ALKALINE LINES BROADENING IN STARS.

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ABSTRACT. Giving new insight for line broadening theory for atoms with more structure than hydrogen in most stars. Using symbolic software to build precise wave functions corrected for δs, δp quantum defects. The profiles obtained with that approach, have peculiar trends, narrower than hydrogen, all quantum defects used are taken from atomic database topbase. Illustration of stronger effects of ions and electrons on the alkaline profiles, than neutral-neutral collision mechanism.

keywords : Stars: fundamental parameters - Atomic processes - Line: profiles.

1. INTRODUCTION

Here we define what is needed for the theory: We introduce the profile function normalized: \( F(\Delta \omega) \) requiring normalization:

\[ \int_{-\infty}^{\infty} F(\Delta \omega) d(\Delta \omega) = 1 \]

The radiant power function, that is the power emitted though unit frequency is:

\[ P(\Delta \omega) = \frac{4 \omega^4}{3c^3} F(\Delta \omega) \]

We recall the two relations defining the Fourier transforms variables: \( \omega \) and \( s \) (time variable) such that \( \omega, s \) is dimensionless.

\[ \Phi(s) = \int_{-\infty}^{\infty} e^{i\Delta \omega s} F(\Delta \omega) d(\Delta \omega) \]

\[ I(\Delta \omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} \Phi(s) e^{i\Delta \omega s} ds \]

2. HYDROGEN FACTS

Recalling some facts on Hydrogen lines broadening: such as Balmer lines H\( \alpha \), and H\( \beta \) or Lyman lines : Ly\( \alpha \), and Ly\( \beta \) \( h\omega_0 \) being the energy gap between levels defining a transition \( i \rightarrow f \) the detuning \( \Delta \omega \) giving rise to \( F(\Delta \omega) \) for hydrogen lines is mainly first order Stark effect: for instance exists for H\( \beta \) whose wavelength at the centre of the \( n_f = 4 \rightarrow n_i = 2 \) transition is: \( \lambda_0 = 486.1nm \).

These Hydrogen lines are broad because of the degeneracy of levels defined by \( |nlm> \) there can exists \( g = 2 \times (2l + 1) \) for an \( l \) defined state such as \( 0 \geq l \leq n - 1 \) for an identified H line such as H\( \beta \) \( n_f = 4 \rightarrow n_i = 2 \) line we have \( N = 4 \times n_f^2 \times n_i^2 \) that is 512 sublevels implied and 128 neglecting the electron spin. Good literature exists for such matters, that is taking
into account for perturbers (ions and electron) effects on the radiating atom. Feautrier (1976).

\[ \Delta E = \frac{3}{2} n \times (n_1 - n_2) eF + O(F^2) \]

\[ \Delta E = \hbar \Delta \omega = \hbar (\omega_0 - \omega) \]

\[ \Delta E = \frac{\hbar^2}{2me} (k_f^2 - k_i^2) \]

These two approaches gives rise to the complete theory of broadening:

1) when the static field \(|F| = \text{Cst}\) is constant relatively to decay rate, in fact a field generated by static heavy charges ions or protons (relatively to the electron). Then the Stark profile has such dependence:

\[ I(\lambda) \simeq |\Delta \lambda|^3 \]

2) The field \(F(t)\) varies quickly before the atom relaxes,

\[ F(t) \simeq \frac{e^2}{r^2(t)} \]

\[ \vec{\rho}(t) \simeq \vec{b} + \vec{v} t \]

The quantum theory of one electron +H (or radiating atom) system Van Regemorter (1972) implies the relation \(\hbar \Delta \omega = \frac{\hbar^2}{2me} (k_f^2 - k_i^2)\) is the good answer to take into account for large \(\Delta \omega\) and replaces the impact parameter semi-classical approach.

