PHYSICAL REVIEW A VOLUME 41, NUMBER 12 15 JUNE 1990

Density-functional approach to the absorption bands in a dense, partially ionized plasma

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(Received 26 October 1989)

Density-functional theory (DFT) for finite temperature (T) is used to account for fluctuations of the transition energies in the average-atom model. These fluctuations lead to absorption bands in the bound-bound contribution to the total spectrum. The transition-energy fluctuations are related to the second derivative of the DFT functional $\Omega[n]$ with respect to the electron density $n(\mathbf{r})$. In the numerical example (the spectrum and opacity of iron plasma at $T=200$ eV and solid density), the Thomas-Fermi (TF) form of $\delta^2\Omega[n]/\delta n(\mathbf{r})\delta n(\mathbf{r}')$ is taken. A comparison with a previous approach based on uncorrelated fluctuations around the TF atom clarifies the meaning of that approach. The numerical results indicate that the inclusion of interactions significantly diminishes the absorption bandwidths.

I. INTRODUCTION

The average-atom approach to the atomic physics of dense, partially ionized plasma close to local thermodynamic equilibrium was initiated a long time ago (see, for instance, Refs. 1–3). The development of the density-functional theory[4,5] (DFT) and, especially, its finite-temperature version[6–8] has provided a further justification to the average-atom models. There are, however, basic problems in applying the DFT approximation to the calculations of atomic photoabsorption cross section due to the fact that the photoabsorption cross section is connected to the density-density time-dependent fluctuations[9] or, in other words, to the frequency-dependent polarization.[10] Only recently have there been some attempts to extend the DFT to the time-dependent phenomena[11] (see also Refs. 10 and 12). Even in Ref. 11, however, the level widths, which are necessary to account for the bound-bound contributions, were taken from outside the DFT formalism. The problem is that independent-electron polarizability $\chi_0(\mathbf{r},\mathbf{r}',\nu)$ (see Sec. III) leads to Dirac-function-like transition lines. For this reason any average-atom model is insufficient in accounting for finite lines or absorption bands observed in dense plasmas. It is known, on the other hand, that the bound-bound contribution to the Rosseland opacity may be dominant, especially in the case of photoabsorption of higher-Z elements. The methods that go beyond average-atom models and introduce detailed atomic configurations lead to rather complex computational schemes.[13,14] For higher Z these schemes have to be additionally supplemented by some elements of statistical treatment like, for instance, the Lanczos collective vector or Monte Carlo methods.[15]

In the case of high-density plasmas and many-electron atoms the photoabsorption cross section is often characterized by many lines that merge into broad bands. If one is not interested in the details of the photoabsorption spectrum but only in a crude model, an alternative way of description may be to use, from the beginning, a fully statistical approach. This idea was at the origin of the papers by Shalitin, Stein, and Ron[16] and Stein, Shalitin and Ron.[17] These authors calculate the electron-density fluctuations around the Thomas-Fermi (TF) average-atom solution[18] to account for the fluctuations in atomic energy levels which, in turn, produce the (postulated) Gaussian line shapes. Their derivation is based on some statistical considerations about as they call it "uncorrelated fluctuations" and they do not use directly the density-functional character of the Thomas-Fermi atomic model. As follows from the comparison with our results (in the simplified TF version), their final expressions for the level widths do not include the Coulomb contribution despite the fact that the Coulomb term may be important (see Sec. V of this paper).

In the present paper we follow the same idea but consequently use the density-functional theory at finite temperature. In Sec. II we present the average-atom model. It is simplified with respect to the DFT atom since, following Refs. 3 and 14 we take the contribution of continuum electron states to the density in the form of the Thomas-Fermi expression. Section III recalls the standard (golden rule) formula for the absorption cross section stemming from the independent-particle approximation which is the usual starting point leading to the bound-bound, bound-free, and free-free contributions.

In Sec. IV we consider the fluctuations around the DFT solution. The average-atom model which gives only the equilibrium quantities such as the potential and electron density may be obtained by minimization of the grand thermodynamic potential. The DFT formalism is based on a functional $\Omega[n]$, which provides a certain approximation to this grand thermodynamical potential in the vicinity of the equilibrium. We use the same functional to calculate the probability of density fluctuations. Our procedure is the standard one:[19] assuming that these fluctuations are small and Taylor expanding the functional around its equilibrium value we relate this probability to the second functional derivative of Ω with respect to the electron density. A brief description of the DFT theory and the formal derivation of $\delta\Omega[n]/\delta n(\mathbf{r})$ and $\delta^2\Omega[n]/\delta n(\mathbf{r})\,\delta n(\mathbf{r}')$, [$n(\mathbf{r})$ is the electron density] is given in the Appendix A.

Our final formula for the line "width" is obtained by averaging the bound-bound cross section with the fluctuation probability. If the dependence of the oscillator strengths and of the Fermi factors upon the density fluctuations is neglected, our procedure leads to Gaussian line shapes. In Sec. V we illustrate the method by taking the Thomas-Fermi form of $\delta^2\Omega[n]/\delta n(\mathbf{r})\,\delta n(\mathbf{r}')$. The numerical example is given for iron plasma of solid density at a temperature of 200 eV. Some details of the Thomas-Fermi formalism may be found in the Appendix B.

II. ATOMIC MODEL

In the self-consistent average-atom model we use the quantum Schrödinger states for the bound-electron density, while the free-electron contribution to the density is treated via the Thomas-Fermi expression[3], i.e., we set for the electron density

$$n(\mathbf{r})=\sum_{i\ \text{bound}} 2(2l_i+1)|\Psi_i(\mathbf{r})|^2 f\left[\frac{E_i-\mu}{T}\right]+n_f(\mathbf{r})\ , \tag{2.1}$$

where

$$n_f(\mathbf{r})=\frac{2}{h^3}\int_{E>0} d\mathbf{p}\, f\left[\frac{1}{T}\left[\frac{\mathbf{p}^2}{2m}-eV_{\text{sc}}(\mathbf{r})-\mu\right]\right]\ , \tag{2.2}$$

with

$$E=\frac{\mathbf{p}^2}{2m}-eV_{\text{sc}}(\mathbf{r})-\mu\ , \tag{2.3}$$

and

$$f(x)=[\exp(x)+1]^{-1}\ . \tag{2.4}$$

The bound states are found from the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2-eV_{\text{sc}}(\mathbf{r})\right]\Psi_i(\mathbf{r})=E_i\Psi_i(\mathbf{r})\ , \tag{2.5}$$

by the phase function method.[20] The self-consistent potential $V_{\text{sc}}(\mathbf{r})$ is

