

Linear response of partially ionized, dense plasmas†

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We propose a new formalism to electronic polarizability of dense, partially ionized plasmas. This formalism is based upon the density functional theory for the electronic equilibrium, the random phase approximation for the density response of electrons, and the cluster expansion in the averaging over ionic configurations. The first term in the final cluster expansion for the imaginary part of electron polarizability corresponds to the Lindhard dielectric function formula. The second term contains the electronic states of the average atom. The additional effects that result from this theory are: channel mixing (screening), “inverse Bremsstrahlung” corrections, and free-bound electronic transitions. Our approach allows the plasma (collective) and atomic physics phenomena to be treated in the frame of one formalism. The theory can be applied for stopping power and opacity calculations.

1. Introduction

In the absorption of energy by a dense, partially ionized plasma, both free and bound electrons can play an important role. We are interested in this article in the theory of the stopping power and opacities of dense plasmas, i.e., of the absorption of energy of ion beams and of the absorption of soft X-ray photons by plasma.

In the case of stopping power, the usual theoretical approaches to this problem are based upon an “additivity” assumption, i.e., the stopping powers due to the bound and free electrons are additive. In consequence, different theories or models are applied to the bound- and free-electron contributions to stopping. The free electrons are taken into account through a plasma-type formula (Nardi, Peleg & Zinamon 1978; Maynard & Deutsch 1982; Deutsch *et al.* 1988; Peter & Meyer-ter-Vehn 1991), while for the bound electrons a Bethe (Garbet, Deutsch & Maynard 1987; Deutsch *et al.* 1988; Peter & Kärcher 1991) expression (with an effective ion charge) is usually applied. There have been in the literature some other attempts to address these problems. Let us mention here as an example Brueckner & Senbetu (1982), where instead of the additivity of the stopping powers the authors advocated the additivity of the dielectric functions connected, respectively, with bound and free (valence) electrons.

Similar problems appear in the calculation of photon absorption cross sections in plasmas (opacities). In this calculation, the difficulty is connected with the dynamic screening of the atomic bound electrons by the plasma. The question of how to take into account the plasma around an average ion (representing the thermodynamic equilibrium) has been discussed in the literature (see, for instance, Stewart & Pyatt 1966; Dharma-Wardana & Perrot 1982; Crowley 1990). A treatment of the dynamic plasma effects on the electronic transi-

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tions in atoms is much more difficult. One may expect also that the interconnection between the dynamics of bound and free electrons should lead, in principle, to a kind of “screening” of plasma electrons by the ionic bound states.

In this article we construct a random phase approximation (RPA) to the total electronic polarizability of a dense, partially ionized plasma. Since the RPA renormalization can describe collective plasma phenomena, we believe that this is the correct way to the inclusion of the mutual dynamic interaction between the bound and free electronic states. This article is organized as follows. In Section 2 we express the stopping power and photoabsorption formulas in terms of the imaginary part of the total electronic polarizability (response function). In Section 3 we will introduce a density functional (DFT) approach (Mermin 1965; Dharma-Wardana & Perrot 1982; see also Błeński-Cichoński 1990) to electron equilibrium for a given ionic configuration. The essential assumption underlying our procedure is the separation of the characteristic time scales of the electronic and ionic responses to an external perturbation. In Section 4 we apply an RPA-type renormalization to the independent-electron polarizability for a given, fixed ionic configuration. The average over all ionic configurations is formally performed in Section 5. The method used is the cluster expansion (see, for example, Cichoński & Felderhof 1988). If the multiion effects are neglected, the obtained averaged, renormalized polarizability consists of two terms. The first (no ions) is the usual homogeneous electron gas term (Gouedard & Deutsch 1978; Maynard & Deutsch 1982). It corresponds to the Lindhard dielectric function formula for the stopping power. The second term is connected with the polarizability of a single average atom submerged in an infinite background consisting of electrons and ions. The electron part of this background is modified in the vicinity of the central ion (scattering solutions). The stopping power formula corresponding to the above two terms is discussed in Section 6.

