-\sigma_{ik} s_k t E_{ki}(\lambda) d\lambda} \quad \text{(A.3.1)}$$

Taking natural logarithm of (A.2.8) and (A.3.1) we can deduce:-

$$P_{ik}(\lambda_k) = \left[P_{ij}(\lambda_j)\right]^{\frac{\sigma_{ik} s_k E_{ki}(\lambda_k) d\lambda_k}{\sigma_{ij} s_j E_{ji}(\lambda_j) d\lambda_j}} \quad \text{(A.3.2)}$$

Where we have distinguished between the two wavelength variables as in practice we will be dealing with a histogram of function values with differing wavelength bin widths.

We can deduce from (A.2.5) that for any two lines of a spectral series

$$s_j \int E_j(\lambda)d\lambda = s_k \int E_k(\lambda)d\lambda = N_i \quad \text{(A.3.3)}$$

or

$$s_j w_j = s_k w_k = N_i \quad \text{(A.3.4)}$$

Where w_j is the equivalent width of the *j* equivalent emission line which is equal to the area of the normalised line as obtained by integrating with respect to wavelength. Substituting into (A.3.2) we obtain:-

$$P_{ik}(\lambda_k) = \left[P_{ij}(\lambda_j)\right]^{\frac{\sigma_{ik} w_k E_{ki}(\lambda_k) d\lambda_k}{\sigma_{ij} w_j E_{ji}(\lambda_j) d\lambda_j}} \quad \text{(A.3.5)}$$

Where we have given the wavelength symbol a single subscript to indicate that they are different wavelength variables. From (A.2.5) we deduce that for any two lines of a spectral series

$$s_j \int E_j(\lambda)d\lambda = s_k \int E_k(\lambda)d\lambda = N_i \quad \text{(A.3.6)}$$

or

$$s_j w_j = s_k w_k = N_i \quad \text{(A.3.7)}$$

Where w_j is the equivalent width of the *j* emission line which is equal to the area of the normalised line as obtained by integrating with respect to wavelength. Substituting into (A.3.5) we finally obtain:-

$$P_{ik}(\lambda_{ik}) = \left[P_{ij}(\lambda_{ij})\right]^{\frac{\sigma_{ik} w_k d\lambda_k}{\sigma_{ij} w_j d\lambda_j}} \quad \text{(A.3.8)}$$

as $E_{ki}(\lambda_{ik}) = 1$ by definition. All factors on the right-hand side of equation (A.3.8) are now known except for the capture cross-sections which we will determine in the following subsection.

Note that from (A.2.9) we have:-

$$s_j t = \frac{-Ln[P_{ij}(\lambda_{ij})]}{\sigma_{ij} d\lambda} \quad \text{(A.3.9)}$$

Substitution from (A.3.7) allows us to determine that:-

$$N_i t = \frac{-w_j Ln[P_{ij}(\lambda_{ij})]}{\sigma_{ij} d\lambda} \quad \text{(A.3.10)}$$

So once σ_{ij} is determined we can also obtain a value for the number of atoms m^{-3} in state *i* multiplied by the photosphere thickness i.e. the column density.

A.4 Einstein Coefficients

Capture and emission processes between two atomic levels with principle quantum numbers i and j (j > i) are governed by the Einstein coefficients. Einstein coefficients can be calculated in various sets of variables we will use:-

- N_i units m^{-3}, is the number density of hydrogen atoms with an electron in the ith energy level at a given point in a photosphere.
- g_i is the electron degeneracy of the ith energy level.
- P_{ij} units $m^{-2}\ s^{-1}$ is the number flux of photons that can induce the i to j transition.
- $\mu(\lambda, T)$ units $m^{-3}\ s^{-1}$, is the Planck distribution photon number flux at temperature T and transition wavelength λ.
- A_{ji} with units s^{-1}, is the Einstein coefficient for spontaneous photon emission from the electron n=j to n=i level transition (j>i).
- B_{ji} units m^2, is the Einstein coefficient for electron stimulated emission from the n=j to n=i level.
- B_{ij} units m^2, is the Einstein coefficient for photon capture resulting in an electron n=i to n=j transition.

