Spin-dependent correlation in two-dimensional electron liquids at arbitrary degeneracy and spin-polarization: CHNC approach

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Abstract

We apply the classical mapping technique developed recently by Dharma-wardana and Perrot for a study of the uniform two-dimensional electron system at arbitrary degeneracy and spin-polarization. Pair distribution functions, structure factors, the Helmholtz free energy, and the compressibility are calculated for a wide range of parameters. It is shown that at low temperatures $T/T_F < 0.1$, $T_F$ being the Fermi temperature, our results almost reduce to those of zero-temperature analyses. In the region $T/T_F \geq 1$, the finite temperature effects become considerable at high densities for all spin-polarizations. We find that, in our approximation without bridge functions, the finite temperature electron system in two dimensions remains to be paramagnetic fluid until the Wigner crystallization density. Our results are compared with those of three-dimensional system and indicated are the similarities in temperature, spin-polarization, and density dependencies of many physical properties.

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I. INTRODUCTION

Two-dimensional electron systems have been investigated by a number of investigators. Their importance seems to have recently increased due to possible applications to spintronics for electronic devices. The properties of two-dimensional electron systems are determined by the Coulomb interaction between electrons and depend crucially on the density, temperature and spin-polarization. In principle, exact results can be obtained by the numerical experiments and are available to some extent at zero temperature. At finite temperatures, however, reliable numerical experiments are still awaited and the importance of theoretical approach is not reduced.

Recently, Dharma-wardana and Perrot have developed a method called classical-map hypernetted-chain method (CHNC). They determine the quantum temperature $T_q$ so that the classical system at the temperature $T_q$ has the same correlation energy as the quantum system at $T = 0$ and assume that the properties of the system at the finite temperature $T$ is given by those of classical system at the temperature

$$T_{cf} = (T_q^2 + T^2)^{1/2}.$$ (1)

One can include the higher-order cluster interactions in classical fluids applying the modified HNC method and taking the bridge function into account.

Various properties of two-dimensional electronic systems at zero-temperature have been examined by Bulutay and Tanatar based on the CHNC method without bridge corrections. We here extend the analysis to finite temperature two-dimensional electronic systems with arbitrary spin-polarization. Confirming that our results reduce to those of Ref. 6 at low temperatures such that $T/T_F \leq 0.1$, we analyze the finite temperature effects for $T/T_F \geq 0.5$, $T_F$ being the Fermi temperature. We observe that the effects are substantial at high densities irrespective of spin-polarization. It is shown that, within our analyses without bridge functions, the two-dimensional electron system remains paramagnetic until the Wigner lattice formation. In Ref. 4, the existence of a ferromagnetic phase before the formation of Wigner lattice is predicted and, in such a domain, one needs careful treatment including the bridge function. The purpose of this paper is to analyze fundamental quantities in a wide domain of density, temperature, and spin-polarization where one may neglect the bridge function as in Ref. 6. In what follows, we adopt the atomic units and take $k_B = 1$. 

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II. CHNC METHOD APPLIED TO TWO-DIMENSIONAL ELECTRON SYSTEM

We consider a two-dimensional fluid of electrons at the temperature $T$ containing two spin species of surface densities $n_1$ and $n_2$ ($n_1 \geq n_2$) with the total density $n = n_1 + n_2$ and spin-polarization $\zeta = (n_1 - n_2)/n$. We determine the Pauli potential for parallel-spin electrons $P_{ii}(r)$ by the relation

$$g_{ii}^0(r) = \exp[-\beta P_{ii}(r) + h_{ii}^0(r) - c_{ii}^0(r)]. \quad (2)$$

Here $\beta$ is determined by the temperature $T_{cf}$ by $\beta = 1/T_{cf}$, $g_{ii}^0(r) = h_{ii}^0(r) + 1$ is the ideal gas pair distribution function for the component $i$,

$$h_{ii}^0(r) = -\frac{1}{n_i^2} \sum_{k_1,k_2} n(k_1)n(k_2) \exp[i(k_1 - k_2) \cdot r] = -[f_i(r)]^2, \quad (3)$$

and $c_{ii}^0(r)$ is the direct correlation function corresponding to $h_{ii}^0(r)$. In (3), $n(k)$ is the Fermi occupation number at temperature $T$. At $T = 0$, $f_i(r) = 2J_1(k_i^F r)/k_i^F r$, where $J_1(x)$ is the Bessel function and $k_i^F$ is the Fermi wave number of species $i$.

