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Electron correlations in quantum and classical plasmas in a layered structure

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We present a theoretical calculation of electron correlations in quantum and classical plasmas in a layered structure. This treatment rests on the solution of the first member of the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy and the fluctuation-dissipation theorem. For arbitrary wave number this leads to a set of coupled integral equations which has to be solved self-consistently. In the long-wavelength limit it is found that the phase velocity of the collective excitation is renormalized due to short-range correlations. Our result is an extension of the earlier theory of K. S. Singwi *et al.* [Phys. Rev. **176**, 589 (1968)] for bulk plasmas to the case of a layered electron gas. Our numerical results show that the correlation function for a layered structure is an oscillatory function of the lattice period, which reflects the interference between the density fluctuations in different layers.

I. INTRODUCTION

The problem of strongly coupled electron plasmas has been attacked by many authors[1-9] through different approaches with a considerable success. The methods can be classified according to whether they rely on the first Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) or on the second BBGKY equation. The former can be characterized as considering the dielectric function to be the central object, deriving an expression for it from the first BBGKY equation, and then guaranteeing self-consistency through the use of fluctuation-dissipation-theorem–type relations. Hubbard,[2] Singwi, Tosi, Land, and Sjoland[1] (STLS) and Golden, Kalman, and Silevech[3] followed this approach in different ways. In the second BBGKY-equation approach the central object is the equilibrium pair-correlation function for which the equation is made self-consistent by the introduction of a decomposition of the triplet correlation function into clusters of pair-correlation functions. Ichimaru *et al.*[6] have pursued this method; their solution depends on the choice of equilibrium triplet correlation which was first suggested by O'Neil and Rostoker.[7] All these approaches have achieved important results. The equilibrium pair-correlation function has been calculated by numerically solving integral equation which result from the theory;[2,6,10,11] equations of state have been obtained[6,11] condition for phase transition have been computed[6] and the theory have been refined to the point that the original inconsistencies concerning the satisfaction of the sum-rule requirements can be removed.[3,6,11]

The generalization of STLS theory to the two-dimensional electron gas (2DEG), such as electrons in the inversion layers and semiconductor heterojunctions, was given by Jonson[12] and Rajagopal.[13] Jonson[12] examined the dielectric function, pair correlation and exchange and correlation energy in 2DEG, taking into account properly the many-body effects. It was pointed out by Jonson[12] that the random-phase approximation (RPA) and Hubbard[2] approximation were less satisfactory approximations for a 2DEG than for a bulk electron gas.

An intermediate situation between bulk electrons and 2DEG is the layered electron gas[14] (LEG). Here, electrons or other mobile particles are confined in planes arranged in a periodic array. To the lowest approximation, this model represents the superlattice structure. Within the RPA, the dielectric function, electronic properties, and the collective excitations were intensively studied during the past decade.[15,16] To lowest order in the plasma parameter the dielectric response depends solely on the self-consistent fields. In a discussion of the many-body effect, Vinter[17] stressed the importance of vertex corrections. In the study of light scattering in LEG, the density-density correlation was calculated and optical properties were investigated.[18,19] However, in the most theoretical studies of LEG the short-range correlations have been neglected. It is expected that the short-range correlations will become important when large wave numbers and low densities are considered.

In this paper we shall present a scheme to calculate the dielectric tenser of LEG including the short-range correlation. We use the solution of the first equation of the BBGKY hierarchy and linear-response theory to find the induced density on the lth layer. Our treatment rests on the ansatz that the two-particle distribution function can be replaced by a product of one-particle distribution functions and a pair-correlation function. The dielectric tensor for a LEG is obtained and collective excitation is discussed. Our formalism is an extension of an earlier theory developed by STLS (Ref. 1) for bulk plasmas, to the case of the layered electron gas. A numerical calculation for local field corrections is presented for several values of the structural parameters.

II. CLASSICAL PLASMAS

We consider here a system consisting periodic layers of electrons. Let the electrons have density per unit area n and mass m, occupying layers which are positioned at $z = la$ (where $l = 0, \pm 1, \pm 2, \ldots$). Here a is the period of the layered structure, i.e., the distance between adjacent layers. The equation of motion for the classical one-particle distribution function in the presence of an external potential $V^{\rm ext}(\mathbf{x},t)$ is given by the first member of the BBGKY hierarchy. For our layered system, we denote the one-particle distribution function on the lth layer as $f_l(\mathbf{r},\mathbf{p},t)$, where $\mathbf{r}$ and $\mathbf{p}$, are, respectively, the position and momentum vectors on the layer. The equation of motion for $f_l(\mathbf{r},\mathbf{p},t)$ can be written as

$$\left[\frac{\partial}{\partial t}+\frac{\mathbf{p}}{m}\cdot\frac{\partial}{\partial \mathbf{r}}-\frac{\partial V_l^{\rm ext}(\mathbf{r},t)}{\partial \mathbf{r}}\cdot\frac{\partial}{\partial \mathbf{p}}\right]f_l(\mathbf{r},\mathbf{p},t)-\sum_{l'}\int d\mathbf{r}'d\mathbf{p}'\frac{\partial}{\partial \mathbf{r}}V^{ll'}(\mathbf{r}-\mathbf{r}')\frac{\partial}{\partial \mathbf{p}}f_{ll'}(\mathbf{r},\mathbf{p};\mathbf{r}',\mathbf{p}';t)=0\ , \quad (1)$$