3. ALKALINE LINES

Dealing with atoms having a structure such as alkalines: Li, Ca, K, Mg, Na or atoms such as He, and O. These atoms can be modelled using what is called since a long time Born (1926) the quantum defect. The optical electron: the one that gives rise to transition (quantum jumps \((\alpha \rightarrow \beta)\) suffers from an additional potential: the polarization potential: \(V_p(r) = -\frac{\alpha_D}{r^4}\), \(\alpha_D\) being the dipolar static polarizibilty. The full theory begins with recent review work Schwerdtfeger (2006) and displays the development of an energy level as orders of the field strength \(F\): (if \(\vec{F}(t) = \vec{E}_0\)) this the well known Stark effect.

\[ E(F) = E_0 + \frac{dE}{dF} dF + \frac{1}{2} \frac{d^2E}{dF^2} dF^2 + O(F^3) \]

The polarization potential varying as \(r^{-4}\) is easily recognized as the second order term \(dF^2\). Let us introduce the way to deal with the \(V_p(r)\) potential.

\[ \vec{\rho} = \alpha_D \vec{E} \]

\[ dV_p = -\vec{\rho} \cdot d\vec{E} \]

\[ dV_p = -\alpha_D \vec{E} \cdot d\vec{E} \]

\[ V_p(r) = -\frac{\alpha_D}{2r^4} \]
3.1. Semi-classical expression. How to deal with: Let’s us start with the semi-classical formula for the profile \( F(\omega) \)

\[
F(\omega) = \lim_{T \to \infty} \int_{-T}^{T} dt \, e^{i \omega t} | < \Psi_{t}(t)|\hat{D}|\Psi_{t}(t)\rangle|^2 \frac{1}{2\pi T}
\]

This equation is put forward in Van Regemorter (1972) in his review of spectral line broadening. I adapt that question to a quite similar way: I need not have \( |\Psi_{t}(t)\rangle \) as a time dependent wave function, but the modified radial \( |\Psi(\vec{r})\rangle \) with no time dependence. Giving for alkaline species, with known quantum defects (there are data from Topbase):

\[
\begin{align*}
\alpha & = n_{s} l_{s} \\
|\Psi_{\alpha}(\vec{r})\rangle & = R_{\alpha} \times Y_{\alpha}(\theta, \phi) \\
\beta & = n_{f} l_{f} \\
|\Psi_{\beta}(\vec{r})\rangle & = R_{\beta} \times Y_{\beta}(\theta, \phi)
\end{align*}
\]

or for Hydrogen the well known basic ket \( |R_{nl}(r) \times Y_{lm}(\theta, \phi)\rangle \)

\[
\begin{align*}
nl & = n_{s} l_{s} \\
|\Psi_{nl}(\vec{r})\rangle & = R_{nl} \times Y_{lm}(\theta, \phi) \\
nl' & = n_{f} l_{f} \\
|\Psi_{nl'}(\vec{r})\rangle & = R_{nl'} \times Y_{lm}(\theta, \phi)
\end{align*}
\]

Our purpose is to define the most efficient way, the \( |\Psi_{\alpha}(\vec{r})\rangle \) using true quantum defects leading to \( n_{s} \): the effective quantum number. Each atomic species has its peculiar quantum defect. These are now available from data base such as Topbase. Now it is a fact that the \( l \) kinetic momentum is defined by eigen value of the spherical harmonics for a pure Coulomb potential, becomes \( l_{s} = l - \delta_{s} \) the degeneracy of the levels disappears. The quantum number set is:\( \alpha \equiv n_{s} = n - \delta_{s}, l_{s} = l - \delta_{s} \). The physical effect produced can be explain this way: the optical electron getting away from the closed shell beneath polarizes the core shell, the higher the levels of the optical electron, the nearest to hydrogenic "states" are the transitions.

\[
L = 0 \equiv S \rightarrow \delta_{s} \quad L = 1 \equiv P \rightarrow \delta_{p} \\
\delta_{s} \equiv \delta_{s} \geq \delta_{p} \geq \delta_{f} \geq \delta_{f} \rightarrow 0
\]

4. Time dependent method

It is seen that one can change the semi-classical formula, into the way suggested by Schiff (1968), with no less generality.

\[
\Psi_{\alpha}(\vec{r}, t) = \Psi_{\alpha}(\vec{r}, 0) \times e^{i \frac{\hbar \omega_{\alpha}}{\hbar} t} \quad \text{the same for the } |\beta\rangle \text{ is: } \Psi_{\beta}(\vec{r}, t) = \Psi_{\beta}(\vec{r}, 0) \times e^{i \frac{\hbar \omega_{\beta}}{\hbar} t}.
\]

The transition probability is proportional to:

\[
| < \Psi_{\alpha}|V(\vec{r})|\Psi_{\beta}\rangle |^2 \propto \omega_{\alpha} \omega_{\beta}.
\]