The rates of change of level populations can be expressed as:-

$$-\frac{dN_j}{dt} = \frac{dN_i}{dt} = A_{ji}N_j - B_{ij}P_{ij}N_i + B_{ji}P_{ij}N_j \qquad \text{(A.4.1)}$$

In equilibrium $-\frac{dN_j}{dt} = \frac{dN_i}{dt} = 0$ therefore we can deduce:-

$$\frac{N_j}{N_i} = \frac{B_{ij}P_{ij}}{A_{ji}+B_{ji}P_{ij}} \qquad \text{(A.4.2)}$$

In thermal equilibrium detailed balance requires $g_iB_{ij} = g_jB_{ji}$ which together with the Boltzmann relation $\frac{N_j}{N_i} = \frac{g_j}{g_i}e^{-\frac{hc}{kT\lambda_{ij}}}$ allows us to deduce in units of m^2:-

$$g_iB_{ij} = \frac{g_jA_{ji}}{P_{ij}\left(e^{\frac{hc}{kT\lambda_{ij}}}-1\right)} \qquad \text{(A.4.3)}$$

To proceed further we need an expression for P_{ij}, now the Planck function can be expressed in two forms:-

1. Energy density $\rho(\lambda, T)d\lambda = \frac{8\pi hc}{\lambda^5}\frac{d\lambda}{e^{\frac{hc}{kT\lambda}}-1}$ J m^{-3}
2. Energy flux $\eta(\lambda, T)d\lambda = \frac{2\pi hc^2}{\lambda^5}\frac{d\lambda}{e^{\frac{hc}{kT\lambda}}-1}$ Wm^{-2}

It seems most appropriate in our case to use form 2 as our absorption model is framed in terms of a flow of photons through a photosphere. Dividing the Energy flux by the photon energy $\frac{hc}{\lambda}$ yields the photon number flux:-

$$\mu(\lambda, T)d\lambda = \frac{2\pi c}{\lambda^4}\frac{d\lambda}{e^{\frac{hc}{kT\lambda}}-1}\ m^{-2}\ s^{-1} \qquad \text{(A.4.4)}$$

Multiplying by a Dirac delta probability function and integrating over all wavelengths yields the result:-

$$P_{ij} = \mu(\lambda_{ij}, T) \qquad m^{-2}\,s^{-1} \tag{A.4.5}$$

Substituting from (A.4.3) into (A.4.1) and using (A.4.2) we obtain:-

$$g_i B_{ij} = \frac{g_j A_{ji}}{\mu(\lambda_{ij},T)\left(e^{\frac{hc}{kT\lambda_{ij}}}-1\right)} = g_j \frac{A_{ji}\lambda_{ij}^4}{2\pi c} \qquad m^2 \tag{A.4.6}$$

We can now relate the Einstein *B* coefficient for an *i* to *j* capture event to the corresponding *A* spontaneous emission constant:-

$$B_{ij} = \frac{g_j}{g_i}\frac{A_{ji}\lambda_{ij}^4}{2\pi c} \qquad m^2 \tag{A.4.7}$$

The *A* Einstein coefficients are readily available in the literature from detailed quantum calculations, Table A.4.1 lists them for transitions of the Hydrogen Balmer series. However if we simply identify the capture cross-sections as $\sigma_{ij} \equiv B_{ij}$, which may be appropriate for the monochromatic case i.e. lasers, the resulting predictions for the relative absorption line amplitudes are in error by many orders of magnitude. Indeed it can be seen from (A.3.5) that relative absorption line amplitudes are extremely sensitive to the capture cross-sections of the lines in question. In addition the relative amplitudes are observed experimentally to be temperature dependent which the $B_{ij}$are most definitely not.

Table A.4.1 Hydrogen Einstein Coefficients A_{ji} s^{-1}

i\j	2	3	4	5	6
1	4.69624	0.55722784	0.1277867	0.04123	0.0164321
2	0	0.44078884	0.0841524	0.0252949	0.0097283
3	0	0	0.0898098	0.0219967	0.0077822
4	0	0	0	0.0269489	0.0077062
5	0	0	0	0	0.0102439

To proceed note that we must have:-

$$\frac{\sigma_{ik}\mu(\lambda_{ik},T)}{\sigma_{ij}\mu(\lambda_{ij},T)} = \frac{N_k}{N_j} \tag{A.4.8}$$

for if (A.4.8) did not hold the level populations over time would depart from their equilibrium values. Thus:-

$$\frac{\sigma_{ik}}{\sigma_{ij}} = \frac{\mu(\lambda_{ij},T)N_k}{\mu(\lambda_{ik},T)\,N_j} \tag{A.4.9}$$

Note both the σ_{ij} and the B_{ij} are functions of the level population and photon field variables and can be explicitly related by eliminating either of the level population or photon field variables if desired.

