Ground state of a two-dimensional charged-boson system

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The ground state of a two-dimensional charged-boson system is investigated over the range of densities $1 \lesssim R_s \lesssim 10$ in the self-consistent-field approximation; $R_s=(a_0^2\pi\rho)^{-1/2}$, where a_0 is the Bohr radius and ρ is the number density. Starting with numerical self-consistent calculations of the static structure factor, the elementary excitation, pair-correlation functions, pressure, and ground-state energy are evaluated. These results are compared with those of the two-dimensional and three-dimensional systems obtained from other methods. The ground-state energy is given as $E_0=-1.2918R_s^{-2/3}+0.03$, which improves the result from the ring-diagram approximation.

I. INTRODUCTION

Since Foldy's pioneering work[1] on the charged-boson system, there has been continuing interest in this system from the viewpoint of real physical systems.[2] It should be pointed out that the special characteristic shared by the charged boson and electron gas is that the properties of the ground state can be described by only a single dimensionless parameter $R_s=r_0/a_0$, where $r_0=(\pi\rho)^{-1/2}$ is the mean particle distance, ρ is the number density, and $a_0=\hbar^2/me^2$ is the Bohr radius of the particle with mass m. The electron gas has been widely investigated for its applications to metals. However, the charged-boson system has been largely ignored because of its nonexistence.

Concerning the ground-state energy (GSE), Foldy first calculated the GSE and elementary excitation spectrum of the charged-boson system in the high-density region ($R_s \lesssim 1$), which was also later evaluated by others.[3] In the intermediate density region ($1 \lesssim R_s \lesssim 100$), Lee,[4] Lee and Ree,[5] and Monnier[6] evaluated the GSE through the variational method with a Jastrow trial wave function. More recently Hansen and Maxighi[7] obtained a variational upper bound to the GSE over a wide range of densities ($1 \lesssim R_s \lesssim 200$) with the use of a variational Jastrow trial wave function, the hypernetted chain integral equation, and the Monte Carlo method, and Hipolito *et al.*[8] investigated the dielectric properties and also the two-dimensional (2D) and three-dimensional (3D) classical electron systems by adopting the self-consistent-field approximation (SCFA) introduced by Singwi *et al.*[9]

Although, in the past two decades, significant progress has been made in the study of the 2D electron systems for the dielectric function, structure factor and pair-correlation function,[10] GSE and specific heat,[11] effective mass,[12] superlattice,[13] quantized Hall effect,[14] and other quantities,[15] there is much less information about the properties of the elementary excitation spectrum, structure factor, pair-correlation function, and the GSE of 2D charged-boson systems. Therefore, in this paper we evaluate the aforementioned quantities of a 2D charged-boson system, which consists of N identical bosons with charge e and mass m, interacting via a Coulomb potential at $T=0$ over the range of densities $1 \lesssim R_s \lesssim 10$. To calculate the preceding quantities we adopt the SCFA given by Singwi *et al.* We survey the basic formula in Sec. II, and starting with the numerical self-consistent evaluation of the static structure factor $S(\mathbf{q})$, we obtain the elementary excitation spectrum, correlation function, and ground-state energy in Sec. III. Finally, in Sec. IV we present our numerical results for the preceding quantities in comparison with other works in terms of graphs and tables.

II. BASIC FORMULAS

The self-consistent-field approximation in the formalism of Singwi *et al.* includes the decoupling of the two-particle distribution function in the Liouville equation into the product of two one-particle distribution functions and a pair-correlation function,

$$f(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}',t)=f_1(\mathbf{r},\mathbf{p}|t)f_1(\mathbf{r}',\mathbf{p}'|t)g(\mathbf{r}-\mathbf{r}') , \tag{2.1}$$

where $\mathbf{r}$ and $\mathbf{p}$ are the position and momentum of each particle and $g(r)$ represents the equilibrium static pair-correlation function. The density-density response function $\chi(\mathbf{q},\omega)$ in Fourier space for an interacting system becomes

$$\chi(\mathbf{q},\omega)=\chi_0(\mathbf{q},\omega)/[1-\psi(\mathbf{q})\chi_0(\mathbf{q},\omega)] . \tag{2.2}$$

