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A simplified approach to line broadening in dense plasmas

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Abstract
A simplified approach is presented for the analysis of broadening and shift of emission lines in hot dense plasmas. The basic approximation which allows this simplified approach is the factorization of the wavefunction for the many-body problem into the wavefunction for the plasma particles, and the wavefunction which describes the internal degrees of freedom.

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1. Introduction

Existing algorithms for evaluating atomic spectral line shapes in plasmas are based on rigorous theoretical derivations and are, experimentally, well established (Griem 1997). Nevertheless, we have found it advantageous to develop a new theoretical approach for the purpose of constructing an opacity code for light ions in dense hot plasmas. The evaluation of atomic spectral line shape in plasmas requires the reduction of the many-body problem of the plasma particles (including internal degrees of freedom) to an equation for the time evolution of the averaged atomic dipole operator, which in frequency space yields the spectrum. In existing theories, this task is performed by using kinetic theory techniques (Hussey *et al* 1975) or by the Zwanzig projection operator method (Smith and Hooper 1967, Boercker *et al* 1987). The first approach focuses on the plasma electrons effect. In the cases where ion motion during the radiation time may be neglected, the theory accounts for the effect of ions by including the interaction of a single realization of (static) ion microfield in the effective Hamiltonian of the radiator and by averaging the dipole operator over all realizations of the ion microfield (Griem 1997). The second approach based on the Zwanzig projection operator method also allows the ion dynamics effect to be included (Boercker *et al* 1987). In the present work, an alternative simplified approach is derived for the evaluation of spectral line shapes. Our approach starts from the factorization of the wavefunction for the many-body problem into a product of two wavefunctions: one describing the plasma particles, and the other accounting for the ion's internal degrees of freedom. A similar approximation was applied in the past (Baranger 1958) using similar factorization also to the plasma wavefunction. In the present work we push this

approach further, avoiding any further approximation to the plasma wavefunction. In section 2, a derivation is described, which reduces the many-body problem to a stochastic differential equation in time. In section 3, the equation for the averaged dipole operator is derived, using the Bourret approximation (Brissaud and Frisch 1974). The averaged equation is solved by treating the time dependence of the ion field (ion dynamics) as a small perturbation. Section 4 is devoted to a summary and discussion of the results.

2. The factorization approximation

We shall start with the picture of a plasma made of point ions and electrons where the plasma Hamiltonian H_p does not involve the internal degrees of freedom in an ion. We shall assume that the wavefunction for the atom–plasma system may be factorized as (Baranger 1958)

$$\Psi = \Psi_A \Psi_P \tag{1}$$

where Ψ_A represents the N_B electrons in the radiating atom (or ion) and Ψ_P represents the perturbers (i.e. plasma which is made of point electrons and ions). The dynamics of Ψ_P is controlled by the Hamiltonian H_p that includes the kinetic energy and the interaction between perturbers. The total wavefunction Ψ is evolved by the Hamiltonian $H_A + H_p + V$, where H_A is the Hamiltonian of the unperturbed emitter and V is the (Coulomb) interaction between the electrons in the emitter and all the perturbers (point ions and electrons). The factorization assumption (1) that is the main approximation in the present work allows the derivation of relatively simple results. This approximation neglects the correlation and exchange interaction between a bound electron and a free electron in the plasma and assumes that the dynamics of the plasma wavefunction Ψ_P is not affected by the evolution of the internal degrees of freedom of the radiator (i.e. Ψ_A). We have checked the effect of correlation and exchange interaction between bound and free electrons in hot plasmas (e.g. F_e at 2 keV and natural density) by comparing the results of a detailed, numerical, electron–ion scattering calculation using a totally anti-symmetric wavefunction to the results of a calculation with the wavefunction of the scattered electron factored as Ψ_P in equation (1). We have found that in typical cases, the factorization approximation (equation (1)) is justified. With this approximation, it is readily found that the dynamics of the internal degrees of freedom of an ion in the plasma is governed by a Hamiltonian of the form $H_A + W$ where

$$W\left(\vec{r}_1 \ldots \vec{r}_{N_B}, t\right) = \sum_{j=1}^{N_B} \int \frac{e}{|\vec{r}_j - \vec{r}'|} (Zen^I(\vec{r}', t) - en^e(\vec{r}', t))\, \mathrm{d}^3\vec{r}' \tag{2}$$

i.e. in the factorization approximation, the interaction potential, W, acting on the bound electrons is a functional of the electron and ion densities, n^I, n^e, in the plasma only. Coordinates of plasma particles and plasma correlations do not appear explicitly in the ion–plasma interaction potential. They do, however, affect the dynamics of n^I and n^e, that is governed by the equation for Ψ_P or by any, possibly quantum (Klimontovich 1982), plasma kinetic equation derived from it.

