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Longitudinal and transverse dielectric functions of a two-dimensional electron system: Inclusion of exchange correlations

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The calculation of the longitudinal dielectric function for a two-dimensional electron system is of importance in discussing the properties of electrons in semiconductor-insulator sandwiches and those confined to the surface of liquid helium. We present here a calculation of this function when exchange processes are included. A variational solution to the vertex equation is used to solve the integral equation. We also compute the plasmon dispersion and the static dielectric function in powers of the wave vector, by solving the appropriate vertex equation exactly in these limits. The latter is important in a theory of gradient expansion for the inhomogeneous counterpart of this two-dimensional system. This may be used in the calculation of the band structure of such systems. We also calculate the transverse dielectric function in the same scheme. From these two, we deduce the orbital susceptibility of the system. As in three dimensions, we find that screening of the electron interactions is essential to give finite values for the orbital susceptibility and the coefficient of the gradient expansion term in the theory of inhomogeneous systems.

I. INTRODUCTION

There has been enormous activity in the study of the electronic properties of (quasi) two-dimensional systems such as found in inversion layers in metal-insulator–semiconductor structures and electron layers on liquid helium.[1] There is much evidence to believe that the many-body effects are more pronounced in these systems than in the three-dimensional systems.[1] Zia[2] calculated the correlation energy of the system in the high-density limit and concluded erroneously that the correlation energy approaches a constant rather than $\ln r_s$. In two separate papers,[3] we shall discuss the correct version of the Gell-Mann–Brueckner theory of this system along with other aspects of the problem. We find[3a] that in the high-density limit, the correlation energy per particle in rydbergs is $-0.38-0.172 r_s \ln r_s$ and not what Zia found, thus invalidating his conclusion. In Ref. 3(b), we have evaluated the correlation energy in the Gell-Mann–Brueckner scheme exactly on a computer and also calculated the pair correlation function that is consistent with the total energy calculation. [r_s is the usual electron-gas parameter related to the system density per unit area $n=(\pi r_s^2 a^2)^{-1}$, where a_0 is the Bohr radius of the three-dimensional hydrogen atom.] Beck and Kumar[4] calculated the contribution to the plasmon dispersion due to exchange correlations and found it to be larger by a factor of 3.2 than what we obtain in the present paper. They also discussed the effect of thickness. Stern[5] calculated the longitudinal dielectric function in the random-phase approximation without including exchange contributions and calculated the asymptotic screened Coulomb potential and the plasmon dispersion. In view of the importance of the problem, we here present calculations of the longitudinal and transverse dielectric functions following the methods employed by us recently in the study of the corresponding functions in three dimensions,[6] which incorporate the exchange contributions appropriately. The longitudinal and the transverse dielectric functions were calculated by a variational procedure for solving the appropriate vertex equations in Ref. 7, whereas in Ref. 6, these were solved exactly in the suitable limits of static and dynamic situations. For instance, we could compute the plasmon dispersion beyond the linear term to find out the effect of exchange. In the static limit, the calculation of the polarizability to second power in the wave vector leads to an expression for the gradient expansion for the inhomogeneous system.[8] The effects of exchange contributions must be handled with care and our formulation is well suited for this. Using a relationship between the magnetic susceptibility and the two dielectric functions, we can deduce the effect of exchange interactions on the orbital susceptibility.[6,7]

In Sec. II we calculate the longitudinal dielectric function in various limits and also give a variational expression for it, valid for all frequencies and wave vectors. In Sec. III we calculate the transverse dielectric function and deduce therefrom the orbital susceptibility in the static long-wavelength limit. A summary of the results is given in Sec. IV.

