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Correlations and plasma oscillations of a two-dimensional classical electron system

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Numerical self-consistent calculations of the static and dynamic properties of a two-dimensional classical electron plasma have been carried out on the basis of the theory derived by Singwi *el al*. In this theory the short-range correlations are present through a local-field correction depending on the pair correlation function. The static structure factor and the density-density response function are determined in a self-consistent scheme. The pair correlation function and the correlation energy obtained are in very good agreement with the numerical experiments carried out by Totsuji. It is found that the onset of short-range order appears at the plasma parameter in the range $14 < \alpha < 15$. The plasmon dispersion relation is determined and is much more accurate than previous theories.

I. INTRODUCTION

The electronic properties of two-dimensional systems have been extensively studied in the last few years both theoretically and experimentally.[1] Electrons trapped on the liquid-helium surface and electrons in the inversion layers in metal-insulator-semiconductor structures are treated as a two-dimensional electron gas. In these systems the electrons are bound perpendicular to the surface in discrete quantum-mechanical states, and their motion parallel to the surface is more or less free. Nevertheless, in spite of this similarity between electrons on liquid helium and in an inversion layer there are some fundamental differences. The most significant one is the accessible range of densities. For electrons on helium, experimental investigations have been carried out with densities between 10^5 and 10^9 cm^{-2}, while typical densities for electrons in inversion-layer semiconductors are $10^{11}-10^{13}$ cm^{-2}. Consequently, the electrons in an inversion layer are Fermi systems, while on liquid-helium surfaces they form classical two-dimensional systems even at temperatures of a few millidegrees Kelvin.

We have studied the static and dynamic properties of such a classical two-dimensional electron gas, interacting via the Coulomb potential, with a Maxwellian distribution of momenta. This system is characterized by the dimensionless plasma parameter $\alpha = 2\pi n e^4/T^2$ or the parameter $\Gamma = (\frac{1}{2}\alpha)^{1/2}$, where n is the density, T the temperature in energy units, and e the effective electronic charge[3] incorporating the effects of the substrate.

Recently, theoretical investigations of the classical model of a two-dimensional electron system have received considerable attention.[2-8] The first attempt to study correlations and plasma oscillations in such a two-dimensional electron gas was made by Fetter,[2] who treated the system in the Debye-Hückel approximation or classical random-phase approximation (RPA). As in the three-dimensional case,[9] the classical RPA is strictly valid in the low-density regime, i.e., for large distances $R > e^2/T$ between particles. The failure of the RPA in the short-range region where electrons are strongly correlated is manifested by the logarithmic divergence of the equation of state. As is well known, the inadequacy of the RPA is much more significant in two- than in three-dimensional systems.[3]

In order to take the short-range correlations into account, Totsuji[3] and Chalupa[4] studied the two-dimensional classical electron systems based on the plasma-parameter expansion in the low-density domain. Their results showed that the short-range correlations are quite important indicating the necessity for improving the RPA in order to make it applicable to systems of higher densities.

The thermodynamic properties of a two-dimensional classical electron gas, neutralized by a uniform background, have very recently been studied by Totsuji[7] with Monte Carlo techniques and by Lado[8] through the hypernetted-chain integral equation. There is very good agreement between the correlation energies obtained by these methods. However, neither approach can describe such dynamic properties as plasma oscillation in these two-dimensional systems.

Two-dimensional plasmon dispersion was

first obtained by Fetter within the framework of the RPA. Subsequent studies by Beck and Kumar[5] and Totsuji[3] have taken into account correlation effects which decrease the coefficient of the $K^{3/2}$ term in the plasmon dispersion relation.

In this work we have investigated the two-dimensional classical electron system based on the self-consistent-field approximation (SCFA) proposed by Singwi *et al.*[10] for a completely degenerate electron gas. Strictly speaking, our calculation is a natural version of both the three-dimensional case of Berggren[9] and the two-dimensional degenerate electron gas studied by Jonson.[11] The approach can be seen as one of the most successful improvements of the RPA, and differs from the other elaborate methods in that it is a dynamic one. The short-range correlations responsible for local-field corrections are calculated in a self-consistent way by making the density-density response functions dependent upon the pair correlation function. For a classical system the approximation consists of replacing the two-particle distribution function in the Liouville equation for the product of two one-particle distribution functions and a pair correlation function.

