

Correlations of a zero-temperature two-dimensional charged Bose gas with $\ln(r)$ interaction

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Some properties of a two-dimensional charged Bose gas interacting with a $\ln(r)$ potential are investigated on the basis of a self-consistent-field formalism which includes the short-range correlations between bosons through a local-field correction depending on the pair correlation function. Numerical results for the static structure factor, pair correlation function, spectrum of elementary excitations, and the response of the system to a static impurity charge are presented. Our results show the same qualitative behavior as those of the three-dimensional analog but the correlation effects are somewhat more pronounced in two dimensions.

I. INTRODUCTION

Over the last few years there has been an active interest of a large number of experimentalists and theorists in studying two-dimensional systems with Coulomb's interaction between particles. In contrast to the three-dimensional analog, there are two different well-defined Coulomb systems in two dimensions. In one case the system consists of charges restricted to motion in a plane and interacting via $1/r$ potential. The second system is made up of charged particles interacting through the logarithmic two-dimensional potential.

The electronic properties of two-dimensional systems, such as electrons trapped on a liquid helium surface and electrons in the inversion layers in metal-insulator-semiconductor structures, have been intensively investigated during the last years.¹ In these systems the electrons are bounded perpendicular to the surface in discrete quantum-mechanical states and interact via a $1/r$ potential in their motion parallel to the surface. Many-body effects in these systems have been studied through the structure factor, pair correlation function, thermodynamic functions, plasma dispersion relation, and ground-state energy, to mention a few.²⁻⁴

On the other hand, a system with a logarithmic Coulomb potential interaction may have applications to real physical situations as a model of two-dimensional superfluidity, for example.⁵⁻⁷ Furthermore, the $\ln(r)$ interaction has recently become quite important in the understanding of dislocations in solids, the Kosterlitz-Thouless transition,⁸ and thin-film superconductors.⁹⁻¹¹

The purpose of the present paper is to investigate some static and dynamical properties of a two-dimensional many-charged boson gas interacting via logarithmic potential over an extensive range of densities.

We use a self-consistent-field approximation,¹² hereaf-

ter called SCFA, proposed by Singwi *et al.* for the degenerate electron gas, which takes into account the short-range correlations arising from the Coulomb repulsion potential. Strictly speaking, the calculations are a natural extension of the three-dimensional charged Bose gas system recently investigated by the authors.¹³ The SCFA method consists of replacing the two-particle distribution function in the Liouville equation for the one-particle distribution function $f_1(\mathbf{r}, \mathbf{p}; t)$ by the product of two one-particle distribution functions and a static pair correlation function as

$$f_2(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}'; t) = f_1(\mathbf{r}, \mathbf{p}; t) f_1(\mathbf{r}', \mathbf{p}'; t) g(\mathbf{r} - \mathbf{r}'), \quad (1)$$

thus terminating the hierarchy of equations. In such a procedure the short-range correlations responsible for the local-field corrections are calculated in a self-consistent way by making the density-density response function dependent upon the pair correlation function. This approach is one of the best improvements of the random-phase-approximation (RPA) formalism and has been successfully employed both for quantum and classical systems.

The SCFA is then applied to calculate the pair-correlation functions, structure factor functions, elementary excitation spectrum, and the screening density around a fixed impurity in a two-dimensional charged Bose system interacting via logarithmic Coulomb potential. The numerical results are compared with those we obtained (as a by product) in the context of RPA and also with the results of the three-dimensional analog. As in the case of the electron gas, we found the correlation effects more pronounced in two than in three dimensions.

This paper is organized as follows. In Sec. II we briefly describe the self-consistent-field approximation. In Sec. III numerical results for the pair correlation functions and structure factor have been obtained for a large range of

densities. The induced charge distribution around a fixed charged impurity is calculated in Sec. IV. In Sec. V the elementary excitation spectrum of energy is determined from the poles of the self-consistent density-density response function, and a brief conclusion concerning the results is presented in Sec. VI.