II. LONGITUDINAL DIELECTRIC FUNCTION

The longitudinal dielectric function is given by

$$\epsilon_L(q) = 1 + V(q)\pi(q) , \tag{1}$$

where the polarization π is given by

$$\pi(q)=2\int\frac{d^2k}{(2\pi)^2}\,\frac{f_0(\vec{k}+\frac{1}{2}\vec{q})-f_0(\vec{k}-\frac{1}{2}\vec{q})}{q_0-\vec{k}\cdot\vec{q}/m}\,\Lambda(k;q)\,. \tag{2}$$

Λ is the irreducible vertex function and obeys the integral equation

$$\Lambda(k;q)=1+\int\frac{d^2k'}{(2\pi)^2}\,V(|\vec{k}-\vec{k}'|)\times\frac{f_0(\vec{k}'+\frac{1}{2}\vec{q})-f_0(\vec{k}'-\frac{1}{2}\vec{q})}{q_0-\vec{k}'\cdot\vec{q}/m}\times\left[\Lambda(k';q)-\left(\frac{q_0-\mathrm{k}'\cdot\vec{q}/m}{q_0-\vec{k}\cdot\vec{q}/m}\right)\Lambda(k;q)\right]. \tag{3}$$

$V(|\vec{k}-\vec{k}'|)$ is the Fourier transform of the effective interaction among electrons and if assumed Coulombic it is $2\pi e^2/|\vec{k}-\vec{k}'|$. We will leave it as a general function until we come to the end of the analysis. $f_0(k)$ is the usual Fermi function, and m is the mass of the electron. We use units with $\hbar=1$. The three vector q stands for $\vec{q}$, q_0 as usual. The *spin susceptibility* in this same scheme is also proportional to $\pi(q)$. Stern[5] computed $\epsilon(q)$ when $\Lambda=1$ in Eq. (2). Equation (3) for Λ incorporates exchange processes both in the one-particle self-energy and in the scattering among the electrons. The methods of Refs. 6 and 8 can be used to study the extreme static and dynamic limits of the function $\pi(q)$ or $\epsilon_L(q)$.

A. Plasmon dispersion

We can solve Eq. (3) exactly as a power series in $k_F q/mq_0$ when this ratio is much less than unity. k_F is the Fermi wave vector. We use the identity

$$f_0(\vec{k}+\tfrac{1}{2}\vec{q})-f_0(\vec{k}-\tfrac{1}{2}\vec{q})\simeq-\frac{\vec{k}\cdot\vec{q}}{m}\left(\delta(E_k-E_F)+\frac{q^2}{8m}\left[\delta'(E_k-E_F)+\tfrac{2}{3}E_k\cos^2\theta_k\,\delta''(E_k-E_F)\right]\right)+\cdots, \tag{4}$$

where the primes denote differentiation of the δ function with respect to the energy $E_k=k^2/2m$. Also note that

$$V(|\vec{k}-\vec{k}'|)=\sum_{l=0}^{\infty}V_l(k;k')\cos l(\theta_k-\theta_{k'})\,,$$
$$V_l(k;k')=\tfrac{1}{2}(1+\delta_{l,0})\int_0^{2\pi}\frac{d\theta}{2\pi}\cos l\theta\, V(|\vec{k}-\vec{k}'|)\,. \tag{5}$$

We first observe that

$$\Lambda(k'q=0,q_0)=1\,. \tag{6}$$

Then using (4), and expanding $(q_0-\vec{k}\cdot\vec{q}/m)^{-1}$ in powers of $(\vec{k}\cdot\vec{q}/mq_0)$, to the order of interest to us, we have $\Lambda(k;q)$ in the form

$$\Lambda(k;q)=1+\sum_{l=0}^{\infty}\left[\left(\frac{k_Fq}{mq_0}\right)^2\Lambda_l^{(2,0)}(k)+\left(\frac{k_Fq}{mq_0}\right)^2q^2\Lambda_l^{(2,2)}(k)+\cdots\right]\cos l\theta_k\,. \tag{7}$$

Substitute this into Eq. (3) along with the other expansions and obtain $\Lambda_l^{(n,m)}(k)$ by equating like powers of $q^n(k_Fq/mq_0)^m$ on both sides of the equation, giving the result

$$\Lambda_l^{(2,0)}(k)=-\frac{m}{4\pi}\{[V_0(k;k_F)-(k/k_F)\tfrac{1}{2}V_1(k;k_F)]\delta_{l,0}+[\tfrac{1}{2}V_2(k;k_F)-(k/k_F)\tfrac{1}{2}V_1(k;k_F)]\delta_{l,2}\}\,. \tag{8}$$