The pair distribution functions (PDF’s) and the direct correlation functions are related via

$$g_{ij}(r) = \exp[-\beta \phi_{ij}(r) + h_{ij}(r) - c_{ij}(r) + B_{ij}(r)]. \quad (4)$$

Here $\phi_{ij}(r)$ is the pair potential between the species $i$ and $j$ defined by

$$\phi_{ij}(r) = P_{ii}(r)\delta_{ij} + V_{\text{Cou}}(r), \quad (5)$$

and $h_{ij}(r) = g_{ij}(r) - 1$, $c_{ij}(r)$, and $B_{ij}(r)$ are the pair correlation, direct correlation and the bridge function, respectively. In the pair potential, $V_{\text{Cou}}(r)$ includes the diffraction effect as

$$V_{\text{Cou}}(r) = \frac{1}{r}[1 - e^{-r k_{th}}], \quad (6)$$

where $k_{th} = (2\pi m^* T_{cf})^{1/2}$, $m^* = 1/2$ is the reduced mass of the scattering electron pair. We also have the Ornstein-Zernike relations between the pair correlation functions and the direct correlation functions:

$$h_{ij}(r) = c_{ij}(r) + \sum_s n_s \int \text{d}r' h_{is}(|r - r'|)c_{sj}(r'). \quad (7)$$

The equations (4) and (7) are exact but are not closed because of the existence of the unknown bridge functions $B_{ij}(r)$. In this paper, however, we neglect the bridge functions as
in Ref. 6 and solve the set of equations (4) and (7). We have analyzed the case of $r_s = 5$
with the bridge function employing the solution of the Percus-Yevick equation for hard disks
with somewhat different formula for $T_q$. The result indicates that the effect of the neglect
of bridge function increases with the temperature and the free energy due to exchange-
correlation is overestimated by at most 5% at $T/T_F = 5$. The results for fundamental
quantities obtained without bridge functions will therefore be still useful in a wide range
of density, temperature, and spin-polarization where the effect of the neglect of the bridge
function is not so subtle.

In the CHNC method, the temperature of the classical fluid $T_{cf}$ is determined by (1).
For the quantum temperature $T_q$, we adopt the one given by Ref. 6,

$$T_q = \frac{1 + a r_s n_1 T_{F1} + n_2 T_{F2}}{b + c r_s} n$$  \hspace{1cm} (8)

where $r_s = (\pi n)^{-1/2}$ with $a = 1.470342$, $b = 6.099404$, and $c = 0.476465$.

The exchange-correlation part of the Helmholtz free energy is calculated by the integration
over the coupling $\lambda$ as

$$\frac{F_{xc}}{n} = \pi n \int_0^1 d\lambda \int dr [g(\lambda; r) - 1]$$  \hspace{1cm} (9)

from the spin-averaged PDF given by

$$g(r) = \frac{1}{4}[((1 + \zeta)^2 g_{11}(r) + 2(1 - \zeta^2)g_{12}(r) + (1 - \zeta^2)g_{22}(r)].$$  \hspace{1cm} (10)

The total Helmholtz free energy $F_{tot}$ is obtained as

$$F_{tot} = F_0 + F_{xc},$$  \hspace{1cm} (11)

where $F_0 = F_{01} + F_{02}$ is the free energy of the ideal electron gas given by

$$F_0^i = n_i \mu_0^i - E_0^i,$$  \hspace{1cm} (12)

$$\mu_0^i = T \ln[e^{E_F^i/T} - 1],$$  \hspace{1cm} (13)

$$E_F^i = (1 \pm \zeta) \pi n,$$  \hspace{1cm} (14)

and

$$E_0^i = \frac{T^2}{\pi} \int_0^\infty \frac{d x x}{\exp[x - \mu_0^i/T] + 1}.$$  \hspace{1cm} (15)

We calculate the exchange part of the Helmholtz free energy $F_x = F_{x1} + F_{x2}$ by the ideal
gas values as

$$\frac{F_{x1}}{n} = \frac{1}{4} \pi n (1 + \zeta)^2 \int dr [g_{11}^0(r) - 1],$$  \hspace{1cm} (16)
\[
\frac{F_x^2}{n} = \frac{1}{4} \pi n (1 - \zeta)^2 \int dr [g_{22}^0(r) - 1],
\]
and define the correlation part by \( F_c = F_{xc} - F_x \). At \( T = 0 \) we have
\[
\frac{F_x}{n} = \frac{E_x}{n} = -\frac{2\sqrt{2}}{3\pi r_s} [(1 + \zeta)^{3/2} + (1 - \zeta)^{3/2}],
\]
\[
\frac{E_0}{n} = \frac{E_0^1 + E_0^2}{n} = \frac{1 + \zeta^2}{2 r_s^2}.
\]

III. RESULTS AND DISCUSSIONS

We have solved the coupled equations (4) and (7) using the Hankel transform as in Refs. 6 and 9 and neglecting the bridge functions for a wide range of density, spin-polarization and temperature, \( 0 \leq r_s \leq 30, 0 \leq \zeta \leq 1, \) and \( 0 \leq t \equiv T/T_F \leq 5 \). Here we summarize the results.

