

Cluster Expansion for Two-Dimensional Electron Liquids

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Synopsis

The pair correlation function and the correlation energy density of two-dimensional electron liquids are calculated on the basis of the Salpeter's Debye-chain type expansion. When the two-dimensional plasma parameter $\epsilon=2\pi n e^4 T^{-2}$ is small, the expansion to the first order gives the correlation energy to the order of $\epsilon^2 \ln \epsilon$. It is shown that experimental results in the domain $\epsilon \leq 0.5$ can be reproduced by taking into account the first and the second order terms in this expansion.

1. Introduction

Electrons in the surface quantum states of dielectric substances such as liquid He make a two-dimensional system, interacting via the Coulomb potential, when the temperature is low enough not to excite the motion perpendicular to the surface [1]. Quantum effects in the two-dimensional motion can be neglected in most experimental conditions and these systems are characterized by the dimensionless plasma parameter defined by $\epsilon=2\pi n e^4 T^{-2}$, where n , e , and T are the surface number density, the effective electronic charge, and the temperature in energy units, respectively.

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Since the positive charges on the metallic plate provide the uniform background, results of experiments on these systems can be compared directly with theories of classical electron liquids. The properties of these two-dimensional systems are of interest also because the relative importance of the individual-particle aspect to the collective aspect is enhanced compared with the case of three dimensions [2].

In addition to experiments on electrons on the surface of liquid He, numerical experiments [3,4] have been useful to analyse detailed properties of two-dimensional electron liquids.

In this paper, we make calculations of the pair correlation function and thermodynamic quantity (the correlation energy density) on the basis of the Salpeter's Debye-chain type expansion [5,6] and compare the results with those of plasma-parameter-expansion analyses [2,7] and recent numerical experiments [4].

2. Debye-Chain Type Expansion

The pair correlation function $g(r)$ is given by the cluster expansion as $g(r)=\exp[-w(r)]-1$, where

$$w(r)=v(r)/T - \sum_{k=1}^{\infty} \beta_k(r)n^k. \quad (1)$$

Here $v(r)$ is the interaction potential and $\beta_k(r)$ denotes the simple irreducible cluster integral including two root points, k field points, and f -bonds, $f(r)=\exp[-v(r)/T]-1$, between them.

For the long-range potential such as the Coulomb potential, each cluster integral diverges, and it is necessary to modify the original cluster expansion by performing some kind of partial summation. Salpeter [5] derived the Debye-chain type expansion introducing the Γ -bond which is the chain sum of f -bonds given by

$$\Gamma(r)=f(r) + n \int d\tilde{r}' f(|\tilde{r}-\tilde{r}'|) \Gamma(\tilde{r}'). \quad (2)$$

To the first order of this expansion, we have

$$w(r) \approx v(r)/T - w_1(r), \quad \text{where } w_1(r) = \Gamma(r) - f(r). \quad (3)$$

There are two kinds of terms in the second order and $w(r)$ is given by

$$w(r) \approx v(r)/T - w_{11}(r) - w_{21}(r) - w_{22}(r),$$

$$w_{21}(r) = n \int d\tilde{r}' \Gamma(|\tilde{r} - \tilde{r}'|) [\Gamma^2(r') - f^2(r')], \quad (4)$$

$$w_{22}(r) = (n^2/2) \int \int d\tilde{r}' d\tilde{r}'' \Gamma(|\tilde{r} - \tilde{r}'|) \Gamma(|\tilde{r}' - \tilde{r}''|) [\Gamma^2(r'') - f^2(r'')].$$

The Γ -bond and the first and the second order terms are shown in Fig.1.

In the case of two-dimensional electron liquids, $v(r) = e^2/T$ and the Fourier transforms of the f -bond and the Γ -bond are given by

$$f(k) = -(4\pi e^2/Tk) J_1(x) K_1(x), \quad (5)$$

$$\Gamma(k) = f(k) / [1 - nf(k)] = -(4\pi e^2/T) J_1(x) K_1(x) / [k + 2k_D J_1(x) K_1(x)]. \quad (6)$$

Here, $x = (2ke^2/T)^{1/2}$, $J_1(x)$ and $K_1(x)$ are the Bessel function and the modified Bessel function of the first order, and $k_D = 2\pi ne^2/T$ denotes the two-dimensional Debye wave number.