We define the time-averaged densities by $\bar{n}^{e,I}(\vec{r})$, and the fluctuations around these averages by $\bar{n}^{e,I}(\vec{r}) = \lim_{\Theta\to\infty} \frac{1}{\Theta} \int_0^\Theta n^{e,I}(\vec{r}, t)\, \mathrm{d}t$ and $\delta n^{e,I}(\vec{r}, t) = n^{e,I}(\vec{r}, t) - \bar{n}^{e,I}(\vec{r})$. Similarly, we also split the plasma potential into the averaged potential $\bar{W}\left(\vec{r}_1 \ldots \vec{r}_{N_B}\right)$ and the fluctuating part $\delta W\left(\vec{r}_1 \ldots \vec{r}_{N_B}, t\right)$.

The static 'smooth' electron or ion density $\bar{n}^{e,I}(\vec{r})$ in the vicinity of a test ion depends on the distance from it and changes as the probability of finding electrons (or ions) at this distance, i.e. it is proportional to the electron–ion (or ion–ion) correlation function (Percus 1962) and

may be obtained by self-consistent field models (see, for example, Liberman 1979). Temporal fluctuations in the density due to passing particles are smoothed out by the averaging process, and appear only in δW. Note that, due to the extraction of the inhomogeneous part $\bar{W}$, the fluctuating component δW is statistically homogeneous in space and time.

The Hamiltonian which governs the dynamics of the internal degrees of freedom of an ion in the plasma, when represented in terms of the eigenfunctions and eigenvalues $\{\phi_a, \varepsilon_a\}$ of $H_A + \bar{W}$, reads as $H_{ab} = \delta_{a,b}\varepsilon_a + \delta W^e_{ab}(t) + \delta W^I_{ab}(t)$ with $\delta W^{e,I}_{ab}(t) = a^{e,I}\int \hbar\Omega_{ab}(\vec{r}')\delta n^{e,I}(\vec{r}', t)\,\mathrm{d}^3\vec{r}'$ where $a^e = -1, a^I = Z$, and Ω_{ab} is the matrix element of the Coulomb interaction between all bound electrons and a point charge in the plasma:

$$\hbar\Omega_{ab}(\vec{r}') = \int \phi_a\big(\vec{r}_{e1}, \ldots, \vec{r}_{eN_B}\big)\left[\sum_{j=1}^{N_B}\int \frac{e^2}{|\vec{r}_{ej} - \vec{r}'|}\right]\phi_b\big(\vec{r}_{e1}, \ldots, \vec{r}_{eN_B}\big)\,\mathrm{d}^3 r_{e1}\ldots\mathrm{d}^3 r_{eN_B}. \quad (3)$$

3. The spectrum

The spectrum is determined by the dipole correlations (Griem 1997):

$$F(\omega) = \sum_{a,b}\frac{1}{2\pi}|d_{ab}|^2\int_0^\theta \mathrm{e}^{\mathrm{i}\omega\tau}[\rho_{ab}(0)\rho^*_{ba}(\tau)]_{\mathrm{av}}\,\mathrm{d}\tau \quad (4)$$

where $\rho = \int \Psi_A\big(\vec{r}_1\ldots\vec{r}_{N_B}, t:\eta\big)\Psi^*_A\big(\vec{r}'_1\ldots\vec{r}'_{N_B}, t:\eta\big)f(\eta)\,\mathrm{d}\eta$ is the atomic density matrix, η denotes the parameters that characterize initial conditions and $\vec{d} = \sum_{j=1}^{N_B} e\vec{r}_j$ is the dipole. The operation $[\cdots]_{\mathrm{av}}$ denotes an averaging over all possible realizations of electron and ion density fluctuations $\delta n^e, \delta n^I$. In the following, we shall also consider averaging over realizations of electron density fluctuations with a fixed single realization of ion density fluctuations. This will be denoted by $[\cdots]_{\mathrm{ave}}$. The averaging over ion realizations will be denoted by $\{\cdots\}_{\mathrm{avi}}$ so that $[\cdots]_{\mathrm{av}} = \{[\cdots]_{\mathrm{ave}}\}_{\mathrm{avi}}$.