2. Formulas for stopping power and photoabsorption cross section in terms of electronic polarizability

Let us consider an ion of energy E , charge z , and velocity v , traversing a partially ionized plasma in thermodynamic equilibrium characterized by a temperature T . If one takes into account only interactions with plasma electrons in the semiclassical approximation [i.e., treats the incident particle as a source of electrostatic potential (Bethe & Jakiv 1986)], then the stopping power of the ion is given by the following formula:

$$\frac{dE}{dx} = -\frac{8\pi e^4 z^2}{v^2} \int_0^\infty d\omega \int_{\omega/v}^\infty \frac{dq}{q^3} \left\{ \frac{1}{V} \left[-\frac{1}{\pi} \operatorname{Im} \chi^R(\mathbf{q}, \mathbf{q}, \omega) \right] \right\}, \quad (1)$$

where Im denotes the imaginary part, V the total volume of the plasma, and $\chi^R(\mathbf{q}, \mathbf{q}, \omega)$ is the double Fourier transform of the frequency-dependent retarded electron polarizability. The exact expression for this polarizability is (Fetter & Walecka 1971):

$$\chi^R(\mathbf{r}, \mathbf{r}', t - t') = -i \operatorname{Tr} \{ \hat{\rho} [\hat{n}_H(\mathbf{r}, t), \hat{n}_H(\mathbf{r}', t')] \} \theta(t - t'), \quad (2)$$

where Tr means the average with the statistical operator:

$$\hat{\rho} \approx \exp \left[-\frac{1}{T} (\hat{H} - \mu \hat{N}) \right], \quad (3)$$

with \hat{H} denoting the Hamiltonian of all interacting electrons and ions and \hat{N} the electron number operator; $\hat{n}_H(\mathbf{r}, t)$ is the electron density operator in the Heisenberg picture.

The semiclassical approximation leads to the same expression for the atomic stopping power as the one given by the Born approximation (Bethe & Jakiv 1986). The conditions for its applicability are, however, different: One should have: (1) $ka \gg 1$, where k is the wave vector of the incident particle and a is a characteristic dimension of the medium (atomic radius); (2) $E \gg V(b)$, where $V(b)$ is the atomic (ionic) potential at the distance of the impact parameter b . For our case, i.e., the stopping in the partially ionized plasma, one may expect that the same two conditions apply. If one substitutes for a the value of the Bohr radius then condition (1) may be rewritten in the following form:

$$\frac{M}{m} \frac{v}{c} \frac{1}{\alpha} \gg 1, \tag{4}$$

where M is the mass of the incident ion, m is the electron mass, c is the light velocity, and α is the fine structure constant. It is the condition given by equation (4) that explains the validity of equation (1) (and the Bethe stopping formula) even for a small ion velocity v (Bethe & Jakiv 1986).

The presence of V , the total volume of the plasma in equation (1), indicates that the stopping power depends upon the polarizability per cm^3 . Let us consider, for example, a homogeneous medium (electron gas). We have then

$$\chi^R(\mathbf{r}, \mathbf{r}', \omega) = \chi^R(\mathbf{r} - \mathbf{r}', \omega) \tag{5}$$

and since (see also Fetter & Walecka 1971)

$$\chi^R(\mathbf{q}, \mathbf{q}, \omega) = V\chi^R(\mathbf{q}, \omega), \tag{6}$$

the total volume disappears from the formula equation (1).

On the other hand, in a situation when one may assume that the total electronic polarizability is a sum of identical electronic polarizabilities characterizing some subsystems (for instance, atoms, as in the case of the Bethe formula for cold materials), one gets (N_{atom} is the total number of atoms):

$$\chi^R(\mathbf{q}, \mathbf{q}, \omega) = N_{\text{atom}}\chi_{\text{atom}}^R(\mathbf{q}, \mathbf{q}, \omega), \tag{7}$$

which, divided by V , which stands in equation (1), leads to the presence of the atomic density in the stopping formula.

Similarly, the opacities, which are total photon absorption cross section per mass unit, are sometimes calculated from the formula (Zangwill & Soven 1980; Grimaldi, Grimaldi-Lecourt & Dharma-Wardana 1985; see also Blenski & Ligou 1989):

$$\sigma_{\text{abs}}(\nu) = -\frac{8\pi\nu e^2}{3c} \text{Im} \int d\mathbf{r} \int d\mathbf{r}' \mathbf{r}' \chi_{\text{atom}}^R(\mathbf{r}, \mathbf{r}', \nu). \tag{8}$$

A generalization to a formula similar to equation (1) is possible.