$$eV_{\text{sc}}(\mathbf{r})=eV_{\text{el}}(\mathbf{r})+V_{\text{xc}}(\mathbf{r})\ ; \tag{2.6}$$

where $V_{\text{el}}(\mathbf{r})$ is the electrostatic part which is determined by the electron and nuclear charges via the Poisson equation

$$\nabla^2 eV_{\text{el}}(\mathbf{r})=4\pi e^2 n(\mathbf{r})\ , \tag{2.7}$$

with the boundary conditions

$$eV_{\text{el}}(\mathbf{r})\underset{|\mathbf{r}|\to 0}{\longrightarrow}\frac{Ze^2}{|\mathbf{r}|}\ , \tag{2.8}$$

$$\frac{dV_{\text{el}}}{dr}(r_0)=0,\quad r\geq r_0\ ; \tag{2.9}$$

with r_0 being the radius of the Wigner-Seitz sphere,

$$r_0=\left[\frac{3}{4\pi n_a}\right]^{1/3}\ , \tag{2.10}$$

and n_a the atomic density. $V_{\text{xc}}(\mathbf{r})$ is the exchange-correlation potential (see Appendix A). In practical calculations we apply the $V_{\text{xc}}(\mathbf{r})$ from Ref. 3 (see also Refs. 21 and 22). The chemical potential μ is found from the condition of neutrality of the atomic sphere.

III. THE PHOTON ABSORPTION CROSS SECTIONS

The golden rule formula (see, for instance, Refs. 1, 10, and 11) gives for the absorption cross section

$$\sigma_a(\nu)=-\frac{8\pi^2\nu e^2}{3c}\operatorname{Im}\int d\mathbf{r}\,d\mathbf{r}'\,\mathbf{r}\mathbf{r}'\chi^R(\mathbf{r},\mathbf{r}',\nu)\ , \tag{3.1}$$

where $\chi^R(\mathbf{r},\mathbf{r}',\nu)$ is the retarded polarization.[9] In the independent-particle approximation

$$\begin{aligned}\chi^R(\mathbf{r},\mathbf{r}',\nu)&=\chi_0^R(\mathbf{r},\mathbf{r}',\nu)\\&=2\sum_{ij}\frac{(f_i-f_j)\Psi_i^*(\mathbf{r})\Psi_j(\mathbf{r})\Psi_j^*(\mathbf{r}')\Psi_i(\mathbf{r}')}{h\nu-(E_j-E_i)+i\eta}\ ,\end{aligned} \tag{3.2}$$

where

$$f_i=f\left[\frac{E_i-\mu}{T}\right]\ .$$

The one-particle states are the bound and free eigenstates of our self-consistent $V_{\text{sc}}(\mathbf{r})$. Equation (3.2) may be written in the form

$$\sigma_a=\sigma_a^{bb}+\sigma_a^{bf}+\sigma_a^{ff}\ ; \tag{3.3}$$

where the superscripts b and f denote to which part of the spectrum (b, bound, or f free) belong the initial and final states (i,j) of Eq. (3.2). This approximation, Eq. (3.2), leads to the δ-line form for the line (bb) transitions:

$$\begin{aligned}\sigma_a^{bb}(\nu)=\frac{8\pi^3\nu e^2}{3c}&\sum_{ij\in\text{bound}}2(f_i-f_j)|\langle\Psi_i|\mathbf{r}|\Psi_j\rangle|^2\\&\times\delta(h\nu-E_j+E_i)\ .\end{aligned} \tag{3.4}$$

Let us note that the cross sections of Eqs. (3.1), (3.3), and (3.4) correspond to net processes, i.e., the correction for stimulated emission is already included.[11]

IV. THE ABSORPTION BANDS CONSIDERED AS DUE TO THE FLUCTUATIONS AROUND THE AVERAGE-ATOM DENSITY

Our statistical approach to the absorption band formation is based on the density-functional theory which may be seen as justifying the average-atom model. As presented in Appendix A the atomic density $n(\mathbf{r})$ [and the self-consistent potential $V_{\mathrm{sc}}(\mathbf{r})$] may be viewed as stemming from the minimum condition

$$\delta\Omega[n(\mathbf{r})]=0\ . \tag{4.1}$$

(In fact, our scheme is not a full DFT one since we take the TF free-electron contribution. We disregard in what follows the difference due to this approximation.) Let us now consider an (assumed small) correction to our average electron density $n(\mathbf{r})$. We set

$$n'(\mathbf{r})=n(\mathbf{r})+\delta n(\mathbf{r})\ . \tag{4.2}$$

According to the fluctuation theory[19] the probability for δn may be expressed as

$$P[\delta n]\sim\exp(-\delta\Omega/T)\ ; \tag{4.3}$$

where $\delta\Omega$ is the change of the grand thermodynamic potential introduced by $\delta n(\mathbf{r})$. We will now assume that $\delta n(\mathbf{r})$ is small and use the expansion

$$\begin{aligned}\delta\Omega[n+\delta n]&\cong\frac{1}{2}\,\frac{\delta^2\Omega}{\delta n'^2}[n]\delta^2 n\\&\equiv\tfrac{1}{2}\int d\mathbf{r}\,d\mathbf{r}'\frac{\delta^2\Omega}{\delta n'(\mathbf{r})\,\delta n'(\mathbf{r}')}[n]\delta n(\mathbf{r})\,\delta n(\mathbf{r}')\ ;\end{aligned} \tag{4.4}$$

since $\delta\Omega/\delta n'[n]=0$. Any $\delta n(\mathbf{r})$ gives the following potential correction:

$$\begin{aligned}e\delta V(\mathbf{r})&=e^2\int d\mathbf{r}'\frac{\delta n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}+\frac{\delta V_{\mathrm{xc}}}{\delta n}[n]\delta n(\mathbf{r})\\&\equiv\int d\mathbf{r}' K(\mathbf{r},\mathbf{r}')\delta n(\mathbf{r}')\end{aligned} \tag{4.5}$$

with

$$K(\mathbf{r},\mathbf{r}')=\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}+\frac{\delta V_{\mathrm{xc}}}{\delta n}[n]\delta(\mathbf{r}-\mathbf{r}')\ . \tag{4.6}$$