In Eq. (2.2), $\chi_0(\mathbf{q},\omega)$ is the density-density response function for a noninteracting charged-boson system at $T=0$ given as

$$\chi_0(\mathbf{q},\omega)=2\rho\varepsilon(\mathbf{q})/[(\omega+i\eta)^2-\varepsilon(\mathbf{q})^2] , \tag{2.3}$$

where $\varepsilon(\mathbf{q})=\hbar^2q^2/2m$ is the free particle energy, η is a positive infinitesimal quantity, and $\psi(\mathbf{q})$ is the self-consistent effective potential,

$$\psi(\mathbf{q})=\phi(\mathbf{q})[1-G(\mathbf{q})] . \tag{2.4}$$

Here, $\phi(\mathbf{q})=2\pi e^2/q$ is the two-dimensional Fourier transform of the Coulomb interaction e^2/r, and $G(\mathbf{q})$ is given by

$$G(\mathbf{q})=-\frac{1}{\rho}\int\frac{\mathbf{q}\cdot\mathbf{k}}{qk}[S(\mathbf{q}-\mathbf{k})-1]\frac{d^2k}{(2\pi)^2}\ . \tag{2.5}$$

In Eq. (2.5) the static structure factor $S(\mathbf{q})$, which is the Fourier transform of the pair-correlation function $g(r)$, can be expressed as

$$S(\mathbf{k})=1+\rho\int d^2r[g(r)-1]e^{-i\mathbf{k}\cdot\mathbf{r}}\ . \tag{2.6}$$

The singularities of the density-density response function represent the energies of the excited states, and the excitation energy of the system is related to $S(\mathbf{q})$ through the Feynman expression

$$E(\mathbf{q})=\varepsilon(\mathbf{q})/S(\mathbf{q})\ . \tag{2.7}$$

We find the ground-state energy to be

$$E_0=\int_0^{e^2}\frac{d\alpha}{\alpha}E_{\rm int}(\alpha)\ , \tag{2.8}$$

where $E_{\rm int}(\alpha)$ is the interaction energy as a function of the coupling constant α, which is a measure of the strength of the coupling between bosons.

III. EXCITATION SPECTRUM, STRUCTURE FACTOR, CORRELATION FUNCTION, AND GROUND-STATE ENERGY

We first investigate the response of the charged-boson system to a static impurity with charge ze located at the origin, where the external potential is

$$\phi_{\rm ext}(\mathbf{q},\omega)=\frac{4\pi^2ze}{q}\delta(\omega)\ . \tag{3.1}$$

The induced charged density, which characterizes the linear response to an external potential from a fixed charge, can be written as

$$\delta\rho(\mathbf{q},\omega)=-\chi(\mathbf{q},\omega)e\phi_{\rm ext}(\mathbf{q},\omega)\ . \tag{3.2}$$

Through the inverse Fourier transform of Eq. (3.2), we obtain the induced charge density at position $\mathbf{r}$ as

$$\delta\rho(\mathbf{r})=-\frac{z}{2\pi r}\int_0^\infty dq\frac{\sin(qr)}{G(\mathbf{q})-(q/\lambda)^3-1}\ , \tag{3.3}$$

where $\lambda^3=8\pi\rho/a_0$. The total induced charge Q is

$$\begin{aligned}Q&=-e\int d^2r\,\delta\rho(\mathbf{r})\\&=ze\int d^2q\frac{\sin(qr)}{G(\mathbf{q})-(q/\lambda)^3-1}=-ze\ .\end{aligned} \tag{3.4}$$

Equation (3.4) indicates that the charged impurity is completely screened at long distances. However, the induced charge density [Eq. (3.3)] diverges at $r=0$. This divergence is due to the fact that the linearized equation of motion for the classical one-particle distribution function is invalid near the charged impurity. The divergence can be avoided by taking quantum effects into consideration.