In order to evaluate the spectrum (4), it is customary to consider the Green function (Sobel'man *et al* 1981) for the density matrix $(\vec{d}_{ab}\rho_{ab}(t))\cdot(\vec{d}_{ba}\rho_{ba}(0)) = \sum G_{aba'b'}(t, 0)\vec{d}_{ab}\cdot\vec{d}_{b'a'}$. Starting with the equation for Ψ_A with the definition of ρ and G, it is readily seen that G obeys the equation $\mathrm{i}\hbar\frac{\partial}{\partial t}G = LG$ with the initial condition $G_{pq}(t', t') = \delta_{p,q}$ or equivalently, it obeys the integro-differential equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}G(t, t') = [L^0 + L^I(t)]G + L^e(t)G^{\mathrm{slow}} + \frac{1}{\mathrm{i}\hbar}\int_0^t \mathrm{d}t_1\, L^e(t)G^{\mathrm{slow}}(t, t_1)L^e(t_1)G(t_1, t'). \quad (5)$$

In the above equation L is the Liouville operator $L_{pq} = H_{aa'}\delta_{bb'} - H_{bb'}\delta_{aa'} = L^0 + L^I + L^e$ where

$$\begin{aligned} L^0_{pq} &= L^0_{aba'b'} = \delta_{aa'}\delta_{bb'}(\varepsilon_a - \varepsilon_b) \\ L^{e,I}_{pq}(t) &= L^{e,I}_{aba'b'}(t) = a^{e,I}\int A_{aba'b'}(\vec{r}')\delta n^{e,I}(\vec{r}', t)\,\mathrm{d}^3\vec{r}' \\ A_{aba'b'} &= \hbar\Omega_{aa'}\delta_{bb'} - \hbar\Omega_{b'b}\delta_{a'a} \end{aligned} \quad (6)$$

$p(a, b) = (a-1)N_B + b$, $q(c, d) = (c-1)N_B + d$, and G^{slow} is the solution of the equation $\mathrm{i}\hbar\frac{\partial}{\partial t}G^{\mathrm{slow}} = (L^0 + L^I)G^{\mathrm{slow}}$ with the initial condition $G^{\mathrm{slow}}_{pq}(t', t') = \delta_{p,q}$.

In terms of G, the spectrum (4) may be written as

$$F(\omega) = \sum_{abcd}\vec{d}_{ab}\cdot\vec{d}_{cd}(\Phi(\omega))_{abcd} \quad (7)$$

where $\Phi(\omega)$ is the Laplace transform of $[G(t, 0)]_{\mathrm{av}}$, i.e. $\Phi(\omega) = \frac{1}{2\pi}\int_0^\infty \mathrm{e}^{\mathrm{i}\omega t}[G(t, 0)]_{\mathrm{av}}\,\mathrm{d}t$.

The only approximation used in the derivation of equation (5) *from the basic equation for* Ψ *is the factorization assumption* (1). In order to reduce it to an equation for the averaged function $[G(t,t')]_{\rm ave}$ we perform the averaging over realizations of electron fluctuations, and further assume that the correlation time for electron fluctuations is much shorter than the typical evolution time of G. This assumption is justified when the plasma frequency $\omega_{pe} = \sqrt{\frac{4\pi\bar{n}^e e^2}{m}}$ (where m is the electron mass) is much larger than the norm of the radiator–plasma coupling matrix $\frac{\delta W^e + \delta W^I}{\hbar}$. In this case we may assume that δn^e and G are statistically independent and use the Bourret approximation (Brissaud and Frisch 1974), i.e.

$$\begin{aligned}[\delta n^e(\vec{r}',t_1)\delta n^e(\vec{r}'',t_2)G(t_2,t')]_{\rm ave} &\approx [\delta n^e(\vec{r}',t_1)\delta n^e(\vec{r}'',t_2)]_{\rm ave}[G(t_2,t')]_{\rm ave} \\ &= \tilde{S}^{ee}(\vec{r}'-\vec{r}'',t_1-t_2)[G(t_2,t')]_{\rm ave} \end{aligned} \tag{8}$$

where $\tilde{S}^{ee}$ is the electron–electron density correlation function.