The potential correction $e\delta V(\mathbf{r})$ leads, in turn, to the first-order corrections to the eigenvalues E_i:

$$\delta E_i=\int|\Psi_i(\mathbf{r})|^2 e\delta V(\mathbf{r})d\mathbf{r}\ ; \tag{4.7}$$

i denotes here any state, bound or free, which we write as $i\in S$ (S is the whole spectrum). Equations (4.5)–(4.7) provide a linear relation between $\delta n(\mathbf{r})$ and δE_i. Since we have

$$P[\delta n]\cong\exp(-\delta^2\Omega/T)\ , \tag{4.8}$$

with $\delta^2\Omega$ given by Eq. (4.4), i.e., bilinear in $\delta n(\mathbf{r})$, the probability of δE_i; $i\in S$, will be a generalized Gaussian:[23]

$$P[\delta E_k,k\in S]\cong\exp\left[-\frac{1}{2}\sum_{ij}A_{ij}\delta E_i\delta E_j\right]\ . \tag{4.9}$$

We have assumed that the operator from Eq. (4.7) is inversible, and set

$$\frac{1}{T}\delta^2\Omega=\tfrac{1}{2}\sum_{ij\in S}A_{ij}\delta E_i\delta E_j\ . \tag{4.10}$$

We will now average the bound-bound transition cross section, Eq. (3.4), upon the density fluctuations. The meaning of this operation may be seen as follows. In the radiative transfer problems one is interested in the spatial and temporal dependence of radiation intensity. The absorption mean free path is a macroscopic quantity orders of magnitude larger in comparison with atomic dimensions. The photons traversing a plasma medium are absorbed by atoms (or ions) which are in different states [we describe these atoms here as fluctuating around an average atom with different electron-density deviations $\delta n(\mathbf{r})$]. On the macroscopic, hydrodynamical spatial scale we may use therefore $\bar{\sigma}_a(\mathbf{r})$, the cross section averaged over all possible fluctuations. In the case of the b-b contribution, this averaging procedure leads to finite linewidths. One should stress, however, that we take into consideration only static fluctuations while dynamic processes (collisions, etc.) are beyond the scope of the present treatment. The statistical approach using the electronic density as the main parameter is also different from the methods which are based on detailed structure of the bound-bound transition arrays.[13,14] This problem has been discussed in Ref. 16. Let us remark finally that the broadening connected with the Stark effect due to the neighboring ions could be, in principle, included in the present statistical approach if one follows Refs. 8 and 24 and introduces the functional $\Omega[n,\rho]$ with $\rho(\mathbf{r})$ being the ionic density inside the correlation sphere.

In order to simplify our model we will neglect the dependence of the oscillator strengths and of the Fermi factor upon the density (or energy) correction. So we will take into account only the Dirac δ's and their dependence on the initial and final energies E_i and E_j. In other words, we set

$$\begin{aligned}\bar{\sigma}^{bb}(\nu)&\equiv\int P[\delta n]d\delta n\,\sigma^{bb}(\nu)\\&\cong\frac{8\pi\nu e^2}{3c}\sum_{ij:\,\mathrm{bound}}2(f_i-f_j)|\langle\Psi_i|\mathbf{r}|\Psi_j\rangle|^2\\&\qquad\times f_{ij}(h\nu-E_j+E_i)\ ,\end{aligned} \tag{4.11}$$

where

$$\begin{aligned}&f_{ij}(h\nu-E_j+E_i)\\&\quad=C\int\prod_{k\in S}d\delta E_k\exp\left[-\frac{1}{2}\sum_{r,s\in S}A_{rs}\delta E_r\delta E_s\right]\\&\qquad\times\delta(h\nu-E_j+E_i-\delta E_j+\delta E_i)\ .\end{aligned} \tag{4.12}$$

C in Eq. (4.12) is the normalization constant.[23] The integration of Eq. (4.12) is performed in Appendix C, and it is found that

$$f_{ij}(x)=\frac{1}{[2\pi(\Delta E_{ij})^2]^{1/2}}\exp\left[-\frac{x^2}{2(\Delta E_{ij})^2}\right]\ , \tag{4.13}$$

where

$$(\Delta E_{ij})^2=(A^{-1})_{ii}-2(A^{-1})_{ij}+(A^{-1})_{jj} \; . \qquad (4.14)$$

In Eq. (4.14) A^{-1} represents the inverse of matrix A from Eq. (4.12). The matrix A^{-1} is the covariance matrix $\langle \delta E_i \delta E_j \rangle$ (see Ref. 23, pp. 13 and 25):

$$\langle \delta E_i \delta E_j \rangle=(A)^{-1}ij \; . \qquad (4.15)$$

Thus ΔE_{ij} is totally determined by the covariance matrix $\langle \delta E_i \delta E_j \rangle$. We will now calculate this average directly using Eqs. (4.5)–(4.8):

$$\langle \delta E_i \delta E_j \rangle=\int\int\int\int d\mathbf{r}\, d\mathbf{r}'\, d\mathbf{r}_1\, d\mathbf{r}_2 |\Psi_i(\mathbf{r})|^2 K(\mathbf{r},\mathbf{r}_1)\langle \delta n(\mathbf{r}_1)\delta n(\mathbf{r}_2)\rangle K(\mathbf{r}_2,\mathbf{r}')|\Psi_j(\mathbf{r}')|^2 \; , \qquad (4.16)$$

where the "covariance matrix" of the density correlations may be identified as

$$\langle \delta n(\mathbf{r}_1)\delta n(\mathbf{r}_2)\rangle=T\left[\frac{\delta^2\Omega}{\delta n'(\mathbf{r}_1)\delta n'(\mathbf{r}_2)}\right]^{-1}=T\chi(\mathbf{r}_1,\mathbf{r}_2) \; ; \qquad (4.17)$$

[see Eq. (A20), Appendix A]. Hence the final conclusion is

$$(\Delta E_{ij})^2=\langle \delta E_i \delta E_i \rangle-2\langle \delta E_i \delta E_j \rangle+\langle \delta E_j \delta E_j \rangle \; ; \qquad (4.18)$$

where

$$\langle \delta E_i \delta E_j \rangle=T\int\int\int\int d\mathbf{r}\, d\mathbf{r}'\, d\mathbf{r}_1\, d\mathbf{r}_2 |\Psi_i(\mathbf{r})|^2 K(\mathbf{r},\mathbf{r}_1)\chi(\mathbf{r}_1,\mathbf{r}_2)K(\mathbf{r}_2,\mathbf{r}')|\Psi_j(\mathbf{r}')|^2 \; . \qquad (4.19)$$

This is our main result. It allows one, in principle, to calculate separately the "linewidth" for each particular transition $i \to j$, provided that the static linear-response function $\chi(\mathbf{r}_1,\mathbf{r}_2)$ is known. Let us note, however, that even in the DFT with local expression for V_{xc}, the calculation of $\chi(\mathbf{r},\mathbf{r}')$ and even of $\chi^{-1}(\mathbf{r},\mathbf{r}')$ is not straightforward since in order to get it one should invert $\chi_0(\mathbf{r},\mathbf{r}')$ [Eq. (A13)]. In the numerical example below we will focus our attention on the Thomas-Fermi approximation to $\chi_0(\mathbf{r},\mathbf{r}')$.

