Collisional broadening by hydrogen for stellar spectroscopy - extension towards high-lying states

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Contents

1 Introduction 2

2 Background 3
   2.1 Theory ...................................................... 3
   2.2 The tables .................................................. 4
   2.3 Appearance of the tables ................................. 5

3 Method 5
   3.1 Computation and data reduction .......................... 5

4 Results 6
   4.1 Explanation of the plots .................................. 6
   4.2 Unexpected results ........................................ 7

5 Recalculating old lines 8

6 Suggestions 10

7 Conclusion 10

8 Appendix 11
   8.1 Bash script for D-F transition ............................. 11
   8.2 Data reduction python script ............................... 11
   8.3 Excerpt of Matlab program for plotting ................ 12
   8.4 Additional graphs ......................................... 13
Abstract

The object of this thesis is to extend the current tables for two useful quantities when calculating collisional broadening, the cross-section of interaction and the velocity parameter. These quantities, which have hitherto been tabulated for lower states, have now been calculated for higher lying states and are used in the ABO - model for spectral line broadening. Having larger tables for these values enables broadening calculations for more spectral lines and this thesis shows examples of calculations which benefited from this. During the calculations of the tables some unexpected behaviour in the distribution of values arose which has not been seen previously. This could point to an unknown underlying mechanism.

1 Introduction

Measuring stellar abundances of different elements is of importance to many branches of stellar physics and astronomy in general. In stars similar to the sun the hydrogen number density is orders of magnitude larger than the electron number density, therefore the collisional broadening effects of collisions with hydrogen is of utmost importance for abundance measurements of strong lines (Barklem, O’Mara, and Anstee 1998). In order to do the required modelling of stellar atmospheric spectra it is important to have a good theory for the effects of pressure broadening due to collisions with hydrogen (Anstee and O’Mara 1991). These abundance determinations is made by fitting the damping wings to strong lines, where the f-values are generally known precisely (Anstee and O’Mara 1995). This proves difficult however, since most strong lines are broadened by collisions with hydrogen (Anstee and O’Mara 1995). In order to calculate the collisional broadening it is also important to have knowledge of the interaction energy between the absorbing and perturbing atom in order to calculate the collisional broadening. Assuming that the interaction happens at very large distance this leads to the van der Waals broadening theory, which has been know to be too low by order of a factor 2 (Holweger 1971). The theory continued to see use, however, because of its simplicity and the possibility to include a semi-empirical enhancement factor to mitigate this problem.
2 Background

2.1 Theory

In order to simplify calculations several assumptions have to be made, out of which three have been removed by Anstee and O’Mara (1991). The first assumptions, which is retained, is often called the Unsöld approximation (Unsöld 1927) which means that the energy expression in the second order perturbation theory can be replaced with a suitable average energy (Anstee and O’Mara 1991). This means that the equations can be simplified

\[ V_i = \langle i|V|i \rangle + \sum_{i \neq j} \frac{\langle i|V|j \rangle \langle j|V|i \rangle}{E_i - E_j} \]

\[ \implies V_i \approx \langle i|V|i \rangle + \frac{1}{E_p} \left[ \langle i|V^2|i \rangle - \langle i|V|i \rangle^2 \right] \]  

(1)

It is also important to assume that the interaction between the hydrogen atom and the perturbed atom is weak enough for perturbation theory to work. Most important, however, are the two assumptions that were removed by Anstee and O’Mara (1991). These assumptions were that the first order energy contributions could be ignored and that the interaction could be averaged over different orientations (Anstee and O’Mara 1991). Since the ABO theory does not have a simple velocity dependence, like that van der Waals theory does, it is also assumed that the cross section obeys the power law

\[ \sigma(v) = \sigma(v_0) \left( \frac{v}{v_0} \right)^{-\alpha} \]

(2)

For the calculations of the cross-section \( \sigma(v) \) a complex dimensionless efficiency factor \( \langle \Pi(b,v) \rangle_{av} \) is introduced, where \( b \) is the collision impact parameter and \( v \) is velocity (Anstee and O’Mara 1995). However, for very small values of \( b \) the \( \langle \Pi(b,v) \rangle_{av} \) starts to oscillate rapidly and becomes impossible to integrate. Therefore a cutoff \( b_0 \) is chosen based on test calculations. The cross section, which can be computed as

\[ \sigma(v) = 2\pi \int_0^\infty \text{Re} \left( \langle \Pi(b,v) \rangle_{av} \right) bdb \]