As the polarizability may be expressed by the density–density correlations, equation (2), equations (1) and (8) are connected to the fluctuation–dissipation theorem (see, for example, Hansen & McDonald 1986, p. 235).

The physical meaning of the electronic polarizability $\chi^R(\mathbf{r}, \mathbf{r}', t)$ is the following. If our plasma at the thermodynamic equilibrium is perturbed by an external potential $e\Phi^{\text{ext}}(\mathbf{r}, t)$, coupled to the electronic charge through the Hamiltonian:

$$\int d\mathbf{r} \hat{n}_H(\mathbf{r}, t) e\Phi^{\text{ext}}(\mathbf{r}, t),$$

then the linear electron density response $\delta n(\mathbf{r}, t)$ may be expressed as:

$$\delta n(\mathbf{r}, t) = \int d\mathbf{r}' \int dt' \chi^R(\mathbf{r}, \mathbf{r}', t - t') e\Phi^{\text{ext}}(\mathbf{r}', t'). \quad (9)$$

We will use equation (9) in our construction of the average electronic polarizability.

3. DFT description of the electronic equilibrium

As we already mentioned, the underlying assumption will be the separation of the time scales characterizing the electronic and ionic movement. We consider all possible ionic configurations and assume that the electrons have enough time to achieve equilibrium around each given ionic configuration. The probability of every ionic configuration is supposed, at the moment, to be known. The average over all ionic configurations will be performed in Section 5. According to the main idea of DFT (see, e.g., Vashista & Kohn 1983), the electronic equilibrium is constructed from the one-particle Kohn–Sham Schrödinger states:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 - eV(\mathbf{r}) \right] \Psi_i(\mathbf{r}) = \epsilon_i \Psi_i(\mathbf{r}), \quad (10)$$

where the index i runs over all states, bound and free, so we may have $\epsilon_i \geq 0$ or $\epsilon_i < 0$. The main quantity is the electron density $n(\mathbf{r})$, formed from the eigenstates of equation (10):

$$n(\mathbf{r}) = 2 \sum_i f_i |\Psi_i(\mathbf{r})|^2, \quad (11)$$

where the factor 2 corresponds to two possible spin states and

$$f_i = \left[\exp\left(\frac{\epsilon_i - \mu}{T}\right) + 1 \right]^{-1} \quad (12)$$

is the Fermi factor with the chemical potential μ . The potential V is a sum of the electrostatic and exchange correlation parts:

$$eV(\mathbf{r}) = eV_{\text{electr}}(\mathbf{r}) + V_{xc}[n(\mathbf{r})], \quad (13)$$

where the Poisson equation for $V_{\text{electr}}(\mathbf{r})$ closes our self-consistent model:

$$\nabla^2 eV_{\text{electr}}(\mathbf{r}) = -4\pi e^2 \left[\sum_j Z_j \delta(\mathbf{r} - \mathbf{r}_j) - n(\mathbf{r}) \right]. \quad (14)$$

In equation (14), the sum is over all nuclei whose instantaneous positions are \mathbf{r}_j and charges Z_j . The local density approximation (Dharma-Wardana & Perrot 1982) is used for the exchange correlation potential.

Among the bound states of the total potential, given by equation (13), there may exist bound states attached to a particular ion but also bound states belonging to two, three, or more ions. Similarly, the free states will be influenced by all particles of the plasma. The presence of ionic centers leads, in principle, to multiscattering problems.

4. Linear electron density response in RPA approximation

As in Section 2 [see equation (9)], we consider a time-dependent external potential $e\Phi^{\text{ext}}(\mathbf{r}, t)$. It perturbs the electrons being in equilibrium around a fixed ionic configuration. A simplest approximation to the electronic polarizability may be obtained if one treats now the electron Schrödinger states as independent quasiparticles (i.e., one forgets for the

moment that they are determined from a self-consistent potential in which some of the interactions have been included). For noninteracting electrons in a fixed ionic configuration, one can use the definition, equation (2) and get:

$$\chi_0(\mathbf{r}, \mathbf{r}', \omega) = 2 \sum_{ij} \frac{(f_i - f_j) \Psi_i^*(\mathbf{r}) \Psi_j(\mathbf{r}) \Psi_i(\mathbf{r}') \Psi_j^*(\mathbf{r}')}{\hbar\omega - (\epsilon_j - \epsilon_i) + i\delta}, \tag{15}$$

where the indices i and j corresponds to all electronic states, bound and free, and δ is a positive infinitesimal that has its origin in the causality principle, already present in the definition, equation (2). Taking the imaginary part of the double Fourier transform of this polarizability, we arrive at double sum over the one-particle transition probabilities or, in other words, the oscillator strengths:

$$\text{Im } \chi_0(\mathbf{q}, \mathbf{q}, \omega) = -2\pi \sum_{ij} (f_i - f_j) |\langle \Psi_i | \exp(i\mathbf{q}\mathbf{r}) | \Psi_j \rangle|^2 \delta(\hbar\omega - \epsilon_j + \epsilon_i). \tag{16}$$

The difference of the Fermi factors result from the fact that these polarizabilities correspond to the net effects, i.e., the processes like stimulated emission, in the case of opacities, have already been included. Indeed, we have:

$$f_i - f_j = f_i(1 - f_j) - f_j(1 - f_i) \tag{17}$$

and

$$(f_i - f_j) \delta(\hbar\omega - \epsilon_j + \epsilon_i) = \left[1 - \exp\left(-\frac{\hbar\omega}{T}\right) \right] f_i(1 - f_j) \delta(\hbar\omega' - \epsilon_j + \epsilon_i), \tag{18}$$

where the last equation contains the probability of the initial state multiplied by the availability of the final state.

For nonzero temperatures, even if one considers an idealized situation where all bound states belong to one ion only the occupation of free electron states leads to problems if one wants to write the polarizability, equation (15), as a sum of atomic (ionic) polarizabilities (the index α_{atom} runs over all ions):

$$\chi_0^R(\mathbf{q}, \mathbf{q}, \omega) = \sum_{\alpha_{\text{atom}}} \chi_{0, \alpha_{\text{atom}}}^R(\mathbf{q}, \mathbf{q}, \omega) \tag{19}$$

since the free states do not belong to a particular atom or ion. One may then try to separate the double sum of equation (15) or (16) in the following way:

$$\chi_0^R(\mathbf{q}, \mathbf{q}, \omega) = \sum_{\substack{ij \\ \text{at least one of } i, j \text{ bound}}} (\dots) + \sum_{\substack{ij \\ \text{both } i, j \text{ free}}} (\dots) \tag{20}$$

and use the plane waves in the free-free expression:

$$\Psi_{\mathbf{k}}(\mathbf{r}) = (2\pi)^{3/2} \exp(i\mathbf{k}\mathbf{r}). \tag{21}$$

This gives for the free-free part of the independent-particle polarizability the well-known Lindhard function (Gouedard & Deutsch 1978; Maynard & Deutsch 1982)

$$\chi_0^{\text{ff, plane waves}}(\mathbf{q}, \mathbf{q}, \omega) = V \chi_0^{(0)}(\mathbf{q}, \omega) \tag{22}$$

$$\chi_0^{(0)}(\mathbf{q}, \omega) = \frac{2}{(2\pi)^3} \int d\mathbf{k} \frac{f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}}{\hbar\omega - \frac{\hbar^2}{2m} [(\mathbf{k} + \mathbf{q})^2 - \mathbf{k}^2] + i\delta}. \tag{23}$$

We know, however, that plasma (collective) effects appear only if a renormalization procedure (RPA) is applied to the Lindhard polarizability (Gouedard & Deutsch 1978). On the other hand, by taking the plane waves in the free-free polarizability we neglect the inverse Bremsstrahlung processes. The inverse Bremsstrahlung is a three-body interaction involving free electron, photon, and ion. It is therefore clear that it is the correction to the plane wave functions, induced by the scattering centers (ions), that is essential for the inclusion of the inverse Bremsstrahlung processes.

