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Linear response of a variational average atom in plasma: Semi-classical model

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ABSTRACT

The frequency-dependent linear response of a plasma is studied in the finite-temperature Thomas–Fermi approximation, with electron dynamics described using Bloch hydrodynamics. The variational framework of average-atoms in a plasma is used. Extinction cross-sections are calculated for several plasma conditions. Comparisons with a previously studied Thomas–Fermi Impurity in Jellium model are presented. An Ehrenfest-type sum rule, originally proposed in a full quantum approach is derived in the present formalism and checked numerically. This sum rule is used to define Bremsstrahlung and collective contributions to the extinction cross-section. It is shown that none of these is negligible. Each can constitute the main contribution to the cross-section, depending on the frequency region and plasma conditions. This result obtained in the Thomas–Fermi–Bloch case stresses the importance of the self-consistent approach to the linear response in general. Some of the methods used in this study can be extended to the linear response in the quantum case.

1. Introduction

Modeling of dense plasma optical properties is necessary to calculate opacity and conductivity, widely needed in inertial confinement fusion, and astrophysics. For this purpose, Average-Atom (AA) models often constitute a first approach thanks to their relative simplicity and low computing cost. We may use AA models to study problems relative to the treatment of the plasma environment including screening and other density effects. Among the main difficulties in these problems are the presence and the appropriate treatment of the "free" or delocalized electrons and of the non-central ions. AA models are a good test bed for such studies. Particularly, we mean the thermodynamic coherence of the models of atoms in plasma. The main issue here is the formulation of models in a correct variational framework taking into account the ionization degree i.e. the number of delocalized electrons per atom as a variational variable.

In recent years there has been progress, which resulted in the "Variational Average-Atom in Quantum Plasma" (VAAQP) approach that was used in both the non-relativistic and relativistic AA as well as in the superconfiguration in plasma model [1–7]. It was also shown that in the case of the quasi-classical description of electron density the VAAQP approach led to the classical Thomas–Fermi (TF) atom at finite temperature proposed in Ref. [8]. In all these cited references the ion correlation was accounted for in a heuristic way, typical for all preceding AA models, see Refs. [9–13]. This ion correlation has been included using the Heaviside function corresponding to the Wigner–Seitz cavity (see Ref. [10] and the discussion in Ref. [7]). The inclusion of non-central ions into a general variational scheme still remains an open problem despite some interesting ideas suggested in Ref. [14].

The AA in plasma models can be used to study frequency-dependent electron properties. This can be done in the framework of the dynamic Linear Response (LR) theory of the AA variational equilibrium. Such studies may give information on whether and at which plasma conditions the collective electron dynamic phenomena may be important. This may have practical implications since the absorption and resistivity can be calculated directly from the LR theory. An important problem for LR when used for quantum models is the treatment of all electrons on an equal footing. The LR frequency-dependent theory of the AA quantum model has been proposed in Refs. [15,16], where the idea was to use the formalism of the cluster expansion that was first introduced in the case of polarizable suspensions [17]. The cluster expansion formalism allows one to solve the problem of

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localization of the AA response by the subtraction of the homogeneous plasma response.

The frequency-dependent LR based on the cluster expansion in the case of the quasi-classical TF ion immersed in plasma has been investigated in detail in a series of publications [18–23]. The problem was the finite temperature extension of the classical paper [24], that was motivated by the earlier results of Refs. [25,26] on the collective oscillations in atoms. The electron dynamic in these studies was based on the Bloch hydrodynamics leading to the Thomas–Fermi–Bloch (TFB) approach. As shown in Refs. [18–23], the cluster expansion automatically cancels some divergent terms in free electrons contribution appearing due to the fact that free electrons do not belong to atoms but to the plasma as a whole. In this way the cluster expansion approach leads formally to a finite expression for the atomic response. However, the TFB LR studied in these publications cannot be considered as the LR of the Thomas–Fermi AA but rather as the response of an impurity ion immersed in hot dense plasma [27,28]. The important contribution of this series of papers on the TFB LR theory and its applications was the understanding of the general LR formalism and the development of an original method allowing one to solve the first order TFB LR equations taking into account the asymptotic behavior of the first-order quantities. This method is highly efficient and provides directly the induced atomic dipole. It gives access to the general aspects of the frequency-dependent LR theory of atoms in plasma that are important for future possible quantum extensions of the LR theory.

In the present paper we report the first calculation of the frequency-dependent LR of the finite temperature Thomas–Fermi AA of Ref. [8] considered in the framework of the VAAQP approach. The fact that the VAAQP variational approach leads in an unique way to the classical Thomas–Fermi AA from Ref. [8] was understood in Ref. [1]. The method we use to solve the TFB set of equations is the same as the one proposed in Ref. [21].