(3)

can be rewritten using a cutoff of \( b_0 \) and becomes

\[ \sigma(v) \approx \pi b_0^2 + \int_{b_0}^\infty \text{Re} \left( \langle \Pi(b,v) \rangle_{av} \right) bdb \]

(4)

where \( b_0 = 3 \) [bohr] and \( \text{Re} \langle \Pi(b,v) \rangle_{av} \) is the real part of the complex efficiency factor averaged over all orientations of the perturbed atom (Barklem, O’Mara, and Anstee 1998). Using the impact approximation and the Lorentz profile the FWHM (full width half maximum) can be calculated as

\[ w = N \int_0^\infty v f(v) \sigma(v) dv \]

(5)
where \( N \) is the hydrogen number density, \( v \) the relative collision speed and \( f(v) \) is the Maxwellian speed distribution. Dividing by \( N \) and assuming that the power law form is a function of velocity then yields

\[
\frac{w}{N} = \left( \frac{4}{\pi} \right)^{\alpha/2} \Gamma \left( \frac{4 - \alpha}{2} \right) v_0 \sigma(v_0) \left( \frac{\bar{v}}{v_0} \right)^{1-\alpha} \left[ \frac{FWHM/2}{\text{number density}} \right]
\]  

(6)

where \( \bar{v} = (8kT/\pi\mu)^{1/2} \), \( \mu \) is the reduced mass, \( \Gamma \) is the gamma-function, \( k \) is the Boltzmann constant and \( T \) is temperature. The relative collision speed is \( v_0 = 10^4 \text{ [ms}^{-1}] \). Since a typical value for \( \alpha \) is around 0.25 that gives a temperature dependence of \( T^{0.38} \) because of

\[
\left( \frac{\bar{v}}{v_0} \right)^{1-\alpha} = \left( \frac{(8kT/\pi\mu)^{1/2}}{v_0} \right)^{1-\alpha} \Rightarrow CT^{(1-\alpha)/2} \approx CT^{0.375}
\]

for values of \( \alpha \approx 0.25 \). \( C \) is a constant introduced to simplify the expression.

2.2 The tables

In order to determine the line broadening cross section from the tabulated data it is necessary to know the effective principal quantum number \( n^* \) (Barklem, Piskunov, and O’Mara 2000). Computing \( n^* \) requires knowledge of the excitation energy of the optical electron as well as the parent configuration. This can be done by computing the correct series limit as the sum of the ionization limit and the excitation of the parent configuration

\[
E_{\text{limit}} = E_{\text{ion}} + E_{\text{parent configuration}}
\]

(7)

and then applying it to the Rydberg formula for neutral atoms

\[
n^* = \sqrt{\frac{109678.8}{E_{\text{limit}} - E_{nl}}}
\]

(8)

where 109678.8 is the Rydberg constant in \([cm^{-1}]\) and \( E_{nl} \) is the excitation energy of the optical electron and \( E_{\text{limit}} \) is the series limit. For cases where the parent core is in its ground state this is of course the usual ionization energy \( E_{\text{ion}} \). A more comprehensive explanation of the series limit and how to use it can be found in Barklem, Piskunov, and O’Mara (2000).

The cross-sections are then computed for relative collision speeds ranging from 3000 to 18000 \([ms^{-1}]\) in steps of 1000 \([ms^{-1}]\) and the velocity parameters are then calculated by linear regression (Anstee and O’Mara 1995), where the coefficient of regression is the slope.
2.3 Appearance of the tables

In three articles written by Anstee and O’Mara (1995) and Barklem and O’mara (1997) and Barklem, O’mara, and Ross (1998) where the tables were calculated, two-dimensional plots were also made to show the general behaviour of the cross-sections and velocity parameter inside the chosen intervals of $n^*$. Below are plots made in Matlab for purposes of showing the appearance of the $\sigma$ and $\alpha$ parameters.

In order to make sure that the values calculated by the script were the same as the ones previously calculated and plotted in the above articles the complete tables were constructed. This enabled a simple reality check for the values in the cases where they appeared unusual, as will be discussed later.

It is also worth noting that not all points in the surfaces necessarily correspond to physical transitions but have been included for the sake of completeness of the tables. For instance, the transitions corresponding to $n^*_F$ – state $= n^*_D$ – state in figure 1 does not exist physically as a transition but is still shown in the plots. These can usually be seen as a ”fold” in the surface (see figure 1). The plots themselves were made using the contour and surface functions in MatLab.