where $V^{ll'}(\mathbf{r}-\mathbf{r}')$ is the Coulomb interaction potential between two charged particles on lth and l'th layers which is given as

$$V^{ll'}(\mathbf{r}-\mathbf{r}')=\frac{e^2}{[(\mathbf{r}-\mathbf{r}')^2+(l-l')^2a^2]^{1/2}} \quad (2)$$

and $f_{ll'}(\mathbf{r},\mathbf{p};\mathbf{r}',\mathbf{p}';t)$ is the two-particle distribution function. The equation of motion of the two-particle distribution function contains, in turn, the three-particle distribution function and so on. We terminate this infinite hierarchy of equations by making the *ansatz* (see Ref. 1)

$$f_{ll'}(\mathbf{r},\mathbf{p};\mathbf{r}',\mathbf{p}';t)=f_l(\mathbf{r},\mathbf{p}t)f_{l'}(\mathbf{r}',\mathbf{p}',t)g_{ll'}(\mathbf{r}-\mathbf{r}')\ , \quad (3)$$

where $g_{ll'}(\mathbf{r}-\mathbf{r}')$ is taken to be the equilibrium, static pair-correlation function. The ansatz [Eq. (3)] takes care, in an approximate way, of the short-range correlations between the charged particles, through a function which has a simple physical meaning. The function $g_{ll'}(\mathbf{r}-\mathbf{r}')$ tends to unity for large value of its arguments $(\mathbf{r}-\mathbf{r}')$ and $(l-l')$, while for small values of its arguments, it is expected to be finite and smaller than unity. The assumption $g_{ll'}(\mathbf{r}-\mathbf{r}')=1$ for all values of its arguments corresponds to the approximation leading to the Landau-Vlasov[20] equation in layered structure.

Now we apply the linear-response theory to our system by writing

$$f_l(\mathbf{r},\mathbf{p},t)=f_l^0(\mathbf{p})+f_l^1(\mathbf{r},\mathbf{p},t)\ , \quad (4)$$

where $f_l^0(\mathbf{p})$ denotes the thermal equilibrium distribution and $f_l^1(\mathbf{r},\mathbf{p}t)$ denotes the deviation from the thermal equilibrium induced by the weak external potential. After linearization we obtain the following equation for $f_l^1(\mathbf{r},\mathbf{p},t)$:

$$\left[\frac{\partial}{\partial t}+\frac{\mathbf{p}}{m}\cdot\frac{\partial}{\partial \mathbf{r}}\right]f_l^1(\mathbf{r},\mathbf{p},t)-\left[\frac{\partial V_l^{\rm ext}(\mathbf{r},t)}{\partial \mathbf{r}}+\sum_{l'}\int d\mathbf{r}'d\mathbf{p}'\frac{\partial}{\partial \mathbf{r}}V^{ll'}(\mathbf{r}-\mathbf{r}')g_{ll'}(\mathbf{r}-\mathbf{r}')f_{l'}^1(\mathbf{r}',\mathbf{p}',t)\right]\cdot\frac{\partial f_l^0(\mathbf{p})}{\partial \mathbf{p}}=0\ . \quad (5)$$

Now let us define an effective interaction for the layered structure including the short-range correlations by the relation,[1]

$$\frac{\partial}{\partial \mathbf{r}}U^{ll'}(\mathbf{r}-\mathbf{r}')=g_{ll'}(\mathbf{r}-\mathbf{r}')\frac{\partial}{\partial \mathbf{r}}V^{ll'}(\mathbf{r}-\mathbf{r}')\ . \quad (6)$$

Its Fourier transformation in momentum space can be obtained as

$$U_q^{ll'}=V_q^{ll'}+\frac{1}{n}\int\frac{d^2q'}{(2\pi)^2}\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}V_q^{ll'}(S^{ll'}(\mathbf{q}-\mathbf{q}')-1)\ , \quad (7)$$

where

$$V_q^{ll'}=\frac{2\pi e^2}{q}e^{-q|l-l'|a} \quad (8)$$

and $S^{ll'}(q)$ is the usual static structural factor which is defined by

$$S^{ll'}(q)=\delta_{ll'}+n\int d\mathbf{r}\,e^{i\mathbf{q}\cdot\mathbf{r}}[g_{ll'}(q)-\delta_{ll'}]\ . \quad (9)$$

This structural factor is related to the dielectric function of the layered structure through the exact relation[21]

$$S_{ll'}(q)=-\frac{T}{\pi^2e^2n}\int_0^\infty\frac{d\omega}{\omega}{\rm Im}[\epsilon_{ll'}^{-1}(q,\omega)]\ . \quad (10)$$

Here the inverse of the dielectric tensor $\epsilon_{ll'}^{-1}(q,\omega)$, which will be defined shortly, is a functional of $S_{ll'}(q)$. Equation (10) impose a self-consistent requirement on $S^{ll'}(q)$ and $\epsilon_{ll'}^{-1}(q,\omega)$. Note that $\epsilon_{ll'}^{-1}(q,\omega)$ is the inverse of the dielectric tensor $\epsilon_{ll'}(q,\omega)$ (see Ref. 16).

