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Dynamic linear response of atoms in plasmas and photo-absorption cross-section in the dipole approximation

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ABSTRACT

We report results on the self-consistent linear response theory of quantum average-atoms in plasmas. The approach is based on the two first orders of the cluster expansion of the plasma susceptibility. A change of variable is applied, which allows us to handle the diverging free-free transitions contribution in the self-consistent induced electron density and potential. The method is first tested on the case of rare gas isolated neutral atoms. A test of the Ehrenfest-type sum rule is then performed in a case of an actual average-atom in a plasma. At frequencies much higher than the plasma frequency, the sum rule seems to be fulfilled within the accuracy of the numerical methods. Close to the plasma frequency, the method seems not to account for the cold-plasma dielectric function renormalization in the sum rule, which was correctly reproduced in the case of the Thomas–Fermi–Bloch self-consistent linear response. This suggests the need for a better accounting for the outgoing waves in the asymptotic boundary conditions.

1. Introduction

The study of photo-absorption (PA) in dense plasmas is relevant as a part of fundamental research on strongly coupled Coulomb systems. PA spectra are among the quantities that can be measured in such plasmas and compared to the ones calculated from models, allowing one to test theories of such systems. Knowledge of the PA cross-sections is also required in inertial fusion research as well as in astrophysics since radiative transfer is often the main energy transport mechanism in dense plasmas typical for these applications. In the present paper, we will consider plasmas in which a significant number of electrons remain bound to the ions even at relatively high temperatures and densities. This is the case in practically all plasmas of interest in these fields, provided the considered element has a moderate or high atomic number.

We address in the present paper an approach to the PA in plasmas which is based on the frequency-dependent linear response theory. This linear response is considered in the framework of a relatively simple equilibrium plasma model. It is the Variational Average-Atom in Quantum Plasma (VAAQP) model [1–6] in which bound and free electrons are treated on the same footing. This property is essential in the equilibrium theory of dense plasmas, especially in order to address the warm dense matter regime, as using separate approaches for bound and free electrons lead to inconsistencies in the case of pressure ionization (see, for instance Ref 7.). Such unified description of the bound and free electrons is also necessary in the PA theories if one aims to include the channel mixing effects (see Refs 8,9.), as for instance the configuration interaction involving bound and free electron configurations, which can be important in atomic physics. The self-consistent screened atomic potential in the VAAQP model accounts for free electrons and also includes non-central ions using the Wigner–Seitz (WS) cavity hypothesis [10,11].

From a theoretical point of view, interaction of photons with a partially ionized plasma is a much more complex process than interaction with individual (isolated) atoms or ions. In some of the equilibrium plasma models, a part of many-body correlations is included which should be then also accounted for in the dynamic linear response theory. However, in the dynamic response of the plasma additional difficulties appear. The delocalized or "free" electrons may participate in atomic processes, for instance, the Bremsstrahlung or its inverse process but also in collective ones. In atomic processes, a well known difficulty appears since delocalized electrons can belong to both initial and final states of the plasma. The idea to calculate PA cross-sections for each atom of the plasma faces the problem of divergences stemming from the fact that delocalized electrons cannot be associated with a particular ion center. This difficulty is often circumvented in practical opacity calculations, making the assumption that the PA cross-section may be split into a sum of three contributions corresponding to the bound-bound, bound-free and free-free electron transitions, respectively. Such a division is however only valid in the independent particle model. Once this division is

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postulated, the bound-bound and bound-free transitions may be then treated using some more sophisticated methods of traditional atomic physics including the fine structure levels obtained by diagonalization of the atomic Hamiltonian limited to bound electrons. The free-free transitions remain treated within the independent-electron approximation and their dipole matrix elements are "localized" using the acceleration form that stems from the Ehrenfest relation. However, in such approaches the channel mixing effects or the configuration interaction including free configurations cannot be accounted for. Also, collective effects including those of atomic nature (i.e. collective effects in which participate free electron wave functions that are modified by ion centers) are disregarded within the independent electron approximation.

