

## 2D Electron Gas at Arbitrary Spin Polarizations and Coupling Strengths: Exchange-Correlation Energies, Distribution Functions, and Spin-Polarized Phases

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We use the classical mapping of quantum fluids [Phys. Rev. Lett. **84**, 959 (2000)] for a study of the uniform 2D electron gas. The “quantum temperature”  $T_q$  of the *classical* 2D Coulomb fluid having the same correlation energy  $E_c$  as the quantum fluid is determined as a function of the density parameter  $r_s$ . Using this  $T_q$ , spin-dependent pair-distribution functions are determined, and an analytic fit to the  $E_c$  is given. The  $T_q$  for 2D and 3D electron fluids is found to be approximately the same universal function of the classical coupling constant  $\Gamma$ . The coupling  $\Gamma$  increases more rapidly with density in 2D; hence, we present a scheme for including bridge terms in the 2D hypernetted-chain method. The Helmholtz free energies of the spin-polarized and unpolarized phases are calculated, and the existence of a ferromagnetic phase near  $r_s \sim 30$  is found to be a marginal possibility.

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The past three decades have established the two-dimensional electron gas (2DEG) as a goldmine of new physics and novel technologies [1]. The 2DEG, ranging from a classical to a quantum system, occurs on liquid-He surfaces, semiconductor heterointerfaces, and in the CuO layers of high- $T_c$  superconductors. The interest in the quantum Hall effect, the metal-insulator transition, Kosterlitz-Thouless-type transitions [2], and applications to nanotechnology and spintronics widens its importance. The exchange-correlation energy ( $E_{xc}$ ) of the 2DEG is important in its own right as an input to the density-functional theory of inhomogeneous 2D systems.

The physics of the 2DEG depends crucially on the “coupling parameter”  $\Gamma = (\text{potential energy})/(\text{kinetic energy})$  arising from the Coulomb interactions. The  $\Gamma$  for the 2DEG at  $T = 0$  and mean density  $n$  is equal to the mean-disk radius  $r_s = (\pi n)^{-1/2}$  per electron. In the absence of a magnetic field or disorder effects, the density parameter  $r_s$ , the spin polarization  $\zeta$ , and the temperature  $T$  are the only relevant physical variables. A major problem in the 2DEG is the need for a theoretical method applicable at *arbitrary* values of  $\Gamma$ ,  $\zeta$ , and  $T$ . As in the 3D electron gas (3DEG), various perturbation methods, equations-of-motion methods, e.g., those of Singwi *et al.* (STLS) [3], work for relatively weak coupling, but lead to negative pair-distribution functions (PDFs) even at moderate  $r_s$ . In spite of a large effort, the calculation of the 2DEG  $g_{ij}(r)$ , where  $i, j$  are spin species, at arbitrary spin-polarization  $\zeta$ ,  $r_s$ , and  $T$  is unsolved, except by direct quantum simulation techniques. Such “quantum Monte Carlo” (QMC) methods [4], as well as Feenberg techniques [5], assume a trial wave function  $\psi = FD$ , where  $F$  is a correlation factor and  $D$  is a Slater determinant. The variational Monte Carlo method [6], and the fixed-node Green-function Monte Carlo method (GFMC) have been applied to the 2DEG, providing the exchange-correlation energy,  $E_{xc}(r_s)$  at  $T = 0$  in a

parametrized form [6]. Finite- $T$  systems involve excited states as well as the ground state. While it is easy to get good  $E_{xc}(r_s)$  at  $T = 0$ ,  $\zeta = 0$ , the same is not true for most properties such as the PDFs, local-field corrections, and xc energies at finite  $T$ , spin polarization  $\zeta$ , and at strong coupling.

Recently we presented a computationally simple, conceptually novel *classical* method for calculating the PDFs and other properties (e.g., static response) of the 3DEG at arbitrary coupling, spin polarization, and temperature [7]. The method is based on identifying a “quantum temperature”  $T_q$  such that the correlation energy of a corresponding *classical* Coulomb fluid at  $T_q$  is equal to that of the quantum fluid at  $T = 0$ . Our only “many-body” input is a set of values of  $E_c(r_s)$  for determining  $T_q$ . Once  $T_q(r_s)$  is known, many properties inaccessible to standard methods become readily calculable. A discussion of the  $T = 0$  and finite- $T$  3DEG was presented earlier [7,8].