From the text book of L.I. Schiff, we use his \( g(t) \) plateau function to transform and the relation \( T = 1 - S \):

\[
< \beta|(S-1)|\alpha\rangle = -\frac{i}{\hbar} < \alpha |T| \beta > \int_{-\infty}^{\infty} g(t) e^{i \omega_{\alpha} t}.
\]

The \( \rho(\Delta \omega) \) function is then proportional to:

\[
w_{\alpha \beta} \propto | < \alpha |T| \beta > |^2 \text{ the transition probability}.
\]
The following operators are the same:

\[ A(t) = \left| \langle \Psi_\alpha(\vec{r},t) \mid \hat{D} \mid \Psi_\beta(\vec{r},t) \rangle \right|^2 \text{ and} \]

\[ B(t) = \left| \langle \Psi_\alpha(\vec{r}) \mid \hat{D} \mid \Psi_\beta(\vec{r}) \rangle \right|^2 \times g(t,t_0) \]
5. Toward the global theory.

It is clear that one can obtain the wave functions of these alkaline elements such as MgI neutral with some quantum defects:

\[ \delta_s = 1.52 \text{ and } \delta_p = 1.04 \text{ and } \delta_f = 0.56 \text{ S=0 (Singlet)} \]
\[ \delta_s = 1.63 \text{ and } \delta_p = 1.12 \text{ and } \delta_f = 0.17 \text{ S=1 (Triplet)} \]

see Ref. Born (1926), pp 190

There the \( I_k \) is the Kostelecký index, taking values such as 1 or 2 Kostelecký (1984). The quantum analog to the classical Born atomic model, with the precession of the ellipse, is obtained by Bates (1949). The good quantum theory needs to consider a modification of the \( Y_{lm}(\theta, \phi) \rightarrow Y_{lm}^*(\theta, \phi) \) It is useful to compare two transitions such as: \( \text{MgI}_3p \rightarrow 4s \) triplet quantum defects to consider whose wavelength is \( \lambda_{sf} = 517.83 \text{nm} \) with an Hydrogen line such as \( H3p \rightarrow 4s \lambda_{sf} = 1875.11 \text{nm} \).

All data taken from [NBS] (1969). The ratio of the intensities is given by:

\[ R = \frac{\left| \langle \alpha n_{s, l_s} | r | \cos(\theta) \rangle \beta n'_{s, l'_{s}} \right|^2}{\sum_{m=-l}^{l} \left| \langle n, l, m, | r | \cos(\theta) \rangle n', l \pm 1, m \right|^2} \]

The ratio \( R \) can be considered as the ratio of the Einstein \( A_k \) of the two lines, for such two lines : \( R = 0.56 \times 10^{-6} \).

For most ionic species, whose single or optical electron gains high distances < \( r > = n^2 a_0 \geq 20a_0 \), the quantum defects disappear, leading to simple hydrogenic behaviour, the wave functions turn to those of Hydrogen.

5.1. Toward the global theory. We use the upward definition for the line shape:

\[ F(\omega) = \int_{-\infty}^{\infty} |\langle \alpha n_{s, l_s} | D.f(t) | \beta n'_{s, l'_{s}} \rangle|^2 dt \]
\[ g(t) = f(t),f(t) \]
\[ F(\omega) = \int_{-\infty}^{\infty} e^{-i\omega t} g(t) dt \]

These Fourier transforms are easily performed with "Mathematica", and I write here the \( g(t, t_0) \) \( t_0 \) being the width of the "plateau" in seconds.

\[ g(t, t_0) = e^{-|t-t_0|} H(t-t_0) + H(-t + t_0) + H(t-t_0) + e^{(t-t_0)} H(-t + t_0) \]

Here is the picture of the distribution function \( g(t, t_0) \):

It is really interesting to have fast symbolic software such as "Mathematica", to perform the Fourier Transform of the function \( g(t, t_0) \) assuming that \( t_0 \geq 0 \) to get \( F(\omega, t_0) \), and have
it as a good analytical function:

\[ F(\omega, t_0) = \frac{1}{\sqrt{\pi \omega}} \frac{1}{1 + \omega^2} \sqrt{\omega} \left( 1 - e^{-t_0 \omega} + 2 \omega \cos(\omega t_0) \right) \]

(38)

It is interesting to look at the behaviour of the profile function \( F(\omega, t_0) \), this function oscillates because of the phases contained in the expression.

