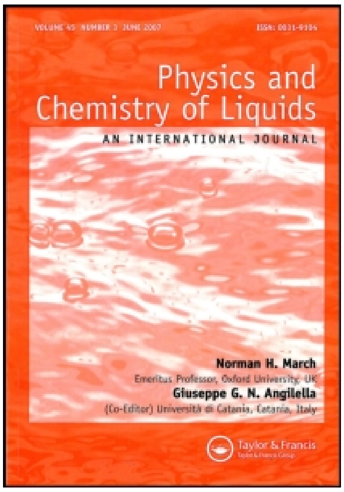

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Sum Rules and Density Response of A Two-Dimensional Charged Bose Fluid

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SUM RULES AND DENSITY RESPONSE OF A TWO-DIMENSIONAL CHARGED BOSE FLUID

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The density response of a two-dimensional charged Bose fluid at absolute zero temperature is studied beyond the random-phase approximation by including the many-body correlation effects. The correlations are accounted for through a static local-field correction obtained by satisfying in an approximate way the third frequency-moment sum rule of the density response function. The static structure factor, the pair-correlation function, the elementary excitation spectrum, and the ground-state energy are calculated over a wide range of boson number density. Wherever available, the results are compared with the recent diffusion Monte Carlo data and the calculation based upon the theory of Singwi *et al.* We also present a comparison between the results of electron and charged Bose fluids for pair-correlation function and elementary excitation spectrum.

Keywords: Structure; elementary excitations; Bose fluids

1. INTRODUCTION

The charged Bose fluid model, comprising a system of charged point-like spinless bosons embedded in a rigid uniform neutralizing background, has drawn considerable interest in the recent years. The model represents the Bose counterpart of the electron jellium and was proposed by Schafroth [1] in connection with the superconducting phenomenon even prior to the BCS theory. It may also have some astrophysical relevance in relation to the cores of white dwarf stars

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consisting of pressure-ionized helium [2]. The charged Bose fluid, however, unlike its electron analog, has not been studied much mainly because it has not been so far realized in the laboratory. Nevertheless, there exists interest in this system, since it offers a ground for studying together the effects related to the many-body correlations and the Bose-Einstein statistics. As a pioneering work for the charged bosons at absolute zero, Foldy [3] calculated the ground-state energy and the elementary excitation spectrum in the high density limit by following a method due to Bogoliubov. Since then, many attempts [4] have been made theoretically to extend this study over a wide range of boson number densities. In addition to the theory, the computer simulation ex-periments [5] have provided useful information on the boson ground state.

The problem of charged bosons has also been considered in the two-dimensions (2D), where the dynamics of particles is restricted to the plane. The 2D charged Bose system had been of course first studied about two decades ago [6], it has recently drawn renewed interest due to its recognition as a possible model for a high-T_c superconductor [7]. The possibility has grown mainly due to the failure of the BSC theory to account for the unusual behavior exhibited by the high-T_c superconductors. Moreover, there are some experimentally observed facts which are theoretically well explained in terms of the charged Bose fluid model. In this respect, the study of a two-dimensional charged Bose fluid (2DCBF) has become an important subject. However, it is not our aim in the present work to deal with the superconducting behavior of the CBF, rather we intend to investigate the effect of many-body correlations on its ground state.