We will now apply the RPA renormalization to all bound-bound, bound-free, free-bound, and free-free transitions present in the independent-particle polarizability, equation (15). This procedure may be performed using a diagram technique (Fetter and Walecka 1971) but, instead, we will use here the usual, heuristic derivation. We will consider the perturbing potential, $e\Phi^{\text{ext}}(\mathbf{r}, t)$, with the following dependence upon time:

$$e\Phi^{\text{ext}}(\mathbf{r}, t) = e\Phi_0(\mathbf{r})\delta(t), \quad (24)$$

and look for the electronic polarizability from the linear response formula:

$$\delta n(\mathbf{r}, \omega) = \int d\mathbf{r}' \chi^R(\mathbf{r}, \mathbf{r}', \omega) e\Phi_0(\mathbf{r}'). \quad (25)$$

This density correction, $\delta n(\mathbf{r}, \omega)$, leads to an induced potential:

$$\delta\Phi^{\text{ind}}(\mathbf{r}, \omega) = \int d\mathbf{r}' \frac{e^2 \delta n(\mathbf{r}', \omega)}{|\mathbf{r} - \mathbf{r}'|} + \frac{dV_{xc}[n(\mathbf{r})]}{dn(\mathbf{r})} \delta n(\mathbf{r}, \omega). \quad (26)$$

We will use from now on an obvious notation in which equation (25) and (26) take the form:

$$\delta\bar{n} = \hat{\chi} e\bar{\Phi}_0, \quad (25a)$$

$$e\bar{\Phi}^{\text{ind}} = \hat{K} \delta\bar{n}. \quad (26a)$$

The effective potential is the sum of the external and induced ones:

$$e\bar{\Phi}^{\text{eff}} = e\bar{\Phi}^{\text{ind}} + e\bar{\Phi}_0. \quad (27)$$

We postulate now (see Zangwill & Soven 1980) that the effective potential and the density correction be related through the independent-particle polarizability $\chi_0(\mathbf{r}, \mathbf{r}', \omega)$, given in equation (15):

$$\delta\bar{n} = \hat{\chi}_0 e\bar{\Phi}^{\text{eff}}. \quad (28)$$

The physical interpretation of equation (28) is the following: The dynamic response of the electrons may be approximately calculated as the response of independent particles perturbed by an effective (mean) field. Substituting now equation (27) and (26a) into (28) and comparing with (25) yields:

$$\hat{\chi} = \frac{1}{1 - \hat{\chi}_0 \hat{K}} \hat{\chi}_0, \quad (29)$$

or

$$\hat{\chi} = \hat{\chi}_0 \frac{1}{1 - \hat{K} \hat{\chi}_0}. \quad (29a)$$

This is our final result for renormalized electron polarizability in a fixed ionic configuration.

In the case of the homogeneous electron gas of density n_0 (when there are no ions except a uniform, positive background), the inversion of operators in equations (29) and (29a) may be easily performed in the Fourier space and one gets

$$\chi^{(0)}(q, \omega) = \frac{\chi_0^{(0)}(q, \omega)}{1 - K(q)\chi_0^{(0)}(q, \omega)}, \tag{30}$$

where $\chi_0^{(0)}(q, \omega)$ is the Lindhard function, equation (23), and

$$K(q) = \frac{4\pi e^2}{q^2} + \frac{dV_{xc}}{dn}(n_0). \tag{31}$$

Taking the imaginary part of equation (30), one obtains the known dielectric-function formula investigated in a series of articles by Deutsch and collaborators (Gouedard & Deutsch 1978; Maynard & Deutsch 1982; Deutsch *et al.* 1988). (The only difference is the exchange-correlation part of the potential.)

$$\text{Im}\chi^{(0)}(q, \omega) = \frac{1}{K(q)} \text{Im} \frac{1}{\epsilon(q, \omega)}, \tag{32}$$

where

$$\epsilon(q, \omega) = 1 - K(q)\chi_0^{(0)}(q, \omega). \tag{32a}$$

Unfortunately, in the case of the situation considered in this section, i.e., that of a non-homogeneous electron equilibrium in the field of a given ionic configuration, such a simple method of inverting the operator $1 - \hat{\chi}_0 \hat{K}$ does not exist and we are left with the operator formulas, equations (29) and (29a).

5. Average over ionic configurations: The cluster expansion

Our results, equation (29a), will now be averaged over all possible ionic configurations. This average on the ionic positions is present in the exact formula, equation (2), where Tr means the sum over all possible states of the interacting electrons and ions with the probability given by the statistical operator, equation (3), which involves the total Hamiltonian.

