

## Exchange and correlation effects on screening in a two-dimensional electron gas

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A simple expression for the screening constant in a two-dimensional electron gas (2D EG) of finite thickness is obtained within the framework of a 2D version of the linearized Thomas-Fermi-Dirac equation, which includes effects of the exchange-correlation energy. For the case of 2D EG in an  $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$  system the role of the correlation energy is shown to be small compared to that of exchange. Effect of the exchange energy on the screening constant decreases with the increasing surface concentration  $n$  of electrons. For  $n \approx 10^{11} \text{ cm}^{-2}$  the screening constant increases by 50% compared to its value calculated for noninteracting particles.

### I. INTRODUCTION

Behavior of an electron gas in inhomogeneous electric fields, in particular the effect of screening, represents an important and complex problem, for which a number of effective methods have been developed. One of the rigorous formulations is given by the density-functional theory of Hohenberg and Kohn.<sup>1</sup> In the three-dimensional case, simple practical realization of this theory is possible in two limiting cases of (1) *weak* and (2) *smooth* inhomogeneities. The first limit, corresponding to the case when deviations of the electron density from its average value are small, allows one to describe the electron gas in terms of a wave-vector-dependent static dielectric constant and thus consider short-wavelength effects such as the Friedel oscillations.<sup>2</sup> The second limit corresponds to slow (though not necessarily small) potential variations on the characteristic scale of electronic wavelengths. If exchange-correlation energy is neglected, then this limit reduces to the well-known Thomas-Fermi method. As discussed by Lang,<sup>3</sup> inclusion of the exchange energy leads to the so-called Thomas-Fermi-Dirac (TFD) equation,<sup>4</sup> and correlation corrections to a generalized TFD (Gombas) equation.<sup>5</sup>

Implementation of a similar program for a two-dimensional (2D EG) electron gas encounters considerable difficulties, associated with the fact that variations of the quantum-well energy levels cannot be related to those in the local self-consistent potential. Neither of the above limits separately leads to a tractable approximation. Indeed, even assuming a smoothly varying 2D concentration and ignoring exchange effects, one does not obtain a 2D version of the nonlinear Thomas-Fermi equation. (This difficulty is, of course, rooted in the fact that the 3D density of a homogeneous 2D EG is not a smooth function of the coordinates.) On the other hand, no simple description of a real 2D EG in terms of a wave-vector-dependent static dielectric constant is available in the limit of a *weak* inhomogeneity—except for the case of an “ideal” 2D EG, corresponding to the case

of an infinitesimal thickness of the quantum well. The latter case, first considered by Stern<sup>6</sup> for noninteracting particles and extended by Maldague<sup>7</sup> to include the exchange and correlation energies, is tractable because the bottom of the 2D energy band follows precisely the local value of the self-consistent potential.

Thus, in order to obtain a *local* description of the response of a real 2D EG to external fields, one has to make *both* of the above approximations, namely assume that the perturbing potential varies little on the scale of  $k_F^{-1}$  [where  $k_F = (2\pi n)^{1/2}$  and  $n$  is the electron concentration per unit area of the 2D EG] and that its effect on the quantum-well energy levels can be adequately treated in a first-order perturbation theory. This was first done by Stern and Howard<sup>8</sup> for the case of noninteracting electrons. In the present work, their results are generalized to include the exchange and correlation corrections. It should be noted that this generalization is achieved without any additional approximations beyond those made in Ref. 8, except for the fact that our consideration is limited to the case of a *degenerate* electron gas in the quantum electronic limit (one subband occupation). The Stern-Howard theory<sup>8</sup> represents a linearized version of the Thomas-Fermi equation extended to the case of a real 2D EG; our results correspond to a similar extension of the Thomas-Fermi-Dirac method.