In a strictly-2D system, the particles interact through ln (r) potential. However, in a real physical situation, if it exists, the particle wave function will not be confined to the plane. To be consistent with the 3D nature of wave function, most of the earlier studies assume that the particles interact with the 3D Coulomb potential, i.e., $1/r$, where r is the 2D separation. We shall confine our discussion to the latter class only. Hines and Frankel [6] first studied such 2DCBF to calculate its dielectric response and the elementary excitation spectrum within the random-phase approximation (RPA). However, the applicability of the RPA appears to be restrictive in the high density limit as it neglects completely the short-range correlations between charged bosons. As an important manifestation of the neglect of correlation effects, the pair-correlation function $g(r)$ in RPA has been found to become negative at small separation. The role of correlations beyond the RPA have recently been explored by us [8] within the self-consistent field approximation of Singwi, Tosi, Land, and Sjölander (STLS) [9] and by Gold [10] within the so-called sum rule version of STLS. The STLS theory describes correlations as giving rise to a region of depleted charge density around each particle in the fluid and quantitatively, this effect is accomplished through a static local-field correction. Results of $g(r)$ thus obtained satisfy the positive definiteness condition at least in the intermediate fluid density range. It may be mentioned here that the STLS theory had originally been proposed for the degenerate electron gas and there also exist some alternative schemes [11] to correlations differing in the method of calculation for the local-field correction. It will be useful to study correlation effects in the 2DCBF in these schemes and to examine the results in comparison with the other theories and the recent diffusion Monte Carlo (DMC) calculation [12]. This forms one of the motivation for the present work. It may be added here that at the time we performed the STLS treatment of 2DCBF, the DMC results were not available for comparison. We also intend to draw a comparison between the screening behavior of charged Bose fluid and its Fermi counterpart, i.e., a fluid of electrons.

In this paper, we use the Pathak-Vashishta (PV) theory [11] for studying the effect of many-body correlations beyond RPA. The PV theory has recently been used by Hong and Choi [13] for studying the ground state of 3DCBF. In the PV approach, a mean-field expression is assumed for the density response function $\chi(q, \omega)$ and the local-field correction is determined by satisfying the third-frequency-moment sum rule of $\chi(q, \omega)$. In Sec. II, we present in brief the PV theory. As in the STLS theory, the local-field correction has to be obtained numerically in a self-consistent way. From the calculation of $\chi(q, \omega)$, we can deduce the various static and dynamic properties of the Bose fluid. The physical properties of our interest are the static structure factor, the pair-correlation function, the elementary excitation spectrum, and the ground-state energy. In Sec. III, we present numerical results for these over the density range $1 \leq r_s \leq 10$; r_s is the dimensionless density parameter defined by $r_s = 1/[a_0\sqrt{n\pi}\,]$ where n is the boson number density and a_0 is the Bohr atomic radius.

Results are discussed in comparison with the STLS theory and the DMC calculation. In Sec. IV, we present a comparison between the results of charged Bose and electron fluids in terms of static correlation functions and the elementary excitation spectrum. In Sec. V, we make the concluding remarks.

2. THEORETICAL PROCEDURE

Consider a fluid of N point-like spinless bosons each of charge e confined to move within the plane in the presence of a rigid uniform neutralizing background. The system is described by the Hamiltonian

$$\mathcal{H} = \sum_i \frac{p_i^2}{2m} + \frac{1}{2}\sum_{\boldsymbol{q}} V(q)(\rho_{\boldsymbol{q}}\rho_{-\boldsymbol{q}} - N), \tag{1}$$

where $V(q) = 2\pi e^2/q$, is the 2D Fourier transform of the Coulomb potential $V(r) = e^2/r$ and $\rho_{\boldsymbol{q}} = \Sigma_i e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_i}$, is the density fluctuation operator. We consider the response of the fluid to an external potential $V^{\text{ext}}(q, \omega)$ that couples to the density fluctuations in the system. Within the linear response theory, the dynamic density response function $\chi(q, \omega)$ is given by

$$\chi(q,\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i\omega t}\chi(q,t), \tag{2}$$

where

$$\chi(q,t) = -\frac{i\theta(t)}{h}\langle [\rho_{\boldsymbol{q}}(t), \rho_{-\boldsymbol{q}}(0)]\rangle. \tag{3}$$

In above Eq., $\theta(t)$ is the unit step function and the angular brackets denote the equilibrium ensemble average appropriate to the system Hamiltonian. $\chi(q, \omega)$ requires for its calculation the knowledge of dynamics of $\rho_q(t)$ and this in turn amounts to solve the complicated many-body problem. In principle, the time evolution of $\rho_q(t)$ can be expressed as an infinite hierarchy of non-linear coupled differential equations, but it is practically impossible to solve this hierarchy. In the effective mean-field approximation, $\chi(q, \omega)$ is written as

$$\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1 - \psi(q)\chi_0(q,\omega)}. \tag{4}$$