II. FORMALISM

In the self-consistent-field approximation formalism corresponding to the ansatz given by Eq. (1), the two-dimensional charged Bose system interacting via logarithmic potential is described by the density-density response function as

$$\chi(\mathbf{q}, \omega) = \chi_0(\mathbf{q}, \omega) / [1 - \psi(\mathbf{q})\chi_0(\mathbf{q}, \omega)], \quad (2)$$

where $\chi_0(\mathbf{q}, \omega)$ is taken to be the zero-temperature density-density response function of the noninteracting system and is simply given by

$$\chi_0(\mathbf{q}, \omega) = 2\rho\epsilon(\mathbf{q}) / [(\hbar\omega + i\eta)^2 - \epsilon(\mathbf{q})^2], \quad (3)$$

where $\rho = N/V$ is the numerical density of the system, $\epsilon(\mathbf{q}) = \hbar^2 q^2 / 2m$ is the free-single-particle energy, m is the mass of the boson, and $\hbar\omega$ is the energy of the quasiparticle associated with the frequency ω of small oscillations of the gas about equilibrium.

The effective self-consistent potential $\psi(\mathbf{q})$ is a functional of the static structure factor function $S(\mathbf{q})$ through the following expression:

$$\psi(\mathbf{q}) = \phi(\mathbf{q})[1 - G(\mathbf{q})], \quad (4)$$

where $\phi(\mathbf{q}) = 2\pi e^2 / q^2$ is the two-dimensional Fourier transform of the Coulombic particle-particle interaction potential as obtained from Poisson's equation and $G(\mathbf{q})$ is the local-field correction which is given in terms of $S(\mathbf{q})$ as

$$G(\mathbf{q}) = -\frac{1}{\rho} \int \frac{d^2\mathbf{k}}{(2\pi)^2} \frac{\mathbf{q} \cdot \mathbf{k}}{q^2} \frac{\phi(\mathbf{k})}{\phi(\mathbf{q})} [S(\mathbf{q} - \mathbf{k}) - 1]. \quad (5)$$

The structure factor, on the other hand, is related to the imaginary part of $\chi(\mathbf{q}, \omega)$ by the dissipation-fluctuation theorem as¹⁴

$$S(\mathbf{q}) = -\frac{\hbar}{\rho} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \text{Im}\chi(\mathbf{q}, \omega), \quad (6)$$

closing then the self-consistent scheme.

It is interesting to note that the expression for the density-density response function in the RPA is recovered if we neglect the local-field corrections, that is, if we set $G(\mathbf{q}) = 0$ which corresponds to take the effective potential interaction as $\psi(\mathbf{q}) = \phi(\mathbf{q})$.

By means of the Kramers-Krönig relation, the integral in Eq. (6) can be easily performed and the result for the structure factor function turns out to be

$$S(\mathbf{q}) = [1 + 2\rho\psi(\mathbf{q})/\epsilon(\mathbf{q})]^{-1/2}, \quad (7)$$

which is much simpler than the corresponding expression for the structure factor function of the quantum degenerate electron gas.

III. PAIR CORRELATION FUNCTION AND STRUCTURE FACTOR

The pair correlation function $g(r)$ which represents the probability of finding one particle at a distance r from another is related to the Fourier transform of the structure factor $S(\mathbf{q})$ and in two-dimensions is given by

$$g(r) = 1 + \frac{1}{2} \int dq q J_0(qr) [S(q) - 1], \quad (8)$$

where $J_0(x)$ is the zeroth-order Bessel function of the first kind and

$$S(q) = \left[1 + \frac{8r_s^2}{q^4} [1 - G(q)] \right]^{-1/2}, \quad (9)$$

with the local-field correction $G(q)$ given by

$$G(q) = -\frac{1}{2} \int dk k [S(k) - 1] \theta(q - k), \quad (10)$$

where $\theta(x)$ is the step function defined as $\theta(x) = 0$ for $x < 0$ and $\theta(x) = 1$ for $x > 0$. In the equations above r is expressed in units of $r_0 = (\pi\rho)^{-1/2}$, the average interparticle separation. The density of the system is expressed through the parameter $r_s = r_0/a_0$, where a_0 is the Bohr radius.

The numerical solutions of the integral equation, Eq. (9), were obtained by an iterative procedure. From an initial guess for $S(q)$, we calculated $G(q)$ from Eq. (10) and the result was inserted in Eq. (9) generating a new $S(q)$, and so on. In the high-density regime the convergence of this self-consistent method is very easy to obtain. For $r_s < 5$ the numerical precision in the self-consistent $G(q)$ was typically one part per million while a much higher accuracy in $S(q)$ was obtained. In decreasing densities the convergence of the iterative process becomes quite poor. The results for the self-consistent structure factor $S(q)$, determined as mentioned above, as a function of wave vector for several values of r_s along with the RPA results are shown in Fig. 1. It should be noted that the correlation effects which are taken into account in the present calculation increase with decreasing densities and also more pronounced as compared to the three-dimensional case. The overall behavior of $S(q)$, however, is similar to the three-dimensional analog,¹³ as well as to the two-dimensional quantum electron gas.⁷

