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Polarisability of a two-dimensional electron gas including fluctuation effects

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Abstract. Stern's result, for the response of a two-dimensional electron gas (2DEG) to a longitudinal electric field in the random phase approximation (RPA) calculation, is generalised to include fluctuation effects. A generalised RPA dielectric function for the 2DEG, which is analytic for all wavevectors and frequencies, in contrast to Stern's expression, is presented. The analyticity facilitates numerical calculations. The results are used to study the influence of fluctuations on the screened Coulomb potential and the plasma dispersion for a 2DEG in a realistic system.

There has been a burgeoning interest in the theory of a two-dimensional electron gas (2DEG), particularly because of the relevance of such studies to the properties of the inversion layer in metal–insulator–semiconductor structure and the electrons trapped in the quantum wells of semiconductor heterostructures and superlattices (Ando *et al* 1982, O'Connell 1982). Fundamental to all theories of the 2DEG is the calculation of the dielectric function $\varepsilon(q, \omega)$ and its properties.

Stern (1967) was the first to calculate the lowest-order polarisability $\chi^0(q, \omega)$ for a 2DEG in the random phase approximation (RPA), which he used to study the screening behaviour of the system, and he found that the plasmon frequency ω_p goes as $q^{1/2}$ at the long-wavelength limit. Since then many efforts have been made to improve Stern's result, so as to extend to the layered electron gas (Visscher and Falicov 1971), to include exchange processes (Rajagopal 1977), to apply the self-consistent scheme (Jonson 1976), to calculate the dynamical local field effect (Czachor *et al* 1982), and to incorporate the electronic scattering effects (Das Sarma and Vinter 1981, Ando 1982, Das Sarma 1983, Giuliani and Quinn 1984, Belitz and Das Sarma 1986). From these studies more important properties of the 2DEG have been discovered. For example, the plasmon dispersion relation (Rajagopal 1977, Czachor *et al* 1982) is found to be

$$\omega_p^2 = (2\pi ne^2/m^*)q(1 + Pq/k_F)$$

with

$$P = [3(\sqrt{2})/4r_s]\{a_B^* - [10r_s/9(\sqrt{2})\pi]\}$$

(see equation (13) and discussions), and the mobility of electrons depends on the impurity density n_i through the $(an_i + bn_i^2)^{-1}$ law (Das Sarma 1983). On the other hand,

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Stern's function and its improvements have the well known non-analytic problem such as the sudden jump of the static dielectric function at $q = 2k_F$, where k_F is the Fermi momentum. This feature remains in the phenomenological approaches as well as in the self-consistent method used to incorporate scattering effects on the screening of the 2DEG. In addition, it was noted (Mermin 1970), that in the process of incorporating scattering effects on the longitudinal dielectric function of the electron gas, in order to retain the conservation of the local electron number more careful work is needed.

In this paper we generalise Stern's polarisation function of 2DEG to include fluctuation effects. In particular, we find that our generalised function does not have the non-analytic problem at $q = 2k_F$. In addition, we study the dielectric screening and the plasmon dispersion as an application of our generalised version of the polarisation function of the 2DEG. A parallel work for the three-dimensional case will be reported elsewhere.

Recently, we have developed a new approach to quantum transport based on the use of a generalised quantum Langevin equation (Hu and O'Connell 1987, 1988). In our approach, the many-body memory function associated with the total momentum of the centre of mass of the electron gas is expressed as a function of the density–density response function of the relative electrons. Since we derive the memory function directly in the process of solving the Heisenberg equations for the centre of mass and relative electrons, expressions for the response function and conductivity are obtained simply as a by-product. We found that when the fluctuation of the coordinates of the centre-of-mass electrons is included, the structure of the response function is changed significantly. In the linear case, our expression for the density–density response function of the non-interacting electrons is (Hu and O'Connell 1988)

$$\chi^0(\boldsymbol{q}, \omega) = \sum_{k,\sigma} \frac{f(\boldsymbol{k}) - f(\boldsymbol{k}+\boldsymbol{q})}{\hbar\omega - (\varepsilon_{k+q} - \varepsilon_k) + \mathrm{i}Dq^2} \tag{1}$$