A method which works in 3D does not necessarily work in reduced dimensions. A first objective of this Letter is to show that the same ideas apply to the challenging problems of the 2DEG. In addition, this study reveals previously unexpected aspects of the quantum temperature  $T_q$ , exposes the long-range nature of the Pauli exclusion effect in the 2D system, and provides new results for the partially polarized 2D electron liquid. It is found to be numerically precise enough, even at  $r_s = 30$ , to selectively favor newer QMC calculations [9]. We also examine the stability of spin-polarized phases of the 2DEG at finite  $T$  and sufficiently large  $r_s$ .

The PDFs of the 3DEG could be accurately calculated using the hypernetted-chain (HNC) approximation [10]. The 2D system requires that bridge-type cluster corrections to the HNC approximation be included. A comparison of the 2DEG and 3DEG forms of  $T_q(r_s)$  reveals that the quantum temperature is approximately a universal function of the classical-fluid coupling constant.

The essence of our method is to start from the quantum mechanical  $g^0(r)$  of the noninteracting problem and build up the interacting  $g(r)$  by classical methods.

Consider a fluid of mean density  $n$  containing two spin species with concentrations  $x_i = n_i/n$ . We deal with the physical temperature  $T$  of the 2DEG, while the temperature  $T_{cf}$  of the classical fluid is  $1/\beta$ . Since the leading dependence of the energy on temperature is quadratic, we assume that  $T_{cf} = \sqrt{T^2 + T_q^2}$ . This is clearly valid for  $T = 0$  and for high  $T$ , and was justified in more detail in Ref. [8]. In this Letter the main effort is to study the 2DEG near  $T = 0$  and at zero magnetic field by determining  $T_q$ . The equations for the PDFs of a classical fluid, and the Ornstein-Zernike (OZ) relations, are

$$g_{ij}(r) = \exp[-\beta\phi_{ij}(r) + h_{ij}(r) - c_{ij}(r) + B_{ij}(r)], \quad (1)$$

$$h_{ij}(r) = c_{ij}(r) + \sum_s n_s \int d\mathbf{r}' h_{i,s}(|\mathbf{r} - \mathbf{r}'|) c_{s,j}(\mathbf{r}'). \quad (2)$$

Here  $\phi_{ij}(r)$  is the pair potential between the species  $i, j$ . For two electrons this is just the Coulomb potential  $V_{cou}(r)$ . If the spins are parallel, the Pauli principle prevents occupation of the same spatial orbital. As before [7,] we introduce a ‘‘Pauli potential,’’  $\mathcal{P}(r)$ . Thus  $\phi_{ij}(r)$  becomes  $\mathcal{P}(r)\delta_{ij} + V_{cou}(r)$ . The function  $h(r) = g(r) - 1$  is related to the structure factor  $S(k)$  by a Fourier transform. The  $c(r)$  is the ‘‘direct correlation function (DCF)’’ of the OZ equations. The  $B_{ij}(r)$  in Eq. (1) is the ‘‘bridge’’ term due to certain cluster interactions. If this is neglected, Eqs. (1) and (2) form a closed set defining the HNC approximation. The HNC is sufficient for the 3DEG for the range of  $r_s$  studied previously [7]. The classical coupling constant of the 2DEG is found to increase with  $r_s$  more rapidly than in the 3DEG. Thus, although  $\mathcal{P}(r)$  restricts clustering effects in the case of  $g_{ii}$ , bridge contributions (which contain irreducible three-body and higher terms) are found to be important for  $g_{12}$ . The inclusion of a bridge term into the HNC equations, usually via a ‘‘hard-sphere’’ model [11], is well known in 3D problems, but is less explored for 2D systems. In this context, it is noteworthy that Kwon *et al.* had to include three-body correlations in QMC trial functions [9,12].