We remark finally that the Gaussian form of lines [Eq. (4.13)] is due to the approximation when we neglect all dependence of $\sigma^{bb}(\nu)$ upon $\delta n(\mathbf{r})$ except that of E_i and E_j in the Dirac δ's. In general, if the full dependence of the oscillator strengths and of the Fermi factors upon $\delta n(\mathbf{r})$ is taken into account, the line-shape function may be different from the Gaussian one.

V. EXAMPLE: THOMAS-FERMI FORM OF $\chi_0(\mathbf{r},\mathbf{r}')$

The Thomas-Fermi theory leads to (Appendix B)

$$(\chi_0^{\text{TF}})^{-1}(\mathbf{r},\mathbf{r}')=\frac{\delta eV}{\delta n'}\delta(\mathbf{r}-\mathbf{r}') \; , \qquad (5.1\text{a})$$

$$\frac{\delta eV}{\delta n'}=\frac{2\pi}{h^3}(2m)^{3/2}T^{1/2}I_{-1/2}\left[\frac{eV_{\text{sc}}(\mathbf{r})+\mu}{T}\right] . \qquad (5.1\text{b})$$

According to Eq. (A20) (Appendix A) we set for the inverse of the linear-response function

$$\chi^{-1}(\mathbf{r},\mathbf{r}')=(\chi_0^{\text{TF}})^{-1}(\mathbf{r},\mathbf{r}')+\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}+\frac{\delta V_{\text{xc}}}{\delta n'}\delta(\mathbf{r}-\mathbf{r}') \; . \qquad (5.2)$$

The exchange-correlation potential V_{xc} at nonzero temperature has been calculated in Ref. 21 (see also Ref. 22). We use, however, the simpler expressions taken from Ref. 3 (the exchange correction interpolated between $T=0$ and $T=\infty$, asymptotic values of the correlation correction at $T=0$), since, as our numerical example indicates, the contribution of dV_{xc}/dn to the statistical broadening seems to be small. By keeping only the first terms in Eq. (5.2) and neglecting consequently the exchange-correlation part of Eq. (4.6), we get from Eqs. (4.18)–(4.19) the result derived by Shalitin, Stein, and Ron.[16] These authors have obtained it in a different way with no direct reference to the formalism of the DFT. For instance, they do not get the Gaussian form of $f_{ij}(x)$, Eq. (4.13), and only suppose it because of the statistical nature of their considerations. From the point of view of our derivation Shalitin *et al.* took into account only the noninteracting part of electron response treated in TF approximations [$\chi_0^{\text{TF}}(\mathbf{r},\mathbf{r}')$]. Actually, the Coulomb part [the second term in Eq. (5.2)] cannot be neglected as we will see later on. This Coulomb term complicates the calculation since $\chi^{-1}(\mathbf{r},\mathbf{r}')$, given in Eq. (5.2), cannot be so easily inverted as the independent-particle part $(\chi_0^{\text{TF}})^{-1}(\mathbf{r},\mathbf{r}')$. If one neglects the second and third terms in Eq. (5.2) one gets immediately

$$\chi_0^{\text{TF}}(\mathbf{r},\mathbf{r}')=\frac{\delta n(\mathbf{r})}{\delta eV}\delta(\mathbf{r}-\mathbf{r}') \; ; \qquad (5.3)$$

with $\delta n/\delta eV(\mathbf{r})$ being the inverse of the right-hand side (rhs) of Eq. (5.2). This leads to the result of Ref. 16. When the full form of Eq. (5.2) is retained the inverse of $\chi^{-1}(\mathbf{r},\mathbf{r}')$ has to be calculated numerically. In order to do it let us first simplify our problem by taking the squares of the wave functions [Eq. (4.19)] already averaged with respect to the magnetic quantum numbers m_i and m_j. That is we take

$$|\Psi_i|^2=\frac{1}{2l_i+1}\sum_{m_i=-l_i}^{+l_i}|\Psi_{n_i l_i m_i}(\mathbf{r})|^2=\frac{1}{4\pi}R^2_{n_i l_i}(r) \; , \qquad (5.4)$$

where $R_{n_i,l_i}(r)$ denotes the radial wave function. This step seems to be justified since anyway the Thomas-Fermi $\chi_0^{\text{TF}}(\mathbf{r},\mathbf{r}')$, with its local $\delta(\mathbf{r}-\mathbf{r}')$-like dependence cannot give a realistic model of the splitting of lines [we believe that $\chi_0(\mathbf{r},\mathbf{r}')$ from DFT, Eqs. (A13), may be more useful for this purpose]. Another point is that we are interested in transition lines as provided by the average-atom model which obviously leads to the degeneracy with respect to the magnetic quantum number. Now it is easy to see from the form of Eq. (4.19), that the approximation, Eq. (5.4), reduces our problem to a spherically symetric one. Denoting symbolically integral operators V and H,

$$(Vf)(r)\equiv\int dr'r'^2V(r,r')f(r')\ , \tag{5.5}$$

$$(Hf)(r)\equiv\int dr'r'^2H(r,r')f(r')\ , \tag{5.6}$$

where $f(r)$ denotes any function and

$$V(r,r')=\frac{1}{\max(r,r')}+\frac{\delta V_{\mathrm{xc}}[n]}{\delta n}\ \frac{1}{4\pi e^2r^2}\delta(r-r')\ , \tag{5.5$'$}$$

$$H(r,r')=\frac{1}{e^2}\ \frac{\delta eV}{\delta n(r)}\ \frac{\delta(r-r')}{4\pi r^2}\ , \tag{5.6$'$}$$

we write Eq. (4.17) as

$$\langle\delta E_i\delta E_j\rangle=e^2T\int dr\,r^2\int dr'\,r'^2R^2_{n_i,l_i}(r)[V(V+H)^{-1}V](r,r')R^2_{n_j,l_j}(r')\ . \tag{5.7}$$

The most convenient representation for calculating the operator product in square brackets will be of course $[R_{n_i,l_i}(r)]^2$, with n_i,l_i belonging to the whole spectrum. It corresponds to the expansion

$$\delta n(\mathbf{r})=\sum_{n_i,l_i\in b,f}\alpha_{n_i,l_i}\frac{|R_{n_i,l_i}(r)|^2}{4\pi}\ , \tag{5.8}$$

which may be viewed as natural, with α_{n_i,l_i} being the correction to the Fermi-Dirac occupation number [see Eq. (2.1)].