A systematic approach to the dynamic linear response of atoms in plasmas has been proposed in Ref. 12. This approach was based on the idea of a cluster expansion introduced in Ref. 13, and its principal objective was to deal with the divergence problem due to the free-free transitions in situations where channel mixing is non-negligible. A modified version of this approach was proposed in Ref. 14. It leads to a practical method Ref. 15, allowing one to obtain the dynamic linear response in the framework of the quasi-classical Thomas–Fermi–Bloch (TFB) theory (see Refs. 16–18). The method was applied in Refs 19,20 to calculate PA in some examples of an impurity immersed in a plasma. However, this method relies on the TFB theory and its extension to the case of a quantum atom in a plasma seemed difficult. Further studies on the quantum linear response resulted in a new sum rule [21] which is a generalization of the Ehrenfest theorem to the dynamic linear response of an atom in a plasma. On the other hand, it was shown [1] that the classical Thomas–Fermi atom at finite temperature model of Ref. 16 can be considered as a special case of the VAAQP model, i.e. that it can be obtained in the framework of the cluster expansion method of Refs. 1–6. In Ref. 22, it was proven that the sum rule of Ref. 21 applies also to the dynamic response of atoms in plasmas treated in the framework of the quasi-classical TFB theory. In the same paper, the new sum rule in the TFB case was also checked for the first time by direct numerical calculations. The values of the induced frequency-dependent atomic dipoles obtained using the method of Refs. 19,20 appeared to be the same as the dipole values stemming from the sum rule.

In this paper, we present an approach to the linear frequency-dependent response applied to the VAAQP model and some results obtained using this approach. In section II we discuss the formalism of the linear susceptibilities and the method of the Green functions that is used in the self-consistent calculation of the induced first-order electron density and potential. The Ehrenfest-like sum rule of Refs. 21 and 22 is recalled in section III. In this section, an example of the validation of the sum rule in the TFB case is also displayed. The method used in the self-consistent calculations is applied in section IV to compute the PA cross-section of rare gases neutral atoms. Section V presents calculations in some cases of a chosen quantum plasma performed in order to check the Ehrenfest-like sum rule in that cases. Main conclusions are presented in the last section.

2. Cluster expansion of the photo-absorption cross-section

The plasma susceptibility $\chi(\vec{r},\vec{r}',\omega)$ is the time Fourier transform of the plasma density response-function with respect to an external potential:

$$\delta n_{\text{exact}}(\vec{r},\omega)=\int \overrightarrow{dr'}\chi(\vec{r},\vec{r}',\omega)(-e)\phi_{\text{ext}}(\vec{r}',\omega) \tag{1}$$

where $\delta n_{\text{exact}}(\vec{r},\omega)$ is the time Fourier transform of the exact electron density displacement in the first order of the external potential, and $\phi_{\text{ext}}(\vec{r}',\omega)$ is the time Fourier transform of that potential.

The plasma susceptibility can be calculated using the cluster expansion [12,13] which gives, limiting the expansion to the zeroth and first orders:

$$\chi(\vec{r},\vec{r}',\omega)=\chi^{(0)}(\vec{r}-\vec{r}',\omega)+n_i\int \overrightarrow{dR}\left(\chi^{(1)}(\vec{r},\vec{r}',\omega,\vec{R})-\chi^{(0)}(\vec{r}-\vec{r}',\omega)\right) \tag{2}$$

In (2), $\chi^{(0)}(\vec{r}-\vec{r}',\omega)$ corresponds to the susceptibility of a homogeneous electron gas neutralized by a rigid, homogeneous ion background (zeroth order system), n_i is the ion density and $\chi^{(1)}(\vec{r},\vec{r}',\omega,\vec{R})$ is the susceptibility of an infinite inhomogeneous electron gas modified by the presence of one ion placed at the position $\vec{R}$ (first-order system).