Also, to this order, we find

$$\epsilon_L(q;q_0)\cong1-2V(q)\frac{m}{4\pi}\left(\frac{k_Fq}{mq_0}\right)^2\times\left[1+\left(\frac{k_Fq}{mq_0}\right)^2\left[\tfrac{3}{4}+\Lambda_0^{(2,0)}(k_F)+\tfrac{1}{2}\Lambda_2^{(2,0)}(k_F)\right]\right]. \tag{9}$$

Using the solution (8) for $\Lambda_l^{(2,0)}(k_F)$ we obtain

$$\epsilon_L(q;q_0)\cong1-2V(q)\frac{m}{4\pi}\left(\frac{k_Fq}{mq_0}\right)^2\left[1+\left(\frac{k_Fq}{mq_0}\right)^2\times\{\tfrac{3}{4}-(m/8\pi)[2V_0(k_F;k_F)+\tfrac{1}{2}V_2(k_F;k_F)-3\times\tfrac{1}{2}V_1(k_F;k_F)]\}\right]. \tag{10}$$

If we employed the bare Coulomb interaction for the two-dimensional system, we obtain ($n=k_F^2/2\pi$ is the number of electrons per unit area)

$$\epsilon_L(q;q_0)\simeq1-\left(\frac{2\pi ne^2}{m}\right)\frac{q}{q_0^2}\left[1+\frac{k_F^2q^2}{m^2q_0^2}\left(\frac{3}{4}-\frac{5}{6}\frac{me^2}{\pi k_F}\right)\right], \tag{11}$$

or the plasmon dispersion is

$$q_0^2(q)\cong\left(\frac{2\pi ne^2}{m}\right)q\left[1+\left(\frac{q}{k_F}\right)\left(\frac{k_F}{me^2}\right)\left(\frac{3}{4}-\frac{5}{6}\frac{me^2}{\pi k_F}\right)\right]. \tag{12}$$

The first two terms were obtained by Stern.[5] The last term is due to the exchange correlations. It was estimated to be $8ne^2/3\pi k_F$ by Beck and Kumar,[4] which is 3.2 times larger than our result. These authors, it appears, took into account only the exchange contribution to self energy and did not include a contribution of the same order to the vertex function.

B. Static limit

For purposes of the gradient expansion in a theory of inhomogeneous systems,[8] we need $\pi(q;0)$ to order q^2:

$$\pi(q;0) \cong \pi^{(0)}(0;0) + q^2 \pi^{(2)}(0;0). \tag{13}$$

Using the same type of methods, we find this time

$$\Lambda(k;\vec{q},0) = \sum_{l=0}^{\infty} [\Lambda_l^{(0)}(k) + q^2 \Lambda_l^{(2)}(k) + \cdots] \cos l\theta_k. \tag{14}$$

Employing (4), and following the same methods, we can solve for $\Lambda_l^{(0)}(k)$ and $\Lambda_l^{(2)}(k)$. Before doing this, let us calculate $\pi^{(0)}(0;0)$ and $\pi^{(2)}(0;0)$. We find

$$\pi^{(0)}(0;0) = \frac{m}{\pi} \Lambda_0^{(0)}(k_F), \tag{15a}$$

$$\pi^{(2)}(0;0) = \frac{m}{\pi}\Big[\Lambda_0^{(2)}(k_F) + \frac{1}{8m}\Big(-\frac{d}{dE_k}\Lambda_0^{(0)}(k) + \frac{1}{3}\frac{d^2}{dE_k^2}E_k \times [\tfrac{1}{2}\Lambda_2^{(0)}(k) + \Lambda_0^{(0)}(k)]\Big)\Big]_{E_k=E_F} \tag{15b}$$

From this we note we need only $\Lambda_0^{(0)}$, $\Lambda_0^{(2)}$, and $\Lambda_2^{(0)}$. We obtain after some algebra

$$\Lambda_l^{(0)}(k) = \Gamma\tilde{\Gamma}(k)\delta_{l,0}, \tag{16}$$

where

$$\Gamma = \{1 - (m/2\pi)[V_0(k_F;k_F) - \tfrac{1}{2}V_1(k_F;k_F)]\}^{-1}, \tag{17}$$

$$\tilde{\Gamma}(k) = \Big(1 - \frac{m}{2\pi}[V_0(k_F;k_F) - V_0(k;k_F)] + \frac{m}{2\pi}\frac{V_1(k_F;k_F)}{2}\Big)\Big(1 + \frac{m}{2\pi}\frac{k}{k_F}\tfrac{1}{2}V_1(k;k_F)\Big)^{-1}, \tag{18}$$