where $f(\boldsymbol{k})$ is the Fermi distribution function, $\varepsilon_k = \hbar^2 k^2/2m$ is the electron energy, $\boldsymbol{q}$ is the wave vector associated with the electron density, σ denotes the sum over electron spins, D is the diffusion constant for the centre-of-mass coordinate defined by

$$D = \lim_{t\to\infty} (1/2t)\overline{\delta\boldsymbol{R}^2(t)}$$

and $\delta\boldsymbol{R}(t)$ is the fluctuation of the centre-of-mass coordinate $\boldsymbol{R}(t)$. In this paper, D will be treated as a controlled parameter. The $\mathrm{i}Dq^2$ term in (1), which is new, introduces a damping effect on the electron response. In the original Stern function, this term is replaced by an $\mathrm{i}\delta$ term, where δ is infinitesimally small. Also, the dielectric function in the RPA approximation is

$$\varepsilon(\boldsymbol{q}, \omega) = 1 - V(\boldsymbol{q})\chi^0(\boldsymbol{q}, \omega) \tag{2}$$

where $\chi^0(\boldsymbol{q}, \omega)$ is defined by (1) and $V(\boldsymbol{q}) = 2\pi e^2/q$ is the Fourier transform of the Coulomb energy of a 2DEG in a vacuum. The corresponding formula for $V(\boldsymbol{q})$ for a realistic system consisting of a semiconductor and insulator (with κ_{sc} and κ_{ins} as dielectric constants, respectively) is

$$V(\boldsymbol{q}) = (2\pi e^2/\kappa q)F(\boldsymbol{q}) \tag{3}$$

with $\kappa = (\kappa_{sc} + \kappa_{ins})/2$ and the form factor $F(\boldsymbol{q}) = 1$ will be used in this paper; this corresponds to the strict two-dimensional limit (Ando *et al* 1982).

By using (1) and (2), after some straightforward algebra we obtain a new version of

the RPA dielectric function $\varepsilon = \varepsilon_1 + i\varepsilon_2$. The real part is

$$\begin{aligned}\varepsilon_1(x,y) = 1 + [(r_s/a_B^*)/(\sqrt{2})x]F(x)\{1 - [\mathrm{sgn}(\nu_-)/(2\sqrt{2})x]\{\nu_-^2 - b^2x^2 - 1 \\ + [(\nu_-^2 - b^2x^2 - 1)^2 + 4b^2x^2\nu_-^2]^{1/2}\}^{1/2} \\ - [\mathrm{sgn}(\nu_+)/(2\sqrt{2})x]\{\nu_+^2 - b^2x^2 - 1 \\ + [(\nu_+^2 - b^2x^2 - 1)^2 + 4b^2x^2\nu_+^2]^{1/2}\}^{1/2}\}\end{aligned} \tag{4}$$

where $F(x)$ is defined by (3), and

$$\begin{aligned} x = q/2k_F \qquad y = \hbar\omega/4\varepsilon_F \qquad r_s = (\sqrt{2})/k_F \\ a_B^* = \kappa\hbar^2/m^*e^2 \qquad b = 2mD/\hbar \qquad \nu_\pm = x \pm y/x. \end{aligned} \tag{5}$$

The imaginary part is

$$\begin{aligned}\varepsilon_2(x,y) = [(r_s/a_B^*)/4x^2]F(x)\{\{1 + b^2x^2 - \nu_-^2 \\ + [(1 + b^2x^2 - \nu_-^2)^2 + 4b^2x^2\nu_-^2]^{1/2}\}^{1/2} \\ - \{1 + b^2x^2 - \nu_+^2 + [(1 + b^2x^2 - \nu_+^2)^2 + 4b^2x^2\nu_+^2]^{1/2}\}^{1/2}\}.\end{aligned} \tag{6}$$

Although the dielectric functions (4) and (6) are quite complicated, it is easy to see that when $b = 0$, they reduce to Stern's result. Also, they satisfy the conductivity sum rule discussed in Stern (1967). In addition to these properties, the most important fact is that our dielectric functions (4) and (6) are analytic for all frequencies and wavenumbers, in contrast to Stern's expressions, which in turn facilitates numerical calculations. This analyticity is introduced rigorously through the fluctuation effects. Thus, we are motivated to study the fluctuation effects on the dielectric screening and the plasmon dispersion by using (4) and (6) in the following.