In Eq. (4), $\chi_0(q, \omega)$ is the density response function of the noninteracting charged Bose gas and at absolute zero, it is given by [3]

$$\chi_0(q,\omega) = \frac{2n\varepsilon_q}{[(\omega + i\eta)^2 - \varepsilon_q^2]}, \tag{5}$$

where $\varepsilon_q = \hbar^2 q^2/2m$, is the free particle energy, n is the areal boson number density, η is a positive infinitesimal quantity, and $\psi(q)$ is the mean effective potential given by

$$\psi(q) = V(q)[1 - G(q)]. \tag{6}$$

$G(q)$ is the local-field correction factor describing the correlations between charged bosons. In the PV theory, $G(q)$ is calculated by satisfying the low-order frequency moments of $\chi(q, \omega)$. In the high-frequency limit, $\chi(q, \omega)$ can be expanded as

$$\chi(q,\omega) = -\frac{nq^2}{m}\frac{1}{\omega^2} - \frac{nq^2}{m}\left[\varepsilon_q^2 + \frac{3q^2}{m}\langle KE\rangle_0 + \omega_p^2(q)(1 - G(q))\right]\frac{1}{\omega^4} - O\left(\frac{1}{\omega^6}\right), \tag{7}$$

where $\omega_p(q) = (2\pi ne^2 q/m)^{1/2}$, is the 2D plasmon frequency and $\langle KE\rangle_0$ is the kinetic energy per particle of the non-interacting Bose gas. Further, since $\chi(q, t)$ is analytic in the upper half of complex-ω plane, we can write

$$\chi(q,\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''(q,\omega')}{\omega' - \omega - i\eta}. \tag{8}$$

The large-frequency expansion of $\chi(q, \omega)$ is obtained from Eq. (8) as

$$\chi(q,\omega) = -\frac{\langle\omega^1\rangle}{\omega^2} - \frac{\langle\omega^3\rangle}{\omega^4} - O\left(\frac{1}{\omega^6}\right), \tag{9}$$

where

$$\langle\omega^{2l-1}\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{\pi}\omega^{2l-1}\chi''(q,\omega), \tag{10}$$

are the odd frequency-moments of the spectral function $\chi''(q, \omega)$. It is easy to calculate the low-order moments and are given by

$$\langle\omega^1\rangle = \frac{nq^2}{m}, \tag{11}$$

$$\langle\omega^3\rangle = \frac{nq^2}{m}\left[\varepsilon_q^2 + \frac{3q^2}{m}\langle KE\rangle + \omega_p^2(q) + I(q)\right], \tag{12}$$

where $\langle KE\rangle$ is the kinetic energy per particle for the interacting charged Bose gas and $I(q)$ is defined by

$$I(q) = \frac{1}{m}\sum_{\boldsymbol{q}'\neq\boldsymbol{q}}(\boldsymbol{q}'.\hat{\boldsymbol{q}})^2 V(q')[S(\boldsymbol{q}'-\boldsymbol{q}) - S(\boldsymbol{q}')], \tag{13}$$

where $S(q)$ is the static structure factor. Comparing Eqs. (7) and (9), the first moment is automatically satisfied and the third moment will be satisfied if

$$G(q) = -\frac{1}{\omega_p^2(q)}\left[I(q) + \frac{3q^2}{m}(\langle KE\rangle - \langle KE\rangle_0)\right]. \tag{14}$$

For charged bosons, at absolute zero, $\langle KE\rangle_0 = 0$ and $\langle KE\rangle$ is related to the ground-state energy E_{gs} through the Virial theorem as

$$\langle KE\rangle = -\frac{d}{dr_s}(r_s E_{\mathrm{gs}}). \tag{15}$$

$$E_{\mathrm{gs}} = \int_0^{e^2} d\lambda \frac{E_{\mathrm{int}}(\lambda)}{\lambda}, \tag{16}$$

where λ measures the strength of the boson-boson interaction and $E_{\mathrm{int}}(\lambda)$ is given by

$$E_{\mathrm{int}}(e^2) = \frac{1}{N}\sum_q \frac{\pi n e^2}{q}[S(q) - 1]. \tag{17}$$