and

$$\Lambda_0^{(2)}(k_F) = \frac{\Gamma^2}{16\pi}\Big\{-\frac{d}{dE_k}\Big[\tilde{\Gamma}(k)V_0(k;k_F) - \Big(\frac{E_k}{E_F}\Big)^{1/2}\frac{V_1(k;k_F)}{2}\Big] + \frac{1}{3}\frac{d^2}{dE_k^2}E_k\Big[V_0(k;k_F)\tilde{\Gamma}(k) + \frac{1}{2}\Big(\frac{E_k}{E_F}\Big)^{1/2}\frac{V_3(k;k_F)}{2} - \frac{3}{2}\Big(\frac{E_k}{E_F}\Big)^{1/2}\frac{V_1(k;k_F)}{2}\Big]\Big\}_{E_k=E_F}. \tag{19}$$

From (15a) then we finally obtain

$$\pi^{(0)}(0;0) = (m/\pi)\Gamma, \tag{20}$$

$$\pi^{(2)}(0,0) = \frac{m}{\pi}\Big[\Lambda_0^{(2)}(k_F) + \frac{\Gamma}{8m}\Big(-\frac{d}{dE_k}\tilde{\Gamma}(k) + \frac{1}{3}\frac{d^2}{dE_k^2}[E_k\tilde{\Gamma}(k)]\Big)\Big|_{E_k=E_F}\Big]. \tag{21}$$

As a very useful approximation for other regions of q, we may solve Eq. (3) by a variational method.[9] For the sake of completeness we present the answer here

$$\pi_v(q) = 2[\pi_0(q)]^2/[\pi_0(q) - J(q)], \tag{22}$$

where

$$\pi_0(q) = \int \frac{d^2k}{(2\pi)^2}\frac{f_0(\vec{k}+\frac{1}{2}\vec{q}) - f_0(\vec{k}-\frac{1}{2}\vec{q})}{q_0 - \vec{k}\cdot\vec{q}/m} \tag{23}$$

and

$$J(q) = \int\int \frac{d^2k\,d^2k'}{(2\pi)^4} V(|\vec{k}-\vec{k}'|) \times \frac{f_0(\vec{k}+\frac{1}{2}\vec{q}) - f_0(\vec{k}-\frac{1}{2}\vec{q})}{q_0 - \vec{k}\cdot\vec{q}/m} \times \frac{f_0(\vec{k}'+\frac{1}{2}\vec{q}) - f_0(\vec{k}'-\frac{1}{2}\vec{q})}{q_0 - \vec{k}'\cdot\vec{q}/m} \times \Big[1 - \Big(\frac{q_0 - \vec{k}'\cdot\vec{q}/m}{q_0 - \vec{k}\cdot\vec{q}/m}\Big)\Big]. \tag{24}$$

It may be of interest to point out here that from this expression we get the *same* plasmon dispersion relation calculated to the same order as in Eq. (12). In the static limit, while $\pi_v^{(0)}(0;0)$ is the same as the exact calculation, $\pi_v^{(2)}(0;0)$ is slightly different, and the answer is

$$\pi_v^{(2)}(0;0)=\frac{m^2}{16\pi^2}\left\{-\frac{d}{dE_k}\left[2V_0(k;k_F)-\left(\frac{E_k}{E_F}\right)^{1/2}\frac{V_1(k;k_F)}{2}-\left(\frac{E_F}{E_k}\right)^{1/2}\frac{V_1(k;k_F)}{2}\right]\right.$$
$$+\frac{1}{3}\frac{d^2}{dE_k^2}E_k\left[2V_0(k;k_F)+\frac{1}{2}\left(\frac{E_k}{E_F}\right)^{1/2}\frac{V_3(k;k_F)}{2}\right.$$
$$\left.\left.-\frac{3}{2}\left(\frac{E_k}{E_F}\right)^{1/2}\frac{V_1(k;k_F)}{2}-\left(\frac{E_F}{E_k}\right)^{1/2}\frac{V_1(k;k_F)}{2}\right]\right\}_{E_k=E_F}. \tag{25}$$

We will postpone the discussion of these results to Sec. IV.