The space Fourier transform of $\chi(\vec{r},\vec{r}',\omega)$ can be written as:

$$\chi(k,\omega)=\chi^{(0)}(k,\omega)+n_i\left\langle\vec{k}\left|\left(\chi^{(1)}(\omega,\vec{R}=\vec{0})-\chi^{(0)}(\omega)\right)\right|\vec{k}\right\rangle \tag{3}$$

where we use the following $\vec{k}$-representation of the operators:

$$\left\langle\vec{k}\left|A\right|\vec{k}'\right\rangle=\int \overrightarrow{dr}\overrightarrow{dr'}e^{-i\vec{k}\cdot\vec{r}}A(\vec{r},\vec{r}')e^{-i\vec{k}'\cdot\vec{r}'} \tag{4}$$

with A having the $\vec{r}$-representation: $\langle\vec{r}|A|\vec{r}'\rangle=A(\vec{r},\vec{r}')$

The plasma electric-field energy absorption cross-section can also be written in the cluster expansion, which gives at the first order:

$$\sigma(k,\omega)=\sigma^{(0)}(k,\omega)+\sigma^{(1)}(k,\omega)+\ldots \tag{5}$$

The zeroth order term $\sigma^{(0)}(k,\omega)$ can be related to the zeroth order susceptibility:

$$\sigma^{(0)}(k,\omega)=-\frac{4\pi e^2\omega}{k^2c_{\text{eff}}}\text{Im}\,\chi^{(0)}(k,\omega) \tag{6}$$

where $c_{\text{eff}}=c\sqrt{\varepsilon_{\text{eff}}(\omega)}$ is the effective light velocity in the plasma. The first order term $\sigma^{(1)}(k,\omega)$ is connected to the first order susceptibility [14]:

$$\sigma^{(1)}(k,\omega)=-\frac{4\pi e^2\omega}{k^2c_{\text{eff}}}n_i\,\text{Im}\left\langle\vec{k}\left|\left(\chi^{(1)}(\omega,\vec{0})-\chi^{(0)}(\omega)\right)\right|\vec{k}\right\rangle \tag{7}$$

In the present paper, we will limit ourselves to the dipole approximation in which the external potential has the form:

$$\phi_{\text{ext}}(\vec{r},\omega)=E_0(\omega)z \tag{8}$$

Expanding $\left\langle\vec{k}\left|\left(\chi^{(1)}(\omega,\vec{0})-\chi^{(0)}(\omega)\right)\right|\vec{k}\right\rangle$ in the low-k limit, we obtain:

$$\left\langle\vec{k}\left|\left(\chi^{(1)}(\omega,\vec{0})-\chi^{(0)}(\omega)\right)\right|\vec{k}\right\rangle = k^2\int \overrightarrow{dr}\overrightarrow{dr'}z\left(\chi^{(1)}(\vec{r},\vec{r}',\omega,\vec{0})-\chi^{(0)}(\vec{r},\vec{r}',\omega)\right)z' \tag{9}$$

The zeroth-order term in Eq. (9) is equal to zero due to the particle conservation.

Using Eq. (9) in Eq. (7), and substituting Eq. (8), we get:

$$\sigma^{(1)}(\omega)=-\frac{4\pi\omega}{c\sqrt{\varepsilon_{\text{eff}}}E_0}\text{Im}\,p_z(\omega)=\frac{4\pi\omega}{c\sqrt{\varepsilon_{\text{eff}}}}\text{Im}\,\alpha(\omega) \tag{10}$$

where we define the dipole $p_z(\omega)$ and polarizability $\alpha(\omega)$ as:

$$\alpha(\omega)=\frac{p_z}{-E_0}=\frac{e}{E_0}\int \overrightarrow{dr}z\left(\delta n^{(1)}(\vec{r},\omega)-\delta n^{(0)}(\vec{r},\omega)\right)=\frac{e}{E_0}\int \overrightarrow{dr}\left(z\delta n(\vec{r},\omega)\right) \tag{11}$$

where:

$$\delta n^{(0)}(\vec{r},\omega)=\int \overrightarrow{dr'}\chi^{(0)}(\vec{r},\vec{r}',\omega)(-e)\phi_{ext}(\vec{r}',\omega) \tag{12}$$