From (A.4.9) we can deduce:-

$$\sigma_{ij} = \frac{K_i}{\mu(\lambda_{ij},T)} \frac{N_j}{N_i} \qquad \text{(A.4.10)}$$

Where K_i, for all lines of a given spectral series, is a constant with units s^{-1}. We will define the K_i in terms of the Einstein coefficients via:-

$$\mathrm{K_i} \equiv \frac{\alpha}{N_i} \sum_{k=i+1}^{\infty} A_{ik} N_k \qquad \text{(A.4.11)}$$

where α is the fine structure constant. So we can finally write:-

$$\sigma_{\mathrm{ij}} = \frac{\alpha}{N_i^2} \frac{N_j}{\mu(\lambda_{ij},T)} \sum_{k=i+1}^{\infty} A_{ik} N_k \qquad m^2 \qquad \text{(A.4.12)}$$

Whilst (A.4.10) has been fully justified (A.4.11) does need more consideration. The summation term in (A.4.11) represents the total emission rate and so is a reasonable factor to employ as a "Lego brick" to construct the factor $\mathrm{K_i}$. Including this factor means the capture cross-sections are being expressed as proportions of the total emission rate.

Regarding the inclusion of the factor α, this factor often appears in equations describing the interaction between photons and electrons so is again a reasonable inclusion. Up to this point these observations are the only justifications for choosing to define $\mathrm{K_i}$ as written in (A.4.11). However, it is demonstrated in the main body of this paper that the capture cross-sections so defined lead to acceptable predictions for known properties of the Sun.

Appendix B: Spectral Line Synthesis Model

B.1 Thermal Spectral Line Broadening

The probability of a fluctuation ΔE from the mean energy in a system in thermal equilibrium at absolute temperature T is:-

$$P(\Delta E) = P_0 e^{-\frac{\Delta E}{kT}} \quad \text{(B.1.1)}$$

As $\Delta E = \frac{1}{2} m \Delta V^2$ this corresponds to an atomic velocity fluctuation (ΔV) probability of:-

$$P(\Delta V) = P_0 e^{-\frac{m \Delta v^2}{2kT}} \quad \text{(B.1.2)}$$

Which, as $\Delta V = c \frac{\Delta \lambda}{\lambda_0}$, in turn corresponds to a Doppler shift (Δλ) probability of:-

$$P(\Delta \lambda) = P_0 e^{-\frac{mc^2 \Delta \lambda^2}{2kT \lambda_0^2}} \quad \text{(B.1.3)}$$

i.e. a Gaussian distribution:-

$$P(\lambda, \lambda_0) = P_0 e^{-\frac{(\lambda - \lambda_0)^2}{2\sigma^2}} \quad \text{(B.1.4)}$$

with $\sigma = \sqrt{\frac{kT}{mc^2}} \lambda_0$ and $P_0 = \frac{1}{o\sqrt{2\pi}}$

FWHM: $P(\Delta \lambda_{\mathrm{FWHM}}) = \frac{P_0}{2}$ i.e.:-

$$\frac{1}{2} = e^{-\frac{\Delta \lambda_{\mathrm{FWHM}}^2}{2\sigma^2}} \quad \text{(B.1.5)}$$

Therefore

$$\mathrm{FWHM} = 2\Delta \lambda_{\mathrm{FWHM}} = \sqrt{8\, ln2}\, \sigma \quad \text{(B.1.6)}$$

B.2 Pressure Spectral Line Broadening

Spectral line widths are affected by pressure, the more frequent atomic collisions are the more a given spectral line will be broadened. This is a resonance process and follows a Lorentzian distribution ("Atomic Astrophysics and Spectroscopy " Anil K. Pradhan and Sultana N. Nahar):-

$$\int_0^\infty L(\omega) d\omega = \frac{1}{\pi} \int_0^\infty \left\{ \frac{\left(\frac{\Gamma}{2}\right)}{(\omega - \omega_0)^2 + \left(\frac{\Gamma}{2}\right)^2} \right\} d\omega = 1 \quad \text{(B.2.1)}$$