In the noninteracting system at temperature  $T$ ,  $n = n_1 + n_2$ ,  $x_i = n_i/n$ , the anti-||  $g_{12}^0(r, T)$  is unity while

$$h_{11}^0(\mathbf{r}) = -\frac{1}{n_1^2} \sum_{\mathbf{k}_1, \mathbf{k}_2} n(k_1)n(k_2)e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r}} = -[f(r)]^2.$$

Here  $\mathbf{k}, \mathbf{r}$  are 2D vectors and  $n(k)$  is the Fermi occupation number at the temperature  $T$ . At  $T = 0$ ,  $f(r) = 2J_1(k_i r)/k_r$ , where  $J_1(x)$  is a Bessel function. The Pauli exclusion potential is defined by

$$\beta\mathcal{P}(r) = h_{11}^0(r) - c_{11}^0(r) - \ln[g_{11}^0(r)], \quad (3)$$

where, e.g.,  $c_{ii}^0(r)$  is the spin-|| DCF of the OZ equation. At  $T = 0$  it may be shown that  $\beta\mathcal{P}(r) \sim -2\ln(r)$  for

$r \rightarrow 0$ ,  $\beta\mathcal{P}(r) \sim \pi/rk_F$  for  $r \rightarrow \infty$ ,  $\beta\mathcal{P}(k) \sim -4\pi/k^2$  for  $k \rightarrow \infty$ . Only the product  $\beta\mathcal{P}(r)$  is determined. The classical fluid ‘‘temperature’’  $T_{cf} = 1/\beta$  is still undefined. The Pauli potential is a universal function of  $rk_F$ , and limited to about a thermal wavelength  $\lambda_{th}$  at finite  $T$ .

The next step in the method is to use the full  $\phi_{ij}(r)$ , and solve the coupled HNC and OZ equations for the binary (up and down spins) *interacting* fluid. The Coulomb potential  $V_{cou}(r)$  for two point-charge electrons is  $1/r$ . However, an electron at the temperature  $T$  is localized to within a thermal wavelength. Thus, for the 3DEG we used a ‘‘diffraction corrected’’ form [13]:

$$V_{cou}(r) = (1/r)[1 - e^{-rk_{th}}], \quad (4)$$

where  $k_{th}$  was taken to be  $k_{th}^0 = (2\pi m^* T_{cf})^{1/2}$  as in Minoo *et al.* [13]. Here  $m^* = 1/2$  is the reduced mass of the electron *pair*. In the case of the 2DEG we have determined  $k_{th}$  by numerically solving the Schrödinger equation for a pair of 2D electrons in the potential  $1/r$  and calculating the electron density in each normalized state [14]. Assuming that the diffraction correction has the same form as before, i.e.,  $V_d(r) = \exp(-k_{th}r)/r$ , it was found that  $k_{th}/k_{th}^0 = 1.158T^{0.103}$ , where  $T$  is in a.u.

As in the 3DEG, we need the quantum temperature  $T_q$  for each  $r_s$  of the 2DEG, such that the classical 2D fluid has the same  $E_c(r_s)$  as the quantum fluid. Unlike in the 3DEG, an additional complication in the 2DEG is the need for a bridge function. In the ||-spin case, if the hard-disk radius of the bridge function is smaller than the range of the Pauli potential, we may neglect the bridge term. In the anti-|| case, we need a bridge term  $B_{12}$  explicitly included, say, via a hard-disk model [15]. The same bridge term enters the paramagnetic PDF,  $g(r) = 0.5(g_{11} + g_{12})$ , via the  $g_{12}$ . We can decouple the determination of  $T_q$  and  $B_{12}$  by obtaining  $T_q$  from the *fully spin-polarized* system as the bridge function is negligible in this case. Using the analytic fit of  $E_c(r_s, \zeta = 1)$  given by Tanatar and Ceperley [6],  $t = T_q/T_F$  is found to be fitted by

$$t = 2/[1 + 0.86413(r_s^{1/6} - 1)^2]. \quad (5)$$

This looks very different from the  $T_q(r_s)$  mapping for the 3DEG. However, when  $T_q$  is plotted as a function of the *classical* coupling constant  $\Gamma_c = 1/T_q r_s$  (cf. Table I), the 3DEG and 2DEG maps are seen to be almost a single universal function [Fig. 1(a)]. This result is *conceptually very interesting* since  $T_q$  is really a single-parameter representation of the density-functional correlation energy of the electron gas, irrespective of dimensionality.