Our formulas Eqs. (4.14), (4.15), and (5.7) allow one to calculate independently the linewidth ΔE_{ij} for each pair i,j. We have found moreover that the matrix operations of Eq. (5.7) are in practice independent of the number of elements of the basis $R^2_{n_i,l_i}(r)$, $i\in S$. In particular, the results for ΔE_{ij} have been found to be independent of the presence of the $R^2_{n_i,l_i}(r)$ belonging to the free spectrum. This part of the basis has therefore been neglected and we took only $R^2_{n_i,l_i}(r), i\in$ bound states.

Below we present some results obtained for iron plasma at $T=200$ eV and of solid density: $\rho=\rho_0=7.8$ g/cm^3. In Table I we list the following.

(i) The energies of transitions.

(ii) ΔE^s_{ij}, the linewidths calculated from the expression corresponding to that of Shalitin, Stein, and Ron[16] with

$$\langle\delta E_i\delta E_j\rangle^s=e^2T\int dr\,r^2\int dr'\,r'^2R^2_{n_i,l_i}(r)(V^sH^{-1}V^s)(r,r')R^2_{n_j,l_j}(r')\ , \tag{5.9}$$

where

$$(V^sf)(r)\equiv\int dr'\,r'^2V^s(r,r')f(r')\ , \tag{5.10a}$$

$$V^s(r,r')\equiv\frac{1}{\max(r,r')}\ . \tag{5.10b}$$

(iii) ΔE_{ij}, the linewidths obtained with the full expression, Eq. (5.7).

(iv) ΔE^*_{ij}, the linewidths obtained from Eq. (5.7) but with the exchange term in Eq. (5.5′) neglected:

$$\langle\delta E_i\delta E_j\rangle^*=e^2T\int dr\,r^2\int dr'r'^2R^2_{n_i,l_i}(r)[V^s(H+V^s)^{-1}V^s](r,r')R^2_{n_j,l_j}(r')\ . \tag{5.11}$$

TABLE I. Transition energies and half-widths ΔE^s_{ij} [Eqs. (4.14) and (5.9)], ΔE_{ij} [Eqs. (4.14) and (5.7), and ΔE^*_{ij} [Eqs. (4.14) and (5.11)].

Nr	$i\to j$	Energy (eV)	ΔE^s_{ij} (eV)	ΔE_{ij} (eV)	ΔE^*_{ij}
1	$1s\to2p$	6339	72.1	57.7	65.6
2	$1s\to3p$	7128	126.1	97.3	104.6
3	$1s\to4p$	7307	158.9	117.6	123.9
4	$2s\to2p$	97.8	10.72	7.65	9.21
5	$2s\to3p$	886.5	59.54	41.4	45.4
6	$2s\to4p$	1066	100.42	67.7	71.8
7	$3s\to3p$	31.4	2.13	1.46	1.65
8	$3s\to4p$	210.8	43.70	27.8	30.0
9	$4s\to4p$	10.96	2.80	1.76	1.81
10	$2p\to3s$	757.2	70.4	49.8	54.1
11	$2p\to4s$	957.1	106.5	73.1	77.3
12	$2p\to3d$	834.7	62.9	45.3	49.1
13	$3p\to4s$	168.4	43.2	27.5	29.9
14	$3p\to3d$	46.0	7.74	4.30	6.07
15	$3d\to4p$	133.5	52.1	32.7	36.1

The inclusion of the operator V^s into the linear response [compare Eqs. (5.9) and (5.11)] lowers all the "half-widths." This is obvious since both operators H and V^s are positive definite. The contribution coming from the operator H [Eq. (5.6)] is dominant. This effect is even more visible at higher temperatures. For instance, at $T=1000$ eV and at $\rho=\rho_0$ the difference between ΔE_{ij}^s and ΔE_{ij}^* is mainly of the order of 5–10 % of ΔE_{ij}^s. We have tested the domain of temperatures T, 10–1000 eV, and densities ρ, $\rho_0/10$–$10\rho_0$, and found that for most cases and transitions this difference was smaller (but of the same order) than ΔE_{ij}^s. A typical value was 20–70 %; however, there were still some transitions with 100% and more.

The local exchange-correlation term also diminishes the bandwidths. The difference between ΔE_{ij} and ΔE_{ij}^* is of the order of 10%. The same order of contribution due to the local exchange-correlation part of the linear response has been observed in Ref. 10 where the authors used the DFT formalism to approximate the frequency-dependent polarization.

In Table II we present some opacity results calculated using the b-b contribution obtained from the above values of "level widths" (ΔE_{ij}). The description of the numerical methods and the formulas for the b-f and f-f cross sections may be found elsewhere.[25,26] The formulas for the total Planck (k_p) and Rosseland (k_R) mean opacities[1] (see, also, Refs. 25 and 26) are

$$k_p=\frac{15}{\pi^4}\left[\frac{h}{T}\right]^4\int_0^\infty\frac{d\nu\,\nu^3 k'(\nu)}{\exp(h\nu/T)-1}\ ,$$

$$k_R^{-1}=\frac{15}{4\pi^4}\left[\frac{h}{T}\right]^5\int_0^\infty\frac{d\nu\,\nu^4\exp(h\nu/T)}{[\exp(h\nu/T)-1]^2k'(\nu)}\ ,$$

where $k'(\nu)=[\sigma_a(\nu)+\sigma_{\text{scat}}]/m_a$. In our example the scattering term is very small and in fact can be neglected. The absorption cross section $\sigma_a(\nu)$ consists of the bound-bound (bb), bound-free (bf), and free-free (ff) contributions [see Eq. (3.3)]. The importance of these contributions may be inferred from the Rosseland and Planck mean opacities calculated with some of these contributions neglected. As follows from Table II the dominant are the bound-bound transitions (see, for instance, Ref. 13). The result from the SESAME Astrophysical Library[27] is k_R (Rosseland opacity) $=2679$ (cm^2/g) and k_C (Rosseland opacity without the contribution of lines) $=988$ (cm^2/g) (see Ref. 28). The agreement seems to be relatively good.

TABLE II. Planck (k_P) and Rosseland (k_R) opacities for iron ($Z=26$) at $T=200$ eV, $\rho=\rho_0=7.8$ g/cm^3. The transitions taken into consideration are listed in the first column. b denotes "bound," f is "free." The values from the Astrophysical Library SESAME (Ref. 27) are (see Ref. 28) $k_R=2679$ cm^2/g, k_C (without lines) $=988$ cm^2/g.