The elementary excitation spectrum $E(\mathbf{q})$ is determined from the pole of the density-density response function $\chi(\mathbf{q},\omega)$, which yields

$$[\omega(\mathbf{q})+i\eta]^2-\varepsilon^2(q)-2\rho\varepsilon(\mathbf{q})\psi(\mathbf{q})=0\ , \tag{3.5}$$

and thus the excitation energy $E(\mathbf{q})=\hbar\omega(\mathbf{q})$ can also be written as

$$E(\mathbf{q})=[\varepsilon(\mathbf{q})^2+2\rho\varepsilon(\mathbf{q})\psi(\mathbf{q})]^{1/2}\ . \tag{3.6}$$

We notice that the elementary excitation spectrum in the ring-diagram approximation[16] (RDA) can be obtained under the condition $\psi(\mathbf{q})=\phi(\mathbf{q})$, i.e., the neglection of the local corrections in Eq. (3.6). Making use of the following expression for the structure in the long-wavelength approximation,

$$S(\mathbf{q}-\mathbf{k})=S(\mathbf{q})-q\cos\theta\frac{\partial S(k)}{\partial k}+\cdots\ , \tag{3.7}$$

the local-field correction $G(\mathbf{q})$ becomes

$$G(\mathbf{q})=\gamma q \tag{3.8}$$

and

$$\gamma=-\frac{R_s^2}{4}\int_0^\infty d^2q[S(\mathbf{q})-1]\ . \tag{3.9}$$

Then the excitation spectrum can be expressed as

$$E(\mathbf{q})=\hbar\Omega\left[1-\frac{\gamma}{2}q+\frac{\hbar^2q^4}{8m^2\Omega^2}\right]\ , \tag{3.10}$$

where $\Omega=(2\pi\rho e^2q/m)^{1/2}$ is the two-dimensional plasma frequency. In the case of three dimensions the excitation spectrum in the long-wavelength approximation is given by

$$E(\mathbf{q})=\hbar\omega_p\left[1-\frac{\gamma}{2}q+\frac{\hbar^2q^4}{2m^2\omega_p^2}\right]\ , \tag{3.11}$$

where $\omega_p=(4\pi\rho e^2/m)^{1/2}$ is the 3D plasma frequency. We remark that one of the authors has obtained the excitation spectrum of the 2D charged-boson system through the RDA in the long-wavelength approximation as[17]

$$E(\mathbf{q})=\hbar\Omega\left[1+\frac{\hbar^2q^4}{2m^2\Omega^2}\right]\ . \tag{3.12}$$

The short-range correlation functions occuring in the Coulomb interaction between the charged bosons are expressed by the pair-correlation function $g(r)$, which represents the probability of finding two boson particles separated by a distance r. The inverse Fourier transform of the structure factor yields

$$g(r)=1+\frac{R_s^2}{2}\int dq\,qJ_0(qr)[S(\mathbf{q})-1]\ , \tag{3.13}$$

and from Eqs. (2.4), (2.7), and (3.6) the structure factor becomes

$$S(\mathbf{q})=\left[1+\frac{8}{R_s^2q^3}[1-G(\mathbf{q})]\right]^{-1/2} \tag{3.14}$$

with

$$G(\mathbf{q})=\frac{R_s^2}{\pi}\left[\int_0^q dk\, kE\left[\frac{k}{q}\right][S(k)-1]+q\int_q^\infty dk\left\{\left[1-\left[\frac{k}{q}\right]^2\right]K\left[\frac{k}{q}\right]+\left[\frac{k}{q}\right]^2 E\left[\frac{k}{q}\right]\right\}[S(k)-1]\right], \tag{3.15}$$