$\Gamma = \gamma + \frac{1}{t_0}$, where γ is a quantum mechanical "damping" factor which can be assumed negligible compared to $\frac{1}{t_0}$ which is the average collision frequency, so we have:-

$$\Gamma = \frac{1}{t_0} \tag{B.2.2}$$

Changing variable to wavelength using $\omega = \frac{2\pi c}{\lambda}$ we can deduce:-

$$\int_0^\infty L(\lambda)\, d\lambda \approx \frac{1}{\pi}\int_0^\infty \left\{ \frac{\left(\frac{\Gamma'}{2}\right)}{(\lambda-\lambda_0)^2+\left(\frac{\Gamma'}{2}\right)^2} \right\} d\lambda = 1 \tag{B.2.3}$$

where:-

$$\frac{\Gamma'}{2} = \frac{\lambda^2 \frac{\Gamma}{2}}{4\pi c} \tag{B.2.4}$$

And the approximately equal sign ≈ occurs in B.2.3 as we have approximated the term $\lambda\lambda_0$ to λ_0^2 in the change of variable calculation. This results in a symmetric distribution function and introduces negligible errors if, as is the case, the width of a line is small compared with the wavelength. So we have:-

$$L(\lambda) = \frac{1}{\pi}\left\{ \frac{\left(\Gamma'/_2\right)}{(\lambda-\lambda_0)^2+\left(\Gamma'/_2\right)^2} \right\} \tag{B.2.5}$$

The half height (wavelength half width) occurs when $(\lambda - \lambda_0) = \pm \Gamma'/_2$.

The book referenced above goes on to deduce:-

$$\frac{\Gamma}{2} = N v_0 (\pi \rho_0)^2 \tag{B.2.6}$$

where *N* is the number density of atoms, ρ_0 is an impact parameter (units m) and v_0 is the relative mean velocity between impacting particles. For a Maxwellian distribution of velocities we have:-

$$v_0 = 4\left[\frac{kT}{\pi M}\right]^{0.5} \tag{B.2.7}$$

where *M* is the mass of the identical impacting particles.

If we simply substitute from B.2.6 into B.2.4 to obtain an expression for Γ' we find that we have introduced a dependence on the emitted wavelength into the wavelength distribution. However, when expressed in terms of emitted frequency, there is no dependence of the width of the distribution on the emitted frequency. To restore this property to B.2.5 and to obtain the correct dimensionality, we must express the impact parameter as a function of wavelength specifically:-

$$\rho_0 = \frac{2\rho^2}{\lambda}\sqrt{\frac{c}{\pi}} \tag{B.2.8}$$

where ρ is a constant. Substituting into B.2.4 we obtain:-

$$\frac{\Gamma'}{2} = \frac{\lambda^2}{4\pi c} N v_0 (\pi \rho_0)^2 = N v_0 \rho^4 \tag{B.2.9}$$

To proceed further we can either:-

1. Investigate the impact parameter ρ_0 in a detailed theoretical analysis as discussed in the book referenced above.
2. Consider ρ as a fitting parameter.

Option 1 is a complex undertaking beyond the simple scope of this work. Therefore we shall adopt option 2 and compare predictions from our simple theory to the known properties of the sun, when applied to other stars, errors are to be expected that grow as the star under consideration becomes more dissimilar to the Sun.

B.3 Convolution of Two Distributions

Given a histogram starting distribution vector (V_0) with known (not necessarily uniform) bin widths $(\Delta\lambda_\mathrm{i})$ we can apply a second spreading distribution to yield the resultant distribution vector (V_1) via the matrix operation:-

$$MV_0 = V_1 \qquad \text{(B.4.1)}$$

where $m_{ij} = D(\lambda_\mathrm{j} - \lambda_\mathrm{i})\left(\frac{\Delta\lambda_\mathrm{j}}{\Delta\lambda_\mathrm{i}}\right)$ and D is the second distribution function.