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Interaction potentials for spectral line shapes in plasma

N. Ben Nessib

Groupe de Recherche en Physique Atomique et Astrophysique, Faculté des Sciences de Bizerte, 7021 Zarzouna, Tunisia
e-mail: nebil.bennessib@planet.tn

Abstract. In the standard formalism of Stark impact broadening of spectral lines and of cross sections, the electrostatic Coulomb potential is used to describe the interaction between the perturbing electrons and the emitting atom. Electronic correlations (screening effects) are usually taken into account by introducing a cut-off in the interaction when the electron-atom distance exceeds the Debye radius. A more consistent treatment to describe collective effects is the Debye-Hückel potential where the two-particle Coulomb field is shielded by the ensemble of the surrounding electrons. This is a good approximation only for high temperature and low density plasmas (weakly non ideal plasmas), while for strongly non ideal plasmas, the Coulomb cut-off potential or the ion sphere potential are more appropriate. These potentials, which can be written as the Coulomb potential with one or two correcting terms, are used for Stark impact broadening. New semi-classical collisional functions are derived for both the transition probability and the cross section, using the classical path approximation. The Coulomb potential is expanded in multipolar components and only the long range part is retained in the perturbation theory and in addition only the dipole term is retained for the calculation of the cross-sections between the levels that are dipolar electric transitions. Using the parametrization of the straight path trajectory in the collision frame, the semiclassical collisional functions for isolated neutral lines $A(z)$ and $a(z)$ are expressed in terms of the modified Bessel functions $K_0(z)$ and $K_1(z)$, these functions are revised when the cutoff or ion sphere potential is used. We have compared the effects of the Coulomb, cut-off and ion sphere potentials on the different collisional functions. The numerical results show that the increase in the screening leads to a decrease in these functions, especially for the lower values of the impact parameter. We investigate also a full quantum model based on quasiparticles treatment to describe the electron ion interaction in a non ideal plasma. We developed this simplified quantum formalism of the emission which take into account the interaction between particles such that it becomes applicable to a weakly non ideal plasma. We give analytic expression of the line width and explain the non linearity of the width via the density observed in some experiments.

Key words. atomic processes – Stars: atmospheres

1. Introduction

Collisions between atoms (or ions) and electrons play an important role in Astrophysics

Send offprint requests to: N. Ben Nessib

for the interpretation of line spectra and for the modellisation of stellar interiors. Correlation effects and plasma shielding effects are not negligible in the physical conditions of white dwarfs atmospheres, owing to their high density. They also play a role in the case of rather cool stars.

In a non-correlated plasma, the interaction is described by the electrostatic Coulomb potential. It is well known, however, that the extreme conditions of some plasma environments can drastically alter transition rates from their values for the corresponding isolated systems. Long-range Coulomb interactions are screened by plasmas, leading to shorter-range interactions.

In the case of a weakly coupled plasma, the amount of the Coulomb forces in the interaction energy may be defined by the Debye-Hückel theory which corresponds to a classical treatment of the charged particle interactions (Debye & Hückel 1923).

2. Coulomb potential and semiclassical formalism for ideal plasma

Stark broadening parameter calculations have been performed within the semiclassical perturbation method (Griem, H. R. 1974; Sahal-Bréchot 1969a,b).

Stark full width (W) at the intensity half maximum (FWHM) and shift (d) of an isolated spectral line, may be expressed as (Sahal-Bréchot 1969a,b):

$$W = N\int v f(v)dv \times \left(\sum_{i'\neq i}\sigma_{ii'}(v) + \sum_{f'\neq f}\sigma_{ff'}(v) + \sigma_{el}\right) \quad (1)$$

$$d = N\int v f(v)dv \int_{R_3}^{R_D} 2\pi\rho d\rho \sin 2\phi_p \quad (2)$$

where N is the electron density, $f(v)$ the Maxwellian velocity distribution function for electrons, ρ denotes the impact parameter of the incoming electron, i and f denote the initial and final atomic energy levels, and i', f' their corresponding perturber levels. The inelastic cross section $\sigma_{j,j'}(v)$ can be expressed by an integral over the impact parameter of the transition probability $P_{jj'}(\rho, v)$ as:

$$\sum_{i'\neq i}\sigma_{jj'}(v) = \frac{1}{2}\pi {R_1}^2 + \int_{R_1}^{R_D}\sum_{j\neq j'}P_{jj'}(\rho, v),\ j = i, f \quad (3)$$

and the elastic cross section is given by

$$\sigma_{el} = 2\pi R_2^2 + \int_{R_2}^{R_D} 8\pi\rho d\rho \sin^2\delta \quad (4)$$

$$\delta = (\phi_p^2 + \phi_q^2)^{1/2} \quad (5)$$

The phase shifts ϕ_p and ϕ_q due respectively to the polarisation potential (r^{-4}) and to the quadrupolar potential (r^{-3}), are given in Section 3 of Chapter 2 in Sahal-Bréchot (1969a). R_D is the Debye radius. All the cut-offs R_1, R_2, R_3 are described in Section 1 of Chapter 3 in Sahal-Bréchot (1969b).

The transition probabilities are related to the collisional functions $A(z)$ by:

$$P_{ij}(\rho, v) = \frac{4I_H^2}{E(E_j - E_i)}\frac{m}{m_e}f_{ij}\frac{a_0^2}{\rho^2}A(z) \quad (6)$$

where f_{ij} is the oscillator strength, I_H the ionization energy of hydrogen, a_0 the Bohr radius, m_e the electron mass and E the energy of the perturber of reduced mass m

$A(z)$ is expressed in term of the modified Bessel functions:

$$A(z) = z^2[K_0^2(z) + K_1^2(z)] \quad (7)$$

This can be written also as:

$$A(z) = A_0(z) + 2A_{\pm}(z) \quad (8)$$

where

$$A_0(z) = z^2K_0^2(z) \quad (9)$$

and

$$A_{\pm}(z) = \frac{1}{2}z^2K_1^2(z) \quad (10)$$

3. Potentials for non ideal plasma

3.1. Non-ideality factor γ

Depending on their temperature T and their electronic density N_e, plasmas may be classified into different families (Ben Nessib et al. 1997).

We define the non-ideality factor γ as the ratio of potential energy E_p between charged particles and kinetic energy E_k :

$$\gamma = \frac{E_p}{E_k} \tag{11}$$

The non-ideality factor is expressed as follows

$$\gamma = 1.80 \times 10^{-3} \frac{(N_e)^{1/3}}{T} \tag{12}$$

where the electronic density N_e is expressed in cm^{-3} and the plasma temperature T in Kelvin.

3.2. Debye-Hückel potential

This potential is often a good approximation for high temperature and low density plasmas, but it is no longer valid in the limit of low temperatures and high densities, where the mean electrostatic interaction energy is much greater in magnitude than the mean kinetic energy of the ions.

This potential can be expressed as (Debye & Hückel 1923):

$$V_{DH}(t) = -Z_p e^2 \sum_{i=1}^{N} \frac{1}{r_{ip}} e^{-\frac{r_p}{R_D}} \tag{13}$$

and the collision function is modified as (Cooper et al. 1971):

$$A(z) = z^2 K_0^2(\beta) + \beta^2 K_1^2(\beta) \tag{14}$$

where $\beta = \sqrt{z^2 + \frac{z^2}{z_D^2}}$ and $z_D = \frac{R_D \omega_{ij}}{v}$.

3.3. Cut-off potential

In a high density and low temperature plasma, the cutoff potential is reliable to describe the interaction process. For these non ideal plasmas conditions, the Cut-off potential is more suitable to describe the interaction between the perturber and the emitter, since it adds a corrective term as follows (Ben Nessib et al. 1997):

$$V_c(t) = \begin{cases} -Z_p e^2 \sum_{i=1}^{N} \frac{1}{r_{ip}}(1 - \frac{r_p}{r_c}), r_p \leq R_c \\ 0, r_p \geq R_c \end{cases} \tag{15}$$

where R_c designates a cut-off parameter assumed to be equal to the Ion Sphere radius $R_c = (3Z/4\pi N_e)^{1/3}$.