where r, q, and k are expressed in units of the Bohr radius a_0 and a_0^{-1}, respectively, and $K(x)$ and $E(x)$ are the complete elliptic integrals of the first and second kinds. The numerical solution of Eq. (3.14) can be obtained by the method of iteration. The 3D structure factor[8] in the long-wavelength approximation is given by

$$S(\mathbf{q})=\left[1+\frac{12}{R_s^2 q^4}(1-\gamma q^2)\right]^{-1/2} \tag{3.16}$$

with

$$\gamma=-\frac{2R_s^3}{9\pi}\int_0^\infty dq\,[S(\mathbf{q})-1]\,. \tag{3.17}$$

Comparing Eqs. (3.9) and (3.17), we find that both forms are similar to each other, with the dependence of the spatial dimensionality on the dimensionless parameter R_s.

From the pair-correlation function or structure factor, we can calculate the ground-state energy of the charged-boson system. We may write the interaction energy as

$$E_{\rm int}(\alpha)=\pi N\rho\int_0^\infty dr\,\phi(r,\alpha)[g(r)-1]r \tag{3.18}$$

or

$$E_{\rm int}(\alpha)=\frac{N}{2}\int_0^\infty dq\,\alpha[S(\alpha,\mathbf{q})-1]\,. \tag{3.19}$$

Expressing the wave number and the density in units of $(2\pi\rho a_0^2)^{1/4}$ and R_s, we can write the ground-state energy per particle in Rydbergs as

$$E_0=2^{1/3}R_s^{-2/3}\int_0^1 d\alpha\int dq\,[S(\alpha,q)-1]\,. \tag{3.20}$$

We note that the 3D ground-state energy per particle in Rydbergs is given by

$$E_0=\frac{2}{\pi}3^{1/4}R_s^{-3/4}\int_0^1 d\alpha\int_0^\infty dq\,[S(\alpha,q)-1]\,. \tag{3.21}$$

IV. RESULTS AND DISCUSSION

In the previous sections we have evaluated the elementary excitation spectrum, pair-correlation functions, and the ground-state energy of the charged-boson system from the determination of the structure factor in the self-consistent-field approximation. Figure 1 illustrates the elementary excitation spectrum as a function of qr_0 for various values of R_s. We see that the third term in the large parentheses of Eq. (3.10) is dominant in the high-momentum region, and thus the excitation energy is almost identical with that of a free particle. As R_s increases, the excitation energy reduces more rapidly to the free-particle case. We notice that in the low-momentum region the 3D excitation energy obtained from the SCFA decreases as q increases, and this reduction is quite significant with increasing R_s. This reduction does not appear in the 2D case for the range of densities $1\lesssim R_s\lesssim 10$. A comparison of Eqs. (3.6) and (3.12) shows that the results in the SCFA gives a correction to Eq. (3.12) derived from the RDA.

In Fig. 2 we have given the numerical calculation of Eq. (3.14) as a function of qr_0 of various values of R_s by the iteration method. The structure factor converges very rapidly to unity as R_s increases. We have compared the 2D structure factor to the 3D case in Fig. 3. The 2D