III. TRANSVERSE DIELECTRIC FUNCTION

The transverse dielectric function is given by[6,7]

$$\epsilon_T(q)=1+\frac{4\pi c}{q_0^2}K_T(q)\left(\frac{q_0^2-c^2q^2}{q_0^2-c^2q^2-4\pi cK_T(q)}\right), \tag{26}$$

where $K_T(q)$ is expressed in terms of an appropriate vertex function $\Lambda_T(k;q)$, which obeys the integral equation

$$\Lambda_T(k;q)=-k\sin\theta_k+\int\frac{d^2k'}{(2\pi)^2}V(|\vec{k}-\vec{k}'|)\times\frac{f_0(\vec{k}'+\frac{1}{2}\vec{q})-f_0(\vec{k}'-\frac{1}{2}\vec{q})}{q_0-\vec{k}'\cdot\vec{q}/m}\times\left[\Lambda_T(k';q)-\left(\frac{q_0-\vec{k}'\cdot\vec{q}/m}{q_0-\vec{q}\cdot\vec{k}/m}\right)\Lambda_T(k;q)\right]. \tag{27}$$

By employing the same methods we can compute $\epsilon_T(q)$ in the various limits. But the static long-wavelength limit is of interest as it is related to the orbital susceptibility of the system. We present this calculation now. This orbital susceptibility is

$$\chi_{\mathrm{orb}}(0;0)=\lim_{q\to 0}\frac{e^2}{m^2c^2q^2}\times\left(-nm-2\int\frac{d^2k}{(2\pi)^2}k\sin\theta_k\times\frac{f_0(\vec{k}+\frac{1}{2}\vec{q})-f_0(\vec{k}-\frac{1}{2}\vec{q})}{-(kq/m)\cos\theta_k}\times\Lambda_T(k;q)\right). \tag{28}$$

From Eq. (27) we note that for $q_0=0$, $\Lambda_T(k;q,0)$ has the symmetry $\Lambda_T(-\vec{k};\vec{q},0)=-\Lambda_T(\vec{k};\vec{q},0)$. We therefore seek an expression of the form

$$\Lambda_T(k;\vec{q},0)=\sum_{l=1}^{\infty}[\Lambda_{T0}^{(l)}(k)+q^2\Lambda_{T2}^{(l)}(k)]\sin l\theta_k. \tag{29}$$

The same procedures as above lead to the answers

$$\Lambda_{T0}^{(l)}(k)=-k\delta_{l,1} \tag{30}$$

$$\Lambda_{T2}^{(l)}(k)=\frac{m}{2\pi}\left\{\left[\tfrac{1}{2}V_l(k;k_F)\Lambda_{02}^{(l)}(k_F)-\left(\frac{E_F}{E_k}\right)^{1/2}\frac{V_1(k;k_F)}{2}\Lambda_{02}^{(l)}(k)\right]+\delta_{l,1}\frac{(2m)^{1/2}}{24m}\frac{d^2}{dE_{k'}^2}\left[E_{k'}^{3/2}\left(\frac{V_1(k;k')}{2}-\frac{V_3(k;k')}{2}\right)\right]_{E_{k'}=E_F}\right\}. \tag{31}$$

And finally

$$\chi_{\mathrm{orb}}(0,0)=-\frac{e^2}{12\pi mc^2}[1+6k_F\Lambda_{T2}^{(1)}(k_F)]. \tag{32}$$

From Eq. (31), we obtain

$$\chi_{\mathrm{orb}}(0;0)=-\frac{e^2}{12\pi mc^2}\left\{1+\frac{m(E_F)^{1/2}}{4\pi}\frac{d^2}{dE_k^2}\left[E_k^{3/2}\left(\frac{V_1(k;k_F)}{2}-\frac{V_3(k;k_F)}{2}\right)\right]\right\}_{E_k=E_F}. \tag{33}$$

The effect of interaction is then contained in the second term in Eq. (33). We can also solve the Λ_T equation by the variational method for all q and the result is not given here. We may point out that this calculation also gives the same result as Eq. (33) in the static long-wavelength limit. We will discuss the results obtained in Sec. IV.