A. Pair distribution function and structure factor

The spin-averaged PDF \( g(r) \) for \( r_s = 1 \) and \( T/T_F = 0, 1 \) in two cases \( \zeta = 0, 1 \) is shown in Fig.1. Our results for \( T/T_F = 0 \) are in good agreement with those given in Ref. 6. We observe that the finite temperature effect considerably reduces the exchange-correlation hole around electrons in both cases of \( \zeta = 0 \) and \( \zeta = 1 \) and we may estimate the behavior of the pair distribution function in the case of arbitrary spin polarization from these results.

In Fig. 2, we show the spin-averaged structure factor defined by
\[
S(q) = 1 + n \int dr [g(r) - 1] e^{i \mathbf{q} \cdot \mathbf{r}}
\]
for \( r_s = 1, T/T_F = 0, 1, \) and \( \zeta = 0, 1. \) At \( T/T_F = 0, \) the structure factor is consistent with the one given in Ref. 6. We observe the finite temperature effect for the cases of spin-polarization \( \zeta = 0, 1. \)

B. Total free energy

We have calculated the total Helmholtz free energy for finite temperatures \( 0 \leq T/T_F \leq 5 \) and spin-polarizations \( 0 \leq \zeta \leq 1. \) The results are shown as a function of the density parameter \( r_s \) and spin-polarization \( \zeta \) in Figs. 3 and 4, respectively.
At low temperatures \( T/T_F \leq 0.1 \), our results reduce to those of Ref. 6. When \( T/T_F \geq 1 \), the finite temperature effects become considerable at high densities for all cases of spin-polarization. Our results indicate that the two-dimensional electron system remains to be in the paramagnetic fluid phase until the Wigner crystallization densities even at high temperatures.

The dashed-dotted line in Fig. 4 represents the total free energy for \( T/T_F = 1 \) and \( r_s = 1 \). It is seen from the figure that the spin-polarization effect is more pronounced at higher temperatures and densities.

C. Exchange-correlation free energy

To compare the electron correlation effects in two and three dimensions, we plot the exchange-correlation and correlation free energies as a function of temperature in Figs. 5 and 6. We find that our results of the temperature dependence of the free energy in two dimensions are similar to those in three dimensions.

To check the validity of the CHNC scheme used in this paper, we compare our exchange-correlation energy with Monte Carlo (MC) and Singwi-Tosi-Land-Sjölander scheme (STLS) results given in Refs. 10, 11, and 12. The exchange-correlation energies computed by different schemes are listed in Table I. We observe that the difference between our results and STLS results is considerable (about 10%) only at high temperatures \( (T > T_F) \). This may be because we have used the expression for quantum temperature \( T_q \) fitted to MC data at \( T = 0 \). To obtain better agreements with STLS results for \( T > T_F \) we may need to include the bridge term and use the results of finite temperature STLS scheme given in Ref. 12 for fitting procedure.

As for the exchange-correlation free energy at high densities, the agreement with MC and other values can be improved by interpolating \( T_q \) more accurately. For example, the set \( a = 24.936526 \), \( b = 87.221405 \), and \( c = 8.455547 \) gives better fitting for \( T_q \) as shown in Fig. 7 and better agreement as listed on the last line in Table I.
TABLE I: Exchange-correlation energy per electron (in a.u.) of unpolarized 2DEG, $F_{xc}$. For comparison, the MC results of Tanatar and Ceperley\textsuperscript{10} and the STLS results of Jonson\textsuperscript{11} and Schweng and Böhm\textsuperscript{12} are given (denoted by a, b, and c, respectively). The results for fully polarized 2DEG are shown in brackets. The last line is the values based on improved interpolation for $T_q$.

| $T/T_F$ | 0.0 | 0.0\textsuperscript{a} | 0.0\textsuperscript{b} | 0.1 | 0.1\textsuperscript{c} | 0.5 | 0.5\textsuperscript{c} | 1.0 | 1.0\textsuperscript{c} | 5.0 | 5.0\textsuperscript{c} |
|---------|-----|-----------------|-----------------|----|-----------------|----|-----------------|----|-----------------|----|-----------------|
| $r_s = 1$ | 0.688 | 0.708 | 0.705 | 0.686 | 0.708 | 0.641 | 0.685 | 0.583 | 0.633 | 0.359 | 0.399 |
|         | 0.167 | 0.168 | 0.167 | 0.167 | 0.163 | 0.167 | 0.158 | 0.163 | 0.121 | 0.127 |
|         | (0.181) | (0.180) | 0.089 | 0.089 | 0.089 | 0.089 | 0.088 | 0.086 | 0.073 | 0.071 | 0.063 |
|         | (0.091) | (0.092) | 0.696 | 0.708 | 0.705 | 0.693 | 0.708 | 0.646 | 0.685 | 0.585 | 0.633 | 0.359 | 0.399 |