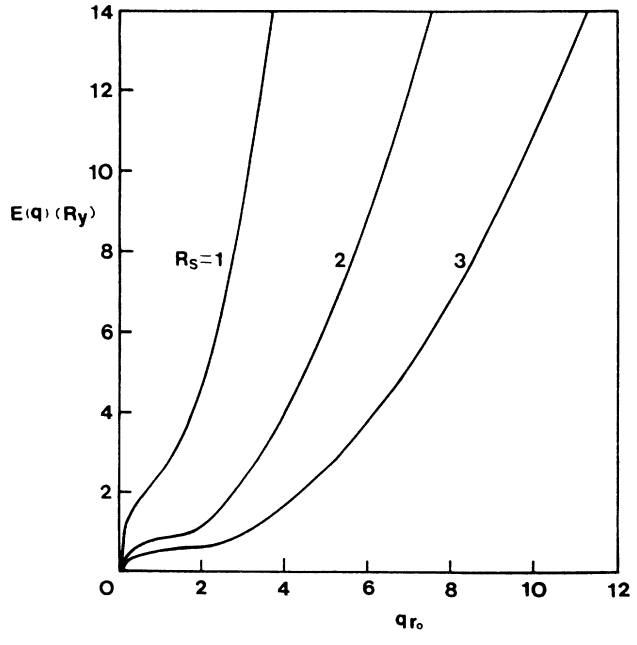

FIG. 1. Excitation energy vs the dimensionless parameter qr_0 in units of the Rydberg at several values of R_s.

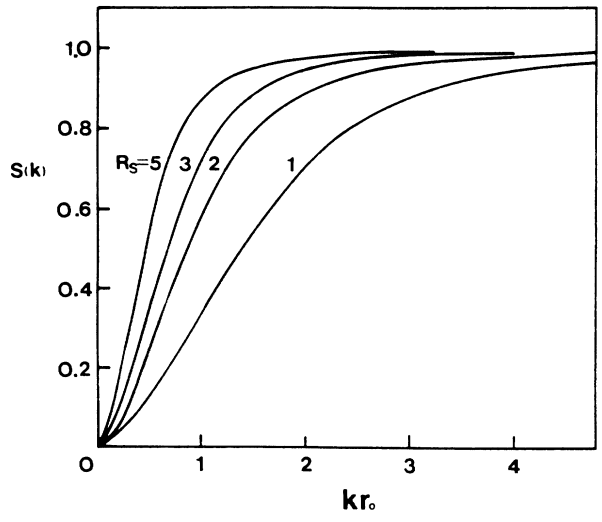

FIG. 2. Structure factor vs kr_0 at various values of R_s.

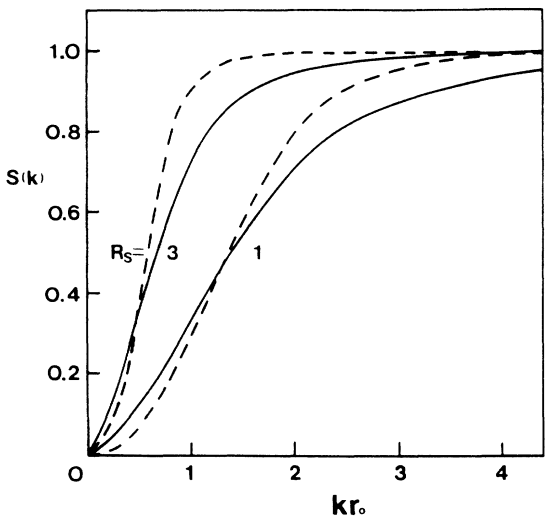

FIG. 3. Structure factor vs kr_0. The solid and dashed lines correspond to two and three dimensions for $R_s = 1$ and 3.

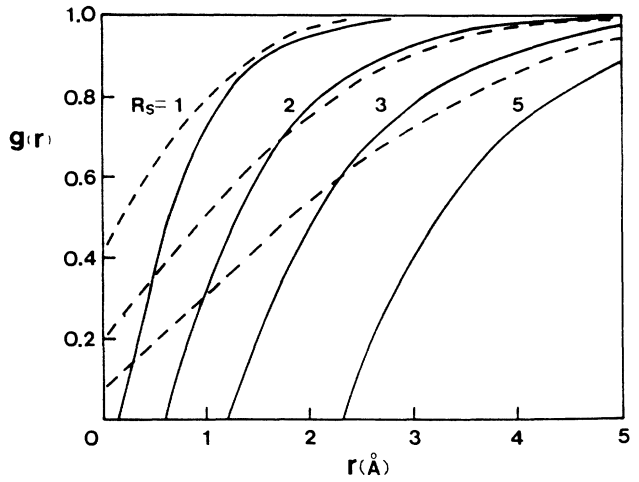

FIG. 4. Pair-correlation function $g(r)$ vs r for various values of R_s. The solid and dashed lines correspond to two and three dimensions.

structure factor increases more slowly than the 3D structure factor in the short-wavelength region but more quickly in the long-wavelength region as qr_0 is varied.