Further, $S(q)$ is related to the imaginary part, $\chi''(q, \omega)$, of $\chi(q, \omega)$ through the fluctuation-dissipation theorem as

$$S(q) = -\frac{\hbar}{n\pi}\int_0^{\infty} d\omega\chi''(q,\omega). \tag{18}$$

By using the Kramers-Kronig relation, the integral in Eq. (18) is simplified to give $S(q)$ as

$$S(q) = 1/[1 + 2n\psi(q)/\varepsilon_q]^{1/2}, \tag{19}$$

which is the famous Feynman-Biji formula. Eqs. (14)–(19) impose the self-consistent condition on $G(q)$ and it seems numerically difficult to obtain the self-consistent solution. The difficulty appears to arise in the calculation of $\langle KE\rangle$ from Eqs. (15)–(17) during each step in the iterative scheme. However, if we assume that $\langle KE\rangle$ is small enough to be negligible, the self-consistency imposed by Eqs. (15)–(17) is relaxed. This assumption is equivalent to state that the Coulomb interactions between charged bosons cause negligible change in the ideal Bose-Einstein distribution function. It seems from the recent DMC calculation of boson distribution function in 3D [14] that this may be a reasonable approximation at low Coulomb coupling strength (r_s). The correlational contribution to the kinetic energy was also neglected in the PV theory proposed originally for the electron fluid. In the next section, we solve Eqs. (14) and (19) self-consistently by taking $\langle KE\rangle = 0$ and present numerical results for the various quantities of interest.

3. RESULTS AND DISCUSSION

In the numerical calculations and the results presented, we use a system of units in which $\hbar = 1$ and lengths are expressed in units of q_s^{-1} with $q_s = \sqrt{2}/[r_s a_0]$.

3.1. Pair-Correlation Functions

Expressed in above units, Eqs. (19) and (14) become

$$S(q) = 1\bigg/\left[1 + \frac{2^{3/2} r_s}{q^3}(1 - G(q))\right]^{1/2}. \tag{20}$$

$$G(q) = -\frac{1}{2\pi q}\int_0^{\infty} dk k \int_0^{2\pi} d\phi \left[\frac{(q+k\cos\phi)^2}{(q^2+k^2+2qk\cos\phi)^{1/2}} - k\cos^2\phi\right][S(k)-1]. \tag{21}$$

Eqs. (20) and (21) are solved numerically in a self-consistent way by taking the RPA ($G(q) = 0$) structure factor as the initial guess. A self-consistent solution is obtained within a tolerance of about 0.01% in about 10–20 iterations depending upon the value of r_s. Results for the self-consistent structure factor are plotted in Figure 1 for $r_s = 1, 3, 5, 10$. Also shown in the same figure are the STLS results at $r_s = 1$ and 10. The DMC results are not readily available for $S(q)$, rather, its real-space transform, i.e., the pair-correlation function $q(r)$, is known at various r_s values. $g(r)$ can be determined from $S(q)$ by taking its inverse Fourier transform as

$$g(r) = 1 + \int_0^{\infty} dq\, qJ_0(qr)[S(q) - 1]. \tag{22}$$

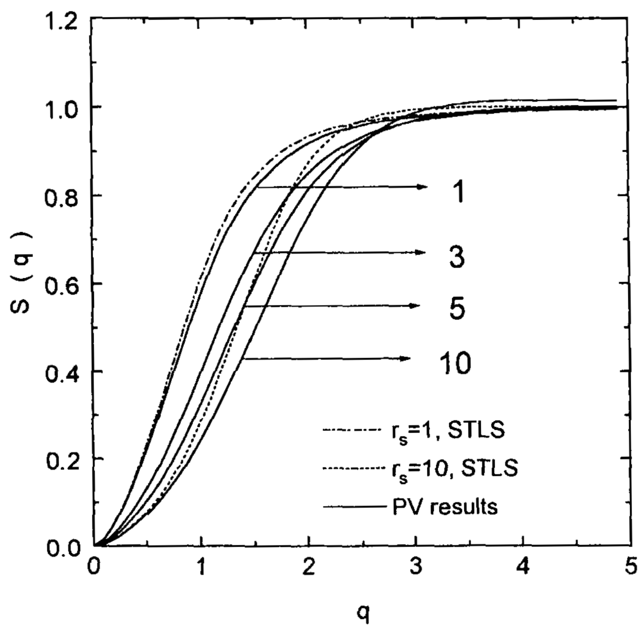

FIGURE 1 The static structure factor $S(q)$ vs q at various values of r_s in comparison with the STLS results at $r_s = 1$ and 10.