The collision function for transition probability becomes:

$$\begin{aligned} A_c(z) &= A(z) - \pi \frac{z^2}{z_c} e^{-z} \left[K_0(z) + K_1(z)\right] \\ &+ \frac{\pi^2}{2} \frac{z^2}{z_c^2} e^{-2z} \end{aligned} \tag{16}$$

3.4. Ion sphere potential

For a strongly non-ideal plasma, the ion sphere model is found to be more suitable:

$$V^{IS}(t) = \begin{cases} -Z_p e^2 \sum_{i=1}^{N} \frac{1}{r_{ip}}(1 - \frac{3}{2}\frac{r_p}{R_c} + \frac{1}{2}\frac{r_p{}^3}{R_c{}^3}), r_p \leq R_c \\ 0, r_p \geq R_c \end{cases}$$

The collision function becomes (Ben Chaouacha et al. 2004, 2005):

$$A^{IS}(z) = A_0^{IS}(z) + 2A_{\pm}^{IS}(z) \tag{17}$$

where

$$\begin{aligned} A_0^{IS}(z) &= \left[zK_0(z) - \frac{3}{2}\frac{\pi z}{2z_c} e^{-z} \right. \\ &\left. + \frac{1}{2}\left(\frac{z}{z_c}\right)^3 \left(\frac{\sin(x_c z)}{z^2} - \frac{x_c \cos(x_c z)}{z}\right)\right]^2 \end{aligned} \tag{18}$$

and

$$\begin{aligned} A_{\pm}^{IS}(z) &= \frac{1}{2}\left[zK_0(z) - \frac{3}{2}\frac{\pi z}{2z_c} e^{-z} \right. \\ &\left. + \frac{1}{2}\frac{z^2}{z_c^3} \sin(x_c z)\right]^2 \end{aligned} \tag{19}$$

4. Line shapes in weakly non ideal plasma

If we consider a plasma with ions and electrons in interactions, the hamiltonian of the system can be written in the form (Eleuch et al. 2004):

$$H = H_0 + H_F + H_{int} + H_{nl} \tag{20}$$

where

$$H_0 = \hbar\omega_0 b^+ b \tag{21}$$

with b^+ and b the bosonic creation and annihilation operators, verifying the relation of commutation $[b, b^+] = 1$.

$$H_F = \hbar\omega_0 a^+ a \tag{22}$$

a^+ and a are the creation and annihilation operators of a photon verifying the commutation relation $[a, a^+] = 1$.

$$H_{int} = \hbar g(a^+ b + b^+ a) \tag{23}$$

where g is the coupling constant.

$$H_{nl} = \alpha\hbar(b^+ b^+ bb) \tag{24}$$

where α is the interaction constant.

Using the Master equation, in interaction representation, the line profile as the Fourier transform of the auto-correlation function will be:

$$I(\omega) = \frac{\gamma n_{th}}{\left(\frac{g^2}{\Delta\omega + 2\alpha N} - \Delta\omega\right)^2 + \left(\frac{\gamma}{2}\right)^2} \tag{25}$$

For weakly non ideal plasmas, the values of the coupling and the non linear interaction are weakly compared to the dissipation of the system:

$$g^2 \ll \left(\frac{\gamma}{2}\right)^2$$

and

$$(\alpha N)^2 \ll \left(\frac{\gamma}{2}\right)^2$$

For the N perturbers, the full width at half maximum (FWHM) is then

$$w = \gamma_1 N - \gamma_2 N^3 \tag{26}$$

where

$$\gamma_1 = \gamma + \frac{16g^2}{\gamma} \tag{27}$$

and

$$\gamma_2 = \frac{4\alpha^2}{\gamma} \tag{28}$$

This simplified quantum formalism (Eleuch et al. 2004) of a line profile in a weakly non ideal plasma, gives a Lorentzian profile with modified width, when interactions between constituents of the plasma are very weak.

5. conclusion

The choice of cut-off or ion sphere potentials describing the interaction of the perturber with the emitter are good models for describing correlations in non ideal plasma.
The simplified quantum formalism allows to explain the variations of the line widths with the density in a weakly non ideal plasma.

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