Since the relevant integration time in equation (5) is limited by the electron–electron correlation time $\tau_e \sim \frac{1}{\omega_{pe}}$ that is always much shorter than the variation time of the ion field $\tau_i \sim \frac{1}{\omega_{pi}}$, the effect of temporal variation of the ion field on $G^{\rm slow}(t,t_1)$ may be neglected. With these approximations, equation (5) when averaged over realizations of electron fluctuations is reduced to

$$\begin{aligned}\left\{\mathrm{i}\hbar\frac{\partial}{\partial t} - (L^0 + L^{SI})\right\}[G(t,t')]_{\rm ave} - \frac{1}{\mathrm{i}\hbar}\int_0^t K(t-t_1)[G(t_1,t')]_{\rm ave}\,\mathrm{d}t_1 \\ = \{L^I(t) - L^{SI}\}[G(t,t')]_{\rm ave} \end{aligned} \tag{9}$$

where $K(t)$ represents the electron 'collision' operator

$$K(t) = \int \frac{\mathrm{d}^3\vec{k}}{(2\pi)^3} A(\vec{k}) \left[\int \mathrm{d}^3\vec{r}\,\mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{r}}\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(L^0+L^{SI})t}\,\tilde{S}^{ee}(\vec{r},t)\right] A(-\vec{k}). \tag{10}$$

In writing equation (9) we have replaced the ion interaction $L^I(t)$ on the left-hand side by its static approximation, L^{SI}, and compensated for that in the right-hand side of the equation (no approximation is involved in this rearrangement). In this way, the right-hand side represents the ion dynamics correction. We are interested in the cases where the ion interaction is predominantly static, i.e. the right-hand side of equation (9) may be considered as a small correction. This enables us to solve the equation by iteration. We start with the zero-order approximation which neglects the ion dynamics term. This yields $G^{(0)}$ that depends only on the time difference $t_1 - t'$, higher order corrections are obtained by the iteration

$$\begin{aligned}\left[-\mathrm{i}\left(\omega - \frac{(L^0+L^{SI})}{\hbar}\right) + \Gamma(\omega)\right][\tilde{G}^{(n)}(\omega)]_{\rm ave} \\ = I + \frac{\mathrm{i}}{2\pi\hbar}\int_{-\infty+\mathrm{i}\xi}^{\infty+\mathrm{i}\xi} \Delta L^I(\omega-\omega',\beta)[\tilde{G}^{(n-1)}(\omega')]_{\rm ave}\,\mathrm{d}\omega' \end{aligned} \tag{11}$$

with $\Gamma(\omega,\alpha) = \int_0^\infty \mathrm{e}^{\mathrm{i}\omega t} K(t,\alpha)\,\mathrm{d}t$ and $\Delta L^I(\omega) = \frac{L^{SI}}{\omega-\omega'} - \int_0^\infty \mathrm{e}^{\mathrm{i}\omega t} L^I(t)\,\mathrm{d}t$.

In the zero-order approximation we get

$$\Phi^0(\omega) = \left(\int (\Im(\omega,\alpha))^{-1} D f^{SI}(\alpha)\,\mathrm{d}\alpha\right) \tag{12}$$

where

$$\Im(\omega,\alpha) = (\tilde{G}^{(0)}(\omega,\alpha))^{-1} = -\mathrm{i}\left(I\omega - \frac{1}{\hbar}L^0 - \frac{1}{\hbar}L^{SI}(\alpha)\right) + \Gamma(\omega,\alpha) \tag{13}$$

α denotes the set of parameters that characterize a realization of static ion fluctuation $\delta n^{SI}(\alpha)$ (which in practice should be transformed to the field at the radiator point) and $f^{SI}(\alpha)$ is the probability for this realization (ion microfield distribution).

Correcting to first order we get

$$[\tilde{G}(\omega)]_{\text{ave}} = \left[-\mathrm{i}\left(\omega - \frac{(L^0 + L^{SI}(\alpha))}{\hbar}\right) + \Gamma(\omega, a)\right]^{-1} \times \left[I + \frac{\mathrm{i}}{2\pi\hbar}\int_{-\infty+\mathrm{i}\xi}^{\infty+\mathrm{i}\xi} \Delta L^I(\omega - \omega', \beta)[\tilde{G}^{(0)}(\omega', \alpha)]_{\text{ave}}\,\mathrm{d}\omega'\right] \tag{14}$$

where β denotes the set of parameters that characterize the correction $\delta n^I(\vec{r}, t) - \delta n^{SI}(\vec{r})$ and ξ is chosen so that all the poles in the integrand are below the contour of integration.