Denoting all the ionic positions by the $3N$ vector $\mathbf{R} = \{\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_N\}$ where N is the number of ions, we write the polarizability averaged over \mathbf{R} as:

$$\langle \hat{\chi} \rangle_{\mathbf{R}} = \left\langle \hat{\chi}_0 \frac{1}{1 - \hat{K}\hat{\chi}_0} \right\rangle_{\mathbf{R}}. \tag{33}$$

The ions have a probability distribution W , for which we use the shorthand notation:

$$W(\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_N) = W(1, 2, \dots, N), \tag{34}$$

and one may introduce the partial distribution functions:

$$n_s(1, 2, \dots, S) = \frac{N!}{(N - S)!} \int \dots \int d(S + 1) \dots dN W(1, 2, \dots, N), \tag{35}$$

with $n_1^{(1)}$ denoting ion density, $n_2^{(1,2)}$ containing ion correlation, etc. For a function $f(\mathbf{R})$, that depends upon the number of ions taken into consideration and on their distribution, one defines the cluster expansion in the following way (Cichocki-Felderhof 1988):

no ions: $f(\emptyset) = g(\emptyset)$ (36a)

one ion: $f(1) = g(\emptyset) + g_1(1)$, (36b)

two ions: $f(1,2) = g(\emptyset) + g_1(1) + g_1(2) + g_2(1,2)$, etc. (36c)

The average of $f(\mathbf{R})$ over all \mathbf{R} , with the probability distribution $W(\mathbf{R})$, may be found in the form of the cluster expansion:

$$\langle f(\mathbf{R}) \rangle_{\mathbf{R}} = \int d1 \dots dN W(1, \dots, N) f(\mathbf{R}) = g(\emptyset) + \int d\mathbf{R}_1 n_1(\mathbf{R}_1) g_1(\mathbf{R}_1) + \int d\mathbf{R}_1 \int d\mathbf{R}_2 n_2(\mathbf{R}_1, \mathbf{R}_2) g_2(\mathbf{R}_1, \mathbf{R}_2) + \dots \quad (37)$$

Using the cluster expansion for our polarizability, equation (33), and neglecting multiion effects [i.e., taking only “no ion” and “one ion” terms in this expansion, equation (37)], we get:

$$\begin{aligned} \langle \hat{\chi} \rangle_{\mathbf{R}} &\equiv \hat{\chi}(\emptyset) + \int d\mathbf{R}_1 n_1(\mathbf{R}_1) [\hat{\chi}(\mathbf{R}_1) - \hat{\chi}(\emptyset)] \\ &= \hat{\chi}(\emptyset) + n_{\text{atom}} \int d\mathbf{R}_1 [\hat{\chi}(\mathbf{R}_1) - \hat{\chi}(\emptyset)]. \end{aligned} \quad (38)$$

In equation (38), the first term, $\hat{\chi}(\emptyset)$, is the homogeneous gas polarizability given by equation (30). $\hat{\chi}(\mathbf{R}_1)$ is the polarizability of one ion, with its center in \mathbf{R} , submerged in a plasma consisting of the electron gas and a neutralizing, positive background.

It is clear that the above averaging procedure over the ionic positions makes the partially ionized plasma homogeneous, i.e., its polarizability, given by equation (33) or (38), depends only upon the difference $\mathbf{r} - \mathbf{r}'$ when written in the coordinate representation. Taking this remark into account, we calculate the Fourier transform of equation (38):

$$\langle \chi \rangle_{\mathbf{R}}(q, \omega) \equiv \chi^{(0)}(q, \omega) + \chi_1(q, \omega), \quad (39)$$

where the first term in equation (39) is given by equation (30) and the second equals

$$\begin{aligned} \chi_1(q, \omega) &= n_{\text{atom}} \int d(\mathbf{r} - \mathbf{r}') \exp[iq(\mathbf{r} - \mathbf{r}')] \int d\mathbf{R}_1 [\chi^{(1)}(\mathbf{r}, \mathbf{r}', \omega; \mathbf{R}_1) - \chi^{(0)}(\mathbf{r} - \mathbf{r}', \omega)] \\ &= n_{\text{atom}}(\mathbf{q} | \hat{\chi}^{(1)}(\mathbf{R}_1 = 0) - \hat{\chi}^{(0)} | \mathbf{q}) \\ &\equiv n_{\text{atom}}(\mathbf{q} | \hat{\chi}^{(1)} - \hat{\chi}^{(0)} | \mathbf{q}). \end{aligned} \quad (40)$$