Unlike in the 3DEG, we need the bridge function for  $g_{12}$  in order to implement the method. We include only the anti-||  $B_{12}(r)$ , and, hence, a one-component hard-disk packing fraction  $\eta$  is needed. The effective coupling constant,  $\Gamma_{eff} = \phi(r_s)/T_{cf}$ , is a function of  $r_s T_q$  and  $k_{th} r_s$ . That is,  $r_s/t$  and  $t^3/r_s$ , where  $t = T_q/T_F$ . The Gibbs-Bogoliubov expression for the free energy of the

TABLE I. Relevant parameters and a comparison of the QMC correlation energies (a.u.) of Tanatar and Ceperley (TC), Rapisarda and Senatore (RS), with those from the classical map-HNC (CHNC) for the paramagnetic 2DEG.

$r_s$	$T/T_F$	$\Gamma_c$	$\eta$	$-E_c(\text{TC})$	$-E_c(\text{RS})$	$-E_c(\text{CHNC})$
1	2.000	0.500	0.235	0.10850	...	0.10838
5	1.849	2.704	0.372	0.04775	0.0489	0.04910
10	1.682	5.946	0.425	0.03034	0.0302	0.03023
20	1.468	13.62	0.469	0.01758	0.0174	0.01739
30	1.331	22.54	0.486	0.01251	0.0124	0.01245

one-component hard-disk system has the same dependence. Also, at large  $r_s$  the packing fraction should tend to a finite limit. Since  $t$  decreases as  $r_s^{-1/3}$ , we consider the simple functional form  $\eta = \theta t r_s^{1/3}$ . Here  $\theta$  is a “global” parameter valid for the whole range of  $r_s$ , and, hence, the procedure does not involve fitting at each  $r_s$ . A constant value,  $\theta = 0.1175$ , proved to be applicable to the range  $r_s = 1-30$  studied here. Values of the packing fraction  $\eta$ , the QMC, and classical-map HNC (CHNC) values of  $E_c(r_s, \zeta = 0)$  for the unpolarized 2DEG are given in Table I. Our  $E_c(r_s, \zeta = 1)$  agrees with Tanatar-Ceperley spin-polarized QMC by construction. It is common for  $\eta$  to approach  $\sim 0.49$  at the liquid-solid transition. The trend in the value of  $\eta$  seen in Table I is consistent with the finding of Tanatar and Ceperley that the 2DEG becomes a Wigner solid for  $r_s = 37 \pm 5$ .

Using the  $T_q$  and the hard-disk bridge parameter  $\theta$ , we can calculate  $E_c(r_s, \zeta, T)$  at any  $\zeta$ . Our results (at  $T = 0$ ) can be presented via a “polarization function”:

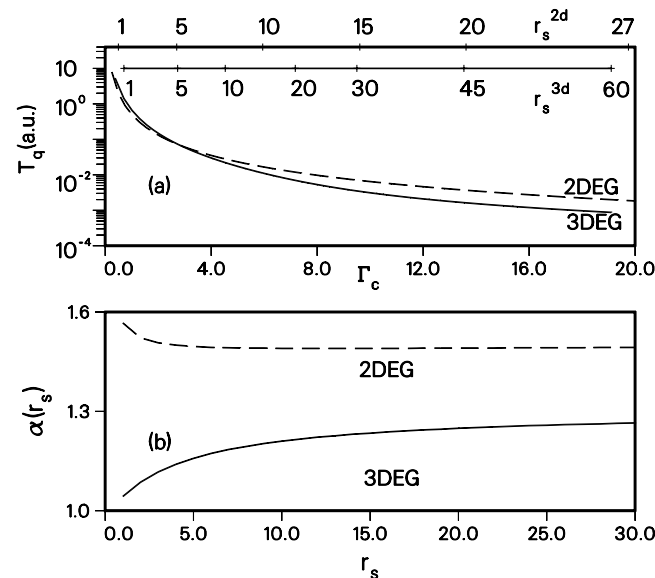


FIG. 1. (a) The quantum temperature  $T_q$  for the 2DEG (dashes) and the 3DEG (solid line) as a function of the classical coupling constant  $\Gamma = \beta/r_s$ . (b) The  $r_s$  dependence of the 2DEG (dashes) and 3DEG (solid line) polarization functions at  $T = 0$ .