### II. THOMAS-FERMI-DIRAC THEORY OF SCREENING IN 2D EG

Accounting for the exchange and correlation corrections, the single-electron energies of a homogeneous 2D EG, referred to an absolute “vacuum” level, can be written in the form

$$E(k, n) = \frac{\hbar^2 k^2}{2m} + E^{xc}(k, n) + E_0^H, \quad (1)$$

where  $k$  is the magnitude of the electron wave vector,  $E^{xc}$  is the exchange-correlation energy, and  $E_0^H$  is the bottom energy of the lowest subband, calculated in the

Hartree approximation. The energy  $E_0^H$  can be regarded as a functional of the self-consistent potential  $\phi$  of the external charges and the other electrons in the 2D EG. It should be noted that  $E_0^H$  is not the true bottom energy  $E_0$  of the lowest subband since the latter also contains an exchange-correlation correction:

$$E_0 = E_0^H[\phi] + E^{xc}(0, n). \quad (2)$$

The energy  $E(k, n)$  can be represented as a sum of (2) and the total single-electron energy counted from the level  $E_0$ , i.e., the kinetic energy (cf. Fig. 1),

$$E^{\text{kin}}(k, n) = \frac{\hbar^2 k^2}{2m} + E^{xc}(k, n) - E^{xc}(0, n).$$

According to (1), the Fermi energy of the 2D EG is given by

$$\begin{aligned} E_F &\equiv E(k_F, n) = \frac{\hbar^2 k_F^2}{2m} + E^{xc}(k_F, n) + E_0^H[\phi] \\ &= \frac{\pi \hbar^2 n}{m} + E_F^{xc}(n) + E_0^H[\phi]. \end{aligned} \quad (3)$$

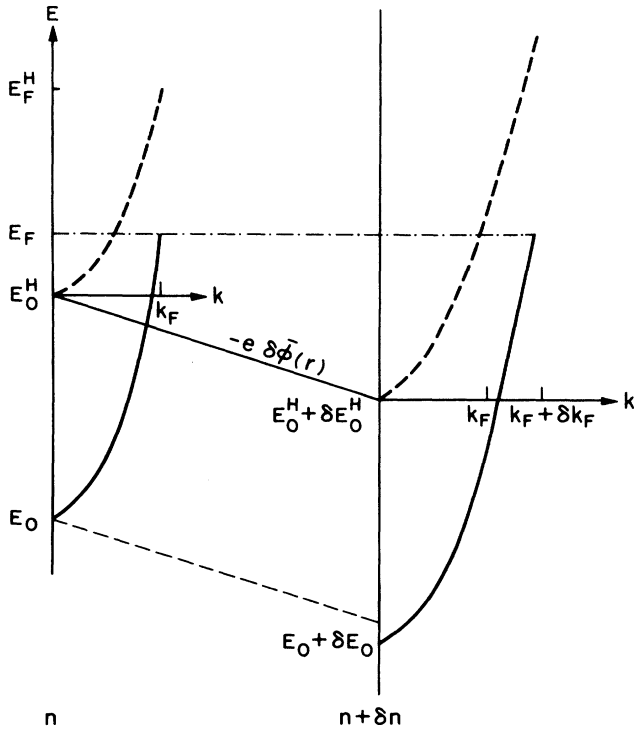


FIG. 1. Schematic illustration of the energies contributing to the formation of a uniform Fermi level in the presence of an inhomogeneous self-consistent "potential"  $\bar{\phi}(\mathbf{r})$ . The diagrams shown correspond to two spatially separated points at which the local concentration differs by  $\delta n$ . Dashed lines show the kinetic energy  $\hbar^2 k^2/2m$  of noninteracting particles, solid lines the true dispersion dependence of the single-electron energy. The figure illustrates the difference between the shift of the true subband bottom  $\delta E_0$ , which includes many-body effects, and the corresponding level  $\delta E_0^H$  calculated in the Hartree approximation.