Transitions included	k_P (cm^2/g)	k_R (cm^2/g)
bb, bf, ff, scattering	6644	2956
bb, bf, scattering	5854	2543
bf, scattering	2958	1098
ff, scattering	790	55

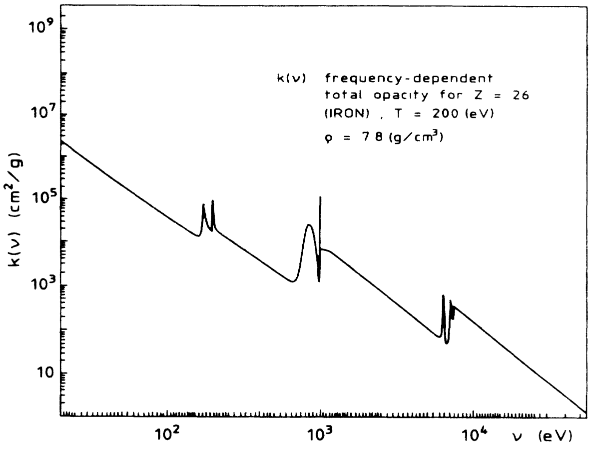

FIG. 1. Frequency-dependent total absorption spectrum $k(\nu)=[\sigma_a(\nu)/m_a]/[1-\exp(-h\nu/T)]$ for $Z=26$ (iron), $T=200$ eV, $\rho=\rho_0=7.8$ (g/cm^2). $k(\nu)$ is in cm^2/g and ν in eV.

In Fig. 1 we show the total absorption $k(\nu)$ $=[\sigma_a(\nu)/m_a]/[1-\exp(-h\nu/T)]$ (with m_a the atomic mass) in cm^2/g as a function of the photon frequency ν (in eV).

VI. CONCLUSIONS

We present a statistical approach to the absorption bands in dense, partially ionized plasma. Our formalism is based on the finite-temperature density-functional theory. It allows us to preserve a consistent model in which the probability of fluctuations around the average atom is obtained from the density dependence of the DFT functional $\Omega[n]$. This functional is minimized with respect to the electron density $n(\mathbf{r})$ when one looks for the DFT equilibrium solution, i.e., the average-atom model.

In the simplest version of DFT, which is the Thomas-Fermi expression of $\Omega[n]$, the presented formalism leads to closed formulas for the ΔE_{ij}—the widths of the transition lines. In this case, when the Coulomb and exchange-correlation contribution to $\delta^2\Omega[n]/\delta n(\mathbf{r})\delta n(\mathbf{r}')$ is neglected, our results reduce to that of Shalitin, Stein, and Ron.[16] The numerical example of iron at $T=200$ eV and solid density shows, however, that especially the Coulomb contribution is non-negligible. Our formalism may lead to interesting conclusions when a more involved form of the linear-response function $\chi_0(\mathbf{r},\mathbf{r}')$ is retained. The inclusion of the dependence of the oscillator strength and of the Fermi factors upon the density perturbation can lead, in principle, to non-Gaussian shapes of lines.

In its simplest Thomas-Fermi version the formalism allows us to estimate the bound-bound contribution to the opacity of dense, partially ionized plasma close to the local thermodynamic equilibrium.

ACKNOWLEDGMENTS

One of the authors (T.B.) gratefully acknowledges the financial support of the Swiss National Science Fund through Subsidy No. 2000-5-527.

APPENDIX A: THE FORMALISM OF DENSITY-FUNCTIONAL THEORY AT FINITE TEMPERATURE AND THE FORMULA FOR $\delta^2\Omega[n]/\delta n(\mathbf{r})\delta n(\mathbf{r}')$

As proved in Refs. 6 and 7 in a grand-canonical ensemble at a given temperature T the density distribution $n(\mathbf{r})$ uniquely determines the quantity $ev(\mathbf{r})+\mu$ (e positive) where v is the external potential and μ is the chemical potential. For a given $v(\mathbf{r})$ and μ there exists a functional of $n'(\mathbf{r})$:

$$\Omega_{ev+\mu}[n'(\mathbf{r})]=-\int[ev(\mathbf{r})+\mu]n'(\mathbf{r})d\mathbf{r}'+F[n'(\mathbf{r})]\ , \tag{A1}$$

which has an absolute minimum for $n'(\mathbf{r})=n(\mathbf{r})$ [the correct density corresponding to $v(\mathbf{r})$ and μ]. This minimum value is equal to the grand potential.

As proved in Ref. 6 for any $n'(\mathbf{r})$ different from $n(\mathbf{r})$,

$$\Omega_{ev+\mu}[n'(\mathbf{r})]>\Omega_{ev+\mu}[n(\mathbf{r})]\ .$$

In the local-density approximation one writes $F[n'(\mathbf{r})]$ as

$$F[n'(\mathbf{r})]=G_s[n'(\mathbf{r})]+\frac{e^2}{2}\int d\mathbf{r}\,d\mathbf{r}'\frac{n'(\mathbf{r})n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}+F_{\mathrm{xc}}[n'(\mathbf{r})]\ , \tag{A2}$$

where

$$G_s[n'(\mathbf{r})]=C_s[n'(\mathbf{r})]-TS_s[n'(\mathbf{r})]\ ; \tag{A3}$$

is the $F[n'(\mathbf{r})]$ corresponding to the noninteracting electron gas where $S_s[n'(\mathbf{r})]$ denotes its entropy. This electron gas may be described in terms of one-electron Schrödinger states:

$$\left[-\frac{1}{2}\frac{\hbar^2}{m}\nabla^2-ev'(\mathbf{r})\right]\Psi_i'(\mathbf{r})=E_i'\Psi_i'(\mathbf{r})\ , \tag{A4}$$

where the relation between $n'(\mathbf{r})$ and $v'(\mathbf{r})$ is given through

$$n'(\mathbf{r})=2\sum_i f_i'|\Psi_i'(\mathbf{r})|^2\ , \tag{A5}$$

$$f_i'\equiv f_i(E_i'-\mu')=\left[\exp\left[\frac{E_i'-\mu'}{T}\right]+1\right]^{-1}\ . \tag{A6}$$

The entropy of the ideal electron gas is

$$S_s[n']=-2\left[\sum_i f_i'\ln f_i'+(1-f_i')\ln(1-f_i')\right]\ . \tag{A7}$$

$F_{\mathrm{xc}}[n'(\mathbf{r})]$ is the correction so that $F_s[n'(\mathbf{r})]+F_{\mathrm{xc}}[n'(\mathbf{r})]$ gives the full exact $F[n'(\mathbf{r})]$. It is approximated here by a *local* expression. From the above formulas one may calculate formally

$$\frac{\delta\Omega}{\delta n'(\mathbf{r})}=ev'(\mathbf{r})+\mu'-ev(\mathbf{r})-\mu+e^2\int d\mathbf{r}'\frac{n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}+\frac{\delta F_{\mathrm{xc}}}{\delta n'}[n']\ . \tag{A8}$$