$$p(r_s, \zeta) = \frac{E_c(r_s, \zeta) - E_c(r_s, 0)}{E_c(r_s, 1) - E_c(r_s, 0)} = \frac{\zeta_+^{\alpha(r_s)} - \zeta_-^{\alpha(r_s)} - 2}{2^{\alpha(r_s)} - 2}$$

$$\alpha(r_s) = C_1 - C_2/r_s + C_3/r_s^{2/3} - C_4/r_s^{1/3}. \quad (6)$$

Here  $\zeta_{\pm} = (1 \pm \zeta)$ . In Hartree-Fock, the exponent  $\alpha(r_s)$  is a constant,  $\alpha = (d + 1)/d$ , where  $d$  is the dimensionality. Hence, for the 2DEG, the Hartree-Fock value of  $\alpha$  is 1.5. The coefficients  $C_1-C_4$  are 1.540 39, 0.030 544 1, 0.296 208, and 0.239 047, respectively. A comparison of the 2D and 3D  $\alpha(r_s)$  is given in Fig. 1(b).

Our classical mapping of the 2DEG uses the GFMC spin-polarized xc-energy fit of Tanatar and Ceperley [6].

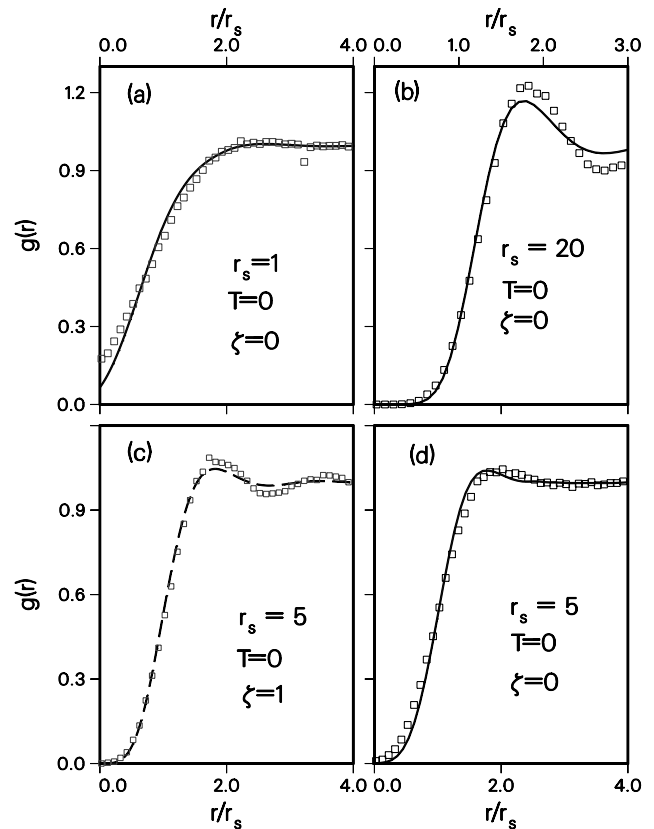


FIG. 2. Here the HNC  $g(r)$  are compared with GFMC simulations of Tanatar and Ceperley. Solid lines: HNC, boxes: GFMC, panels (a) and (b) unpolarized case ( $\zeta = 0$ ),  $r_s = 1$ , and  $r_s = 20$ . Panels (c) and (d)  $r_s = 5$  spin-polarized ( $\zeta = 1$ ) and unpolarized systems.

