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Spin-resolved Dielectric Functions of Spin-Polarized Electrons

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Spin-resolved dielectric functions are formulated for a spin-polarized electron gas. Correlation effects are taken into account in terms of Hartree-Fock local-field corrections and self-consistent local-field correction, respectively. The self-consistent spin-resolved static dielectric functions have positive and finite values when an induced spin is parallel with a perturbing spin, whereas they have singular behaviors when the induced spin is anti-parallel with the perturbing spin.

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I. INTRODUCTION

Dielectric function $\epsilon(q,\omega)$ is a basic quantity of great importance in dealing with an interacting many-electron system. It enables one to calculate the responses of the system to external electromagnetic disturbances and to examine the excitation spectrum *via* the fluctuation-dissipation theorem [1]. Spin-resolved dielectric functions $\epsilon_{\sigma\sigma'}(q,\omega)$ play a key role in describing the charge-spin responses in a spin-polarized electron gas (SPEG), such as the electrons in a dilute-magnetic semiconductor (DMS). Here, the index σ (σ') denotes the spin state, up ($\uparrow$) or down ($\downarrow$). Electrons of the SPEG are correlated to each other *via* electromagnetic force and the Pauli exclusion principle, and therefore proper inclusion of correlation effects has been a demanding problem in dielectric functions [2].

The most widely used models of dielectric functions are the Thomas-Fermi model, random-phase approximation (RPA), and local-field correction [2]. Most of the studies were limited to spin-averaged systems of vanishing spin polarization. The Thomas-Fermi model is a static model representing a local screening charge density as the difference between a local electron density and the overall equilibrium electron density. The local electron density is obtained from the Fermi-Dirac distribution function when electron energy is the sum of kinetic energy and the effective potential energy, which is due to both external and screening charges. When the total potential energy is slowly varying in space and small enough compared with the chemical potential, the screening charge density can be approximated to the first order in the total potential energy [2,3]. In the RPA, a screening charge is usually taken to be proportional to the self-consistent effective charge. Thus, one can obtain the screening charge density by using the first-order perturbation method. The RPA neglects all other components of the wave vector different from that of the external charge in evaluating the self-consistent effective charge. The RPA result reduces to the Thomas-Fermi one in the long-wavelength limit, and also the RPA method has the advantage that it can easily be extended to a dynamic model when external charge density has time dependence [2]. Hubbard introduced a correction factor to the RPA, which we now call a local-field correction. This originally takes the exchange-hole effects into account in deriving the equation of motion of a screening charge [2]. Singwi *et al.* improved Hubbard's idea to include the correlation-hole effects [4]. Niklasson derived a quantum version of the local-field correction by using the equation of motion of the one-particle Wigner distribution function [5]. Recently, we developed self-consistent approaches to a quantum version of spin-resolved local-field corrections of an SPEG [6]. The spin-resolved local-field corrections come into susceptibility functions in the linear response calculation, and the susceptibility functions are linked to structure factors by the fluctuation-dissipation theorem. Therefore, three quantities make a self-consistent loop, and we can obtain convergent results by iterating the loop. Instead of taking the self-consistent loop, if we use analytically known Hartree-Fock structure factors we can get spin-resolved Hartree-Fock local-field corrections which take only exchange-hole effects into account [6]. On the basis of recent work [6–10], we formulate spin-resolved dielectric functions $\epsilon_{\sigma\sigma'}(q,\omega)$ including correlation effects *via* local-field corrections in an SPEG under a weak external field and present numerical results of the spin-resolved static dielectric functions $\epsilon_{\sigma\sigma'}(q)$.

Two parameters, dimensionless density parameter r_s and spin polarization ζ, are useful in describing an SPEG. We define $r_s = (9\pi/4)^{1/3}(a_0 q_{F_0})^{-1}$, where $a_0 = \hbar^2/me^2$ is the Bohr radius and q_{F_0} is the Fermi wave