We have used here the definition:

$$(\mathbf{q} | A | \mathbf{q}) = \int d\mathbf{r} \int d\mathbf{r}' \exp[iq(\mathbf{r} - \mathbf{r}')] A(\mathbf{r}, \mathbf{r}'). \quad (41)$$

Equations (39) and (40) indicate the correct approach one should apply to construct the dynamic polarizability of a partially ionized plasma using the average (Rozsnyai 1972) [or DFT (Dharma-Wardana & Perrot 1982; Błeński & Cichoński 1990)] atomic model. The one-ion polarizability $\hat{\chi}^{(1)}$ and no-ion polarizability $\hat{\chi}^{(0)}$ are to be constructed according to equation (29a), i.e.,

$$\hat{\chi}^{(1,0)} = \hat{\chi}_0^{(1,0)} \frac{1}{1 - \hat{K}_{(1,0)} \hat{\chi}_0^{(1,0)}}, \quad (42)$$

where $\hat{\chi}_0^{(0)}$ is the noninteracting polarizability operator for the homogeneous electron gas [its Fourier representation is the Lindhard function of equation (23)] while $\hat{\chi}_0^{(1)}$ has the following form in the coordinate representation:

$$\chi_0^{(1)}(\mathbf{r}, \mathbf{r}', \omega) = 2 \sum_{ij} \frac{(f_i - f_j) \Psi_i^{(1)*}(\mathbf{r}) \Psi_j^{(1)}(\mathbf{r}) \Psi_i^{(1)}(\mathbf{r}') \Psi_j^{(1)*}(\mathbf{r}')}{\hbar\omega - (\epsilon_j - \epsilon_i) + i\delta}. \tag{43}$$

Equation (43) has the same form as equation (15); however, the Kohn–Sham eigenstates correspond now to one DFT (or average) ion placed at the origin. The self-consistent potential of this atom, which for the strongly correlated plasmas has practically a finite range (Dharma-Wardana & Perrot 1982), may have bound states. All the free states, normalized to the plane waves at infinity, are taken into account by the double sum of equation (43), which means that the atom is submerged in the infinite electron gas with a neutralizing, positive background. The sense of our result, equation (40), is the following: The dynamic response of the homogeneous electron gas is already present in the first term of equation (39). Therefore, as results from the cluster expansion, one should correctly subtract this response while constructing the localized atomic polarizability [second term of equation (39)]. Far from the atom, the polarizability $\hat{\chi}^{(1)}$ is the same as that of the homogeneous electron gas $\hat{\chi}^{(0)}$. One may also note that the double Fourier transform of each of these operators separately would be divergent [see equation (6)].

The approximation, equation (38) and the following, in which we take into account only the two first terms in the cluster expansion and neglect further terms including ion correlation and multiion effects, is justified in the situations when the overlapping of ionic spheres (or potentials) is not very important (Crowley 1990). The scheme of cluster expansion indicates, at least in principle, the way for constructing $\hat{\chi}^{(2)}$ and higher-order terms. Nevertheless, these terms can contain nonspherical, quasimolecular electronic states belonging to two and more ions and, besides the problem of how to calculate these eigenstates, the average over ionic configurations for such situations would be difficult.

6. Consequences for the stopping power formula

We now briefly discuss what additional effects may appear when our results, equations (39)–(43), are substituted in the stopping formula, equation (1). The renormalization, connected to the inversion of the operators in equation (42), is called channel mixing (Zangwill & Soven 1980). These effects are responsible for the plasma collective phenomena [equation (30); see Maynard & Deutsch 1982 and Gouedard & Deutsch 1978]. It is an open question what is the importance of the channel mixing as concerns the atomic transitions in plasmas, i.e., of the second term of equation (39). Zangwill & Soven (1980) found that these effects are important in the photoabsorption cross section for rare gases. Their calculation has been performed in the case of single atoms without any surrounding plasma. One may expect that the channel mixing including free electrons, according to our formulas, equations (39)–(40), may be even more important. An extension of Zangwill & Soven’s approach to finite temperatures has been proposed by Grimaldi, Grimaldi-Lecourt & Dharma-Wardana (1985). These authors consider a finite temperature DFT atom but in their channel mixing the free–free transitions are completely neglected. Their article also does not take into account the separation of the polarizability due to the local, atomic transitions from the polarizability of free electrons (plasma).