When $\omega = 0$, it is straightforward to see from (6) that $\varepsilon_2(x, y) = 0$. Hence, from (4) we obtain

$$\varepsilon(x) \equiv \varepsilon_1(x, y = 0) = 1 + [(r_s/a_B^*)/(\sqrt{2})x]F(x)L(x) \tag{7}$$

where

$$L(x) = 1 - (1/\sqrt{2}x)\{x^2 - b^2x^2 - 1 + [(x^2 - b^2x^2 - 1)^2 + 4b^2x^4]^{1/2}\}^{1/2}. \tag{8}$$

The usual RPA static dielectric constant is obtained from (7) and (8) when $b = 0$. As is well known, it is not analytic at $x = 1$. By contrast, our dielectric function (7), supplemented by (8), is analytic. To illustrate the general features of the function $\varepsilon(x)$ and $L(x)$ of (7) and (8), we plot $\varepsilon^{-1}(x)$ and $L(x)$ in figure 1. The figure shows that the $b \neq 0$ analytic functions $\varepsilon^{-1}(x)$ and $L(x)$ deviates from its Stern's ($b = 0$) counterparts mainly in the vicinity of $x = 1$, and the deviation is significant even for b as small as 0.001, where the sharp drop of the $L(x)$ of the $b = 0$ case at $x = 1$ is dramatically rounded in the $b = 0.001$ case. How is the magnitude of $b = (2m/\hbar)D$ arrived at? In general, D is complicated and field dependent, but in the classical limit we can use the Einstein relation $D = k_BT\tau/Nm$, where τ is the momentum transport time, to obtain $b = 2k_BT\tau/\hbar$. Then, for example, if we choose $T = 1$ K, $\tau = 4 \times 10^{-12}$ s and $N = 1.2 \times 10^3$ (corresponding, for instance to a surface density of electrons of 0.5×10^{12} cm^{-2} and a sample area 0.5 μm^2) we obtain $b = 10^{-3}$. In general, the fluctuation effect is more significant for smaller systems and smaller densities.

Next, we study the screening charge density $n_s(r)$ for a static impurity of unit charge

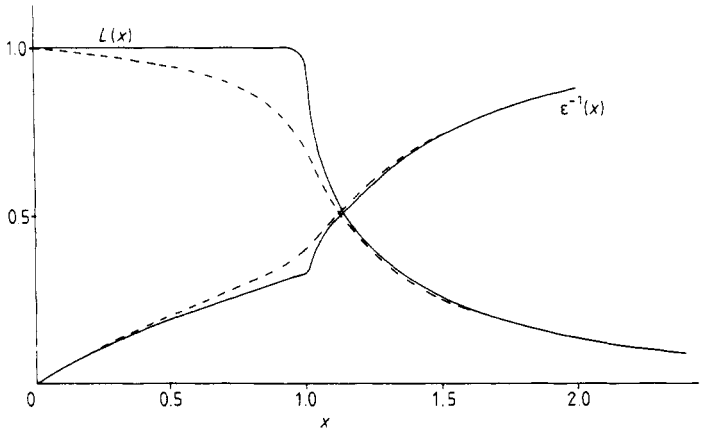

Figure 1. The inverse of the static dielectric function $\varepsilon^{-1}(x)$ and the function $L(x)$ versus $x = q/2k_F$, for $r_s/a_B^* = 3$ at selected values of b, where $b = 2mD/\hbar$. Full curve, $b = 0.001$; broken curve, $b = 0.1$.

inside the plane of the 2DEG. The screening charge density at a distance r from this static unit charge is given by (Vissher and Falicov 1971).