Because of the linearity of Eq. (5) we can construct a general solution from the response to an external field with single frequency and wave number, respectively. We write

$$V^{\rm ext}(\mathbf{r},t)=\int d\mathbf{q}\,e^{i\mathbf{q}\cdot\mathbf{r}}e^{-i\omega t}V^{\rm ext}(\mathbf{q},\omega)+{\rm c.c.} \quad (11)$$

Taking the Fourier transformation of Eqs. (5) and (6) with respect to $\mathbf{r}$, we find

$$(\omega-\mathbf{q}\cdot\mathbf{v})f_l^1(\mathbf{q},\mathbf{p},\omega)-V^{\rm ext}(\mathbf{q},\omega)\mathbf{q}\cdot\frac{\partial f_l^0(\mathbf{p})}{\partial \mathbf{p}}+\sum_{l'}\mathbf{q}\cdot\frac{\partial f_l^{(0)}(\mathbf{p})}{\partial \mathbf{p}}U_q^{ll'}\int d\mathbf{p}'f_{l'}^1(\mathbf{q},\mathbf{p}',\omega)\ . \quad (12)$$

The induced charge density on the lth layer is defined as

$$\rho_l(\mathbf{q},\omega)=\int d\mathbf{p}\,f_l^1(\mathbf{q},\mathbf{p},\omega) \quad (13)$$

and its explicit integral equation can be obtained from Eq. (12)

$$\rho_l(\mathbf{q},\omega)=Q^l(\mathbf{q},\omega)\left[V^{\rm ext}(\mathbf{q},\omega)+\sum_{l'}U_q^{ll'}\rho_{l'}(\mathbf{q},\omega)\right]\ , \quad (14)$$

where

$$Q^l(\mathbf{q},\omega)=\int\frac{d\mathbf{p}}{4\pi^2}\frac{\mathbf{q}\cdot[\partial f_l^0(\mathbf{p})/\partial\mathbf{p}]}{\omega-\mathbf{q}\cdot\mathbf{v}+i\delta}\ . \quad (15)$$

If we define the element of the dielectric tensor of the layered structure as

$$\epsilon_{l'l}(q\omega)=\delta_{ll'}-U_q^{ll'}Q_l(q,\omega)\ , \quad (16)$$

we can write

$$\sum_{l'} \rho_{l'}(q,\omega)\epsilon_{l'l}(q,\omega)=Q^{1}(q,\omega)V^{\text{ext}}(q,\omega) \ . \tag{17}$$

The inverse of the dielectric tensor can then be found through the relation

$$\sum_{l''}\epsilon^{-1}_{l'l''}(q,\omega)\epsilon_{l''l}(q,\omega)=\delta_{ll'} \ . \tag{18}$$

For a periodic layered structure, the number of elements of the dielectric tensor is infinite and therefore it is difficult to find its inverse. However, if we introduce the discrete Fourier transform in the z direction, we can find the following relation:

$$\sum_{l'}\epsilon_{ll'}(q,\omega)e^{ik_z(l-l')a}=\epsilon(q,k_z,\omega) \tag{19}$$

and

$$\sum_{l'} \epsilon^{-1}_{ll'}(q,\omega)e^{ik_x(l-l')a}=\frac{1}{\epsilon(q,k_z,\omega)} \ , \tag{20}$$

where use has been made of the fact that all functions here only depend on the quantity $(l-l')$. It is easy to show, by direct substitution, that Eqs. (19) and (20) are consistent with Eq. (18). To find $\epsilon(q,k_z,\omega)$ we would like to use the fact that a layered structure is completely periodic in the z direction with periodicity a. Therefore we can use following *Ansatze* for Eq. (14):

$$\rho_l(q,\omega)=\rho(q,\omega)e^{ik_z la}$$

and

$$Q^l(q,\omega)=Q(q,\omega)e^{ik_z la} \ .$$

The "wave number" k_z that labels the induced density fluctuation in the periodic system is restricted within the first Brillouin zone of the layered structure, i.e., $0<k_z<2\pi/a$. With these *Ansatze* Eq. (14) becomes

$$\rho(q,k_z,\omega)=\frac{Q(q,\omega)V^{\text{ext}}(q,\omega)}{1-Q(q,\omega)U(q,k_z)} \ , \tag{21}$$

where $U(q,k_z)$ is the Fourier transform of the effective interaction

$$U(q,k_z)=\sum_{l'} U^{ll'}(q)e^{ik_z(l-l')a}$$
$$=V(q,k_z)+\frac{2\pi e^2}{q}G(q,k_z) \ , \tag{22}$$

with $V(q,k_z)$ the bare Coulomb interaction

$$V(q,k_z)=\frac{2\pi e^2}{q}\frac{\sinh(qa)}{\cosh(qa)-\cos(k_z a)}=\frac{2\pi e^2}{q}F(q,k_z) \tag{23}$$

and $G(q,k_z)$ the local field correction. To find $G(q,k_z)$ we insert Eq. (7) into Eq. (22), taking the inverse Fourier transform for $V_q^{ll'}$ and $S^{ll'}(\mathbf{q}-\mathbf{q}')$, summing over l', we then obtain