The condition for minimum is obviously

$$\frac{\delta\Omega}{\delta n'(\mathbf{r})}[n]=0\ , \tag{A9}$$

which leads to the self-consistent scheme by connecting $ev_{eq}(\mathbf{r})+\mu_{eq}$ to the electron density $n(\mathbf{r})$:

$$-ev_{eq}(\mathbf{r})-\mu_{eq}=-ev(\mathbf{r})-\mu+e^2\int d\mathbf{r}'\frac{n'(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|}+V_{\mathrm{xc}}[n(\mathbf{r})]\ ; \tag{A10a}$$

where

$$V_{\mathrm{xc}}[n(r)]=\frac{\delta F_{\mathrm{xc}}}{\delta n'}[n(r)]\ . \tag{A10b}$$

In the case of the atom $v(\mathbf{r})=Ze/|\mathbf{r}|$. Following Ref. 7 we note that the condition Eq. (A10a) leads to the equation for $ev'(\mathbf{r})+\mu'$ and not for $ev'(\mathbf{r})$ alone.

Using Eq. (A8) we get for the second derivative[29]

$$\frac{\delta^2\Omega}{\delta n'(\mathbf{r})\delta n'(\mathbf{r}')}=\frac{\delta[ev'(\mathbf{r})+\mu']}{\delta n'(\mathbf{r}')}+\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}+\frac{\delta^2 F_{\mathrm{xc}}}{\delta n'(\mathbf{r})\delta n'(\mathbf{r}')}\ . \tag{A11}$$

The first term on the rhs of Eq. (A11) may be written explicitly. $ev'(\mathbf{r})$ is the trial (external) potential and $n'(\mathbf{r})$ the inhomogeneous density of an noninteracting electron gas immersed in the field of this potential. Hence we have

$$\delta n'(\mathbf{r})=\int d\mathbf{r}'\chi_0(\mathbf{r},\mathbf{r}')e\delta v'(\mathbf{r}')\ , \tag{A12}$$

where $\chi_0(\mathbf{r},\mathbf{r}')$ is the static linear-response function of noninteracting electron gas. It may be calculated as the real part of retarded polarization at $\omega=0$:[9]

$$\chi_0(\mathbf{r},\mathbf{r}')=\mathrm{Re}\Pi^R(\mathbf{r},\mathbf{r}',\omega=0)=2\sum_{i\neq j}\frac{\Psi_i^*(\mathbf{r})\Psi_j(\mathbf{r})\Psi_j^*(\mathbf{r}')\Psi_i(\mathbf{r}')(f_i-f_j)}{(E_i-E_j)}\ , \tag{A13}$$

where $\Psi_j(\mathbf{r})$ are the eigenstates of the potential $v_{eq}(\mathbf{r})$. A useful relation used in Ref. 30 (see also Ref. 10) is

$$\chi_0(\mathbf{r},\mathbf{r}')=-\frac{2}{\pi}\hbar\,\mathrm{Im}\int_{-\infty}^{+\infty}d\omega\,f(\hbar\omega)G_0^R(\mathbf{r},\mathbf{r}',\omega)G_0^R(\mathbf{r}',\mathbf{r},\omega), \tag{A14}$$

relating $\chi_0(\mathbf{r},\mathbf{r}')$ to the retarded noninteracting Green function of the potential $ev_{eq}(\mathbf{r})$:

$$G_0^R(\mathbf{r},\mathbf{r}',\omega)=2\sum_j\frac{\Psi_j^*(\mathbf{r}')\Psi_j(\mathbf{r})}{\omega-(E_j-\mu_{eq})/\hbar+i\eta}\ ; \tag{A15}$$

$$f(\hbar\omega)=\left[1+\exp\left[\frac{\hbar\omega}{T}\right]\right]^{-1}\ . \tag{A16}$$

$G_0^R(\mathbf{r},\mathbf{r}',\omega)$ fulfils the equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2-ev_{eq}(\mathbf{r})-\hbar\omega\right]G_0^R(\mathbf{r},\mathbf{r}',\omega)=-\delta(\mathbf{r}-\mathbf{r}')\ , \tag{A17}$$

with the "outgoing-wave" boundary conditions. Let us also remark that Eq. (A8) may be viewed as

$$\frac{\delta\Omega}{\delta n'(\mathbf{r})}=\delta e v'_{\text{eff}}(\mathbf{r})\equiv e v'(\mathbf{r})-e v_{eq}(\mathbf{r}) \; ; \tag{A8'}$$

(we set $\mu_{eq}=\mu$) and, at $n'(\mathbf{r})=n(\mathbf{r})$;

$$\frac{\delta^2\Omega}{\delta n'(\mathbf{r})\delta n'(\mathbf{r}')}=\frac{\delta e v'_{\text{eff}}(\mathbf{r})}{\delta n'(\mathbf{r}')} \; ; \tag{A11'}$$

(see Ref. 29) where the rhs is the inverse operator to the DFT linear-response function $\chi(\mathbf{r},\mathbf{r}')$ since

$$\frac{\delta n'(\mathbf{r})}{\delta e v'_{\text{eff}}(\mathbf{r}')}[n]=\chi(\mathbf{r},\mathbf{r}') \, . \tag{A18}$$

The inverse operator is defined in the standard way:[29]

$$\int d\mathbf{r}''\chi^{-1}(\mathbf{r},\mathbf{r}'')\chi(\mathbf{r}'',\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}') \, . \tag{A19}$$

From Eqs. (A11), (A11'), and (A12) we get the following relation between the DFT linear-response function $\chi(\mathbf{r},\mathbf{r}')$, the independent electrons response function $\chi_0(\mathbf{r},\mathbf{r}')$, and the second functional derivative of the grand thermodynamic potential with respect to the electron density $\delta^2\Omega[n]/\delta n(\mathbf{r})\delta n(\mathbf{r}')$:

$$\begin{aligned}\frac{\delta^2\Omega}{\delta n'(\mathbf{r})\delta n'(\mathbf{r}')}[n]&=\chi^{-1}(\mathbf{r},\mathbf{r}')\\&=\chi_0^{-1}(\mathbf{r},\mathbf{r}')+\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\\&\quad+\frac{\delta^2 F_{\text{xc}}}{\delta n'(\mathbf{r})\delta n'(\mathbf{r}')} \, .\end{aligned} \tag{A20}$$