In the local-density approximation, corresponding to the limit of a smoothly varying perturbation, Eq. (3) remains valid. Consider the response of the system to a small inhomogeneous perturbation  $\delta\phi(\mathbf{r}, z)$ , where  $\mathbf{r}$  is the coordinate in the plane of the 2D EG and  $z$  is the coordinate in the normal direction. The variation in  $E_0^H$  linear in  $\delta\phi$  is given by the first-order perturbation theory<sup>8</sup>

$$\delta E_0^H = -e \int \delta\phi(\mathbf{r}, z) |\zeta(z)|^2 dz \equiv -e \delta\bar{\phi}(\mathbf{r}), \quad (4)$$

where  $\zeta(z)$  is the envelope wave function of the first subband. In the presence of the inhomogeneous perturbation  $\delta\phi$ , the concentration of electrons is redistributed so as to keep the Fermi level constant. To within linear terms in the variation  $\delta n$  of the concentration we find

$$-\delta E_0^H = \frac{\pi \hbar^2 \delta n}{m} + \frac{dE_F^{xc}}{dn} \delta n, \quad (5)$$

whence we have

$$\delta n(\mathbf{r}) = -\frac{m}{\pi \hbar^2} \frac{\delta E_0^H(\mathbf{r})}{1 + \beta(n)}, \quad (6)$$

where

$$\beta(n) = \frac{m}{\pi \hbar^2} \frac{dE_F^{xc}}{dn}. \quad (7)$$

Let us assume that the perturbation is caused by an external charge of volume density  $\delta\rho(\mathbf{r}, z)$ . The induced charge has the volume density equal  $\delta n(\mathbf{r}) |\zeta(z)|^2$ . Using (6), the Poisson equation for the potential  $\delta\phi(\mathbf{r}, z)$  can be written in the form

$$\nabla^2 \delta\phi(\mathbf{r}, z) - 2s \delta\bar{\phi}(\mathbf{r}) |\zeta(z)|^2 = -(4\pi/\kappa) \delta\rho(\mathbf{r}, z), \quad (8)$$

where  $\kappa$  is the dielectric permittivity of the medium and

$$s = \frac{s_0}{1 + \beta(n)} \quad (9)$$

is the screening constant. In this equation,  $s_0$  is the screening constant for noninteracting electrons,<sup>8</sup> given by

$$s_0 = \frac{2e^2 m}{\hbar^2 \kappa} \equiv \frac{2}{R_B}, \quad (10)$$

where  $R_B$  is the effective Bohr radius. Parameter  $\beta$  defined by (7) is always negative, since the exchange-correlation energy  $E_F^{xc} < 0$  and the magnitude  $|E_F^{xc}|$  increases with the concentration. It therefore follows from (9) that screening is enhanced by the exchange-correlation effects.

### III. EVALUATION OF THE SCREENING CONSTANT

As will be shown in Sec. IV, the correlation corrections to the screening parameters are negligible in range of concentrations of practical interest (e.g., in the range  $n \gtrsim 10^{11} \text{ cm}^{-2}$  for a GaAs inversion layer). In this section we shall confine our consideration to the effects of exchange.

To proceed with the calculation, we must assume a concrete model of the 2D EG. We shall assume the

wave function of the first subband in the usual form<sup>9,10</sup>

$$\xi(z) = \frac{\alpha^{3/2} z}{2^{1/2}} e^{-\alpha z/2}, \quad (11)$$

where the parameter  $\alpha$  is given by (in the case when the background doping charge can be neglected compared to the inversion-layer charge):

$$\alpha^{-1} = R_B (2r_s^2/33)^{1/3}, \quad (12)$$

$$E^x(k, k_F) = \frac{e^2 \alpha^6}{\pi \kappa} \int_0^\infty \frac{dq}{(\alpha^2 + q^2)^3} \ln \left[ \frac{[(q^2 + k_F^2 k^2)^2 - 4k^2 k_F^2]^{1/2} + q^2 + k_F^2 - k^2}{2q^2} \right]. \quad (13)$$

The equivalence of (13) to the expression given by Stern<sup>13</sup> can be shown by a straightforward though somewhat tedious algebra. Letting  $k = k_F$  in Eq. (13), differentiating  $E_F^x(n) \equiv E^x(k_F, k_F)$ , and using (7), we obtain an exact analytic expression for the exchange contribution to  $\beta$ :

$$\beta^x(n) = \frac{2}{\pi R_B k_F} F(\alpha/2k_F), \quad (14)$$

where

$$F(\xi) = \frac{\xi}{8} \left[ \frac{3\pi}{2} - \frac{\xi(2-5\xi^2)}{(1-\xi^2)^2} - \frac{3\xi^5}{(1-\xi^2)^{5/2}} \ln \left[ \frac{1+(1-\xi^2)^{1/2}}{\xi} \right] \right]. \quad (15)$$