For a given \( \omega \) the shorter is the \( t_0 \) width the least the profile \( F(\omega) \) oscillates. To obtain the good former profile function we need to replace in the defined function \( F(\omega, t_0) \) the variable \( \omega \) by the variable \( \Delta \omega = \omega - \omega_0 \). Here are some pictures of the alkaline Mg element:

Here \( \omega_0 \) is the frequency associated with the center of the line \( \omega_0 = \frac{E_\beta - E_\alpha}{\hbar} \).
The parameter $I_1 = |<\Psi_\alpha|\vec{D}|\Psi_\beta>|^2$, should be the intensity at the center of the line that is $\omega = \omega_0$. That definition of $I_1$ shall be modified to take into account the pressure effect.

6. The cut-off radius and its significance upon the profile $F(\Delta \omega, t_0)$.

A simple and efficient way to take into account the pressure effect whose origin comes from external parameter such as density $N_A$, and thus the cut-off is the following $L_A = N_A^{-1/3}$. This cut-off parameter $L_A$ is the one to use when there are no charges, and the surrounding of the emitters is mainly done of atomic species of density $N_A$. If the emitters of the transition $\alpha \rightarrow \beta$ are part of a plasma, with a degree of ionization: $\tau = \frac{N_e}{N_e + N_A}$, the good cut-off could be the shorter of the the two Stehle (1996) that is:

\begin{align}
\lambda_{De} &= \sqrt{\frac{kT_e}{4\pi e^2 N_e}} \\
\lambda_{De} &= 6.9 \times 10^8 \sqrt{\frac{T_e}{N_e}} \left(\text{nm, K, cm}^{-3}\right) \\
\lambda_{Di} &= \lambda_{De} \sqrt{1 + \frac{Z^2 \lambda_e}{Z_e T_e}}
\end{align}

\[ \rho_C = \min(\lambda D(N_e, T), L_A) \]

$\lambda D N_{ions}$ that is the Debye radius to compare the spatial extension $L_A$, because of the distribution of the charges in the plasma.

7. Effect of the cut-off on the value obtained for the dipolar squared matrix element $d_{\alpha\beta} = |<\alpha|\vec{D}|\beta>|^2$

That simple explanation to take into account for pressure effects on radiating atoms, parts of such media, such as exists in Astrophysics: -Star atmospheres, -Dust in interstellar matter, -Molecular clouds. Finding the way to define the upper limit $\rho_C$ for the emitting atoms, and to build the wave functions with their peculiar quantum defects for each species (Li, Na , Al, Ca , Na, Mg and even He) now easily reached with modern symbolic calculation software, I define there the a probability function $P_{\alpha\beta}(x)$:

\[ P_{\alpha\beta}(x, T) = \frac{|\int_0^{x(T)} <\alpha|\vec{r}|\beta>|^2}{|\int_0^{\infty} <\alpha|\vec{r}|\beta>|^2} \]

8. Some results coming from the $P_{\alpha\beta}(x, T)$ function

The variation domain of this function is the-half real axis, strictly positive as suitable for a length.

We can consider such function:

\[ 0 \leq P_{\alpha,\beta}(x(T)) \leq 1 \]

$P_{\alpha\beta}(0) = 0$ void of particle.

$P_{\alpha\beta}(x) = 0$ squeezed state of the optical electron.

$P_{\alpha\beta}(\infty) = 1$ existence of the particule.
9. Analytical Results for $F(\Delta \omega, t_0)$ Taken from $\Phi(t)$.

In such matter we dealt with: two distincts problems are solved: The non hydrogenic behaviour of the emitters or absorbers (He, Li, O, Mg, Ca, Na, K) and their ionized species, is modelled with the quantum defects from which exist a large litterature and even databases such as Topbase. The correct building of the wave functions is a solved problem. de Ker-

Setting $\Delta \omega = \omega - \omega_0$.

Fixing the $t_0$ parameter that is the width of the smooth function $g(t, t_0)$.

