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Spectral description of fluctuating electromagnetic fields of solids using a self-consistent approach

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ABSTRACT

A new way to evaluate the spectral-correlation properties of thermal fields of solids is suggested. The principal element here is the surface linear response function of an inhomogeneous electron subsystem of solids. Along with straightforward calculations using the known response functions, the suggested method allows calculating the response functions self-consistently based on the time dependent density functional theory. The self-consistent calculation of the linear response function followed by an application of the fluctuation–dissipation theorem yields spectral power densities of the fluctuating electromagnetic fields.

1. Introduction

Theory of fluctuating electromagnetic (FEM) fields of solids is grounded on the Maxwell's equations with the fluctuation–dissipation theorem (FDT) [1–8]. The key point of this theory is to solve the boundary-value problem of the phenomenological electrodynamics. Knowledge of the Green's tensor of the boundary-value problem together with the FDT enables us to evaluate the spectral and correlation properties of thermal fields of solids [9–16]. It should be emphasized that in accordance with such formulation of the problem, it is clear that the interface is simply an abstract mathematical line between material domains. It is true despite the local or nonlocal description of optical properties. At the same time, an adequate calculation of subsurface physical and chemical processes requires more detailed description of an interface as some transition layer between materials with a variable chemical and structural composition. Obviously, it can be achieved only by quantum mechanical means. The interface transition layer consists of the electron subsystem, the nuclear lattice (regular or irregular) subsystem, and the regular and fluctuating electromagnetic fields. Here we deal with thermally stimulated fluctuating electromagnetic fields originating from charge fluctuations within the material domain. It is well known that the near-field zone in the heterogeneous system "solid–vacuum" is composed mostly by so-called evanescent electromagnetic waves. The spectra of thermal electromagnetic fields consist of series of resonances relating to the surface electromagnetic waves (surface polaritons) within the spectral ranges where such surface eigenstates can be excited.

It should be noted that the surface electromagnetic states play an important role in different physical processes including van der Waals interactions, heat transfer between the bodies at small distances, continuous growth of crystals, Raman-scattering, capture of atoms, molecules, and coherent material states, photochemistry, surface phenomena such as the adsorption and desorption, heterogeneous chemical catalysis, etc. In practice, surface polaritons can be excited by laser radiation and by a beam of particles, or by internal thermal fluctuations inside a body. Thermally excited electromagnetic fields within a body, which appear due to charge and current fluctuations, partially reflect on the vacuum–sample interface and return back to the body, and partially penetrate into a vacuum region outside the body, where these waves form the electromagnetic background in the near- and far-field regimes. Properties of the propagating and evanescent electromagnetic fluctuating fields are crucially different [9–16]. In the near field the energy density can be much larger in magnitude than in the far field. The matter is that the optical properties and sample geometry have a strong influence on the characteristics of thermally excited near fields. As a result, the noise spectra in the near-field region differ essentially from the noise spectra in the far-field zone. Moreover, the coherence properties of thermal electromagnetic fluctuations in a near field regime are extremely different from those of the propagating waves. The above described results were obtained within the framework of the electrodynamics of continuous media, which excludes a description of microprocesses at interatomic distances.

Needless to say, that the phenomenological approach is valid only at comparatively large distances from solids, at least larger

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than the interatomic distance in the sample lattice. Along with the above, we have a different way to evaluate the spectral-correlation properties of thermal fields of solids without use of the theory developed in [1–8]. In addition to the complete description of thermal fields it is possible to determine in detail the properties of the interface transition layer which separates a bulk region from the vacuum region. The principal foundation here is the static version of the density functional theory (DFT) [17,18] for zero and nonzero [19] temperatures, and the time dependent density functional theory (TDDFT) [20–25]. TDDFT allows for calculating the linear response function of an arbitrary inhomogeneous electron system of solids. The application of the fluctuation–dissipation theorem then yields the spectral power densities of the charge and current correlation functions. In the final step of this scenario, the spectral-correlation properties of thermal fields of solids at any distances (including those within the solids) will be calculated. It should be noted that some microscopic models for the subsurface region were discussed in [26–29], and general ideas how to calculate field correlations near an interface can also be found, for example in [30–32].

The Letter is organized as follows. In Section 2 we provide theoretical basis to calculate the spectral-correlation characteristics of thermal fields using TDDFT. Analytical formulas in the hydrodynamic approach for the spectral power densities of the components of thermal fields in the particular case of a linear response function for a half-space and corresponding illustrations are presented in Section 3, Subsection 3.1. Numerical results for distance dependence of the spectral power densities of thermal fields in case of the self-consistent approach including comparison to the phenomenological approach are demonstrated in Section 3, Subsection 3.2. Our conclusions are given in Section 4. Finally, in appendixes we provide some accepted definitions and details of the self-consistent solution of the Kohn–Sham system of equations.

2. Formalism

Here, we formulate the problem of calculating the spectral-correlation tensors of thermal fields via the linear response functions of spatially inhomogeneous systems. Phenomenological theory adequately describes the fluctuating electromagnetic fields at comparatively large distances from the surface of a body. That is why we restrict our consideration to the subsurface domains at distances much smaller than typical wavelengths of thermal spectra of solids. Thus, we consider the quasistationary (evanescent) fields. In general, the heated body of interest has an arbitrary form and volume V. The sources of thermal fields are the fluctuating charges $\rho(\vec{r},t)$ and currents $\vec{j}(\vec{r},t)$ within this volume. The formulas for the field's components are as follows

$$E_i(\vec{r},t) = -\int_V d^3r'\,\rho(\vec{r}',t)\frac{\partial}{\partial x_i}\frac{1}{|\vec{r}-\vec{r}'|},$$
$$H_i(\vec{r},t) = \frac{1}{c}\int_V d^3r'\,e_{ik\ell}\frac{\partial}{\partial x_k}\frac{j_\ell(\vec{r}',t)}{|\vec{r}-\vec{r}'|}, \tag{1}$$