The AA TF equilibrium is presented in Section 2. The cluster expansion and the TFB set of equations are derived in Section 3. In Section 4 we prove that the Ehrenfest-Type Atom-in-Plasma Sum Rule (ETAPSR) that was previously derived in the quantum AA case [7] remains valid in the TFB LR model. The numerical solution of the LR TFB set of equations allows us for the first time to check this sum rule and discuss its physical meaning. The numerical results for the extinction cross section are analyzed in Section 5. The VAAQP formalism introduces the presence of the WS cavity, which is neutral in the Thomas–Fermi case. This has an impact on the values of the AA absorption cross-section especially close to the plasma frequency. The ETAPSR allows us also to distinguish two terms in the induced atom dipole and in the extinction cross-section. The first term we call the "Bremsstrahlung"-like term since it leads to the Bremsstrahlung term in the independent electron approach (see, for example, [29]) and the second term we call the "collective" like term. The contribution of these two terms to the extinction cross-section as a function of the plasma parameters and frequency range is discussed. The conclusions are given in Section 6.

2. Equilibrium description: Thomas–Fermi atom

An approach to plasma modeling consists of treating locally electrons as an ideal Fermi gas. The term locally means here that the electron density $n(\mathbf{r})$ only depends on the local potential value $\phi(\mathbf{r})$. This is the usual Thomas–Fermi (TF) hypothesis. In the considered non-relativistic case:

$$n(\mathbf{r}) = 2\int \frac{\mathrm{d}\mathbf{p}}{h^3} \frac{1}{\exp\left(\beta\left(\frac{p^2}{2m} - \mu_0 - e\phi(\mathbf{r})\right)\right) + 1}. \tag{1}$$

Here, μ_0 stands for the chemical potential, β is the inverse of the temperature $1/k_BT$, m is the electron mass, and e is the electron absolute charge.

A first approach of this kind to atoms in condensed matter appeared in Ref. [30]. In this reference, the Wigner–Seitz (WS) polyhedron cell resulting from the periodic structure of metal at zero temperature was replaced by a sphere of radius r_{WS} such that:

$$\frac{4}{3}\pi r_{\mathrm{WS}}^3 = \frac{1}{n_i}. \tag{2}$$

where n_i is the atom density. The application of a TF atom contained in the WS sphere to compressed matter and finite temperatures plasma was first proposed in Ref. [8]. In both approaches, the equations for the self-consistent electron density and electrostatic potential are as follows:

$$\nabla^2\phi(\mathbf{r}) = 4\pi e n(\mathbf{r}), \tag{3}$$

$$\phi(r\to 0) = \frac{Ze}{r},\ \phi(r_{\mathrm{WS}}) = 0,\ \left.\frac{\mathrm{d}\phi}{\mathrm{d}r}\right|_{r=R_{\mathrm{WS}}} = 0, \tag{4}$$

where $n(\mathbf{r})$ is given by Equation (1). The boundary conditions Equation (4) account for the central nuclear charge Ze and the neutrality of the WS sphere. In the following we will call this model Thomas–Fermi Average-Atom (TFAA). In the TFAA model, the equilibrium is determined by three parameters: n_i, Z, T.

The TFAA has been widely used in the literature because of its simplicity, thermodynamic consistency, and scaling with respect to the atomic number Z. The results obtained using the TFAA model for a given element can be generalized to other elements thanks to the scaling law in Z of the model. The equations can be made independent of Z, by using the following four quantities:

$$TZ^{-4/3},\ nZ^{-2},\ \phi Z^{-4/3},\ rZ^{1/3}. \tag{5}$$

At finite temperatures, the physical picture of the WS sphere has to be interpreted differently from the idea of Ref. [30] because in a plasma, there is no periodical structure. It stems from the TFAA model that a finite electron density $n_0^{(0)} = n(r_{\mathrm{WS}})$ related to the chemical potential μ_0 is obtained at the WS boundary. One may then consider as in Ref. [10] that beyond the WS sphere is a jellium of electron density $n_0^{(0)}$. This implies the presence beyond the WS sphere of a homogeneous, neutralizing non-central ion background composed of ions of effective charge $Z^* = n_0^{(0)}/n_i$. These non-central ions then have a charge density: $\rho_i(r) = n_0^{(0)} e\Theta(r - r_{\mathrm{WS}})$, which corresponds to a WS cavity.

This picture of one ion in a jellium with a cavity was used in the framework of a cluster expansion [17] in previous works leading to the Variational Average-Atom in Quantum Plasma (VAAQP) model [1,2,5]. It was proved that the TFAA model could also be considered as resulting from the VAAQP approach, if the electron free-energy is taken in the TF approximation. This interpretation is the starting point of the present study.

In Ref. [21] another TF model at finite temperature is studied, corresponding to an impurity in a jellium of a given electron density $n_0^{(0)}$, without any WS cavity. The jellium ion charge density is then $\rho_i = en_0^{(0)}$. We will call this model Thomas–Fermi Impurity in Jellium (TFIJ). Instead of Equation (4) the boundary conditions become in the TFIJ case:

$$\phi(r\to 0) = \frac{Ze}{r},\ \phi(r\to\infty) = 0. \tag{6}$$