In this paper we compare the numerical results for the pair correlation functions and the correlation energies with those recently given by Totsuji[7] and Lado.[8] We present dispersion-relation results for the plasma oscillations in the long-wavelength approximation and analyze their deviation from the RPA and Beck and Kumar[5] calculations.

In Sec. II a brief account of the SCFA is given. In Sec. III the plasmon dispersion, the compressibility, and the compressibility sum rules are presented. Numerical results for the pair correlation functions are presented in Sec. IV, and the thermodynamic quantities in Sec. V. A summary of the results is given in Sec. VI.

II. METHOD

Since the self-consistent-field method has been discussed widely, we summarize here the equations for a two-dimensional classical electron plasma. The density-density response function for the interacting system is written

$$\chi(\vec{K},\omega)=\chi_0(\vec{K},\omega)/[1-\psi(\vec{K})\chi_0(\vec{K},\omega)]\,, \qquad (1)$$

where $\chi_0(\vec{K},\omega)$ is the screened density-density response function, which is taken to be the density-density response function of noninteracting particles with a Maxwellian distribution of momenta. The effective self-consistent potential $\psi(\vec{K})$ is given by

$$\psi(\vec{K})=\phi(\vec{K})[1-G(\vec{K})]\,, \qquad (2)$$

where $\phi(\vec{K})$ is the bare particle-particle interaction, and

$$G(\vec{K})=-\frac{1}{n}\int\frac{\vec{K}\cdot\vec{Q}}{KQ}[S(\vec{K}-\vec{Q})-1]\frac{d\vec{Q}}{(2\pi)^2}\,. \qquad (3)$$

The structure factor $S(\vec{K})$,

$$S(\vec{K})=1+n\int d\vec{R}\,e^{-i\vec{K}\cdot\vec{R}}[g(\vec{R})-1]\,, \qquad (4)$$

is related to the imaginary part of the density-density response function of the system through the well-known dissipation-fluctuation theorem[12]

$$S(\vec{K})=-\frac{\hbar}{n}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\mathrm{Im}\chi(\vec{K},\omega)\coth\left(\frac{\hbar\omega}{2T}\right)\,, \qquad (5)$$

completing the self-consistent scheme.

The density-density response function of a two-dimensional noninteracting particle system is simply

$$\chi_0(\vec{K},\omega)=-\frac{n}{T}W\left[\frac{\omega}{K}\left(\frac{m}{T}\right)^{1/2}\right]\,, \qquad (6)$$

with

$$W(z)=\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}dx\frac{xe^{-x^2/2}}{x-z-i0}\,. \qquad (7)$$

In the classical limit $\hbar\omega \ll T$, and Eq. (5) can be written by means of the Kramers-Kronig relation as

$$S(\vec{K})=K/\{K+K_D[1-G(\vec{K})]\}\,. \qquad (8)$$

where $K_D=2\pi ne^2/T$ is the Debye wave number of the two-dimensional system.

We notice that Eq. (1) reduces to the classical RPA expression for the density-density response function if we neglect the local-field corrections, i.e., if we set $G(\vec{K})=0$. In this sense the structure factor is given by[3]

$$S_{\mathrm{RPA}}(\vec{K})=K/(K+K_D)\,, \qquad (9)$$

and the pair correlation function by

$$g_{\mathrm{RPA}}(\vec{R})=1-\frac{e^2}{TR}\int_0^{\infty}dx\frac{x}{x+K_DR}J_0(x)\,, \qquad (10)$$

where $J_0(x)$ is the Bessel function of the zeroth order.

III. LONG-WAVELENGTH LIMIT

A. Plasma dispersion

From the poles of the density-density response function $\chi(\vec{K},\omega)$ we obtain the plasma dispersion relation $\omega(\vec{K})$ and the damping $\Gamma(\vec{K})$ of the plasma oscillation. In the long-wavelength approximation the local-field correction $G(\vec{K})$ can be written

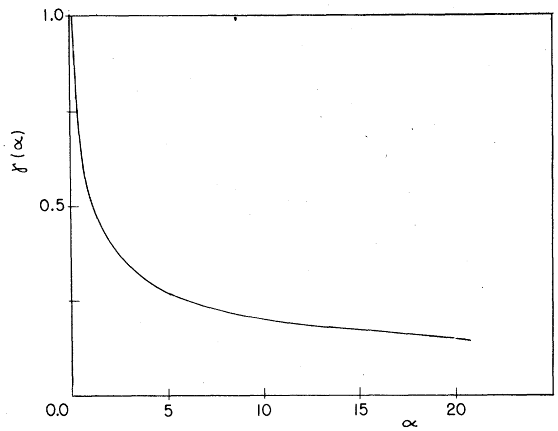

FIG. 1. Values of γ, determined from the self-consistent structure factor, as a function of the plasma parameter α.