$$n_s(r) = \frac{1}{2\pi}\int_0^\infty qJ_0(qr)(1 - 1/\varepsilon(q))\,\mathrm{d}q \tag{9}$$

where $J_0(x)$ is the zeroth-order Bessel function of the first kind. The results obtained with our dielectric function (7) at $r_s/a_B^* = 3$, $b = 0$ and other selected values of b are presented in figure 2. The full line ($b = 0$) represents the usual RPA results where one sees the well known Friedel oscillations (Stern 1967) in the two-dimensional case,

$$n_s(r) \sim (1/r^2)\sin 2k_F r \tag{10}$$

at large values of $k_F r$. This behaviour is often considered to be the direct result of the non-analyticity of the Stern function at $q = 2k_F$. It is then of particular interest to see how it changes when we eliminate the non-analyticity by using the dielectric function (7) at $b \neq 0$, i.e. including the fluctuation effect. Our results show that in general the presence of fluctuations reduces the strength of the Friedel oscillation. When b is less than about 10^{-1}, the oscillation is still present although the amplitude of the oscillation is reduced compared to the $b = 0$ case. However, when b greater than about 10^{-1}, the amplitude of the oscillation decreases dramatically. We will now make some comments on these results.

First, the conservation of the local electron number holds in our calculation, which can be easily seen by integrating the $n_s(r)$ of (9) over the whole r-space. As is well known, this conservation is not easily achieved in phenomenological attempts (Mermin 1970) in the three-dimensional case to improve the Lindhard function (where the ω in (1) is simply replaced by $\omega + \mathrm{i}/\tau$, τ being the relaxation time, and the $\mathrm{i}Dq^2$ term does not appear), and the same remark applies to the case of the 2DEG (Giuliani and Quinn 1984, Belitz and Das Sarma 1986). Our approach is basically from first principles and is rigorous, and so the local electron number is conserved naturally in the calculation.

Secondly, in comparison with the RPA ($b = 0$) results, after we consider the fluctuation

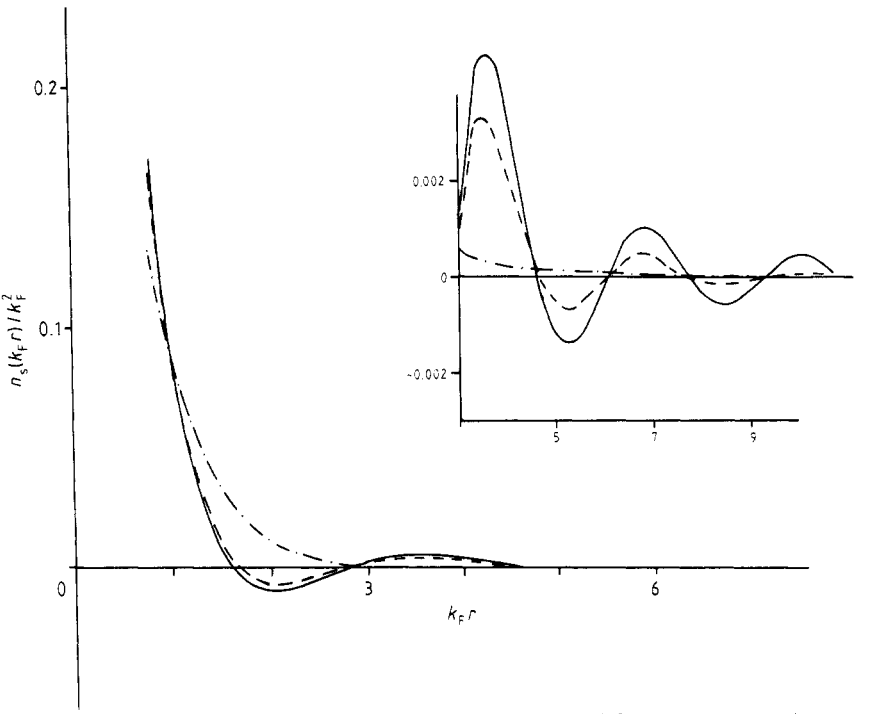

Figure 2. The dimensionless screening charge density $n_s(k_F r)/k_F^2$ versus $k_F r$, for $r_s/a_B^* = 3$ at selected values of b, where $b = 2m D/\hbar$. Full curve, $b = 0$; broken curve, $b = 0.1$; chain curve, $b = 1$.