In Figure 2, $g(r)$ is shown for different r_s values in comparison with the results of the STLS theory and the DMC calculation. It is apparent that the behavior of $g(r)$ in STLS is overall in better agreement with the DMC data and in particular, it fulfills the condition of its positive definiteness for $r_s \leq 5$. On the other hand, in the PV calculations $g(r)$ becomes negative at small r for $r_s \geq 2$. However, it may be noticed that, except at small r, the PV results match reasonably well with the DMC data. The reason for the poor quality of $g(r)$ at small r can be understood as follows: In our calculations, the third-frequency-moment sum rule is satisfied in an approximate way in the sense that we have neglected the q^2-term in the expression for $G(q)$ in Eq. (14).

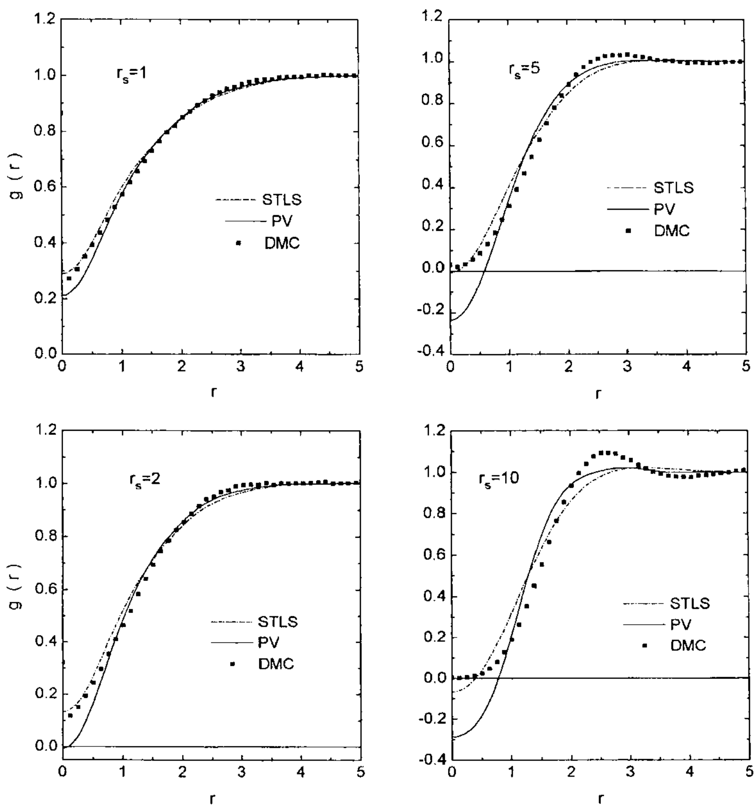

FIGURE 2 The pair-correlation function $g(r)$ vs r at various values of r_s; solid lines, the PV results; dash-dot lines, the STLS results; solid squares, the DMC results.

The assumption appears satisfactory at low vlaues of r_s where one can treat the kinetic energy term $\langle KE \rangle$ as negligibally small. However, with increasing r_s, $\langle KE \rangle$ grows with correlations and as a consequence, the q^2-term should contribute significantly at large values of q. Thus, the approximation used by us seems to be reasonable only in the low-q regime or at large r values. We anticipate an improvement in the small-r behavior of $g(r)$ if the numerical calculations are performed by exactly satisfying the third-moment sum rule, i.e., by taking into account the correlational kinetic energy contribution.