The first-order correction to Φ is linear in the correction ΔL^I that, in turn, is linear in $\delta n^I(\vec{r}, t) - \delta n^{SI}(\vec{r})$. This means that in evaluating $\Delta L^I(\omega - \omega', \beta)$, we may expand $\delta n^I(\vec{r}, t) - \delta n^{SI}(\vec{r})$ in any basis of functions (provided that we know the occurrence probability of every element in the basis). Summations over realizations and over the basis elements making a specific realization commute.

For the basis of plane waves, the probability for an ion density wave of amplitude (complex) having norm a_1 , wave vector of norm k_1 and frequency ω_1 may be estimated by a simple generalization of the method developed by Pines and Bohm (see the appendix in Pines and Bohm (1952)) $f^{DI}(a_1, k_1, \omega_1) = \frac{\mathrm{e}^{-a_1^2/(n_0^2 S^{ii}(k_1,\omega_1))}}{n_0^2 S^{ii}(k_1,\omega_1)}$ where S^{ii} is the ion dynamic structure factor.

With this probability, $\Phi(\omega)$, corrected to first order, is $\Phi(\omega) = \int \Im^{-1}(I + \Re) f^{SI}(\alpha)\,\mathrm{d}\alpha$ where

$$\Re(\omega, \alpha)D = \mathrm{i}\int_0^\infty \nu_0(\omega_1)(\Im(\omega - \omega_1, \alpha))^{-1}\,\mathrm{d}\omega_1$$

$$(\nu_0(\omega))_{aba'b'} = \frac{\sqrt{\pi}}{2} n^0 Z \int \sqrt{S^{ii}(k,\omega)}\left[\frac{\hbar}{(2\pi)^3}\int (\Omega_{aa'}(\vec{k})\delta_{bb'} - \Omega_{b'b}(\vec{k})\delta_{a'a})\,\mathrm{d}\Omega_{\vec{k}}\right] k^2\,\mathrm{d}k.$$

As expected, the dynamic correction $\mathrm{Re}(\omega, \alpha)$ involves coupling between $\tilde{G}(\omega)$ at different frequencies with coupling strength which is directly related to the spectrum of fluctuations in the ion density, $S^{ii}(k, \omega)$.

4. Summary and discussion

Existing algorithms for evaluating line shape are based on rigorous theoretical derivations and are, experimentally, well established (Griem 1997). Nevertheless, we have found it advantageous to develop a new theoretical approach that is suitable for the construction of an opacity code for light ions in dense hot plasmas. The only approximation used in the reduction of the basic equation for the many-body wavefunction Ψ to the stochastic equation (5) for the dipole is the factorization assumption (1). This approximation neglects the exchange and correlation interaction between bound and free electrons and the effect of the bound electrons on the dynamics of perturbers. It does not involve any further approximation concerning the plasma wavefunction Ψ_P, i.e. equation (5) holds also for plasmas within the quantum and strong coupling regimes, as long as the exchange and correlation between bound and free electrons are small.

The spectrum obtained by neglecting ion dynamics effect yields the same formula as obtained by expanding up to second order in electron–perturber interaction (Smith and Hooper 1967, Hussey *et al* 1975). In the present approach it is derived by supplementing

the factorization approximation (equation (1)) with the Bourret approximation (equation (8)). This is justified when the correlation time for electron fluctuations is much shorter than the typical evolution time of the average dipole, i.e. when the plasma frequency is much larger than the norm of the radiator–plasma coupling matrix $\frac{e^2\langle x\rangle^2 n_0 K_B T}{\hbar^2\omega_p^2} \ll 1 \Rightarrow K_B T \ll \frac{1}{2\pi}\frac{\hbar^2}{2m}\frac{1}{\langle x\rangle^2}$, where by the virial theorem, the right-hand side is of the order of the binding energy of electrons in the ion. Unlike existing treatments of ion dynamics (see, for example, Boercker *et al* (1987) and Stamm *et al* (1986)), the present treatment is limited to the case where the static ion effect is dominant. On the other hand, this approximation enables us to avoid further simplifications and to get an explicit formula for the coupling between the Green function at different frequencies (due to ion dynamics) in terms of the spectrum of fluctuations of the ion density.

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