$$G(\vec{K}) = \alpha\gamma K\,, \tag{11}$$

with

$$\gamma = -\tfrac{1}{2}\int_0^\infty dK\,[S(K) - 1]\,, \tag{12}$$

which is determined from $S(\vec{K})$ evaluated self-consistently. Here and in the rest of the paper we use wavevectors in units of K_D. In Fig. 1 we give values of γ as a function of the plasma parameter α. From Eq. (11), together with $W(z)$ in Eq. (7) expanded up to second order, we obtain the plasma dispersion relation

$$\omega(K)/\omega_0 = K^{1/2}[1 + (\tfrac{3}{2} - \tfrac{1}{2}\alpha\gamma)K]\,, \tag{13}$$

where $\omega_0 = (2\pi n e^2 K_D/m)^{1/2}$.

In Fig. 2 plasma dispersion relations are shown for two values of the plasma parameter α, as calculated from Eq. (13) and with γ determined self-consistently. For comparison we have also plotted the classical RPA curve.

It is interesting that the short-range correlations between particles present in the system correct the RPA result by decreasing the coefficient of the $K^{3/2}$ term in the plasmon dispersion relation [Eq. (13)]. This correction expands upon the work of Beck and Kumar,[5] in which the correlation effects become relevant at high densities only.

The plasma damping $\Gamma(K)$ is determined through the imaginary part of the density-density response function of the system $\chi(\vec{K}, \omega)$:

$$\Gamma(K) = -(\tfrac{1}{8}\pi)^{1/2}(1/K - \alpha\gamma)^{3/2} \times \exp[(1/2K + \tfrac{3}{2} - \tfrac{1}{2}\alpha\gamma)]\,\omega(K)\,, \tag{14}$$

which reduces to the Landau damping[3] at $\gamma = 0$.

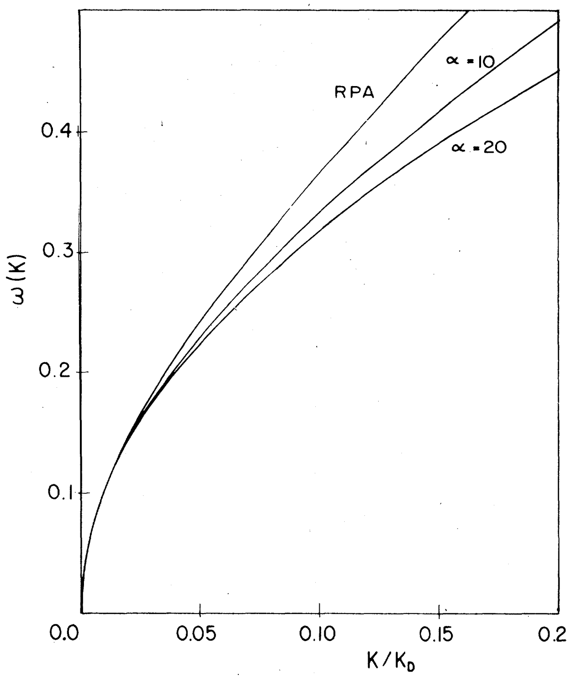

FIG. 2. Long-wavelength plasma dispersion curves for two values of the plasma parameter α, in units of $\omega_0 = (2\pi n e^2 K_D/m)^{1/2}$.

For small values of K, it can be shown that the correction to the Landau damping is negligible. On the other hand, it is known that in this limit the collisional damping is much larger than the Landau damping.[3]

B. Compressibility

The ratio κ_T^0/κ_T of the compressibility of a two-dimensional free system to the interacting one is given by the sum rule[13]

$$\lim_{K\to 0} \epsilon(\vec{K}, 0) = 1 + (1/K)\kappa_T/\kappa_T^0\,. \tag{15}$$

From the density-density response function, Eq. (1) in the long-wavelength limit and for $\omega = 0$, we get the following expression for the dielectric function:

$$\lim_{K\to 0} \epsilon(\vec{K}, 0) = \lim_{K\to 0}\left(1 + \frac{1}{K - G(K)}\right) = 1 + \frac{1}{1-\alpha\gamma}\frac{1}{K}\,, \tag{16}$$

where γ is given by Eq. (12).