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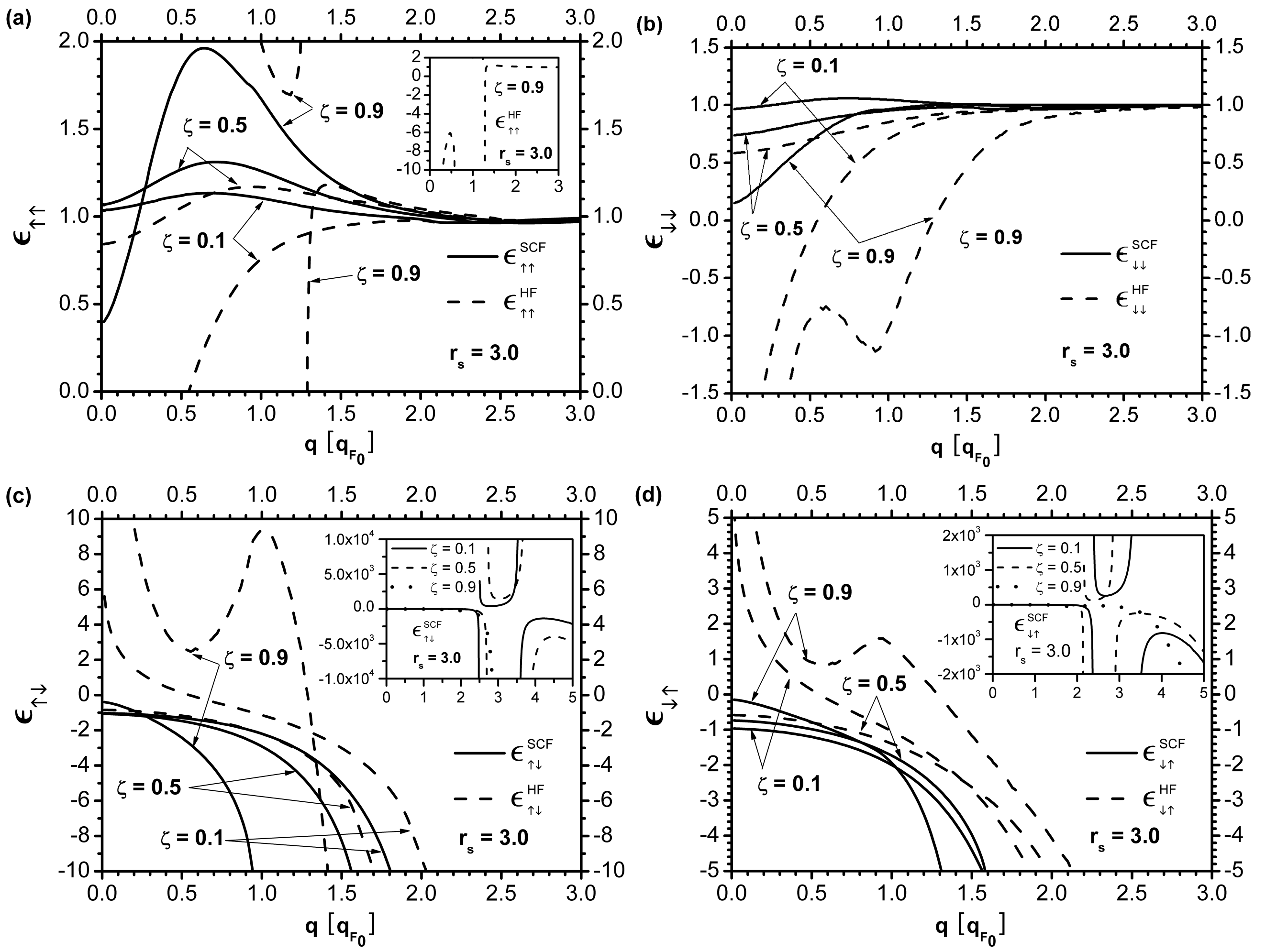

Fig. 1. Spin-resolved static dielectric functions: (a) $\epsilon_{\uparrow\uparrow}(q)$, (b) $\epsilon_{\downarrow\downarrow}(q)$, (c) $\epsilon_{\uparrow\downarrow}(q)$ and (d) $\epsilon_{\downarrow\uparrow}(q)$ for $\zeta = 0.1$, 0.5 and 0.9 and $r_s = 3.0$. Solid lines denote the result with self-consistent local-field corrections (SCF) and dashed lines Hartree-Fock local-field corrections (HF). The wave number q is scaled by q_{F_0}, the Fermi wave number in spin-unpolarized system. Inset in figure (a) is an overview of $\epsilon^{\mathrm{HF}}_{\uparrow\uparrow}(q)$ for $\zeta = 0.9$, and insets in figures (c) and (d) are overviews of $\epsilon^{\mathrm{SCF}}_{\uparrow\downarrow}(q)$ and $\epsilon^{\mathrm{SCF}}_{\downarrow\uparrow}(q)$ for three spin polarizations.

number in a spin-unpolarized case. Spin polarization ζ is defined by $\zeta = (N_\uparrow - N_\downarrow)/(N_\uparrow + N_\downarrow)$ for the SPEG consisting of $N_\uparrow$ and $N_\downarrow$ electrons, in up- and down-spin states, respectively.