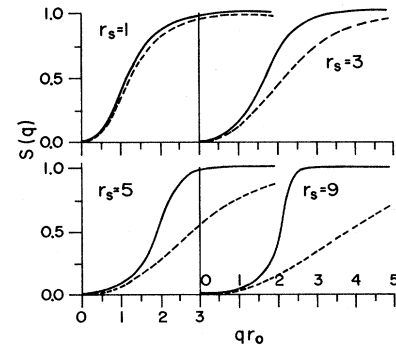


FIG. 1. Structure-factor function $S(q)$ versus qr_0 for various values of r_s . The RPA results (dashed curves) are also plotted for comparison.

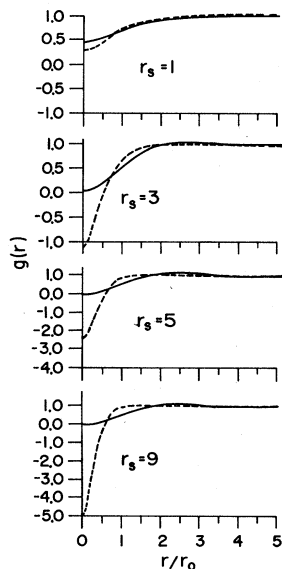


FIG. 2. Pair correlation function $g(r)$ as a function of r/r_0 for several values of r_s . Dashed curves are the RPA results.

With the self-consistent results we have obtained for the structure factor $S(q)$, we have calculated the pair-correlation function $g(r)$ as given by Eq. (8). The results we have obtained are plotted in Fig. 2 for various values of the coupling parameter r_s . For comparison the corresponding results of the RPA are also shown. As we can see, the inadequacy of the RPA is revealed even for small values of r_s with the pair correlation function becoming negative at small distances. In the SCFA, on the other hand, $g(0)$ remains positive even for large values of r_s such as $r_s=9$. This result is similar to the three-dimensional analog but contrasts with the results of the two-dimensional electron gas with $\ln(r)$ interaction where the pair correlation function $g(0)$ becomes negative for $r_s > 2$.

Once again it may be noted that the correlation effects in our two-dimensional system are stronger than the corresponding three-dimensional model but the qualitative behavior is similar in both systems.

IV. IMPURITY SCREENING

In this section we investigate the effects of a static impurity of charge $Q=Ze$ immersed in the two-dimensional charged Bose gas. The screening density around a fixed impurity is given in the linear-response approximation by¹⁵

$$\delta\rho(\mathbf{q},\omega) = -\chi(\mathbf{q},\omega)e\phi_{\text{ext}}(\mathbf{q},\omega), \quad (11)$$

where $\chi(\mathbf{q},\omega)$ is the density-density response function which is obtained by the self-consistent solution of Eqs. (2), (5), and (6), and $\phi_{\text{ext}}(\mathbf{q},\omega)$ is the external potential due to a static impurity charge given by

$$\phi_{\text{ext}}(\mathbf{q},\omega) = \frac{4\pi^2 e^2}{a_0 q^2} \delta(\omega). \quad (12)$$

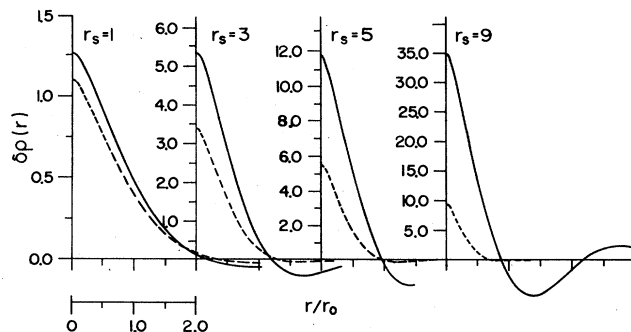


FIG. 3. Screening density $\delta\rho(r)$ plotted as a function of the distance from the impurity r/r_0 for various values of r_s . The dashed curves are the RPA results.

By substituting this external potential into Eq. (11) and taking its inverse Fourier transform we obtain the following expression for the screening density at a distance r :

$$\delta\rho(r) = -Z\rho \int dq \frac{qJ_0(qr)}{\frac{q^4}{4r_s^2} + 2[1-G(q)]}, \quad (13)$$

where $J_0(x)$ is the Bessel function of order zero and length is expressed in units of r_0 , the average interparticle separation.