We can now write the isothermal compressibility ratio as

$$\kappa_T^0/\kappa_T = 1 - \alpha\gamma\,. \tag{17}$$

In Fig. 3 we compare values of the compressibility obtained from Eq. (17) (curve I) with those ob-

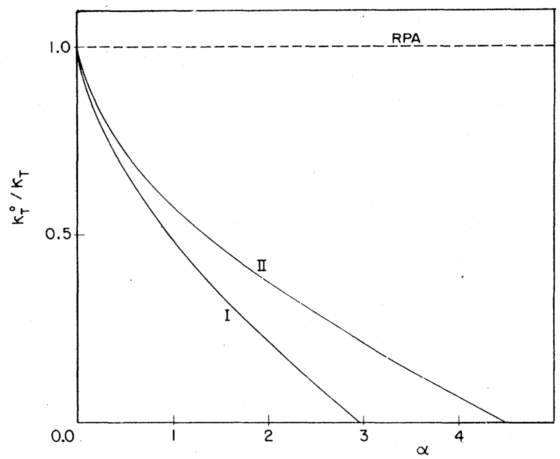

FIG. 3. Ratio of free-electron isothermal compressibility to isothermal compressibility of the two-dimensional classical electron gas vs the plasma parameter. Curve I is obtained from the compressibility sum rule [Eq. (17)] with self-consistent values of γ, and curve II from the second derivative of the correlation energy of the system. The broken line represents the classical RPA result corresponding to $\gamma = 0$.

tained from the second derivative of the correlation energy of the system (curve II). The inconsistency between the two ways of obtaining the isothermal compressibility is characteristic of all perturbation calculations.

According to curve II in Fig. 3 the isothermal compressibility diverges in the vicinity of $\alpha = 4.5$. Beyond this critical value the system becomes thermodynamically unstable. There is complete agreement between our results and those obtained from the Monte Carlo calculations.[7]

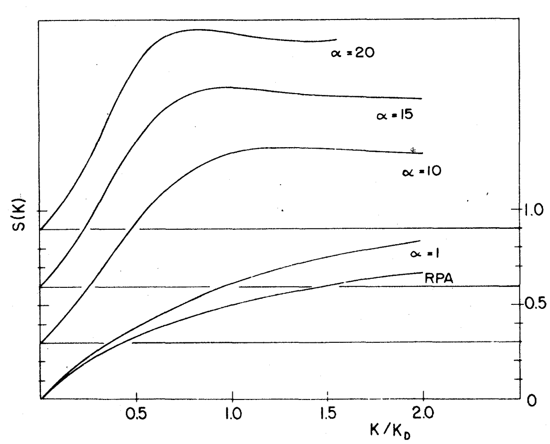

FIG. 4. Self-consistent structure-factor functions $S(\vec{K})$ plotted as a function of K in units of K_D for various values of α. Note that the structure factor overshoots unity with increasing plasma parameter, showing an oscillatory behavior.

IV. CORRELATIONS

Short-range correlations are described directly by the pair correlation function $g(R)$, which is the basic physical quantity derived from the self-consistent-field approximation. It represents the probability of finding one particle at a distance R from another and is obtained from the inverse Fourier transform of the structure factor:

$$g(R) = 1 + \alpha \int_0^\infty dK\, K J_0(\sqrt{2\alpha}\, KR)[S(K) - 1], \qquad (18)$$

where

$$S(K) = K/[1 + K - G(K)], \qquad (19)$$

$$G(K) = -\frac{2\alpha}{\pi}\left(\int_0^K dQ\, Q\mathcal{E}\left(\frac{Q}{K}\right)[S(Q) - 1] + K\int_K^\infty dQ \left\{\left[1 - \left(\frac{Q}{K}\right)^2\right]\mathcal{K}\left(\frac{K}{Q}\right) + \left(\frac{Q}{K}\right)^2 \mathcal{E}\left(\frac{K}{Q}\right)\right\}[S(Q) - 1]\right), \qquad (20)$$

where K and Q are in units of K_D, R in units of $(\pi n)^{-1/2}$, and $\mathcal{K}(x)$ and $\mathcal{E}(x)$ are the complete elliptic integrals of the first and second kinds, respectively.[14]

The self-consistent solution of Eq. (19) is obtained by the standard method of iteration described, for example, in Ref. 9. The results for the structure factor as a function of wave number for several values of the plasma parameter are shown in Fig. 4. We can see from the figure that the structure factor overshoots unity as the plasma parameter α increases. Pronounced peaks in $S(K)$ appear for $\alpha > 10$.