In the long-range domain $k \ll T/e^2$ or $e^2/T \ll r$, $f(k) \approx -2\pi e^2/Tk$ and $\Gamma(k) \approx -(2\pi e^2/T)/(k + k_D)$ or

$$\Gamma(r) \approx -u(r)/T = -(e^2/Tr) \int_0^\infty dx J_0(x) x / (x + k_D r) = -v(r)/T + (\pi e/2) [H_0(k_D r) - N_0(k_D r)], \quad (7)$$

where $J_0(x)$, $N_0(x)$, and $H_0(x)$ are the Bessel functions and the Struve's function of the zeroth order, respectively. In the short-range domain $k_D \ll k$ or $r \ll k_D^{-1}$, $\Gamma(k) \approx f(k)$ or $\Gamma(r) \approx f(r)$ and Eq.(3) reduces to $w(r) \approx v(r)/T \approx u(r)/T$.

When the plasma parameter is small, $|\Gamma(r)| \approx u(r)/T \gg |f(r) + v(r)/T| \approx [v(r)/T]^2$ for $e^2/T \ll r \ll \epsilon^{-1} k_D^{-1}$. Noting that $e^2/T \ll k_D^{-1}$, we have from Eq.(3) the nonlinear Debye-Hückel approximation (for $r \ll \epsilon^{-1} k_D^{-1}$) [2]

$$w(r) \approx u(r)/T. \quad (8)$$

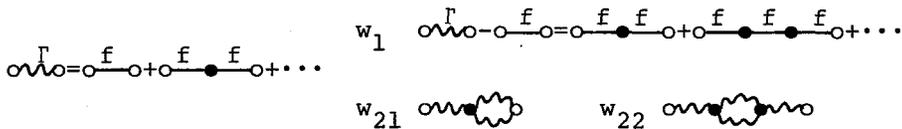


Fig.1 The Γ -bond and the first and the second order terms in the Debye-chain type expansion.

It has been shown [4] that the nonlinear Debye-Hückel approximation reproduces experimental results for $g(r)$ in the domain $\epsilon \leq 0.05$. The correlation energy density E_c normalized by the thermal energy density nT , E_c/nT , is given by this approximation as

$$\begin{aligned} E_c/nT &= (ne^2/2T) \int dr g(r)/r \approx (\pi ne^2/T) \int_0^\infty dr \{ \exp[-u(r)/T] - 1 \} \\ &= (1/2) \epsilon \ln 2\epsilon + (\gamma - 1/2) \epsilon - (1/4) \epsilon^2 \ln^2(\epsilon/2) + (1/2 - \gamma) \epsilon^2 \ln \epsilon + O(\epsilon^2), \end{aligned} \quad (9)$$

where $\gamma = 0.5775 \dots$ is the Euler's constant. The resultant value of E_c/nT , however, is exact only to the order of ϵ ; the exact value is known [2,7] to the order of $\epsilon^2 \ln \epsilon$ as

$$E_c/nT = (1/2) \epsilon \ln 2\epsilon + (\gamma - 1/2) \epsilon - (1/2) \epsilon^2 \ln^2(\epsilon/2) + (1 - 2\gamma) \epsilon^2 \ln \epsilon + O(\epsilon^2). \quad (10)$$

We can improve the nonlinear Debye-Hückel approximation by taking more terms in the Debye-chain type expansion into account. As is shown in the Appendix, the expansion to the first order, Eq.(3), gives the exact result, Eq.(10), and the contributions of the second order terms are of the order of ϵ^2 .

3. Numerical Computation and Comparison with Experimental Results

In the domain where the plasma parameter is not much smaller than unity, analytical evaluations of the terms in the Debye-chain type expansion is not easy nor useful. Here we compute their contributions numerically.

In Figs.2 and 3, we show the values of the pair correlation function and the normalized correlation energy density given by Eqs. (3) and (4) in comparison with experimental results [4] for various values of the plasma parameter. The expansion to the first order reproduces experimental values in the domain $\epsilon \leq 0.1$, and the expansion to the second order, those in the domain $\epsilon \leq 0.5$.

In order to show that the expansion is well-defined for these values of the plasma parameter, we compare the contributions of w_1 , w_{21} , and w_{22} in Fig.4. The Debye-chain type expansion works as an expansion in the domain $\epsilon < 0.5$.