$$G(q,k_z)=\frac{a}{n}\int\frac{d\mathbf{q}'}{4\pi^2}\frac{\mathbf{q}\cdot\mathbf{q}'}{qq'}\left[\int\frac{dk_z'}{2\pi}F(q',k_z')S(\mathbf{q}-\mathbf{q}',k_z-k_z')-F(q',k_z)\right] \tag{24}$$

and

$$S(\mathbf{q},k_z)=\sum_{l} e^{ik_z(l-l')a}S^{ll'}(q) \ . \tag{25}$$

By comparing Eq. (21) with the standard definition for the dielectric function

$$\rho(q,k_z,\omega)=\frac{1}{V(q,k_z)}\left[\frac{1}{\epsilon(q,k_z,\omega)}-1\right]V^{\text{ext}}(q,\omega) \ , \tag{26}$$

we find

$$\epsilon(q,k_z,\omega)=1-\frac{Q(q,\omega)V(q,k_z)}{1-(2\pi e^2/q)Q(q,\omega)G(q,k_z)} \ . \tag{27}$$

The essential point of our result is that the solution of Eqs. (24) and (27) together with the relation

$$S(q,k_z)=-\frac{T}{\pi^2 e^2 n}\int_0^\infty\frac{d\omega}{\omega}\text{Im}[\epsilon^{-1}(q,k_z,\omega)] \tag{28}$$

provide us with a set of equations which, when solved self-consistently, determined the dielectric response for a layered electron gas including short-range correlations.

III. QUANTUM PLASMAS

Our treatment in the case of classical plasmas rests on the ansatz expressed in Eq. (3). Using this ansatz allowed us to calculate the dielectric response of classical plasmas including short-range correlations. However, this *Ansatz* is not applicable for the case of quantum plasmas. Here, in order to find the effects of short-range correlations, we will consider the equation of motion for the density matrix and calculate the dielectric response function.

We begin by defining the Hamiltonian of the system which can be written as (in units $\hbar=1$)

$$H_0=\sum_{\mathbf{p},l}a^\dagger_{\mathbf{p},l}a_{\mathbf{p},l}E_{\mathbf{p},l}+\frac{1}{A}\sum_{\mathbf{p},\mathbf{p}',\mathbf{q}}\sum_{l,l'}V_q^{ll'}a^\dagger_{\mathbf{p}+\mathbf{q},l}a^\dagger_{\mathbf{p}'-\mathbf{q},l'}a_{\mathbf{p}'l'}a_{\mathbf{p},l} \ , \tag{29}$$

where $V_q^{ll'}$ is given by Eq. (8), A is the area of the layer, and $E_{\mathbf{p},l}=p^2/2m$. We consider first the equation of motion for the density operator, which in second quantized notation, is given as

$$\hat{\rho}_l(q)=\sum_{\mathbf{p}}a^\dagger_{\mathbf{p}+\mathbf{q},l}a_{\mathbf{p},l} \ , \tag{30}$$

where $a^\dagger_{\mathbf{p},l}$ and $a_{\mathbf{p},l}$ are, respectively the creation and destruction operator of the electron with momentum $\mathbf{p}$ on the lth layer. Its first time derivative is

$$i\frac{\partial\hat{\rho}_l(q)}{\partial t}=\sum_{\mathbf{p}}\left[\frac{\mathbf{p}\cdot\mathbf{q}}{m}+\frac{q^2}{2m}\right]a^\dagger_{\mathbf{p}+\mathbf{q},l}a_{\mathbf{p},l}\ , \tag{31}$$

which is independent of the Coulomb interaction. However, the second time derivative of $\hat{\rho}_l$ yields an expression including electron-electron interactions:

$$\begin{aligned}\frac{\partial^2\hat{\rho}_l(q)}{\partial t^2}=&-\sum_{\mathbf{p}}\left[\frac{\mathbf{p}\cdot\mathbf{q}}{m}+\frac{q^2}{2m}\right]^2a^\dagger_{\mathbf{p}+\mathbf{q},l}a_{\mathbf{p},l}\\&+\frac{2\pi e^2qn}{m}\sum_{l'}e^{-q|l-l'|a}\hat{\rho}_{l'}(q)\\&+\frac{2\pi e^2}{m}\sum_{\mathbf{q}\neq\mathbf{q}',l'}\frac{\mathbf{q}\cdot\mathbf{q}'}{q'}e^{-q'|l-l'|a}\hat{\rho}_{l'}(q')\hat{\rho}_l(\mathbf{q}-\mathbf{q}')\ .\end{aligned} \tag{32}$$

The first term of the right-hand side (RHS) of the equation represents the single-particle recoil and Doppler shift. The second term in the RHS is due to the long-range part of the Coulomb potential and is proportional to the plasma frequency. The last term on the RHS involves the product of two density operators. Since $\hat{\rho}_l(\mathbf{q}-\mathbf{q}')$, given by $\sum_i e^{i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{r}_l(i)}$ [where $r_l(i)$ represents the electronic coordinate of the ith electron], is a sum of complex exponential terms with differing phases for $\mathbf{q}\neq\mathbf{q}'$ and since the ensemble average of $\hat{\rho}_l(\mathbf{q}-\mathbf{q}')$ vanishes for $\mathbf{q}\neq\mathbf{q}'$ if the system is homogeneous, we expect destructive interference to occur in this term and therefore we drop it from the equation as our first approximation. This gives the original random-phase approximation as proposed by Bohm and Pines.[22] Therefore within the RPA we obtain