The pair correlation functions as obtained from Eq. (18) are shown in Fig. 5 for various values of α. For comparison, the experimental results obtained by Totsuji[7] from the Monte Carlo method are also given. Note that the agreement between theory and numerical experiment is quite satisfactory.

In the range $14 < \alpha < 15$, $g(R)$ exhibits an oscillatory behavior which is interpreted as the onset of the short-range order.

We have also calculated the pair correlation function for $\alpha > 25$ (not shown in Fig. 5). Unfortunately, as in the three-dimensional version[9] $g(R)$ becomes increasingly negative for small values of R. Since this negative behavior cannot be neglected, calculation is terminated at $\alpha = 25$.

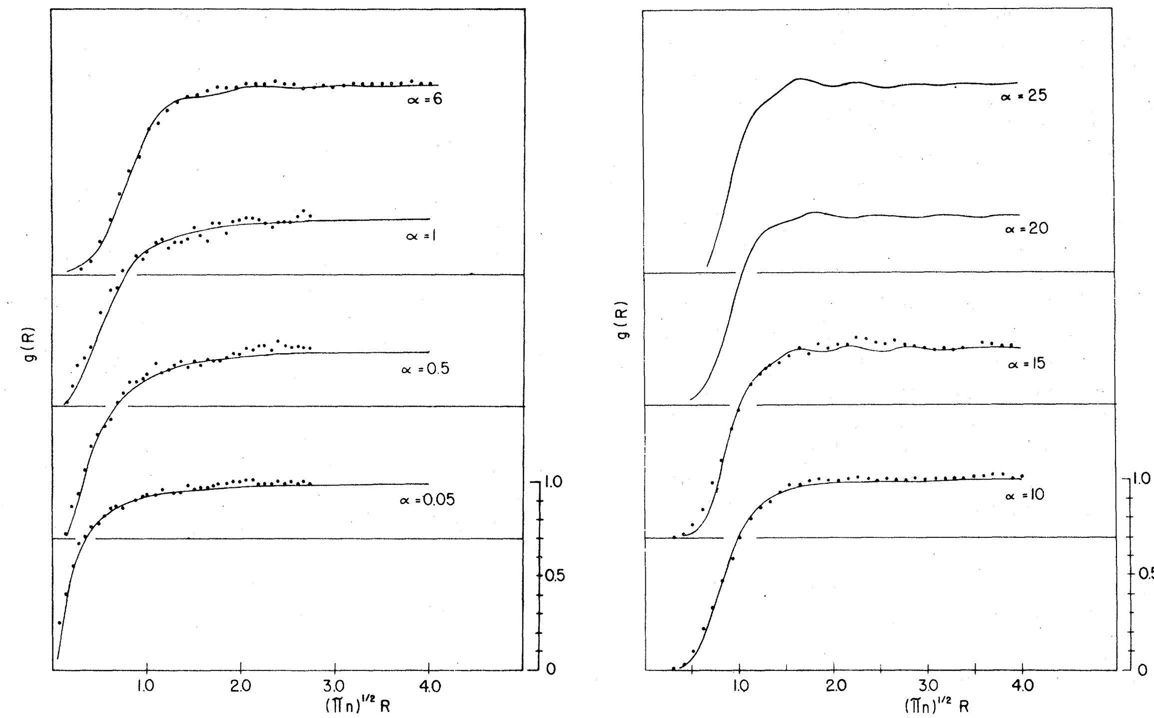

FIG. 5. Pair correlation function $g(R)$ as a function of R in units of $(\pi n)^{-1/2}$ for several values of the plasma parameter. The points represent values given by numerical experiment through the Monte Carlo method (Ref. 7).