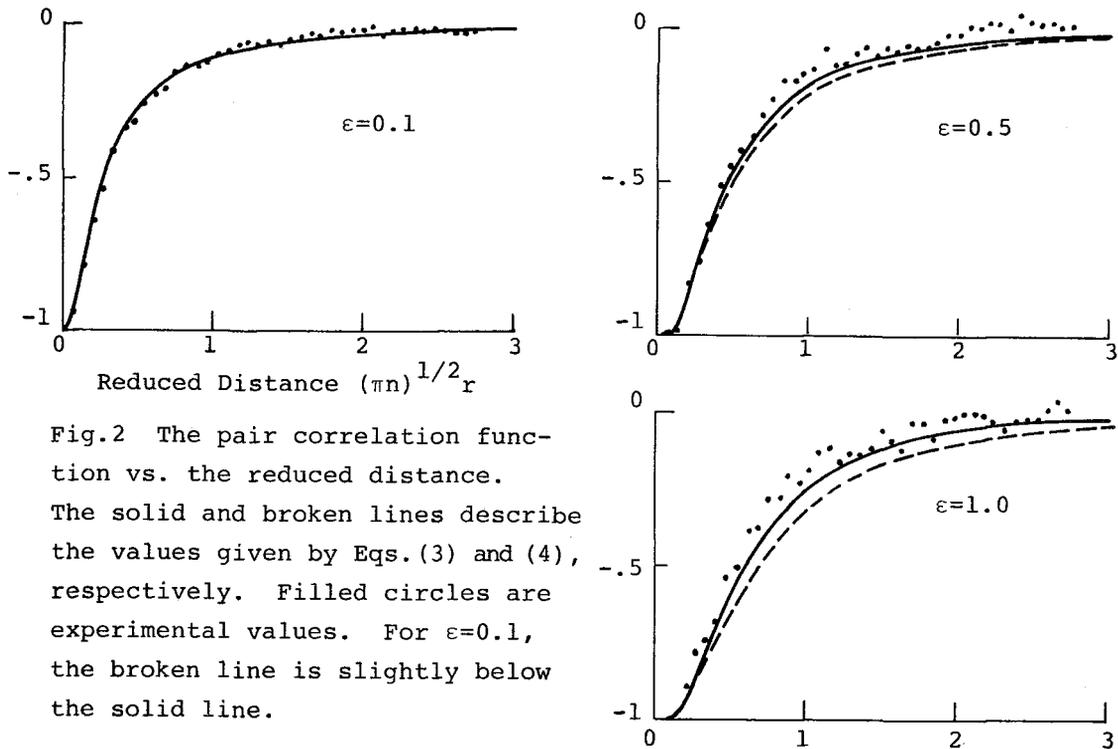


Fig.2 The pair correlation function vs. the reduced distance. The solid and broken lines describe the values given by Eqs. (3) and (4), respectively. Filled circles are experimental values. For $\epsilon=0.1$, the broken line is slightly below the solid line.

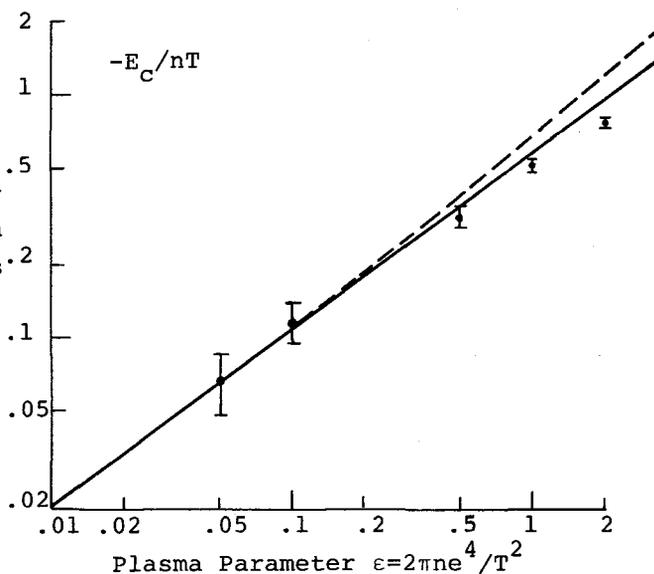
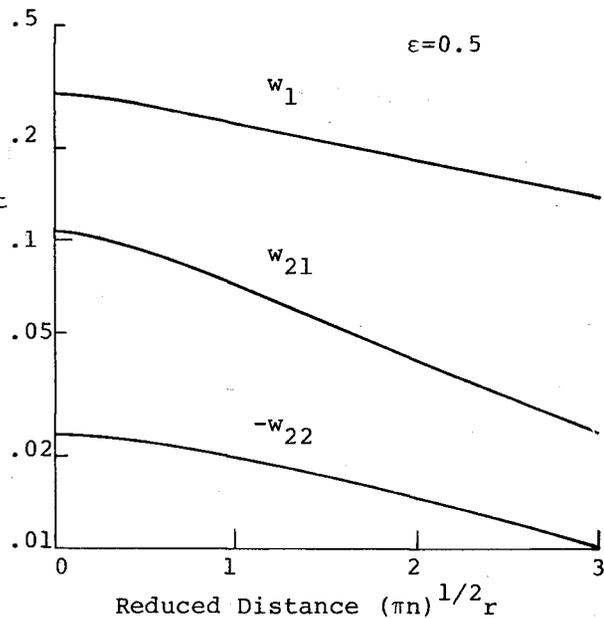


Fig.3 The normalized correlation energy vs. the plasma parameter. The same symbols are used as in Fig.2.