$$\begin{aligned}\frac{\partial^2\hat{\rho}_l(q)}{\partial t^2}=&-\sum_{\mathbf{p}}\left[\frac{\mathbf{p}\cdot\mathbf{q}}{m}+\frac{q^2}{2m}\right]^2a^\dagger_{\mathbf{p}+\mathbf{q},l}a_{\mathbf{p},l}\\&+\omega_p^2\sum_{l'}e^{-q|l-l'|a}\hat{\rho}_{l'}(q)\ ,\end{aligned} \tag{33}$$

where $\omega_p^2=2\pi e^2qn/m$ is the plasma frequency for a 2DEG. It is obvious that for the limit $q\to 0$, the first term in the RHS of Eq. (32) vanishes and the density fluctuation oscillates with the plasma frequency of LEG (Ref. 16) given by $\omega^2_{\rm LEG}=\omega_p^2[qa/1-\cos(k_Za)]$.

To include the short-range correlations, the nonlinear term in Eq. (31) (i.e., the third term in the RHS) must be retained. It can be rewritten if we express $\rho_l(q)$ in terms of the electronic coordinates, i.e., $\rho_l(q)=\sum_i\exp[i\mathbf{q}\cdot\mathbf{r}_i(l)]$, we obtain

$$\begin{aligned}\rho_{l'}(q')\rho_l(\mathbf{q}-\mathbf{q}')=&\sum_{i,j}\exp[i\mathbf{q}'\cdot\mathbf{r}_i(l')]\exp[i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{r}_j(l)]\\=&\sum_i\exp[i\mathbf{q}\cdot\mathbf{r}_i(l')\\&\times\sum_j\exp\{i(\mathbf{q}-\mathbf{q}')\cdot[\mathbf{r}_i(l')-\mathbf{r}_j(l)]\}\ .\end{aligned} \tag{34}$$

If we now replace the sum over j by its static average value, i.e.,

$$\begin{aligned}\sum_j\exp\{i(\mathbf{q}-\mathbf{q}')\cdot[\mathbf{r}_i(l')-\mathbf{r}_j(l)]\}&=\frac{1}{n}\left\langle\sum_{i,j}\exp\{i(\mathbf{q}-\mathbf{q}')\cdot[\mathbf{r}_i(l')-\mathbf{r}_j(l)]\}\right\rangle\\&=S^{ll'}(\mathbf{q}-\mathbf{q}')\ ,\end{aligned} \tag{35}$$

Eq. (32) can be rewritten as

$$\begin{aligned}\frac{\partial^2\hat{\rho}_l(q)}{\partial t^2}=&-\sum_{\mathbf{p}}\left[\frac{\mathbf{p}\cdot\mathbf{q}}{m}+\frac{q^2}{2m}\right]^2a^\dagger_{\mathbf{p}+\mathbf{q},l}a_{\mathbf{p},l}\\&+\frac{q^2n}{m}\sum_{l'}U^{ll'}(q)\hat{\rho}_{l'}(q)\ ,\end{aligned} \tag{36}$$

where

$$U_q^{ll'}=V_q^{ll'}+\frac{1}{n}\int\frac{d^2q'}{(2\pi)^2}\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}V_{q'}^{ll'}[S^{ll'}(\mathbf{q}-\mathbf{q}')-1]\ . \tag{37}$$

Comparing the RPA result, Eq. (33), with Eq. (36) we find that the last term in Eq. (36) has the same structure as the last term of the RPA expression, except that the bare Coulomb potential in Eq. (33) has been replaced by an effective potential $U^{ll'}(q)$. The *Ansatz* for quantum plasmas will therefore be to derive the dielectric response within RPA but to replace the Coulomb interaction $V_q^{ll'}$ by the effective interaction $U_q^{ll'}$. This procedure was first used in STLS (Ref. 1) with considerable success for bulk plasmas.

Let us now consider a layered plasma. In the absence of external disturbance, the dynamics of the system is governed by the Hamiltonian H_0 consisting of kinetic and Coulomb energies. We now apply a weak external potential $V^{\rm ext}(\mathbf{x},t)$ which acts on the layer plasmas. The dynamics of our system are then governed by the Hamiltonian

$$H=H_0+\frac{1}{A}\sum_{\mathbf{p},\mathbf{q},l}a^\dagger_{\mathbf{p}+\mathbf{q},l}a_{\mathbf{p},l}V^{\rm ext}(\mathbf{q},t)\ . \tag{38}$$

In order to obtain the induced density in the external potential we define the single-electron density matrix element between states $\langle\mathbf{p},l|$ and $|\mathbf{p}+\mathbf{q},l\rangle$ as

$$F_l(\mathbf{p}+\mathbf{q},\mathbf{p},t)=\langle a^\dagger_{\mathbf{p},l}(t)a_{\mathbf{p}+\mathbf{q},l}(t)\rangle\ .$$

In the Heisenberg representation, the equation of motion for the single-electron density matrix is

$$i\frac{\partial}{\partial t}F_l(\mathbf{p}+\mathbf{q},\mathbf{p},t)=\langle(a^\dagger_{\mathbf{p},l}a_{\mathbf{p}+\mathbf{q}}H)\rangle\ . \tag{39}$$