3.2. Excitation Spectrum and Ground-State Energy

The energy spectrum of the elementary excitations in the system is determined from the poles of density response function, i.e.,

$$1 - V(q)[1 - G(q)]\chi_0(q,\omega) = 0. \tag{23}$$

Substituting for $\chi_0(q, \omega)$ in above Eq., the excitation energy, $E(q) = \hbar \omega(q)$, turns out to be

$$E(q) = \omega_p(q)\left[[1 - G(q)] + \frac{q^3}{2^{3/2} r_s}\right]^{1/2} \tag{24}$$

In the long-wavelength limit, $E(q)$ is given approximately by

$$E(q) \approx \omega_p(q)\left(1 - \frac{1}{2}q\gamma\right); \quad \gamma = -\int_0^\infty dq\, q[S(q) - 1]. \tag{25}$$

As γ is positive definite, the plasmon dispersion coefficient is negative at all values of r_s. Results for $E(q)$ (in units of $\omega_p(q)$) for different r_s are plotted in Figure 3 alongwith the STLS curves at $r_s = 1$ and 10. The qualitative nature of $E(q)$ in the two theories is the same, but the minima in $E(q)$ is somewhat more pronounced in the STLS theory.

The ground-state energy E_{gs} defined by Eq. (16) can be expressed after some simplification as

$$E_{gs} = \frac{2^{1/2}}{r_s^2}\int_0^{r_s} dr_s' \int_0^\infty dq[S(q; r_s') - 1]. \tag{26}$$

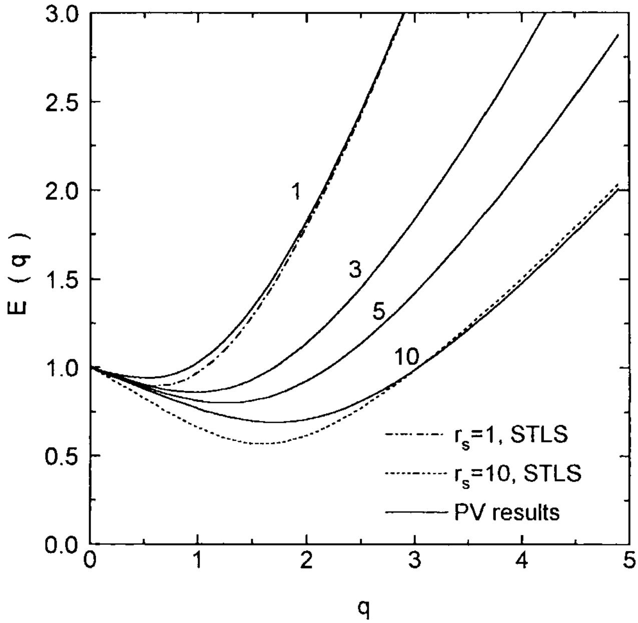

FIGURE 3 The excitation energy $E(q)$ (in units of plasmon frequency $\omega_p(q)$) vs q at various r_s values in comparison with the STLS results at $r_s = 1$ and 10.

In above Eq., E_{gs} is expressed in units of Rydberg ($1\text{Ry} = e^2/2a_0$). Eq. (26) is solved numerically to calculate E_{gs} and the results are given in Table I as a function of density alongwith the DMC values and the results of STLS and variational calculations [15]. The agreement of our results is reasonable with the DMC predictions. Hong and Choi [13] have argued in 3D that the PV theory as applied to the charged Bose system may provide a lower-bound to the ground-state energy. Their argument is based upon the fact that the use of mean-field approximation for $\chi(q, \omega)$, which neglects the frequency-dependence of the local-field correction, seems more reliable for the charged Bose system than for the electron gas since no low-lying continuum single-particle excitations exist in the former system. Further, the local-field factor is determined by satisfying the third-frequency moment of $\chi(q, \omega)$, which is otherwise not satisfied in the STLS theory. From Table I, our results also seem to yield a lower-bound for the ground-state energy, but unless there exists some rigorous proof for it, the

TABLE I The ground-state energy ($-E_{gs}$ in units of Rydberg) as a function of r_s

r_s	*PV*	*DMC*	*STLS*	*Ref.* [*15*]
1	1.1462	–	1.1121	1.1062
2	0.6842	0.6740	0.6519	0.6631
3	0.4998	–	0.4707	–
5	0.3317	0.3190	0.3083	0.3133
10	0.1850	0.1748	0.1725	0.1667

claim for the lower-bound may not be strong. An attempt to provide with an upper-bound on the plasmon dispersion and hence, a lower-bound on the ground-state energy has recently been made by Chiofalo *et al.* [16] for the 3DCBF. Their method has also been based upon the sum-rule arguments, but in a different fashion.

