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Comparison of electron width models for fast line profile calculations

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ABSTRACT

The first non-vanishing term in the perturbation expansion of the electron contribution to the line width, commonly used in spectral line broadening by plasmas, was previously expressed in terms of the thermally averaged bremsstrahlung Gaunt factor. The approximations in the derivation, however, suggest that the result is uncertain. The electron width formula is tested with the hydrogen Balmer series and found suspect. Calculations for the He II Lyman series also display similar difficulties. The limitation of this electron width formulation is traced to the absence of an explicit strong collision cutoff beyond which the second-order theory is invalid.

1. Introduction

Spectral lines provide valuable information [1] and Stark-broadening models have been developed [2–4] to characterize plasmas [5–7]. These models share approximations such as quasi-static ions and impact electrons [1]. Due to the large number of calculations often necessary to analyze spectra, these efforts employ fast algorithms to compute the width contribution from perturbing electrons. One approach expresses the first non-vanishing term in the perturbation expansion of the electron width as the thermally averaged bremsstrahlung Gaunt factor [8]. This formula was successfully tested for transitions involving atomic levels with low principal quantum numbers (PQN) [8]. Contrary to other approaches [2,3,9], the Gaunt factor expression [8] does not include an explicit strong collision cutoff beyond which perturbation theory becomes invalid. Consequently, there remained uncertainty whether the formula extends to spectral lines associated with higher PQNs.

Unfortunately, plasma experiments are challenging and data often contain large uncertainties making it difficult to discriminate among models. One notable exception is the high-precision measurements of the hydrogen Balmer series [10]. The purpose here is to compare two electron width models [2,8] for fast line profile calculations at the conditions of the measured spectra. This requires an extension of the O'Brien–Hooper formalism [8] to neutral radiators readily accomplished from their main results. The comparisons show that the connection to bremsstrahlung used in line profile calculations [4,7,8,11,12] is suspect. A second test for the He II Lyman series yields similar conclusions. Possible consequences in the analysis of recent opacity experiments [6] are entertained. The electron width models are also applied to isolated lines in Li-like systems and compared with measurements [13].

2. Electron widths

The line shape function for an ion emitting or absorbing (the radiator) a photon of energy $\hbar\omega$ while immersed in a plasma is given in the "standard" Stark-broadening theory by [1]

$$I(\omega) = \int_0^\infty dF W(F) J(\omega, F) \tag{2.1}$$

where $W(F)$ is the ion electric microfield probability distribution function and (neglecting lower state broadening to simplify notation)

$$J(\omega, F) = -\pi^{-1} \mathrm{Re} Tr_a \left\{ \vec{d} \cdot \left[i\Delta\omega - i\vec{d}\cdot\vec{F}/\hbar + \phi(\Delta\omega) \right]^{-1} \rho \vec{d} \right\} \tag{2.2}$$

Here, Tr_a denotes a trace over the internal states of the radiator, $\vec{d}$ is the radiator dipole operator, ρ describes the radiator internal state populations, and the matrix elements of the detuning frequency from line center are given by

$$\Delta\omega_{\mu\nu} = \omega - \omega_\mu + \omega_\nu \tag{2.3}$$

with $\hbar\omega_\alpha$, the energy of the radiator internal state α.

The description of electron broadening in ϕ often assumes weak collisions of duration much shorter than the internal radiator state lifetimes involved in the radiative transition [1]. Hence, collisions are treated in perturbation theory retaining only the first non-vanishing term in the electron–radiator interaction simplified to the dipole approximation. The resulting second-order electron width is then given by

$$\phi(\Delta\omega) = -\frac{\vec{d}\cdot\vec{d}}{3\hbar} \int_0^\infty dt\, e^{i\Delta\omega t} Tr_e \left\{ \vec{F}_e \cdot e^{-iH_e t/\hbar} \rho_e \vec{F}_e e^{iH_e t/\hbar} \right\} \tag{2.4}$$

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where Tr_e, ρ_e, and H_e denote a trace, density matrix, and Hamiltonian for an electron gas, respectively, and $\vec{F}_e$ is the electric field produced by the electron gas at the radiator. In the line formulations of interest here, the electron width is rewritten in the form

$$\phi(\Delta\omega) = -\frac{4\pi n_e e^2}{3\hbar}\sqrt{\frac{2m}{\pi T}}\vec{d}\cdot\vec{d}G(\Delta\omega) \tag{2.5}$$

where m, n_e, and T, are the electron mass, number density, and temperature (energy units), respectively, and the G-function is related to the space and time dependent charge-density fluctuations in an electron gas [14]. Two approaches for computing the G-function [2,8] that are commonly used in experimental plasma diagnostics are compared in the present work.

2.1. Lee model

The second-order width can be written in terms of an integral over the momentum transfer in the electron–radiator collision [2,14]. Assuming $\hbar\Delta\omega \ll T$ yields

$$\phi(\Delta\omega) \approx \frac{2e^2T}{3\pi\hbar\Delta\omega}\vec{r}_a\cdot\vec{r}_a\int_o^{k_m} dk k^2 \operatorname{Im}\varepsilon^{-1}(k,\Delta\omega) \tag{2.1.1}$$

leading to

$$G(\Delta\omega) = \int_o^{k_m}\frac{dk}{k}\exp\left\{-\frac{1}{2k^2\lambda_e^2}\frac{\Delta\omega^2}{\omega_p^2}\right\}\frac{1}{|\varepsilon(\Delta\omega,k)|^2} \tag{2.1.2}$$

where λ_e and ω_p are the electron Debye length and plasma frequency,

$$\lambda_e^2 = \frac{T}{4\pi n_e e^2} \tag{2.1.3}$$

$$\omega_p^2 = \frac{4\pi n_e e^2}{m} \tag{2.1.4}$$

e is the elementary unit of electric charge, and $\varepsilon(\omega,k)$ is the dielectric function for a homogeneous electron gas. Thus, the latter neglects the net radiator charge effects on the perturbing electrons. Nevertheless, it is expected to be valid for charged radiators [9].

