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Relation between the super-transition-array method in opacity calculations and the Hartree-Fock approximation at nonzero temperature

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We consider the photoabsorption cross section of dense plasmas in thermodynamic equilibrium. We transform the exact expression of this cross section into a form suitable for the calculation of moments with respect to frequency. We show that the super-transition-array (STA) method, which is successfully applied in opacity calculations, is consistent with the thermal Hartree-Fock approximation. The Hartree-Fock theory justifies the use of the noninteracting partition function inside each superconfiguration, which is an important approximation in the STA method.

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I. INTRODUCTION

The super-transition-array (STA) method proposed in Refs. [1–3] appears to be a very efficient approach to the theoretical calculation of opacities of dense plasmas in local thermodynamic equilibrium. (See, for instance, Ref. [4].) The large number of configurations in case of intermediate- and high-Z (atomic number) elements remains one of the main problems in modeling the bound-bound opacity. It has been shown [1] that the inclusion of transitions involving most probable configurations with the neglect of many other low probability configurations may lead to large errors in opacities. The important problems of term structures seem now to be in large part resolved by the statistical approach developed by Bauche, Bauche-Arnoult, and Klapisch [5].

In the STA method, the arrays of transitions between two group of electronic configurations (called super configurations) are replaced by Gaussian curves characterized by the first two moments of these transitions. One of the most important features of the STA method is the possibility to take into account, within the framework of super transition arrays, all electronic configurations by summing them up analytically. This simplification relies on the use of the noninteracting partition function inside each super configuration. Recently [3], the authors of the STA method have included configuration interaction (CI) in their approach.

The objective of this brief paper is to show that the use of the noninteracting partition function can be justified within the framework of the thermal Hartree-Fock (HF) approximation [6,7]. This approximation leads to the noninteracting partition function with all or a part of configuration interactions still preserved. The strategy of the authors of the STA method is, therefore, consistent with the HF theory.

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II. THE PHOTO ABSORPTION CROSS SECTION

The formula for the photo absorption cross section can be obtained from the expression for the dynamic electron polarizability. (See, for instance, Refs. [8–10].) At nonzero temperature $T=1/\beta$, one gets in the dipole approximation

$$\sigma_a(\omega)=\frac{4\pi^2\omega e^2}{3c}\int d\mathbf{r}\,d\mathbf{r}'\sum_{n_E,m_E}P_{n_E}\langle n_E|\hat{n}(\mathbf{r})\mathbf{r}|m_E\rangle \times\langle m_E|\hat{n}(\mathbf{r}')\mathbf{r}'|n_E\rangle \times\delta(\hbar\omega-E_{m_E}+E_{n_E}) , \quad (1)$$

where E_{n_E} is the energy of the N-electron eigenstate $|n_E\rangle$ of the atomic Hamiltonian and P_{n_E} denotes the eigenvalue of the statistical operator

$$\hat{P}=\exp[-\beta(\hat{H}-\mu\hat{N})]/\mathrm{Tr}\{\exp[-\beta(\hat{H}-\mu\hat{N})]\} , \quad (2)$$

with $\hat{H}$ being the atomic Hamiltonian and $\hat{N}$ the electron number operator. $\hat{n}_H(\mathbf{r},t)$ denotes the electron density operator in the Heisenberg picture.

Since $\delta(\hbar\omega-E_1+E_2)=\int d(\hbar\omega')\delta(\hbar\omega-\hbar\omega'+E_2)\delta(\hbar\omega'-E_1)$, we can rewrite Eq. (1) as

$$\sigma_a(\omega)=\frac{4\pi^2\omega e^2}{3c}\times\int d\mathbf{r}\,d\mathbf{r}'\int d(\hbar\omega')\sum_{n_E}\langle n_E|\hat{P}\delta(\hbar\omega-\hbar\omega'+\hat{H})\times\hat{n}(\mathbf{r})\mathbf{r}\delta(\hbar\omega'-\hat{H})\times\hat{n}(\mathbf{r}')\mathbf{r}'|n_E\rangle . \quad (3)$$

The expression of Eq. (3) being the trace of an operator, we can use an arbitrary basis $|n\rangle$ of atomic states in place of $|n_E\rangle$. Let us use the basis defined as

$$|n\rangle=\hat{a}_{i_1}^{\dagger},\ldots,\hat{a}_{i_N}^{\dagger}|0\rangle , \quad (4)$$

where $\hat{a}_i^{\dagger}$ are creation operators for a basis of one-electron states. The cross section now reads

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$$\sigma_a(\omega)=\frac{4\pi^2\omega e^2}{3c}\int d\mathbf{r}\,d\mathbf{r}'\int d(\hbar\omega')\times\sum_{n,m}\langle n|\hat{P}\delta(\hbar\omega-\hbar\omega'+\hat{H})\hat{n}(\mathbf{r})\mathbf{r}|m\rangle\times\langle m|\delta(\hbar\omega'-\hat{H})\hat{n}(\mathbf{r}')\mathbf{r}'|n\rangle\ , \tag{5}$$

where we inserted back the unit operator $\sum_m|m\rangle\langle m|$, expressed in the new basis.