[For  $\xi > 1$  one should use the principal branch of the function  $F$ , i.e., replace the logarithm by  $\arccos(1/\xi)$  and in the prelogarithmic factor change  $1-\xi^2$  to  $\xi^2-1$ .] The concentration dependence of the screening constant  $s$ , defined by (9) and calculated with (14), is shown in Fig. 2 by the solid line. We see that the screening effect decreases with the concentration. For  $n \approx 10^{11} \text{ cm}^{-2}$  the screening constant is nearly 50% higher than that for noninteracting particles.

#### IV. ESTIMATE OF THE CORRELATION CORRECTION TO THE SCREENING CONSTANT

This estimate will be carried out for an "ideal" 2D EG, corresponding to the limit of an infinitesimally thin quantum well, when  $\alpha \rightarrow \infty$  and  $|\xi(z)|^2 \rightarrow \delta(z)$ . In this limit, the function  $F$  defined by (15) tends to unity and

and  $r_s \equiv 1/(\pi n R_B^2)^{1/2}$  is the dimensionless gap parameter of the 2D EG.

In the framework of this model, the exchange energy,  $E^x(k, n) \equiv E^x(k, k_F)$ , was first considered for an ideal 2D EG by Chaplik<sup>11</sup> and also by Stern.<sup>12</sup> For a finite-thickness 2D EG the problem was treated by Stern<sup>13</sup> who reduced the evaluation of  $E^x$  to a quadrature. It is more convenient for our purposes to use a different quadrature form for  $E^x$ , viz:

hence

$$\beta^x \rightarrow \beta_{\text{ideal}}^x = \frac{2}{\pi R_B k_F}. \quad (16)$$

To estimate the correlation contribution to  $\beta_{\text{ideal}}$ , we shall use the interpolation formula of Jonson and Srinivasan<sup>14</sup> for the total correlation energy per particle of an ideal 2D EG:

$$\epsilon^c = -\frac{1.103}{r_s + 4.41} \quad (17)$$

(in units of  $\hbar^2/2mR_B^2$ ). Although Eq. (17) was obtained<sup>14</sup> by an interpolation between the 2D EG correlation energy calculated at a low value of  $r_s$  and the low-density result corresponding to a 2D electron crystal,<sup>15</sup> it reproduces reasonably well (to within 25% in the range  $0.5 < r_s < 16$ ) the more reliable numerical calculations<sup>14</sup> based on a 2D version of the local-field theory of Singwi *et al.*<sup>16</sup> As seen from Table I, the range of practical interest for  $r_s$  in GaAs/Al<sub>x</sub>Ga<sub>1-x</sub>As systems (where  $10^{11} \lesssim n \lesssim 10^{12} \text{ cm}^{-2}$ ) is  $0.5 \lesssim r_s \lesssim 2$ .

Evaluating the correlation part of the chemical potential  $E_F^c = d(n\epsilon^c)/dn$  with the help of (17) and using Eq. (7) we obtain

$$\beta_{\text{ideal}}^c = -\frac{0.41r_s^3(r_s + 1.47)}{(r_s + 4.41)^3}. \quad (18)$$

The bottom two rows in the table show the values of  $\beta_{\text{ideal}}^x$  and  $\beta_{\text{ideal}}^c$  for several concentrations. We see that the correlation energy plays only a minor role in the many-body enhancement of the screening effect. Even at  $n = 10^{11} \text{ cm}^{-2}$  the correlation contribution is less than 4% of  $\beta_{\text{ideal}}$  and at higher concentrations this contribu-

TABLE I. Typical parameters and results for an Al<sub>x</sub>Ga<sub>1-x</sub>As/GaAs 2D EG system.