This equation can be easily worked out with the help of the commutation rules, and we obtain

$$i\frac{\partial}{\partial t}F_l(\mathbf{p}+\mathbf{q},\mathbf{p},t)=(E_{\mathbf{p}+\mathbf{q}}-E_{\mathbf{p}})F_l(\mathbf{p}+\mathbf{q},\mathbf{p},t)+\sum_{\mathbf{p}',\mathbf{k}}\sum_{l'}V_k^{ll'}\langle a^\dagger_{\mathbf{p}',l'}a_{\mathbf{p}'+\mathbf{k},l'}(a^\dagger_{\mathbf{p},l}a_{\mathbf{p}+\mathbf{q}-\mathbf{k},l}-a^\dagger_{\mathbf{p}+\mathbf{k},l}a_{\mathbf{p}+\mathbf{q},l})\rangle$$
$$-\sum_{\mathbf{k},l'}V_{l'}^{\text{ext}}(\mathbf{k},t)[F_{l'}(\mathbf{p}+\mathbf{q}-\mathbf{k},\mathbf{p},t)-F_{l'}(\mathbf{p}+\mathbf{q},\mathbf{p}+\mathbf{k},t)]\ . \quad (40)$$

This is a complicated equation which, through the Coulomb interaction, couples one- and two-particle operators. To make any progress in solving it one must somehow approximate the latter by simpler functions. The RPA procedure is to replace the two-particle correlations by suitable products of one-particle functions, i.e.,

$$\langle a^\dagger_{\mathbf{p}',l'}a_{\mathbf{p}'+\mathbf{k},l'}a^\dagger_{\mathbf{p},l}a_{\mathbf{p}+\mathbf{q}-\mathbf{k},l}\rangle\sim\langle a^\dagger_{\mathbf{p}',l'}a_{\mathbf{p}'+\mathbf{k},l'}\rangle\langle a^\dagger_{\mathbf{p},l}a_{\mathbf{p}+\mathbf{q}-\mathbf{k},l}\rangle\ ,$$

where the higher order of exchange and nonlinear correlation terms has been neglected. Our scheme to include the short-range correlation is to neglect the exchange and nonlinear correlation terms but replace the bare Coulomb interaction by the effective interaction. We write

$$V_k^{ll'}\langle a^\dagger_{\mathbf{p}',l'}a_{\mathbf{p}'+\mathbf{k},l'}a^\dagger_{\mathbf{p},l}a_{\mathbf{p}+\mathbf{q}-\mathbf{k},l}\rangle\sim U_k^{ll'}\langle a^\dagger_{\mathbf{p}',l'}a_{\mathbf{p}'+\mathbf{k},l}\rangle\langle a^\dagger_{\mathbf{p},l}a_{\mathbf{p}+\mathbf{q}-\mathbf{k},l}\rangle\ . \quad (41)$$

This approximation is similar to the derivation of Eq. (36). With this approximation in mind, Eq. (40) can be written as

$$i\frac{\partial}{\partial t}F_l(\mathbf{p}+\mathbf{q},\mathbf{p},t)=(E_{\mathbf{p}+\mathbf{q}}-E_{\mathbf{p}})F_l(\mathbf{p}+\mathbf{q},\mathbf{p},t)+\sum_{\mathbf{k},l'}U_k^{ll'}\rho_{l'}(k)[F_{l'}(\mathbf{p}+\mathbf{q}-\mathbf{k},\mathbf{p},t)-F_{l'}(\mathbf{p}+\mathbf{q},\mathbf{p}+\mathbf{k},t)]$$
$$-\sum_{\mathbf{k},l'}V_{l'}^{\text{ext}}(\mathbf{k},t)[F_{l'}(\mathbf{p}+\mathbf{q}-\mathbf{k},\mathbf{p},t)-F_{l'}(\mathbf{p}+\mathbf{q},\mathbf{p}+\mathbf{k},t)]\ . \quad (42)$$

The time-dependent function $F_l(\mathbf{p}+\mathbf{q},\mathbf{p},t)$ can be written as $F_l(\mathbf{p}+\mathbf{q},\mathbf{p},t)=F_l(\mathbf{p}+\mathbf{q},\mathbf{p},\omega)e^{i\omega t}$ to represent the response in the external potential which varies as $e^{i\omega t}$. Our next step is to expand all quantities in terms of external perturbation, i.e., $F_l=F_l^0+F_l^1+\cdots$, where subscript 0 and 1 denotes the equilibrium function and linear deviation from equilibrium, respectively. In this approximation $F_l^0(\mathbf{p}+\mathbf{k},\mathbf{p})=f_{\mathbf{p}}\delta_{\mathbf{k},0}$, where $f_{\mathbf{p}}$ is the Fermi distribution function which is independent of layer index

$$f_{\mathbf{p}}=\frac{1}{e^{\beta(E_{\mathbf{p}}-\mu)}+1}\ , \quad (43)$$

β is the inverse temperature in energy units, and μ is the chemical potential. After the linearization we obtain