where $e_{ik\ell}$ is the totally antisymmetric unit pseudotensor of a third rank. Corresponding symmetrized correlation tensors of thermal fields are obtained by composing the components from Eqs. (1), for example,

$$\langle E_i(\vec{r}_1,t)E_k(\vec{r}_2,t+\tau)\rangle^S = (1/2)\big\{\langle E_i(\vec{r}_1,t)E_k(\vec{r}_2,t+\tau) + E_k(\vec{r}_2,t+\tau)E_i(\vec{r}_1,t)\rangle\big\}, \tag{2}$$

and then we have

$$\langle E_i(\vec{r}_1,t)E_k(\vec{r}_2,t+\tau)\rangle^S = \iint_V d^3r'\,d^3r''\langle\rho(\vec{r}',t)\rho(\vec{r}'',t+\tau)\rangle^S \times\frac{\partial}{\partial x_i}\frac{1}{|\vec{r}_1-\vec{r}'|}\frac{\partial}{\partial x_k}\frac{1}{|\vec{r}_2-\vec{r}''|}. \tag{3}$$

Writing the symmetrized functions in Eq. (3) in the following form

$$\langle E_i(\vec{r}_1,t)E_k(\vec{r}_2,t+\tau)\rangle^S = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}g_{ik}^{(E)}(\vec{r}_1,\vec{r}_2;\omega)\exp(-i\omega\tau), \tag{4}$$

and

$$\langle\rho(\vec{r}',t)\rho(\vec{r}'',t+\tau)\rangle^S = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\big(\rho(\vec{r}')\rho(\vec{r}'')\big)_\omega\exp(-i\omega\tau), \tag{5}$$

we have for the spectral power densities

$$g_{ik}^{(E)}(\vec{r}_1,\vec{r}_2;\omega) = \iint_V d^3r'\,d^3r''\big(\rho(\vec{r}')\rho(\vec{r}'')\big)_\omega \times\frac{\partial}{\partial x_i}\frac{1}{|\vec{r}_1-\vec{r}'|}\frac{\partial}{\partial x_k}\frac{1}{|\vec{r}_2-\vec{r}''|}, \tag{6}$$

$$g_{ik}^{(H)}(\vec{r}_1,\vec{r}_2;\omega) = \frac{1}{c^2}\iint_V d^3r'\,d^3r''\,e_{is\ell}e_{kmn}\big(j_\ell(\vec{r}')j_n(\vec{r}'')\big)_\omega \times\frac{\partial}{\partial x_s}\frac{1}{|\vec{r}_1-\vec{r}'|}\frac{\partial}{\partial x_m}\frac{1}{|\vec{r}_2-\vec{r}''|}, \tag{7}$$

$$g_{ik}^{(HE)}(\vec{r}_1,\vec{r}_2;\omega) = -\frac{1}{c}\iint_V d^3r'\,d^3r''e_{is\ell} \times\frac{\partial}{\partial x_s}\frac{(j_\ell(\vec{r}')\rho(\vec{r}''))_\omega}{|\vec{r}_1-\vec{r}'|}\frac{\partial}{\partial x_k}\frac{1}{|\vec{r}_2-\vec{r}''|}, \tag{8}$$

where $(\rho(\vec{r}')\rho(\vec{r}''))_\omega$, $(j_\ell(\vec{r}')j_n(\vec{r}''))_\omega$ and $(j_\ell(\vec{r}')\rho(\vec{r}''))_\omega$ are the symmetrized spectral power densities for the fluctuating charges, currents and crossed characteristics, see Appendix A. Then, taking into account FDT from Eq. (A.5) corresponding to charge fluctuations $(\rho(\vec{r}')\rho(\vec{r}''))_\omega = \hbar\,Coth(\hbar\omega/2k_BT)\,\mathrm{Im}\{\chi(\vec{r}',\vec{r}'';\omega)\}$, it directly follows from Eq. (6), for instance, the spectral power density of electric fluctuations

$$g_{ik}^{(E)}(\vec{r}_1,\vec{r}_2;\omega) = \hbar\,Coth(\hbar\omega/2k_BT)\iint_V d^3r'\,d^3r''\,\mathrm{Im}\big\{\chi(\vec{r}',\vec{r}'';\omega)\big\} \times\frac{\partial}{\partial x_i}\frac{1}{|\vec{r}_1-\vec{r}'|}\frac{\partial}{\partial x_k}\frac{1}{|\vec{r}_2-\vec{r}''|}, \tag{9}$$

where the linear response function $\chi(\vec{r}',\vec{r}'';\omega)$, in its turn, is defined by the following relation between the induced charge ρ_{ind} and external potential ϕ_{ext}

$$\rho_{ind}(\vec{r},\omega) = \int_V d^3r'\,\chi(\vec{r},\vec{r}';\omega)\phi_{ext}(\vec{r}',\omega). \tag{10}$$

The main part of the proposed method of calculation of the spectral and correlation properties of thermal fields of solids is concerned with the time dependent density functional theory [20–25]. In a framework of this method the linear response of an arbitrary spatially bounded system of volume V is a solution of the integral equation

$$\chi(\vec{r}',\vec{r}'';\omega) = \chi^0(\vec{r}',\vec{r}'';\omega) + \iint_V d^3r_1\,d^3r_2\,\chi^0(\vec{r}',\vec{r}_1;\omega)V(\vec{r}_1,\vec{r}_2;\omega) \times\chi(\vec{r}_2,\vec{r}'';\omega), \tag{11}$$