I rewrite down the Fourier Transform with the modified constant $I_1$ changed into a $\Gamma_{i \rightarrow f}$ resulting from the shortening of the radial integration domain or ”incomplete” dipolar squared matrix element.

\[ OpeQDFunction(x, ind, 3, 4) = \int_0^x (e^{2+ind}) \phi_{n=3-\delta_i} (r) \phi_{n=4-\delta_i} (r) dr \]

$a_0$ is the Bohr radius.

\[ I_1 = n_a^3 \times (OpeQDFunction(0.1, 1, 3, 4)^2) a_0^3 \]

The $\Gamma_{i \rightarrow f}$ parameter is always defined by the chosen transition $i \rightarrow f$ is obtained by solving:

\[ g(t, t_0) \times \Gamma_{i \rightarrow f} = OpeQDFunction(t, 1, n_i, n_f) \]

\[ F(\Delta \omega, t_0) = \frac{\Gamma_{i \rightarrow f} \sqrt{\pi} \omega}{\sqrt{\pi} \omega^2} \times \frac{(1-e^{-\omega_0} \theta + 2 \omega \cos(\omega t_0))}{1+\omega^2} \]

This function $F(\Delta \omega, t_0)$ can be integrated on the $\Delta \omega$ variable from $-\infty \rightarrow \infty$. Using the Stehle [1996], as a reference a function such as $F1(\Delta \omega) = \frac{\Gamma}{\Delta \omega}$ can not be normalized when integrated from $-\infty \rightarrow \infty$ while a function such as $F(\Delta \omega, t_0)$ can.

In fact:

\[ \int_{-\infty}^{\infty} F1((\Delta \omega)) d\Delta \omega = 0 \]

\[ \int_{-\infty}^{\infty} F((\Delta \omega, t_0)) d\Delta \omega = \Gamma_{i \rightarrow f} e^{t_0} \sqrt{2\pi} \]
10. Conclusions

This work whose conclusion is a new insight to complex atoms (more structure than Hydrogen) line broadening, lies on two different points. First, the pressure effect is included in the calculation of the probability function $P_{\alpha\beta}(x(T,N))$, where $x(N,T)$ is the cut-off parameter $\rho_C$ to be used. The surrounding of the radiating atom will fix it. It is clear that when $x(N,T) \to \infty$ the isolated atom line profile is obtained, in between the pressure effect is taken into account. The second interesting fact is included in the definition of the width $t_0$ of the smoothed $g(t,t_0)$ distribution function: It can exhibit oscillations of the profile $F(\Delta\omega,t_0)$. The choice of the width $t_0$ should be driven by a sound consideration of the surrounding atoms or ions background. It seems plausible the densest is the medium of the surrounding plasma or bath of neutral perturbers, the shorter the $t_0$ should be! Here are some sketches in Fig.4 and Fig.5 of the $F(\Delta\omega,t_0)$ for different width $t_0$ whose range goes from $t_0 = 1\mu s$ to $t_0 = 20s$.
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Profile function \( F(\Delta \omega, t_0) \) \( \Pi = |\langle \alpha | D | \beta \rangle|^2 = 1 \)

**Figure 2.** 3D Plot of \( F(\Delta \omega, t_0) = \frac{\sqrt{2}(1-e^{-t_0\omega}+2\omega \cos(t_0\omega))}{\pi(\omega+\omega^3)} \) profile function \( \omega_0 = 1.0301^{15} \).

It happens that if \( N_A = N_e \) the cut-off radius \( r_e \) is always smaller \( r_A = N_A^{-1} \). This is a proof that the pressure effects in a plasma with a charge density \( N_e \) is bigger than the pressure effects due to atoms of same densities \( N_A = N_e \).
Figure 3. dark blue line: cut-off radius $r_A = N_A^{-\frac{1}{3}}$ in Bohr unit as function of the atoms density $N_A$ in $cm^{-3}$. light blue curve: cut-off radius $r_e = 6.9 \times 10^8 \sqrt{\frac{T_e}{N_e}}$ for an electronic temperature of $T_e=1000K$ and a density of charges $N_e$. 
Figure 4. Oscillations of the $F(\Delta \omega, t_0)$ function for $t_0$ 1µ, 10µs, 10 ms
Figure 5. Oscillations of the $F(\Delta \omega, t_0)$ function for $t_0$, 0.01 ms, 0.1 s, 1 s, 7 s, 20 s and all profiles.
**FIGURE 6.** Display of cut-off bounds in unit of principal quantum number two approaches $L = N^{-\frac{1}{3}}_A$ yellow compared to $\lambda D$ Debye shielding radius brown. Explanation: for a density of $N = N_A = N_e = 4 \times 10^{21} \text{cm}^{-3}$ the low $n=2$ is obtained for $\lambda D$ and $n=4$ for $L_A = N^{-\frac{1}{3}}_A$. The cut-off $\rho_C$ varies from $4a_0$ to $16a_0$, from charged to neutral surroundings.

**FIGURE 7.** Debye length $\lambda D(N_A, T)$ for several temperatures.