$$(E_{\mathbf{p}+\mathbf{q}}-E_{\mathbf{p}}-\omega)F_l^1(\mathbf{p}+\mathbf{q},\mathbf{p},\omega)=\sum_{l'}[U_q^{ll'}\rho_{l'}^1(\mathbf{q},\omega)+V_{l'}^{\text{ext}}(\mathbf{q},\omega)](f_{\mathbf{q}+\mathbf{q}}-f_{\mathbf{p}})\ , \quad (44)$$

where $\rho_l^1(\mathbf{q},\omega)=\sum_{\mathbf{p}}F_l^1(\mathbf{p}+\mathbf{q},\mathbf{p},\omega)$. Equation (44) is an integral equation for the density matrix F_l^1 and the density fluctuation ρ_l^1. Upon solving it we obtain

$$\rho_l(\mathbf{q},\omega)=Q(q,\omega)V_l^{\text{ext}}(q,\omega)+Q(q,\omega)\sum_{l'}U_q^{ll'}\rho_{l'}(q,\omega)\ . \quad (45)$$

In Eq. (45) $Q(q,\omega)$ is the two-dimensional (2D) polarizability defined as

$$Q(q,\omega)=\int\frac{d^2p}{(2\pi)^2}\frac{f_{\mathbf{p}+\mathbf{q}}-f_{\mathbf{p}}}{E_{\mathbf{p}+\mathbf{q}}-E_{\mathbf{p}}-\omega-i\delta}\quad(\delta\to 0)\ . \quad (46)$$

By taking the Fourier transformation with respect to l in Eq. (45), we obtain

$$\rho(q,k_z,\omega)=\frac{Q(q,\omega)V^{\text{ext}}(q,\omega)}{1-Q(q,\omega)U(q,k_z)}\ . \quad (47)$$

Our expression for $\rho(\mathbf{q},k_z,\omega)$ in Eq. (47) is identical to that of Eq. (21). However, here $Q(q,\omega)$ is the quantum pair fluctuation function. Therefore we conclude that effective interaction alter the dielectric response in an identical way for classical and quantum plasmas, respectively.

As was done for the classical case, by comparing Eq. (47) with Eq. (26) we obtain the dielectric function for quantum plasmas as

$$\epsilon(q,k_z,\omega)=1-\frac{Q(q,\omega)V(q,k_z)}{1-(2\pi e^2/q)Q(q,\omega)G(q,k_z)}\ , \quad (48)$$

where $G(q,k_z)$ again represents the local field correction and is given by

$$G(q,k_z)=\frac{a}{n}\int\frac{d\mathbf{q}'}{4\pi^2}\frac{\mathbf{q}\cdot\mathbf{q}'}{qq'}\times\left[\int\frac{dk_z'}{2\pi}F(q',k_z')S(\mathbf{q}-\mathbf{q}',k_z-k_z')-F(q',k_z)\right]\ . \quad (49)$$

For quantum plasmas $S(q,k_z)$ is related to the dielectric function $\epsilon(q,k_z,\omega)$ by the relation

$$S(q,k_z)=-\frac{\hbar}{2\pi^2e^2n}\int_0^\infty d\omega\coth\left[\frac{\beta\omega}{2}\right]\text{Im}[\epsilon^{-1}(q,k_z,\omega)]\ . \quad (50)$$

Our result for the dielectric function is again given in terms of the self-consistent solution of Eqs. (48)–(50). Here the solution of these equations leads to the determination of the dielectric function and the pair-correlation function, respectively.

Contact with the experiments could be made by comparing the roots of the dielectric function with the plas-

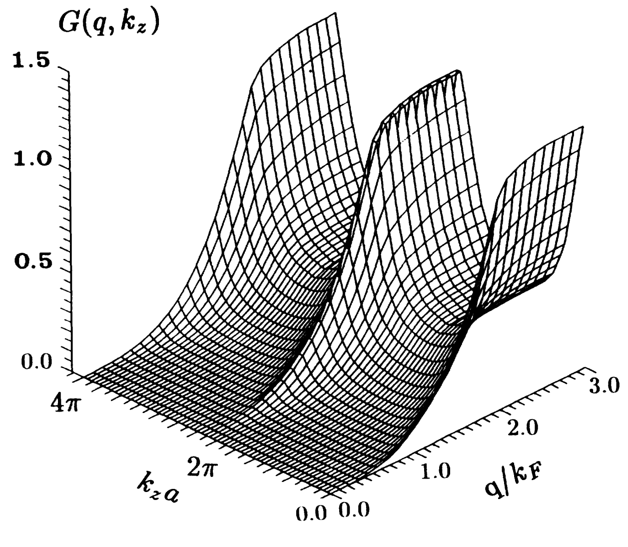

FIG. 1. Plot of the local field correction $G(q,k_z)$ as a function of $k_z a$ and q/k_F, where $a=50$ Å, $r_s=3.0$.