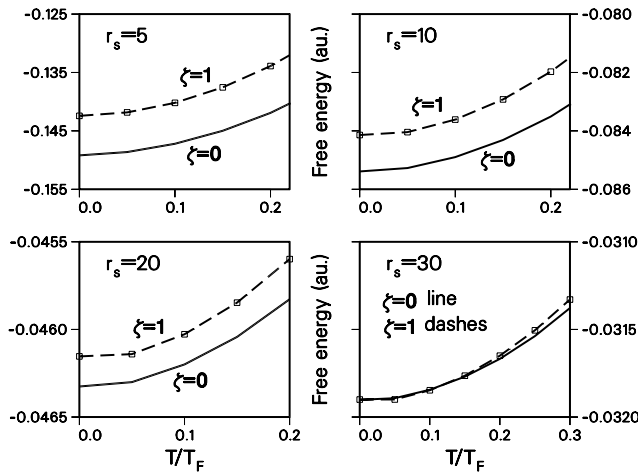


FIG. 3. The total Helmholtz free energy of the unpolarized ( $\zeta = 0$ ) and polarized ( $\zeta = 1$ ) phases of the 2DEG near  $T = 0$  and for  $r_s = 5, 10, 20$ , and  $30$ , as a function of  $T/T_F$ . Solid lines:  $\zeta = 0$ ; dashes with data points (squares):  $\zeta = 1$ .

Our unpolarized energies (Table I) are in better agreement with the more recent QMC results of Rapisarda *et al.* [9]. In Fig. 2 we compare our PDFs with those of GFMC at  $r_s = 1, 5$ , and  $20$  given in Tanatar *et al.*, and find satisfactory agreement.

Equation (6) for  $p(r_s, \zeta)$  provides a comparison with the results of Varsano *et al.* [12], for the correlation energies at partial polarizations, for  $r_s = 20$  and  $30$ . Their  $E_c(r_s, \zeta)$  (a.u.) at  $r_s = 30$  are  $0.01216, 0.01132, 0.00987$ , and  $0.00776$  at  $\zeta = 0.2, 0.4, 0.6$ , and  $0.8$ , while the results from our fit, Eq. (6), are  $0.01219, 0.01134, 0.00989$ , and  $0.00775$ , respectively. Varsano *et al.* suggest that the fully spin-polarized phase is more stable, “by an amount close to the statistical uncertainty.” Instead of using the fit, we have evaluated the relevant PDFs accurately at  $r_s = 30$  and  $T = 0$ . Varsano *et al.* report a stabilization energy of  $-1.185 \times 10^{-5}$  a.u., while ours is even smaller and not significant.

When  $r_s$  is large, the kinetic energy is less important; exchange favors spin polarization and correlation favors the paramagnetic phase. Figure 3 displays the Helmholtz free energy for  $r_s = 5, 10, 20$  and  $30$ . Stable spin-polarized phases in the 3DEG have been reported recently [16]. Studies related to the metal-insulator transition in the 2DEG, and numerical studies of 2D clusters, have increasingly suggested the possibility of ferromagnetic phases of the 2DEG [17]. The 2DEG metal-insulator transition is influenced by the presence of impurities. Our results are for the *pure, uniform* system and there seems to be no stable ferromagnetic phase except perhaps near  $r_s = 30$ . For 2DEGs in GaAs,  $r_s = 30$  and  $T/E_F = 0.1$  corresponds to  $4.7 \times 10^8$  electrons  $\text{cm}^{-2}$  and  $0.019$  K.

The more favorable  $m^*$  of Si brings the densities close to the  $\sim 10^{10}$  electrons  $\text{cm}^{-2}$  range. Details of the finite- $T$  calculations, the effect of impurities on the spin-polarized phase, etc. will be presented elsewhere.

The computer codes used here may be remotely accessed by interested workers by visiting our website [18].

In conclusion, we present a classical calculation of the PDFs, correlation energies, etc. of the 2DEG for any spin polarization and temperature, and find good agreement with quantum Monte Carlo results at  $T = 0$ . The temperature mapping of the quantum effects obtained for 3D and 2D systems is found to be universal, to within the accuracy of the available quantum Monte Carlo exchange-correlation energies. New results for spin-dependent correlation energies and spin-polarized distribution functions are given. A comparison of the free energies of the polarized and unpolarized phases at finite  $T$  is presented.

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