The cutoff k_m, which limits the momentum transfer in a collision and avoids the divergence of the integral, can be estimated by considering the partial wave expansion of the full electron–radiator interaction [15,16], which contains the spherical Bessel function $j_\ell(kr_a)$ [17] with r_a the radial position of the bound electron. In most cases of interest $kr_a \ll 1$ and the lowest order non-vanishing term yields the dipole approximation. Thus, a reasonable upper limit is given by k values that are cutoff by fast oscillations in $j_\ell(kr_a)$ [15],

$$\frac{\hbar^2k_m^2}{2m} \approx E_j \tag{2.1.5}$$

where E_j is the binding energy of the radiator jth level. For hydrogenic systems,

$$k_m^2a_o^2 \approx \frac{Z^2}{n^2} \tag{2.1.6}$$

with Ze the nuclear charge, n the level PQN, and a_o the Bohr radius. Further approximations replace the dielectric function by its $\Delta\omega \to 0$ and ∞ limits to get [2]:

$$G_o = \frac{1}{2}\left\{\ln\left[1+k_m^2\lambda_e^2\right] - \frac{k_m^2\lambda_e^2}{1+k_m^2\lambda_e^2}\right\} \tag{2.1.7}$$

$$G_\infty(\Delta\omega) = \frac{1}{2}E_1\left(\frac{1}{2k_m^2\lambda_e^2}\frac{\Delta\omega^2}{\omega_p^2}\right) \tag{2.1.8}$$

with $E_1(z)$ the exponential integral [17]. Finally, Lee takes [2]

$$G_L(\Delta\omega) = \sigma_n + Min[G_o, G_\infty(\Delta\omega)] \tag{2.1.9}$$

where neglected strong collisions are accounted by $\sigma_2 = 1.5$, $\sigma_3 = 1.0$, $\sigma_4 = 0.75$, $\sigma_5 = 0.5$ and $\sigma_n = 0.4$ for $n > 5$ [9,18]. For large detuning,

$$G_L(\Delta\omega \to \infty) = \sigma_n + k_m^2\lambda_e^2\frac{\omega_p^2}{\Delta\omega^2}\exp\left(-\frac{1}{2k_m^2\lambda_e^2}\frac{\Delta\omega^2}{\omega_p^2}\right) \tag{2.1.10}$$

Thus, a correction is necessary to reproduce the quasi-static limit [2]. The Griem et al. [9] and Calisti et al. [3,18] models are similar to Lee's [2] and need not be considered separately.

The subroutines to compute Stark profiles of one- and two-electron systems with G_L were incorporated into widely used codes for designing and analyzing experiments [19,20]. In addition, the subroutines were generously made available for other applications [21].

2.2. O'Brien–Hooper model

An alternative expression for the G-function is given by the thermal average [8]

$$G_{OH}(\Delta\omega; Z_{net}) = \frac{\pi}{\sqrt{3}}\int_o^\infty\frac{dE}{T}e^{-E/T}g(E,\Delta\omega; Z_{net}) \tag{2.2.1}$$

where $g(E,\Delta\omega; Z_{net})$ is the bremsstrahlung Gaunt factor for absorption of a photon with energy $\hbar\Delta\omega$ by an electron with initial energy E scattering in the Coulomb potential produced by the net radiator charge, $Z_{net}e$. It can be expressed in terms of the radial integrals [8,22–24]

$$\int_o^\infty dr\psi_\ell(r,E)\psi_{\ell\pm1}(r,E+\hbar\Delta\omega) \tag{2.2.2}$$

for partial wave ℓ and boundary conditions for the perturbing electron wave function

$$\psi_\ell(r\to 0,E) \propto r^{\ell+1} \tag{2.2.3a}$$

$$\psi_\ell(r\to\infty,E) \propto \frac{\sin(qr+\delta_\ell)}{qr} \tag{2.2.3b}$$

with wave vector $\hbar^2q^2/2m = E$ and δ_ℓ the phase shift.

In the case of neutral radiators $\psi_\ell(r,E) = j_\ell(qr)$, the spherical Bessel function in the partial wave expansion of plane waves. Thus, the Gaunt factor reduces to the Born approximation [24] with thermal average [25]

$$\begin{aligned} G(\Delta\omega; Z_{net}=0) &= G_{OH}^{Born}(\Delta\omega) \\ &= e^{\hbar\omega/2T}K_o(\hbar\Delta\omega/2T) \end{aligned} \tag{2.2.4}$$

where $K_o(z)$ is the modified Bessel function of the second kind [17]. For large detuning

$$G_{OH}^{Born}(\Delta\omega\to\infty) \propto \Delta\omega^{-1/2} \tag{2.2.5}$$

reproducing the Holtsmark quasi-static limit [2]. The G-function expression in Eq. (2.2.1) describes ideal electrons interacting with the net radiator charge; however, electron-screening effects can be approximated by $G_{OH}(\Delta\omega = \omega_p)$ for $\Delta\omega \le \omega_p$ [26,27]; thus, avoiding the