3 Method

The purpose of this thesis is to calculate the tables of cross-section and velocity parameter for a greater span of values of $n^*$ than done previously by Anstee and O’Mara (1995) and Barklem and O’mara (1997) and Barklem, O’mara, and Ross (1998) at which time they were limited to an upper $n^*$. The choice was considered a bit conservative but there is some evidence of numerical instability for larger values of $n^*$.

There are several reasons to believe that the tables would not be possible to construct for arbitrarily large values for $n^*$. The code that calculates the cross-sections and velocity parameters breaks down for too large values as well as for theoretical reasons in the model which don’t allow arbitrarily large values. For example the code assumes a thousand points for the distance of the electron from the core and the standard maximum distance is set as 100 Bohr radii. For these reasons a maximum of $n^* = 5.5$ was decided except for the D-F transition in which case a highest value of 6 was reached.

3.1 Computation and data reduction

The first, and arguably biggest, problem in executing the plan of increasing the tables is to find a simple way of running the codes that computes them. The program itself requires
several inputs and then outputs around a hundred lines of data. This poses a hurdle since the code has to be run many hundred times in order to make complete tables. Without reasonable data management this would create far too much data to process. For this reason a script was created (see section 8.1) to both run the program continuously and make to necessary data reductions.

The basic idea of the script is a nested for-loop to iterate over all values in both ranges of $n^*$ and in each iteration save only the necessary data into new files for easier management. Since the ABO-cross code was most easily ran through the Mac terminal the script was written in the same terminal using a shell script in the BASH environment.

After the script had run its course the final output was three files, one for the cross-sections, one for the velocity parameter and one for the regression correlation coefficient. However, since BASH lacked some functionality in data reduction another code was written in Python to essentially tidy up the files and make them more readable. The Python code also formated the data in a useful form.

Finally the fully reduced and formated data was input into a Matlab program to make surface and contour plots of the data. The importance of this step is explained in section 2.3.

4 Results

4.1 Explanation of the plots

As can be seen in figure 2 the general trend in the surface cross section plots is that the crossection is increasing with increasing values of $n^*$. This is what creates a typical "fold" in the graph since the larger $n^*$ dominates the appearance. This is further clear by following increasing values for one state while keeping the other fixed. This is what was expected to see. The plots have also been color coded to make it easier to discern changes in magnitude. In figure 2 this can be seen as the larger values of $\sigma$ go towards the yellow part of the spectrum and the lower values towards the blue of the color scale. The color scale does not correspond to the wavelength of the actual spectral lines.

However, many of the graphs deviate from this behaviour of monotonous rise with $n^*$ and this is discussed further below.

Figure 2: Surface plot of the s-p transition
4.2 Unexpected results

After the first run of the scripts plots were created but certain things appeared unusual in a few of the plots. As can be seen in figure 3 the velocity parameter $\alpha$ reaches values as low as zero when the S-state principal quantum number is larger than 3.5 and the P-state is low. This poses somewhat of a problem since the velocity parameter has been analytically calculated to values around 0.3 and while it could be zero it does need to be given a more thorough assessment to make sure it is correct. These low values for $\alpha$ coupled with the outlier values of the coefficient of regression (see section 2.2) means that something unusual might be happening in these areas. One possibility of this behaviour could be explained by the fact that the Coulomb wave-function is not well defined for $(n^* < l + 1)$.

However this is not a complete explanation since the behaviour is not present in all areas where the $n^*$-criteria is met. If this was the full cause it would be expected to show up for all problematic values of $n^*_P$ not just around $n^*_S \approx 3$. Further, two more plots of the initial run raised some interest. Both figure 4 and figure 5 show sharp ridges around $n^* \approx 5.4$ and $n^* \approx 4.4$ respectively. Figure 1 shows a typical distribution of values for the cross-section. In many of the graphs two ridges protrude for higher values of $n^*$. These are then often followed by a small dip in values and then continued growth. This behaviour had not previously been seen since it does not become apparent for smaller values of $n^*$. Since no numerical reason for the appearance could be found the analysis continued into looking for a physical explanation. The full explanation however, is beyond the scope of this thesis and could be followed up on in further research.
Figure 5: Notice the ridge of $\sigma [\text{a.o.}]$ around $s \approx 4.5$

5 Recalculating old lines

Figure 6: The older calculated values. Only five out of the 56 data points could be calculated with the old values. Notice that most of the values are around 2 to 3 times the previous data

In an earlier project by Hultquist (2019), which aimed to make calculations of collisional
broadening, one of the limiting factors to how much could be properly calculated was the size of the tables that are calculated in this thesis. Specifically in the cases of several lines which could not be calculated with the tables of the time gave the idea for this thesis. The results from that project can be seen in figure 6 which compared new to old broadening data for silicon. Most of the data is concentrated around 2, which is what had been expected but only 5 out of the 56 could be calculated. The plots were made with a MatLab program written by Bengtsson (2018).