IV. DISCUSSION OF RESULTS

The main results of this paper are (i) the plasmon dispersion given by $\epsilon_L(q;q_0)=0$, Eq. (10): This extends the work of Starn[5] and corrects that of Beck and Kumar[4]; (ii) the static dielectric function, in the limit $q\to 0$,

$$\epsilon(\vec{q};0)=1+2me^2\Gamma/q=(q+q_s)/q\,,$$

where

$$q_s=\frac{2me^2}{1-(m/2\pi)\{V_0(k_F;k_F)-\frac{1}{2}[V_1(k_F;k_F)]\}} \tag{34}$$

is the two-dimensional screening constant. The result with the denominator set equal to one was earlier given by Stern[5] and Zia.[2] The denominator appears because of exchange corrections. q_s is related to the compressibility of the interacting system and it blows up for the Coulomb system for $r_s=4.4$; (iii) the polarization to order q^2,

$$\pi(q;0)=\pi^{(0)}(0;0)+q^2\pi^{(2)}(0;0)\,,$$

Eqs. (19)–(21); (iv) the orbital susceptibility $\chi_{\rm orb}(0,0)$, Eq. (33); results (iii) and (iv) have not been derived before to the best of our knowledge. We have expressed our results in terms of V_l, the lth Fourier component in the angular distribution of the interaction, as it resembles the Fermi-liquid parameter, which may be determined experimentally. The static long-wavelength spin susceptibility is proportional to $\pi^{(0)}(0,0)$ and shows an interesting divergence for $1=(m/2\pi)(V_0-\frac{1}{2}V_1)$, signalling a ferromagnetic transition.[10]

We may make several comments here. If we use a strictly two-dimensional model for the electron gas with $V(q)$ given by the unscreened Coulomb potential, $2\pi e^2/|\vec{q}|$, we find that $\pi^{(2)}(0,0)$ and $\chi_{\rm orb}(0,0)$ diverge as in the three-dimensional case.[7,8] This can be overcome by screening the Coulomb interaction, in the form $2\pi e^2/(|\vec{q}|+\xi k_F)$, where ξ is a screening constant. In the Thomas-Fermi limit, $\xi=q_s/k_F$ where q_s is given by Eq. (34). More interestingly, the effect of finite size of the electron gas, which we know to be confined to a fairly thin size, may be taken into account by considering them to be in their lowest quantum state as far as the third direction is concerned. This, along with the image forces that keep the electrons confined, lead to an effective interaction of the form[4,11]

$$V(|\vec{q}|)=(2\pi e^2/\epsilon_1 q)f(q)\,, \tag{35}$$

where

$$f(|\vec{q}|)=\int\int_0^\infty dz\,dz'\,|\zeta_0(z)|^2|\zeta_0(z')|^2 \times\left(e^{-q|z-z'|}+\frac{\epsilon_1-\epsilon_2}{\epsilon_1+\epsilon_2}\,e^{-q(z+z')}\right) \tag{36}$$

is a form factor for the thickness of the electron system. Here ϵ_1 and ϵ_2 are the dielectric functions of the two bounding surfaces confining the electrons. Knowing the structure of $f(|\vec{q}|)$ in detail, the various $V_l(k;k')$ can be calculated and used to compute the quantities of interest. This will also remove the divergences alluded to above.

Recently, I received a preprint[12] from Jonson where he reports calculations of correlation energy, dielectric function, and the pair-correlation function of a strictly 2-dimensional system and also the effects of finite thickness in the manner mentioned above on these quantities, based on a scheme due to Singwi. From such studies, it is found that the effect of interactions and finite thickness are competitive at certain electron densities and thicknesses. Jonson, in a private communication, informs me that the correlation energy tends to a constant for $r_s\to 0$ and agrees with our result. He also points out that in the plasmon dispersion, the effect of thickness may be neglected in the low density limit while it dominates for high densities for system parameters corresponding to $Si(100)$-SiO_2 inversion layer. We plan to investigate these and other aspects of the finite thickness (ferromagnetism, etc.) in a subsequent paper. We therefore conclude that the effects of interactions on the system properties have interesting features in them with which the present work is mainly concerned.

In an application of the density-functional formalism to calculate the band structure of these systems, one needs $\pi^{(2)}(0,0)$, Eq. (21), which we hope will be used in the future.

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