The channel mixing effects may be shown more explicitly if we use a symmetry of equation (42) (Zangwill & Soven 1980) and rewrite the imaginary part of $\chi^{(1)}(q, \omega)$ as follows:

$$\text{Im}\chi^{(1)}(q, \omega) = \sum_{ij} (f_i - f_j) (|\Phi_{ij}^{(1)}(\mathbf{q}, \omega)|^2 - |\Phi_{ij}^{(0)}(\mathbf{q}, \omega)|^2) \delta(\hbar\omega - \epsilon_j + \epsilon_i), \tag{44}$$

where $\Phi_{ij}^{(0,1)}(\mathbf{q}, \omega)$ fulfill the equations

$$\Phi_{ij}^{(1,0)}(\mathbf{q}, \omega) = \sum_{rs} M_{ij;rs}^{(0,1)}(\omega) \Phi_{sr}^{(0,1)}(\mathbf{q}, \omega) + \Phi_{ij}^{\text{ext}(0,1)}(\mathbf{q}), \tag{45a}$$

where we have defined

$$\Phi_{ij}^{\text{ext}(0,1)}(\mathbf{q}) = \langle \Psi_i^{(0,1)} | \exp(i\mathbf{q}\mathbf{r}) | \Psi_j^{(0,1)} \rangle \tag{45b}$$

and

$$M_{ij;rs}^{(0,1)}(\omega) = \frac{2(f_r - f_s)}{\hbar\omega + (\epsilon_s - \epsilon_r) + i\delta} \int d\mathbf{r} \int d\mathbf{r}' K(\mathbf{r}, \mathbf{r}') \times \Psi_i^{(0,1)*}(\mathbf{r}) \Psi_j^{(0,1)}(\mathbf{r}) \Psi_r^{(0,1)*}(\mathbf{r}') \Psi_s^{(0,1)}(\mathbf{r}'). \tag{45c}$$

The above form explains the terminology. Equation (45a) shows how the generalized oscillator strengths are mixed by the matrices M . Again, in equation (44), both terms containing the squares of the oscillator strength are divergent (proportional to the total volume) and only their difference is finite.

Our formalism leads to additional contributions to the usual formulas for the stopping power of partially ionized plasma even if one neglects the channel mixing in atomic terms. This additional approximation means that one takes in the formula for $\chi^{(1)}(q, \omega)$ [equation (40)]:

$$\hat{\chi}^{(1,0)} \equiv \hat{\chi}_0^{(1,0)}. \tag{46}$$

The stopping power formula then has four terms:

$$\frac{dE}{dx} = \left(\frac{dE}{dx}\right)_{\text{diel. funct}} + \left(\frac{dE}{dx}\right)_{\text{Bethe } b \rightarrow b, f} + \left(\frac{dE}{dx}\right)_{f \rightarrow b} + \left(\frac{dE}{dx}\right)_{\text{inverse Bremstrahlung}} \tag{47}$$

The first term corresponds to the dielectric function of the homogeneous electron gas [equations (32) and (32a)] The second is the analog of the Bethe stopping power expression for cold material. It contains the bound-bound and bound-free transitions but, as for the zero temperature case where only the bound states are occupied, it does not include the free-bound transitions, which are contained in the third term. The last term has its origin in the deformation of the plane waves in the vicinity of the scattering centers (in the calculation of the opacities, this phenomenon leads to the inverse Bremstrahlung absorption). The last two terms are generally not included in the stopping power formulas one finds in the literature. We have checked (Błeński, Ligou & Morel, in preparation) that the free-bound correction, which is negative, amounts to at most 10% of the total stopping power. The importance of the inverse Bremstrahlung correction and, of course, of the channel mixing effects, needs numerical verification.

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