Although the operator standing in Eq. (5), which contains the convolution with respect to $\hbar\omega'$, is rather complex, we can now work with the simple basis formed by Slater determinants of one-electron eigenstates as in Eq. (4). Besides, the moments with respect to ω of the elements of Eq. (5) have a simple form. Let us also note that Eq. (5) is equivalent to Eq. (1) and that up to now no approximation has been introduced. Only the entire sum over n, m in Eq. (5) has a physical sense. We can, however, consider different parts of Eq. (5) corresponding to transitions between two definite configurations or groups of configurations and apply a statistical approach to them.

III. THE STATISTICAL OPERATOR IN THE HARTREE-FOCK THEORY AT NONZERO TEMPERATURE

Let us now use the one-electron basis, which diagonalizes the HF equilibrium density matrix. As shown by Mermin [6] the HF theory at nonzero temperature is equivalent to the minimization of the grand thermodynamic potential $\Omega=\mathrm{Tr}[\hat{P}(\hat{H}-\mu\hat{N})+T\hat{P}\ln\hat{P}]$ over all trial statistical operators of the form

$$\hat{P}=\exp\left[-\sum\hat{a}_i^\dagger\gamma_{ij}\hat{a}_j\right]\Big/\mathrm{Tr}\left[\exp\left[-\sum\hat{a}_i^\dagger\gamma_{ij}\hat{a}_j\right]\right]\ , \tag{6}$$

where γ is a Hermitian matrix. The Hamiltonian has the form

$$\hat{H}=\sum K_{ij}\hat{a}_i^\dagger\hat{a}_j+\tfrac{1}{2}\sum\langle ij|v_{ee}|kl\rangle\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_l\hat{a}_k\ , \tag{7}$$

where K corresponds to the kinetic energy an the external (nuclear) potential, and $v_{ee}=e^2/|\mathbf{r}-\mathbf{r}'|$ in the coordinate representation.

In equilibrium, after choosing the basis in which γ is diagonal, one gets the self-consistent HF equations for the one-electron states of this basis

$$\varepsilon_i=K_{ii}+\sum\langle in|v|in\rangle\rho_n\ , \tag{8}$$

$$\rho_i=[\exp(\varepsilon_i-\mu)+1]^{-1}\ , \tag{9}$$

where

$$\langle in|v|in\rangle=\langle in|v_{ee}|in\rangle-\langle in|v_{ee}|ni\rangle\ . \tag{10}$$

γ can be expressed in terms of ε_i as follows:

$$\gamma_{ij}=\gamma_i\delta_{ij}=(\varepsilon_i-\mu)\delta_{ij}\ . \tag{11}$$

IV. THE MOMENTS OF TRANSITION ARRAYS AND SUPER TRANSITION ARRAYS

We can consider the ith moment $\mu_i^{CC'}$ of the transition array between two configurations C and C',

$$\mu_i^{CC'}=M_i^{CC'}/M_{i=0}^{CC'}\ , \tag{12}$$

$$M_i^{CC'}=\int d(\hbar\omega)(\hbar\omega)^i\int\int d\mathbf{r}\,d\mathbf{r}'I^{CC'}(\mathbf{r},\mathbf{r}',\omega)\ , \tag{13}$$

where

$$I^{CC'}(\mathbf{r},\mathbf{r}',\omega)=\int d(\hbar\omega')\sum_{n\in C,m\in C'}\langle n|\hat{P}\delta(\hbar\omega-\hbar\omega'+\hat{H})\hat{n}(\mathbf{r})\mathbf{r}|m\rangle\langle m|\delta(\hbar\omega'-\hat{H})\hat{n}(\mathbf{r}'\mathbf{r}'|n\rangle\ . \tag{14}$$

If one uses the HF approximation for the statistical operator $\hat{P}$ in equilibrium, i.e., Eq. (6) with Eq. (11), $|n\rangle$ are eigenstates of $\hat{P}$, and their eigenvalues are identical for any state $|n\rangle$ belonging to a definite configuration C because of the degeneracy of the HF energy eigenvalue ε_i with respect to the magnetic quantum number.

One obtains for $i=0$,

$$M_0^{CC'}=P_C\sum_{n\in C,m\in C'}\left|\langle n|\hat{D}|m\rangle\right|^2\ , \tag{15}$$

where $\hat{D}$ is the electric dipole operator of the atom, i.e., $\hat{D}=-\sum_{k=1}^{N}\mathbf{r}_k$ in the coordinate representation. Similarly one gets for $i\geq 1$,

$$M_1^{CC'}=P_C\int\int d\mathbf{r}\,d\mathbf{r}'\sum_{n\in C,m\in C'}[\langle n|\hat{H}\hat{n}(\mathbf{r})\mathbf{r}|m\rangle\langle m|\hat{n}(\mathbf{r}')\mathbf{r}'|n\rangle-\langle n|\hat{n}(\mathbf{r})\mathbf{r}|m\rangle\langle m|\hat{H}\hat{n}(\mathbf{r}')\mathbf{r}'|n\rangle]\ , \tag{16}$$