V. THERMODYNAMIC PROPERTIES

With the values of the pair correlation function $g(R)$ or the structure factor $S(K)$ obtained in Sec. IV, we can calculate the correlation energy density as

$$E_c = \frac{ne^2}{2}\int_0^\infty [S(K) - 1]dK \,, \tag{21}$$

which can alternatively be written in dimensionless units as

$$E_c/nT = -\alpha\gamma(\alpha) \,. \tag{22}$$

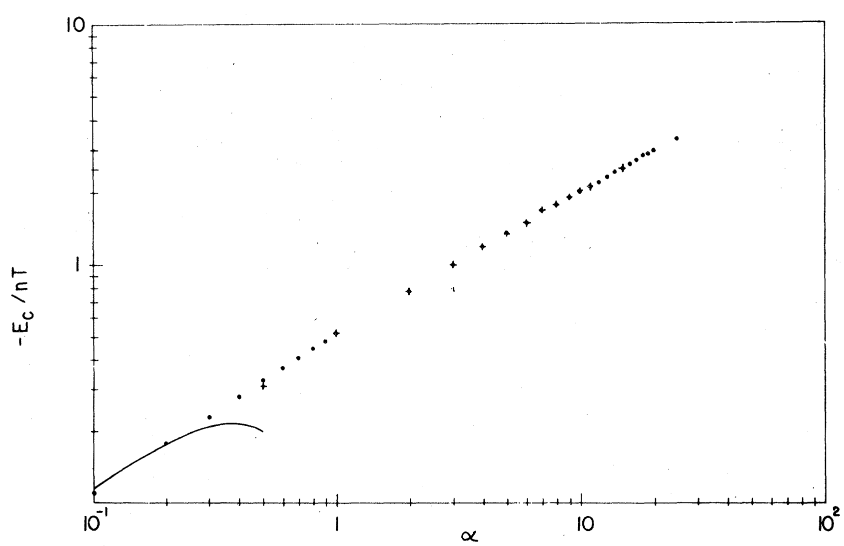

FIG. 6. Correlation energy density normalized by the kinetic energy density E_c/nT vs the plasma parameter α. The full curve is based on the plasma-parameter expansion. Crosses denote the numerical experimental values of Totsuji, and closed circles those found with the self-consistent-field method.

In Fig. 6 we show values of the correlation energy density as a function of the plasma parameter. For comparison, we also plot the numerical experimental results and results based on the plasma-parameter expansion. From Fig. 6 it is clear that our results reproduce the experimental values very well and are also consistent with the plasma-parameter expansion method. Unfortunately, we have only two values of the correlation energy, corresponding to $\alpha=0.02$ and $\alpha=2.0$, to compare with the hypernetted-chain integral-equation calculation. For these values, the results are exactly the same.

Once we have obtained the correlation energy we can calculate the Helmholtz free energy, F, the internal energy E, the specific heat at constant volume C_v, the isothermal compressibility κ_T, and the equation of state of the classical gas as

$$F=F_0+\frac{NT}{2}\int_0^\alpha \frac{d\alpha}{\alpha}\frac{E_c}{nT}, \tag{23}$$

$$E=NT[1+(E_c/nT)], \tag{24}$$

$$C_v=N\left[1+\frac{E_c}{nT}-2\alpha\frac{\partial}{\partial\alpha}\left(\frac{E_c}{nT}\right)\right], \tag{25}$$

$$\frac{\kappa_T^0}{\kappa_T}=1+\frac{1}{2}\left[\frac{E_c}{nT}+\alpha\frac{\partial}{\partial\alpha}\left(\frac{E_c}{nT}\right)\right], \tag{26}$$

and

$$pV=NT[1+\tfrac{1}{2}(E_c/nT)], \tag{27}$$

where F_0 and κ_T^0 are the free energy and isothermal compressibility, respectively, of the noninteracting two-dimensional classical gas, N is the total number of electrons, and p and V are the total pressure and volume of the gas.

VI. SUMMARY

We have shown that the self-consistent-field approximation, which takes into account short-range correlation effects, is indeed capable of describing both the static and dynamic properties of a two-dimensional classical electron gas. Numerical results for the pair correlation functions, structure factor, plasmon dispersion, isothermal compressibility, and thermodynamic quantities were obtained, and the agreement with those of other elaborate methods is very good. It should be stressed that our results for the plasma dispersion relation represent a definite improvement over both the classical RPA and the Beck-Kumar calculations. This is one of the major points of this work. Calculations for a quasi-two-dimensional classical plasma, which take into account the finite thickness of the electron layer, are in progress and we hope to present the results later.

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