![Figure 7: The new calculations show the same five points as previous in the bottom left as well as 13 other points. Here again most of the points are around 2 to 3 times the previous values](image)

As a proof of concept for the value of the extended tables in this thesis the broadening calculations from figure 6 were done again. This time, as can be seen in figure 7, there are 18 lines calculated. This is a significant improvement from the previous five. It shows that the clustering around 2 to 3 is still present but with the addition of two outliers which reach to almost 6.5. The $n^*$ values for these P-S transitions were roughly 2.5 in the lower state and 4 in the upper state which could explain the larger broadening (see figure 5). After additional investigation no problem with the calculations were found. This is not completely unexpected however since the previously expected doubling of spectral broadening does not hold for all values of $n^*$ so 6 or 7 times the values is not necessarily a problem.
6 Suggestions

For further research it could be interesting to investigate the source of the "dip" in, for example, figure 2 as well as the other graphs for cross-section and velocity parameter with similar behaviour. As previously stated it appears to have something to do with the zeroes of the Coulomb wave function but a more full explanation would be necessary. A place to start could be to evaluate the mathematical behavior for the wave functions that are used.

7 Conclusion

The main goal of the thesis, to calculate and evaluate larger values for the cross-section and velocity parameter, which initially appeared to be a coding and data-reduction problem has uncovered previously unknown aspects of the quantities. Beyond the expected usefulness for calculating collisional broadening this thesis may also have raised a few questions regarding the distribution of these quantities that warrant a physical or numerical explanation.

Judging by the appearance of the tables for the largest values evaluated it is unlikely that it would be useful to attempt to extend the tables further. It appears that all the reliable values in the stable regions have been found.
8 Appendix

Below follows full codes or examples or excerpts of the codes used in this projects. Since much of the code is similar between the different transitions, some parts may have been omitted.

8.1 Bash script for D-F transition

```bash
#!/bin/bash
step=0.1
d_low=2.3
d_up=5.0
f_low=3.3
f_up=6.0
for d in $(seq $d_low $step $d_up)
do
    for f in $(seq $f_low $step $f_up)
do
        echo "f-state n-star is $f and d-state n-star is $d"
        printf "$d
$f
100
Table for d$d f$f.txt" | ./cwdf.out
        awk 'FNR == 26 {print $2}' "$Table for d$d f$f.txt"
        >> Sigma_CWDF.txt
        awk 'FNR == 40 {print $3}' "$Table for d$d f$f.txt"
        >> Alpha_CWDF.txt
        rm "Table for d$d f$f.txt"
done
    echo ";" >> Sigma_CWDF.txt
    echo ";" >> Alpha_CWDF.txt
done
```

8.2 Data reduction python script

```python
# File to be copied
import sys
with open('Alpha_CWID.txt', 'r') as rf:
    with open('Alpha_CWID_fixad.txt', 'w') as wf:
        for line in rf:
            if line.endswith(';
'): line = line[:-3]
            wf.write(line.replace('-0.', '.').rstrip())
            wf.write(' '
else:
    line = line[:-2]
    wf.write(line.replace('-0.', '.').rstrip())
    wf.write(' ')
```
8.3 Excerpt of Matlab program for plotting

```matlab
[X,Y] = meshgrid(2.3:0.1:5.0,1.3:0.1:3.9); figure
mesh(Y,X,CWPD) %interpolated
title('Surface Plot of velocity parameter \alpha for P-D transition');
xlabel('P state n*');
ylabel('D state n*');
zlabel('Velocity parameter');
figure
contourf(Y,X,CWPD) %interpolated
axis tight; hold on
```

```matlab
title('Contour Plot of velocity parameter \alpha for P-D transition');
xlabel('P state n*');
ylabel('D state n*');
```
8.4 Additional graphs
References