and so on. Let us notice that although CI's are neglected in the partition function (statistical operator), Eq. (16) (and Eq. (13) for $i\geq 1$) still contains CI's due to the presence of the products of the Hamiltonian and the electron density operator. If CI's are neglected, we obtain the expression of the moments used by Bauche, Bauche-Arnoult and Klapisch [5],

$$\mu_i^{CC'}=\sum_{\tilde{n}\in C,\tilde{m}\in C'}|\langle\tilde{n}|\hat{D}|\tilde{m}\rangle|^2[\langle\tilde{m}|\hat{H}|\tilde{m}\rangle-\langle\tilde{n}|\hat{H}|\tilde{n}\rangle]^i\Big/\sum_{\tilde{n}\in C,\tilde{m}\in C'}|\langle\tilde{n}|\hat{D}|\tilde{m}\rangle|^2\ , \tag{17}$$

where $\tilde{n}$, $\tilde{m}$ diagonalize $\hat{H}$ in C and C', respectively.

Instead of two configurations, we can consider transitions between two super configurations Ξ and Ξ' each containing

a group of configurations, and average Eq. (12) (CI included) or Eq. (17) (CI neglected) over Ξ and Ξ'. This leads to the expressions used by Bar-Shalom *et al.* [1]. The eigenvalue of the statistical operator in both cases equals to

$$P_C=\exp\left[-\beta\sum_{\text{shell } s\in C} q_s(\varepsilon_s-\mu)\right]\Big/\prod_{\text{one-electron state }\lambda}[1+\exp\{-\beta(\varepsilon_\lambda-\mu)\}]\ , \tag{18}$$

where q_s is the occupation number of shell s. This leads to the partition function, Eqs. (15) and (16) in Ref. [1].

Actually, the authors of the STA method calculate the self-consistent potential and one-electron states separately for each of the super configurations. In order to understand this approach, let us rewrite the exact expression, Eq. (5), grouping configurations into super configurations

$$\sigma_a(\omega)=\frac{4\pi^2\omega e^2}{3c}\int d\mathbf{r}\,d\mathbf{r}'\int d(\hbar\omega')\sum_{\Xi,\Xi'}\sum_{C\in\Xi,C'\in\Xi'}\sum_{n_C^\Xi\in C,m_{C'}^{\Xi'}\in C'}\langle n_C^\Xi|\hat{P}\delta(\hbar\omega-\hbar\omega'+\hat{H})\hat{n}(\mathbf{r})\mathbf{r}|m_{C'}^{\Xi'}\rangle$$
$$\times\langle m_{C'}^{\Xi'}|\delta(\hbar\omega'-\hat{H})\hat{n}(\mathbf{r}')\mathbf{r}'|n_C^\Xi\rangle\ . \tag{19}$$

We do not specify for the moment the basis of one-electron states. One can propose a HF-like procedure for each super configuration. In order to do this, γ in the HF approximation for the statistical operator, Eq. (6), should be now minimized according to the constraints that correspond to the structure of each super configuration. The minimization procedure can be performed separately for each super configuration, and the one-electron basis will be different for each super configuration. The partition function will have the noninteracting form, Eq. (18), inside each super configuration. For instance, the first moment corresponding to the super transition arrays has the form

$$M_1^{\Xi\Xi'}=\sum_{C\in\Xi,C'\in\Xi'}P_C\int\int d\mathbf{r}\,d\mathbf{r}'\sum_{n_C^\Xi\in C,m_{C'}^{\Xi'}\in C'}[\langle n_C^\Xi|\hat{H}\hat{n}(\mathbf{r})\mathbf{r}|m_{C'}^{\Xi'}\rangle\langle m_{C'}^{\Xi'}|\hat{n}(\mathbf{r}')\mathbf{r}'|n_C^\Xi\rangle$$
$$-\langle n_C^\Xi|\hat{n}(\mathbf{r})\mathbf{r}|m_{C'}^{\Xi'}\rangle\langle m_{C'}^{\Xi'}|\hat{H}\hat{n}(\mathbf{r}')\mathbf{r}'|n_C^\Xi\rangle]\ . \tag{20}$$

Equation (20) still preserves the CI.

In principle, the cross-section formulas that follow from Eq. (1) contain also the free-free transitions. In the present considerations we have disregarded all problems connected with them. A method that treats these transitions including their mixing with the bound-bound and bound-free transitions has been proposed in Ref. [11]. We also have not discussed the relativistic character of the STA method.

V. CONCLUSION

We have transformed the exact expression of the total photoabsorption cross section of dense plasmas into a form useful for the statistical description of transitions between configurations or super configurations. We have shown that the Hartree-Fock approximation to the statistical operator leads to the noninteracting partition function in the cross-section formula with configuration interactions still preserved. The approach of the super-transition-array method [1–3], in which the use of the noninteracting partition function inside each superconfiguration is an important approximation, is consistent with the Hartree-Fock theory at nonzero temperature.

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