D. Compressibility

The compressibility is obtained by density derivatives of the free energy. In order to check the accuracy of our finite temperature scheme, we have calculated the compressibility as a function of density parameter $r_s$ or spin-polarizations $\zeta$ for different temperatures. We note that at low temperatures our results reduce to those of Ref. 6. Our results shown in Fig. 8 indicate that the temperature effect on the compressibility is remarkable only at low densities and high temperatures such that $T/T_F > 0.3$.

The spin-polarization dependence of the compressibility is displayed in Fig. 9. We observe that the effect of spin-polarization increases with the temperature and electron density.

IV. CONCLUSIONS

Applying the recently proposed classical-map hypernetted-chain (CHNC) method to the two-dimensional electron system, we have calculated the pair distribution function, structure factor, Helmhotz free energy, and compressibility at finite temperatures for a wide range of spin-polarization and density. It is shown that at low temperatures $T/T_F \leq 0.1$, our results are almost identical to those of Ref. 6 at $T = 0$. Our results indicate that correlation characteristics in 2D electron liquids depend remarkably on the temperature, spin-polarization,
and density, similarly to the three-dimensional case.

When $T > T_F$, the finite temperature effects become considerable at high densities irrespective of spin-polarization as concretely shown in various quantities in this paper. We find that the finite temperature 2D electron system remains to be in the paramagnetic fluid phase until the Wigner crystallization density is attained. Though the validity of the conclusion on the phase around $r_s \sim 30$ might depend on that of CHNC applied to two-dimensional electron system and the neglect of bridge functions, results obtained here for $1 < r_s < 30$ will be useful in investigation of the system whose finite temperature properties are important in applications but not exactly known.

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1 M. W. C. Dharma-wardana and F. Perrot, Phys. Rev. Lett. 84, 959(2000).
2 F. Perrot and M. W. C. Dharma-wardana, Phys. Rev. B 62, 16536(2000).
3 F. Perrot and M. W. C. Dharma-wardana, Phys. Rev. Lett. 87, 206404(2001).
4 M. W. C. Dharma-wardana and F. Perrot, Phys. Rev. Lett. 90, 136601(2003).
5 Y. Rosenfeld and N. W. Ashcroft, Phys. Rev. A 20, 1208(1979).
6 C. Bulutay and B. Tanatar, Phys. Rev. B 65, 195116(2002).
7 H. Minoo et al., Phys. Rev. A 23, 924(1981).
8 N. Q. Khanh and H. Totsuji, Solid State Communications 129, 37(2003)
9 F. Lado, J. Chem. Phys. 49, 3092(1968).
10 B. Tanatar and D. M. Ceperley, Phys. Rev. B 39, 5005(1989).
11 M. Jonson, J. Phys. C 9, 3055(1976)
12 H. K. Schweng and H. M. Böhm, Z. Phys. B 95, 481(1994).
FIG. 1: Pair distribution function $g(r)$ for $r_s = 1$, $t = T/T_F = 0, 1$, and $\zeta = 0, 1$.

FIG. 2: Structure factor $S(k)$ for $r_s = 1$, $t = T/T_F = 0, 1$, and $\zeta = 0, 1$. 
FIG. 3: Total Helmholtz free energy as a function of $r_s$ for different temperatures and spin-polarization.

FIG. 4: Total Helmholtz free energy as a function of spin-polarization $\zeta$ for different temperatures and densities.
FIG. 5: Exchange-correlation free energy per electron in units of $\mu_x = -2k_F/\pi$ as a function of temperature for different spin-polarization and densities.

FIG. 6: Correlation free energy per electron in units of $\mu_x = -2k_F/\pi$ as a function of temperature for different spin-polarization and densities.
FIG. 7: Improved fitting for $T_q$ in comparison with the one given in Ref. 6.

FIG. 8: Inverse compressibility of unpolarized ($\zeta = 0$) and fully polarized ($\zeta = 1$) phases normalized by 2D free Fermion value $K_0$ for $t = T/T_F = 0, 0.1, 0.3, 0.5$. 
FIG. 9: Compressibility normalized by paramagnetic value ($\zeta = 0$) as a function of spin-polarization for $t = T/T_F = 0.5, 1$, and $r_s = 1, 5, 10$. 