effects ($b > 0$), the screening charge density $n_s(r)$ in the region very close to the point impurity is reduced and it is compensated by an increase in the intermediate region where $k_F r > 1$. Also, we find a reduction of the amplitude of the Friedel oscillations. We note that the behaviour of this fluctuation contribution to the Friedel oscillations in the RPA calculation is different from other known results in the literature (Czachor *et al* 1982). In the latter studies, in three dimensions as well as two dimensions, the short-range correlations arising from the Coulomb and exchange effects are added to the RPA calculation with the result that the screening charge density is increased for small r, compensated by the increase of the amplitude of the first oscillation peak of the negative charge, and, for large r, the oscillation is unchanged (Singwi *et al* 1970). Furthermore, the spread of $n_s(r)$ at large values of b indicates that the fluctuation effect will tend to make the impurity interaction more long range in character.

Thirdly, the period of the Friedel oscillations is decreased due to inclusion of the fluctuation effects at $b < 1$. Using (7) and (9), one can show the Friedel oscillation behaviour of (10) should be replaced by

$$n_s(r) \sim (1/r^2) \sin[2k_F r(1 + b/3)]. \tag{11}$$

The above expression shows that when b increases (keeping $b < 1$) the period of the Friedel oscillation becomes smaller. This fact is indicated by the inset in figure 2.

We now study the plasmon dispersion relation by means of the dielectric function (4) and (6). As the imaginary part $\varepsilon_2(x, y)$ of (6) is non-zero except at $x = 0$, the plasmon excitation in our scheme is a damped one at $x \neq 0$. It follows that the simple plasmon

equation $\varepsilon_1(x, y) = 0$ for the undamped case should be replaced by the maximum conditions for the inverse of the dielectric function $\varepsilon(x, y)$, which are

$$(\mathrm{d}/\mathrm{d}y)(\varepsilon^{-1}(x, y)) = 0 \qquad \text{and} \qquad (\mathrm{d}^2/\mathrm{d}y^2)(\varepsilon^{-1}(x, y)) < 0. \tag{12}$$

In general, the real part and the imaginary part of these equations will give slightly different plasmon dispersion equations, a point not often appreciated in the literature. We note that when ε_2 is independent of y, equation (12) will be equivalent to the usual Drude result, namely $\varepsilon_1(x, y) = 0$ for a damped plasma. In the present case, we are concerned with the plasmon excitation with a non-vanishing imaginary part of the above equations. Substituting (4) and (6) into (12), we obtain the plasmon dispersion relation of a 2DEG. For $x \to 0$, the result is

$$\omega_p^2 = \frac{2\pi ne^2}{m^*} q \left\{1 + \frac{q}{k_F}\left[\frac{3\sqrt{2}}{4r_s/a_B^*} + \left(\frac{b}{8}\right)^2 \left(\frac{r_s/a_B^*}{\sqrt{2}}\right)\right]\right\}. \tag{13}$$

The last term in (13) is the first-order contribution of the fluctuation effect to the RPA plasmon dispersion. It is interesting to note that this correction term has the same dependence on r_s compared to the contribution due to exchange mentioned at the beginning, except that it has an opposite sign, which implies that the fluctuation contribution will partly cancel the exchange contribution to the plasmon dispersion.

In summary, we have presented a well behaved dielectric function in (4) and (6) for all wavenumbers and frequencies, in contrast to Stern's expression which is non-analytic at $|\nu_\pm| = 1$ (see the definition of $\nu_\pm$ in (5)). The origin of the elimination of the non-analyticity is the inclusion of the effects due to the fluctuations of the electrons in the calculation of the dielectric function. Our study of $\varepsilon(x, 0)$ and $L(x)$ shows that their behaviour changes dramatically even for very small b. We find the screening charge density is more spread out when b gets larger, which indicates that high-mobility material should have a longer impurity interaction range than that of the low-mobility material. In the study of the fluctuation contribution to the plasmon dispersion, we have obtained the criterion (12) for the damped plasmon excitation, and the results given by (13) indicate that the fluctuation will contribute a term which partly cancels the exchange contributions to the plasmon dispersion.

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