$-\beta_{\text{ideal}}^c$	$-\beta_{\text{ideal}}^x$	$\alpha/k_F$	$k_F$ ( $10^6 \text{ cm}^{-1}$ )	$\alpha$ ( $10^6 \text{ cm}^{-1}$ )	$r_s$	$n$ ( $10^{12} \text{ cm}^{-2}$ )
0.1	1.73	1.76	0.82	2.16	1.78	0.03
0.5	0.78	3.02	1.82	1.65	0.35	$3 \times 10^{-3}$
1.0	0.55	3.8	2.58	1.47	0.25	$6 \times 10^{-4}$
1.5	0.45	4.35	3.16	1.38	0.20	$6 \times 10^{-4}$
2.0	0.39	4.79	3.65	1.31	0.18	$4 \times 10^{-4}$

tion is still more negligible. A qualitatively similar situation is expected in any realistic model of the 2D EG. Moreover, judging from the numerical data by Jonson<sup>14</sup> for  $E^c$  of a real 2D EG, the ratio  $\beta^c/\beta^x$  should be even smaller than in the ideal case. For comparison, Fig. 2 also displays the dependence  $s/s_0$  calculated for an ideal 2D EG. It is evident that the effect of exchange on the screening constant is much stronger in the ideal than in the real case.

### V. CONCLUSION

The method of including the many-body effects in 2D EG screening described in this paper is strictly valid in the long-wavelength limit  $q \ll k_F$ , where  $q$  is the characteristic wave number for the inhomogeneity of an external potential. At low temperatures, this inequality turns out to be too restrictive compared to the actual validity range of the results. For an ideal 2D EG in the limit  $q \rightarrow 0$ , the static wave-vector-dependent polarizability  $\chi(q)$  is related to the screening constant  $s$  as follows:

$$q^2\chi(q) = \frac{\kappa s}{2\pi}. \quad (19)$$

Evaluation of  $\chi(q)$  in the noninteracting limit<sup>6</sup> shows that for  $T=0$  the polarizability remains constant with increasing  $q$  up to  $q=2k_F$ . A similarly weak  $q$  dependence is found in the ideal 2D EG including electron-electron interaction effects.<sup>7</sup> This gives us grounds to believe that the simple way of accounting for many-body corrections to the screening length, proposed in this work, should be adequately accurate in the description of various low-temperature phenomena involving screening. At higher temperatures, however, the short-wavelength effects begin to manifest themselves at smaller wave numbers,<sup>7,17</sup> and a user of the long-wavelength approximation must carefully assess the range of  $q$  where

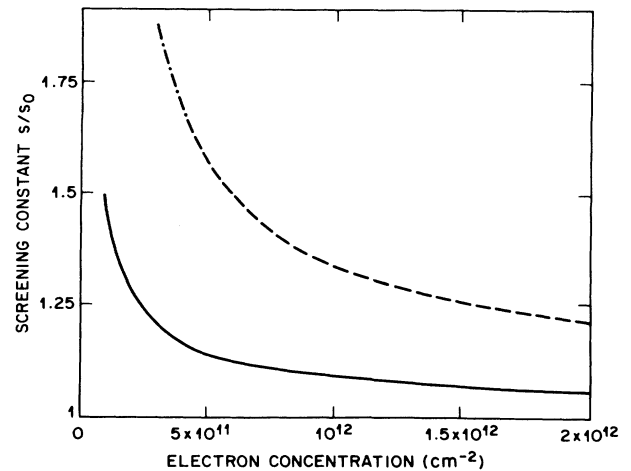


FIG. 2. Dependence of the screening constant  $s$ , normalized by its value  $s_0$  for noninteracting particles, on the electron concentration per unit area of the 2D EG. Dashed line shows the same constant evaluated (Sec. IV) for the "ideal" 2D EG (of infinitesimal thickness,  $\alpha \rightarrow \infty$ ).

the dispersion effects are still small.

In estimating the role of the correlation energy we had assumed the 2D EG parameter values characteristic of an  $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$  system. In a silicon inversion layer, the relative role of correlation effects is *higher* because of the many-valley structure of the conduction band and hence of the 2D EG subbands. Therefore, analysis of the role of correlation energy requires additional consideration on the basis of more detailed calculations of  $\epsilon^c$  and  $\epsilon^x$ —from which one would be able to reliably extract the concentration derivative (7) of the chemical potential which enters Eq. (9).

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