Fig.4 Comparison of the contributions of the first and the second order terms in the Debye-chain expansion for $\epsilon=0.5$.



4. Concluding Remarks

It is shown that thermodynamic properties of two-dimensional electron liquids in the domain $\epsilon \leq 0.5$ are given by the first and the second order terms of the Salpeter's Debye-chain type expansion.

Strongly coupled plasmas with $\epsilon > 1.0$ have no small parameters useful for theoretical analyses, and one of possible approaches is to make some ansatz which satisfies as many boundary conditions as possible and compare the results based on the ansatz with those of experiments [8]. The result of this paper may provide one of boundary conditions for theoretical analyses in strongly coupled domains.

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Appendix

When the plasma parameter is small, the Γ -bond is evaluated as

$$\Gamma(r) \approx \begin{cases} -1 - \epsilon \ln \epsilon, & r \ll e^2/T \\ -u(r)/T \approx -v(r)/T - \epsilon \ln k_D r, & e^2/T \ll r \ll k_D^{-1} \\ -u(r)/T \approx -\epsilon (k_D r)^{-3}, & k_D^{-1} \ll r \end{cases} \quad (A1)$$

Expanding $\exp[-v(r)/T + \Gamma(r) - f(r)] - 1$ as

$$f(r) + \exp[-v(r)/T] \sum_{k=1}^{\infty} (1/k!) [\Gamma(r) - f(r)]^k,$$

we neglect the terms with $k \geq 2$ whose contribution to E_c/nT is estimated to be of the order of ϵ^2 with the aid of Eq. (A1). We thus have

$$\begin{aligned} E_c/nT &= (\pi n e^2/T) \int_0^{\infty} dr \{ f(r) + \exp[-v(r)/T] [\Gamma(r) - f(r)] \} + O(\epsilon^2) \\ &= 2\epsilon \int_0^{\infty} dx JK [-1 + 8\epsilon (JK)^2 / (x^2 + 4\epsilon JK)] / x \\ &\quad - 4\epsilon^2 \int_0^{\infty} dx x (JK)^2 [J_0(x)K_0(x) + J_2(x)K_2(x)] / (x^2 + 4\epsilon JK) + O(\epsilon^2). \end{aligned} \quad (A2)$$

Here $J = J_1(x)$ and $K = K_1(x)$, and we used Eqs. (5), (6), and the relation

$$\int_0^{\infty} dy \exp(-1/y) J_0(x^2 y/2) = 4JK/x^2 - [J_0(x)K_0(x) + J_2(x)K_2(x)].$$

Rewriting Eq. (A2) as

$$\begin{aligned} E_c/nT &= -2\epsilon \int_0^{\infty} dx x JK / (x^2 + 2\epsilon) + 8\epsilon^2 \int_0^{\infty} dx (JK)^2 (2JK - 1) / x(x^2 + 4\epsilon JK) \\ &\quad + 4\epsilon^2 \int_0^{\infty} dx x JK (2JK - 1) / (x^2 + 4\epsilon JK)(x^2 + 2\epsilon) \\ &\quad - 4\epsilon^2 \int_0^{\infty} dx x (JK)^2 [J_0(x)K_0(x) + J_2(x)K_2(x)] / (x^2 + 4\epsilon JK) + O(\epsilon^2), \end{aligned}$$

we divide the first integration by an auxiliary parameter x_0 which satisfies $\epsilon \ll x_0^2 \ll 1$ and use the conditions $x \ll 1$ and $|\epsilon J_1(x)K_1(x)| \ll x^2$ in the domains $0 \leq x \leq x_0$ and $x_0 \leq x$, respectively. The resultant value of the first term is independent of x_0 and is given by

$$(1/2)\epsilon \ln 2\epsilon + (\gamma - 1/2)\epsilon - (1/8)\epsilon^2 \ln^2 \epsilon - (1/8)(4\gamma - 3 - 2 \ln 2)\epsilon^2 \ln \epsilon + O(\epsilon^2). \quad (A3)$$

In the remaining integrals, the main contributions come from the domain $0 < x \ll 1$ and they are evaluated as

$$-(3/8)\epsilon^2 \ln^2 \epsilon - (1/8)(12\gamma - 5 - 6\ln 2)\epsilon^2 \ln \epsilon + O(\epsilon^2). \quad (\text{A4})$$

From Eqs. (A3) and (A4), we obtain the value given by Eq. (10).

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