II. SPIN-RESOLVED DIELECTRIC FUNCTIONS

Let us consider an SPEG under a weak external electric field varying in space and time with the wave number q and the frequency ω. An external potential energy $\Phi^{\mathrm{ext}}_\sigma(q,\omega)$ felt by a test electron of spin σ influenced by the external perturbing field is

$$\Phi^{\mathrm{ext}}_\sigma(q,\omega) = v(q)\rho^{\mathrm{ext}}_\sigma(q,\omega), \tag{1}$$

where $v(q) = 4\pi e^2/q^2$ is the Fourier transform of the Coulomb potential energy and $\rho^{\mathrm{ext}}_\sigma(q,\omega)$ is a number density of electrons with spin σ which is acted on by the external perturbing field [1,11]. The external test charge $\rho^{\mathrm{ext}}_\sigma(q,\omega)$ acted on by the external perturbing field plays the role of a perturbing charge in the SPEG. The perturbation due to $\rho^{\mathrm{ext}}_\sigma(q,\omega)$ induces charge density fluctuations $\Delta n_\sigma(q,\omega)$ and $\Delta n_{\overline{\sigma}}(q,\omega)$, where $\overline{\sigma}$ means the inversion of the spin σ [12]. An effective potential energy $\widetilde{\Phi}_\sigma$ felt by the test charge with spin σ is written as [13]

$$\begin{pmatrix} \widetilde{\Phi}_\uparrow \\ \widetilde{\Phi}_\downarrow \end{pmatrix} = \begin{pmatrix} \Phi^{\mathrm{ext}}_\uparrow \\ \Phi^{\mathrm{ext}}_\downarrow \end{pmatrix} + v \begin{pmatrix} 1-G_{\uparrow\uparrow} & 1-G_{\uparrow\downarrow} \\ 1-G_{\downarrow\uparrow} & 1-G_{\downarrow\downarrow} \end{pmatrix} \begin{pmatrix} \Delta n_\uparrow \\ \Delta n_\downarrow \end{pmatrix}. \tag{2}$$

The arguments q and ω are abbreviated for notational simplicity, and in what follows we shall use this convention, unless specified otherwise. Exchange-correlation holes are reflected into the local-field correction $G_{\sigma\sigma'}$. In the term $1 - G_{\sigma\sigma'}$, 1 denotes the Hartree (direct) part and $G_{\sigma\sigma'}$ denotes the Fock (exchange) and Coulomb correlation part [12].

Since the perturbation induces the number fluctuation of both spin-up and spin-down electrons, the spin-resolved dielectric function $\epsilon_{\sigma\sigma'}$ can be defined by [13]

$$\widetilde{\Phi}_\sigma = \sum_{\sigma'} \frac{\Phi^{\rm ext}_{\sigma'}}{\epsilon_{\sigma\sigma'}}. \quad (3)$$

Here, σ and σ' denote, respectively, the spin of the induced charge and the spin of the perturbing charge. Within the linear response calculation to the time-dependent perturbation, the induced electron number density Δn_σ is related to the effective potential energy $\widetilde{\Phi}_\sigma$ by

$$\begin{pmatrix} \Delta n_\uparrow \\ \Delta n_\downarrow \end{pmatrix} = \begin{pmatrix} \chi^{(0)}_{\uparrow\uparrow} & 0 \\ 0 & \chi^{(0)}_{\downarrow\downarrow} \end{pmatrix} \begin{pmatrix} \widetilde{\Phi}_\uparrow \\ \widetilde{\Phi}_\downarrow \end{pmatrix}. \quad (4)$$

Here, $\chi^{(0)}_{\sigma\sigma}$ is the spin-resolved noninteracting one-particle susceptibility function defined by [6]

$$\chi^{(0)}_{\sigma\sigma}(q,\omega) = \frac{1}{V}\sum_k \frac{n^{(0)}_{k-q/2,\sigma} - n^{(0)}_{k+q/2,\sigma}}{\hbar\omega - (\varepsilon_{k+q/2,\sigma} - \varepsilon_{k-q/2,\sigma})}. \quad (5)$$

In Eq. (5), V, $n^{(0)}_{k,\sigma}$ and $\varepsilon_{k,\sigma}$ are, respectively, the volume of the system, the noninteracting electron density, and the equilibrium energy of an electron with spin σ.