With the use of the aforementioned calculations for the structure factor, we evaluate the pair-correlation function from Eq. (3.13). The result is given and compared with the 3D case in Fig. 4. The pair-correlation function starts oscillating at large distances, which is not displayed in the figures. These oscillations have very small and broad amplitudes. This long-distance behavior is similar to the 3D case. For Bose fluids[18] interacting via a soft potential with a Lennard-Jones-type tail and pseudopotential, in the RDA the pair-distribution functions become negative at short distances and decrease as r^{-3} at large distances. This decrease corresponds to the existence of a phonon spectrum for small momenta. In the RDA the pair-distribution function for the 2D charged boson becomes negative with decreasing R_s and diverges at $r \to 0$. Consideration of the short-range correlation of the charged boson through the local-field correction SCFA improves the result from the RDA, i.e., the value of $g(0)$ obtained in SCFA is negative, but so small that for the practical purposes one can consider $g(0)$ to be zero.

We have evaluated the ground-state energy by a numerical self-consistent solution through Eqs. (3.14) and (3.19) to give

$$E_0 = -1.2918 R_s^{-2/3} + 0.03 \ . \tag{4.1}$$

In the RDA we have obtained the ground-state energy per particle in terms of R_s as

$$E_0 = -1.2918 R_s^{-2/3} \ , \tag{4.2}$$

and for the 3D charged-boson system the ground-state energy per particle is evaluated by various methods:

$$E_0 = -0.8030 R_s^{-3/4} \ \text{(RDA) (Ref. 19)} \ , \tag{4.3}$$

$$E_0 = -0.8030 R_s^{-3/4} + 0.027 \ \text{(VCA) (Ref. 5)} \ , \tag{4.4}$$

$$E_0 = -0.8030 R_s^{-3/4} + 0.032 \ \text{(SCFA) (Ref. 8)} \ , \tag{4.5}$$

The extra numerical terms in Eqs. (4.1), (4.4), and (4.5) are due to the better estimation of the correlation. The numerical data for the ground-state energies in the vari-

TABLE I. Ground-state energies obtained from various methods for the two- and three-dimensional charged-boson system.

	2D			3D	
$-E_0$	SCFA	RDA[a]	SCFA[b]	RDA[c]	VCA[d]
R_s					
1	1.2617	1.2918	0.7712	0.8030	0.7767
2	0.7808	0.8138	0.4472	0.4475	0.4516
3	0.5965	0.6210	0.3231	0.3523	0.3270
5	0.4245	0.4418	0.2129	0.2402	0.2159
10	0.2670	0.2783	0.1188	0.1428	0.1209

[a]Reference 17.
[b]Reference 8.
[c]Reference 19.
[d]Reference 5.

TABLE II. Pressure of the 2D charged-boson system obtained from the SCFA and RDA.

R_s	$-P/\rho$ 2D SCFA	RDA
1	0.4060	0.4306
2	0.2557	0.2713
3	0.1961	0.2070
5	0.1404	0.1473
10	0.0911	0.0928

ous calculations are summarized in Table I, where we see that the SCFA results are an improvement over the RDA results.

Differentiating Eq. (3.20) with respect to R_s, we obtain the pressure of the 2D charged-boson system:

$$\frac{P}{\rho} = -\frac{R_s}{2}\frac{dE_0}{dR_s} . \tag{4.6}$$

The numerical results for the pressure are listed in Table II in comparison with the RDA results.

In conclusion, we remark that the behaviors of the elementary excitation spectrum, structure factor, and pair-correlation functions obtained from the SCFA, which includes the short-range correlations for the 2D charged-boson system, are very much like those of the 3D case. The SCFA results for the ground-state energy are an improvement over the RDA results.

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