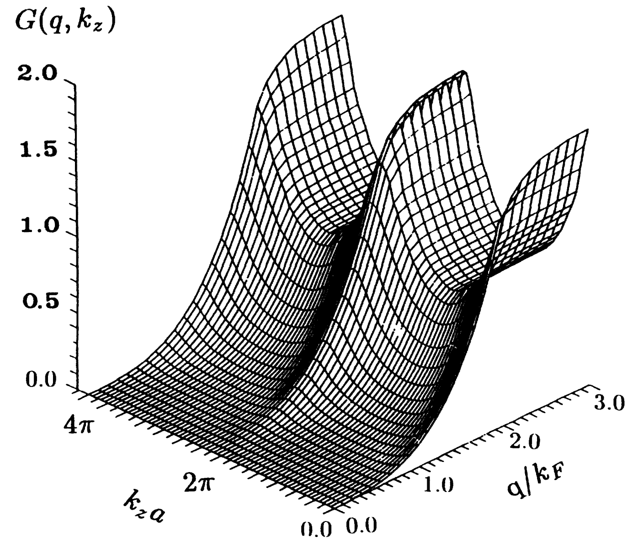

FIG. 2. The plot of local correction $G(q,k_z)$ as a function of $k_z a$ and q/k_F, where $a=100$ Å, $r_s=4.0$.

ma resonance frequencies observed by inelastic light scattering. Here the small-q limit is applicable, and we look for an expression of the dielectric function Eq. (26) in the limit $q\to 0$ for finite ω when $k_z\neq 0$ ($k_z=0$ is not considered here, since it represents a situation equivalent to a bulk electron gas). Our explicit expression for the dielectric function when $q\to 0$ is

$$\epsilon(q,k_z,\omega)=1-\frac{2\pi e^2 n q^2 a}{\omega^2 m[1-\cos(k_z a)}\times\left[1-\frac{2\pi e^2 q n}{m\omega^2}G(q,k_z)\right]^{-1}, \quad (51)$$

with

$$G(q,k_z)=\frac{a}{4\pi^2 n}\int q'dq'd\alpha\cos\alpha\times\left[\int\frac{dk_z'}{2\pi}F(q',k_z')\mathbf{q}\cdot\frac{\partial}{\partial\mathbf{q}'}\times S(q',k_z-k_z')-F(q',k_z)\right], \quad (52)$$

where α is the angle between the directions of $\mathbf{q}$ and $\mathbf{q}'$. Since $F'(q',k_z)$ is independent of the direction of $\mathbf{q}'$, the second term in the above equation vanishes. Integrating over α, we obtain

$$G(q,k_z)=\frac{qa}{4\pi n}\int q'dq'\int\frac{dk_z'}{2\pi}F(q',k_z')\frac{\partial}{\partial q'}S(q',k_z-k_z')=A(k_z)q\ . \quad (53)$$

In the present formalism the quantity $A(k_z)$ has to be determined from the self-consistent solution of $S(q,k_z)$. From Eq. (48) we find that the plasma dispersion relation is given by

$$\omega_p(q)=[1+A(k_z)]^{1/2}q\left[\frac{2\pi e^2 na}{m[1-\cos(k_z a)]}\right]^{1/2}. \quad (54)$$

As is well known, the long-wavelength excitation in a layered structure, when the coupling between layers is strong, is an "acoustic like" plasma wave. Here we found that the effect of short-range correlations is to renormalize the phase velocity of this acousticlike mode.

IV. DISCUSSION

In this paper, we have derived an expression for the dielectric function for both quantum and classical plasmas in a layered structure. Our result goes beyond the RPA treatment for the density fluctuations to include not only the self-consistent field effects but also the effects of short-range correlations. Our result for the dielectric function would provide a more accurate description of the dielectric properties such as the roots of the collective excitations, the determination of the pair-correlation function, and the Coulomb contribution to the ground-state energy for a system of layered electron gas. In terms of the plasma parameter r_s ($r_s=me^2/k_F\hbar^2$ for the quantum case and $r_s=e^2\sqrt{n}/k_BT$ for the classical case), our result approaches the RPA result for vanishing r_s and finite wave number. Our result provides a more realistic description of the dielectric function than the RPA result when finite values of r_s and finite values of wave number are considered. The numerical calculation for $\epsilon(q,k_z,\omega)$ is given in terms of a highly nonlinear integral equation, or by the self-consistent solution of the coupled integral equations for $\epsilon(q,k_z,\omega)$, $S(\mathbf{q},k_z)$, and $G(\mathbf{q},k_z)$ as described in the text. We point out that the numerical solution in our case is more complicated than in the 3D case due to the loss of translational invariance in the z direction. We have carried out numerical calculations for local field correction $G(\mathbf{q},k_z)$ for some typical values of the structural parameter. The method used in our calculation is simply iteration. To achieve a convergent result more than ten iterations are needed. The results are plotted in Figs. 1 and 2. As in the 2D and bulk cases, the correlation effect is very important for large r_s and large momentum transfer in the plane (q is of the order of the Fermi wave vector). The local field correction always vanishes as q approaches zero. The interesting point one can see from present results is the strong interference effect. When the density fluctuations in different layers oscillate in phase ($k_z a = n2\pi$, $n = 0,1,2\ldots$), the correlation effect has its maximum for a fixed value of in-plane momentum. When the density fluctuations in different layers oscillate out of phase ($k_z a = n\pi$, $n = 1,3,5\ldots$), the correlation effect is greatly reduced. The 2D case can be obtained by taking the limit $qa \gg 1$. For $qa \ll 1$ and $k_z a = n2\pi$, the system is equivalent to a bulk material.

In conclusion, we have calculated the dielectric response for a layered structure with short-range correlation included. Our numerical result shows that the effect of short-range correlation is very important if the plasma parameter is large, especially when $k_z a$ equals $2n\pi$.

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