Therefore, from Eqs. (2) – (4), we can derive the spin-resolved dielectric functions of the SPEG including the correlation correction:

$$\epsilon_{\uparrow\uparrow} = \frac{D}{D + \mathcal{N}_{\uparrow\uparrow}}, \quad (6a)$$

$$\epsilon_{\downarrow\downarrow} = \frac{D}{D + \mathcal{N}_{\downarrow\downarrow}}, \quad (6b)$$

$$\epsilon_{\uparrow\downarrow} = \frac{D}{\mathcal{N}_{\uparrow\downarrow}}, \quad (6c)$$

$$\epsilon_{\downarrow\uparrow} = \frac{D}{\mathcal{N}_{\downarrow\uparrow}}, \quad (6d)$$

where

$$\mathcal{N}_{\uparrow\uparrow} = v\chi^{(0)}_{\uparrow\uparrow}\left[(1-G_{\uparrow\uparrow})[1 - v\chi^{(0)}_{\downarrow\downarrow}(1-G_{\downarrow\downarrow})] + v\chi^{(0)}_{\downarrow\downarrow}(1-G_{\uparrow\downarrow})(1-G_{\downarrow\uparrow})\right], \quad (7a)$$

$$\mathcal{N}_{\downarrow\downarrow} = v\chi^{(0)}_{\downarrow\downarrow}\left[(1-G_{\downarrow\downarrow})[1 - v\chi^{(0)}_{\uparrow\uparrow}(1-G_{\uparrow\uparrow})] + v\chi^{(0)}_{\uparrow\uparrow}(1-G_{\downarrow\uparrow})(1-G_{\uparrow\downarrow})\right], \quad (7b)$$

$$\mathcal{N}_{\uparrow\downarrow} = v\chi^{(0)}_{\downarrow\downarrow}\left[(1-G_{\uparrow\downarrow})[1 - v\chi^{(0)}_{\uparrow\uparrow}(1-G_{\uparrow\uparrow})] + v\chi^{(0)}_{\uparrow\uparrow}(1-G_{\uparrow\downarrow})(1-G_{\uparrow\uparrow})\right], \quad (7c)$$

$$\mathcal{N}_{\downarrow\uparrow} = v\chi^{(0)}_{\uparrow\uparrow}\left[(1-G_{\downarrow\uparrow})[1 - v\chi^{(0)}_{\downarrow\downarrow}(1-G_{\downarrow\downarrow})] + v\chi^{(0)}_{\downarrow\downarrow}(1-G_{\downarrow\uparrow})(1-G_{\downarrow\downarrow})\right], \quad (7d)$$

and

$$D = \left[1 - v\chi^{(0)}_{\uparrow\uparrow}(1-G_{\uparrow\uparrow})\right]\left[1 - v\chi^{(0)}_{\downarrow\downarrow}(1-G_{\downarrow\downarrow})\right] - v^2\chi^{(0)}_{\uparrow\uparrow}\chi^{(0)}_{\downarrow\downarrow}(1-G_{\uparrow\downarrow})(1-G_{\downarrow\uparrow}). \quad (8)$$

III. RESULTS AND DISCUSSION

In Figure 1, we show the spin-resolved static dielectric functions $\epsilon_{\sigma\sigma'}(q)$ including the local-field correction for $\zeta = 0.1$, 0.5, and 0.9 and $r_s = 3.0$. Solid lines indicate the results of self-consistent local-field corrections, and dashed lines the Hartree-Fock local-field corrections [6]. Self-consistent dielectric functions for parallel spin responses do not show divergent behavior as illustrated in Figures 1(a) and (b). However, those for the anti-parallel spin responses show divergence at two different values of q as shown in the insets of Figures 1(c) and (d). The inset in Figure 1(a) is an overview of $\epsilon^{\rm HF}_{\uparrow\uparrow}(q)$ for $\zeta = 0.9$, and the insets in Figure 1(c) and (d) are overviews of $\epsilon^{\rm SCF}_{\uparrow\downarrow}(q)$ and $\epsilon^{\rm SCF}_{\downarrow\uparrow}(q)$ for three spin polarizations. A negative value in the dielectric function is known as an overscreening [14]. This means that there is an attractive interaction between perturbing charge and induced charge. All the $\epsilon^{\rm SCF}_{\sigma\sigma'}$ start to have finite values as wave number $q \to 0$. As the compressibility sum rule is related with the divergence of the dielectric function for $q \to 0$ [2], we presume that some correction is needed on the compressibility sum rule in an SPEG.

IV. CONCLUSIONS

In this paper, we derive spin-resolved dielectric functions taking into account correlation effects *via* local-field corrections in the SPEG. We hope that our results can be verified in optical or transport measurements on intriguing spin polarized condensed matter in the presence of an electromagnetic disturbance.

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