The total induced charge Q_T is

$$Q_T = e \int d\mathbf{r} \delta\rho(r) = -Ze \int d\mathbf{q} \frac{2\delta(q)}{\frac{q^4}{4r_s^2} + 2[1-G(q)]} = -Ze \quad (14)$$

which means that the charged impurity is totally screened at large distances.

Since there is no exact analytic solution of Eq. (13) even in the more simple approximation such as the RPA, we have numerically calculated it as a function of the distances r from the impurity for several values of the density of the boson gas. In Fig. 3 we show the results we have obtained along with RPA results. It is seen that the presence of the short-range correlations in the system gives significant enhancement of the screening density over the RPA results. We also observe with increasing r_s that the screening density becomes larger at small distances from the impurity and decreases to zero much faster. The qualitative behavior of the induced screening density is similar to the three-dimensional analog.

V. QUASIPARTICLE ENERGY SPECTRUM

The quasiparticle energy spectrum $E(\mathbf{q}) = \hbar\omega(\mathbf{q})$ is obtained from the poles of the density-density response function $\chi(\mathbf{q},\omega)$ of the system. Thus from Eq. (2) we set

$$[\hbar\omega(\mathbf{q}) + i\eta]^2 - \epsilon(\mathbf{q}) - 2\rho\epsilon(\mathbf{q})\psi(\mathbf{q}) = 0, \quad (15)$$

resulting, for the excitation energy, in the following expression:

$$E(\mathbf{q}) = \{[\epsilon(\mathbf{q})]^2 + 2\rho\epsilon(\mathbf{q})\psi(\mathbf{q})\}^{1/2}, \quad (16)$$

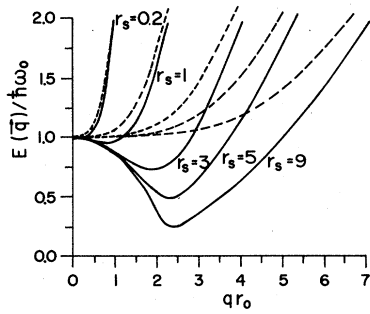


FIG. 4. Elementary excitation spectrum $E(\mathbf{q})$ as a function of qr_0 for several r_s . The corresponding RPA results (dashed curves) are plotted for comparison.

which can be related to the static structure factor $S(\mathbf{q})$ through the well-known Feynman's expression

$$E(\mathbf{q}) = \frac{\epsilon(\mathbf{q})}{S(\mathbf{q})} \quad (17)$$

by integrating the right-hand side of Eq. (6).

The dispersion relation has been numerically obtained and the results are plotted in Fig. (4) in comparison with those of RPA. As we can see, the differences with the RPA results are more pronounced in the low-density region, where the correlations between particles play a fundamental role.

In the long-wavelength limit region, where the oscillations are weakly damped and well defined as quasiparticles, we obtain the following expression for the energy:

$$E(\mathbf{q}) = \hbar\omega_0 \left[1 - \frac{q^2}{4\pi\rho} + \frac{\hbar^2 q^4 a_0}{4m^2 \omega_0^2} \right]^{1/2}, \quad (18)$$

where $\omega_0 = (2\pi\rho e^2 / \hbar^2)^{1/2}$ is the plasma frequency.

As in the three-dimensional system the short-range correlations give a correction to the RPA results by decreasing $E(\mathbf{q})$ while increasing the wave vector \mathbf{q} . The quasiparticle energy reaches a minimum value and increases again asymptotically to the single-particle excitation spectrum at large \mathbf{q} . Nevertheless it may be noted that the correlation effects in decreasing $E(\mathbf{q})$ are much more pronounced in our two-dimensional system than those in the three-dimensional analog.

VI. CONCLUSIONS

In this paper we have applied a self-consistent-field approximation which takes into account the short-range correlation effects, to calculate some of the static and dynamical properties of a two-dimensional charged Bose gas interacting with $\ln(r)$ potential. Numerical results for the induced charge density around a static impurity, pair correlation functions, structure factor, and plasmon dispersion relation have shown significant differences from those given by the RPA. It should be stressed that our results were found to be qualitatively similar to the three-dimensional charged Bose system. Moreover, stronger correlation effects appear in our two-dimensional gas.

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