In the local-density approximation we obviously have

$$\frac{\delta^2 F_{\text{xc}}}{\delta n'(\mathbf{r})\delta n'(\mathbf{r}')}=\frac{\delta^2 F_{\text{xc}}}{\delta n'^2(\mathbf{r})}\delta(\mathbf{r}-\mathbf{r}') \, . \tag{A21}$$

APPENDIX B: THOMAS-FERMI MODEL AS DFT

As noted by Mermin[6] the finite-temperature Thomas-Fermi theory (see Ref. 18) may be obtained through minimization of the following $\Omega[n'(\mathbf{r})]$:

$$\begin{aligned}\Omega[n'(\mathbf{r})]=\frac{2}{h^3}\int d\mathbf{r}\, d\mathbf{p}\Bigg[&T\ln\left\{1-f\left[\frac{1}{T}\left[\frac{\mathbf{p}^2}{2m}-e v'(\mathbf{r})-\mu'\right]\right]\right\}\\&+[e v'(\mathbf{r})-\mu']f\left[\frac{1}{T}\left[\frac{\mathbf{p}^2}{2m}-e v'(\mathbf{r})-\mu'\right]\right]\Bigg]-\int d\mathbf{r}[e v(\mathbf{r})+\mu]n'(\mathbf{r})+\frac{e^2}{2}\int d\mathbf{r}\, d\mathbf{r}'\frac{n'(\mathbf{r})n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \, ,\end{aligned} \tag{B1}$$

with $n'(\mathbf{r})$ and $e v'(\mathbf{r})+\mu$ being connected by

$$n'(\mathbf{r})=\frac{2}{h^3}\int d\mathbf{p}\, f\left[\frac{1}{T}\left[\frac{\mathbf{p}^2}{2m}-e v'(\mathbf{r})-\mu'\right]\right] \, , \tag{B2}$$

where

$$f(x)=\frac{1}{\exp(x)+1} \, . \tag{B3}$$

By straightforward differentiation we get the TF version of Eq. (A20):

$$\frac{\delta\Omega}{\delta n'}[n']=e v'(\mathbf{r})+\mu'-e v(\mathbf{r})-\mu+e^2\int d\mathbf{r}'\frac{n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \, , \tag{B4}$$

where $e v'(\mathbf{r})+\mu$ are the functional of $n'(\mathbf{r})$ because of Eq. (B2). Also

$$e v(\mathbf{r})=\frac{Ze}{|r|}$$

is the potential of the nucleus (Z atomic number). The condition $\delta\Omega[n_{\text{TF}}]/\delta n'=0$ may be easily transformed into the usual form of the TF equation. In the case of a finite, spherically symmetric neutral atom we have

$$\nabla^2 e v_{\text{TF}}(r)=\frac{16\pi^2 e^2(2mT)^{3/2}}{h^3}I_{1/2}\left[\frac{e v_{\text{TF}}(r)+\mu_{\text{TF}}}{T}\right] \, , \tag{B5}$$

where

$$I_n(x)=\int_0^\infty dy\, y^n\frac{1}{\exp(y-x)+1} \, , \tag{B6}$$

with the boundary conditions

$$e v_{\text{TF}}\xrightarrow[r\to 0]{}\frac{Ze^2}{r}, \quad v_{\text{TF}}(r_0)=0, \quad \frac{d v_{\text{TF}}}{dr}(r_0)=0 \, , \tag{B7}$$

and r_0 the atomic radius. Similarly, we get

$$\frac{\delta^2\Omega}{\delta n'(\mathbf{r})\delta n'(\mathbf{r}')}=\frac{\delta e v'(\mathbf{r})}{\delta n'(\mathbf{r}')}\delta(\mathbf{r}-\mathbf{r}')+\frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \; ; \tag{B8}$$

comparing with Eqs. (A11), (A18), and (A20) we get

$$\begin{aligned}\chi_0^{\text{TF}}(\mathbf{r},\mathbf{r}')&=\frac{\delta n'(\mathbf{r})}{\delta e v'(\mathbf{r}')}[n_{\text{TF}}]\delta(\mathbf{r}-\mathbf{r}')\\&=\frac{2\pi(2m)^{3/2}T^{1/2}}{h^3}I_{-1/2}\\&\quad\times\left[\frac{e v_{\text{TF}}+\mu_{\text{TF}}}{T}\right]\delta(\mathbf{r}-\mathbf{r}') \, .\end{aligned} \tag{B9}$$

The independent-electron linear-response operator is local in the Thomas-Fermi model.

APPENDIX C: PROOF OF EQ. (4.13)

A simple way to prove Eq. (4.13) is to make use of the formula (see Ref. 23, p. 25)

$$\int_{-\infty}^{+\infty}\prod_{r=1}^{N} dx_r \exp\left(-\tfrac{1}{2}\mathbf{x}^T\hat{M}\mathbf{x}-\mathbf{B}^T\mathbf{x}\right) =(2\pi)^{N/2}(\det\hat{M})^{-1/2}\exp\left(-\tfrac{1}{2}\mathbf{B}^T\hat{M}^{-1}\mathbf{B}\right)\,, \quad \text{(C1)}$$

where $\hat{M}$ is an $N\times N$ positive definite matrix, and $\mathbf{x}$ and $\mathbf{B}$ are vectors in the R^N space. Equation (C1) may be easily proved by diagonalization of the quadratic form in the exponential.

Substituting the Fourier transform for the Dirac function we get immediately for $f_{ij}(x)$ [Eq. (4.12)]

$$\int dk \int \prod_{t\in S} d\delta E_t \exp\left[-\frac{1}{2}\sum_{r,s}A_{rs}\delta E_r \delta E_s + ik(x-\delta E_j+\delta E_i)\right]\,. \quad \text{(C2)}$$

The term that is linear in $\delta\mathbf{E}$ in the exponential may be written as

$$-ik(\delta E_j-\delta E_i) = -ik\sum_{p\in S} B_p^{(i,j)}\delta E_p\,, \quad \text{(C3)}$$

where the vector $B_p^{(i,j)}$ is defined as

$$B_p^{(i,j)}=\delta_{i,p}-\delta_{j,p}\,. \quad \text{(C4)}$$

We are now able to perform the integration over $\prod_t d\delta E_t$ by applying Eq. (C1). We get

$$f_{ij}(x)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} dk \exp\left[ikx-\tfrac{1}{2}k^2\sum_{r,s}B_r^{(i,j)}(A^{-1})_{r,s}\times B_s^{(i,j)}\right]\,. \quad \text{(C5)}$$

Using again Eq. (C1) in Eq. (C5) we find Eq. (4.13).

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