4. COMPARISON WITH THE 2D ELECTRON FLUID

So far, we have studied the ground state properties of the 2DCBF. In this part of the paper, we discuss briefly the results of the charged Bose fluid in comparison with those of a fluid of charged fermions, namely, the electrons. As one may expect, the difference in the behavior of two fluids will enable one to understand the importance of effects related to the statistics. The physical properties we consider for comparison are (i) the pair-correlation function, (ii) the static structure factor and (iii) the collective density excitation spectrum. We compare only the results of the STLS theory. In Figure 4, $g(r)$ is shown for the electron and Bose fluids at densities corresponding to $r_s = 1$ and 5. As expected, at small separation, $g(r)$ is larger in the Bose fluid than in the electron fluid. The reason underlying our expectation is that the bosons, in contrast to the fermions, do not obey Pauli exclusion principle. We also notice that (i) the difference in $g(r)$ for the two fluids is maximum at separations corresponding to the limit of small approach and at small r_s values and (ii) with increasing r_s, the two results become very close to each other. This implies that the exchange correlation effects associated with the electron statistics become less important with increasing r_s and correlations at large r_s are determined essentially by Coulomb effects. A similar behavior of correlations is also reflected in the static structure factor $S(q)$ and for an illustration, results for $S(q)$ are compared in Figure 5.

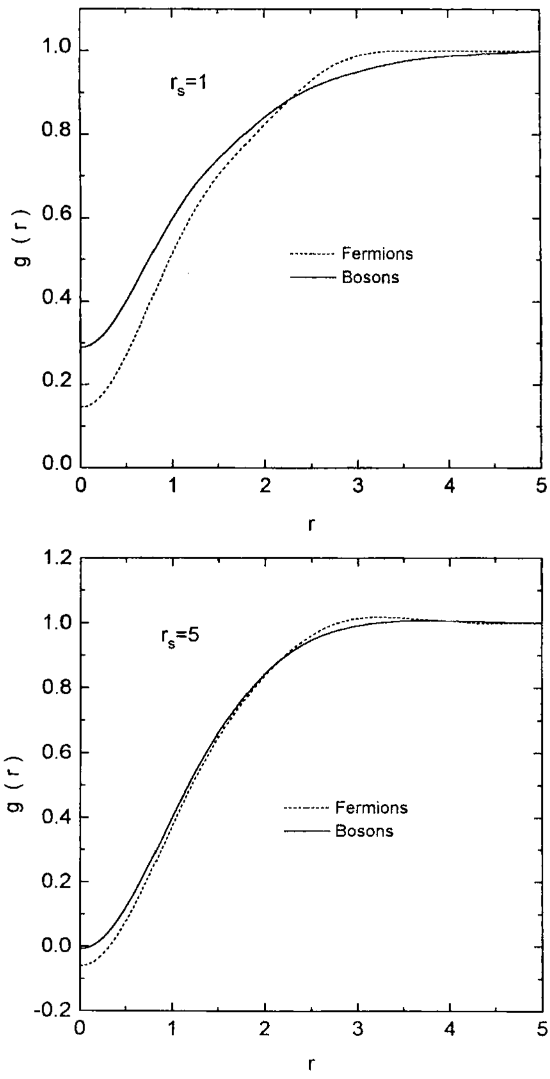

FIGURE 4 The pair-correlation function $g(r)$ vs r for bosons and fermions in STLS at $r_s = 1$ and 5.

Finally, we compare the spectrum of elementary excitations in the two fluids. For the fermion fluid, there exists two kinds of excitations in the system, namely (i) the single particle electron-hole pair excitations and (ii) the collective density (plasmon) excitations. The

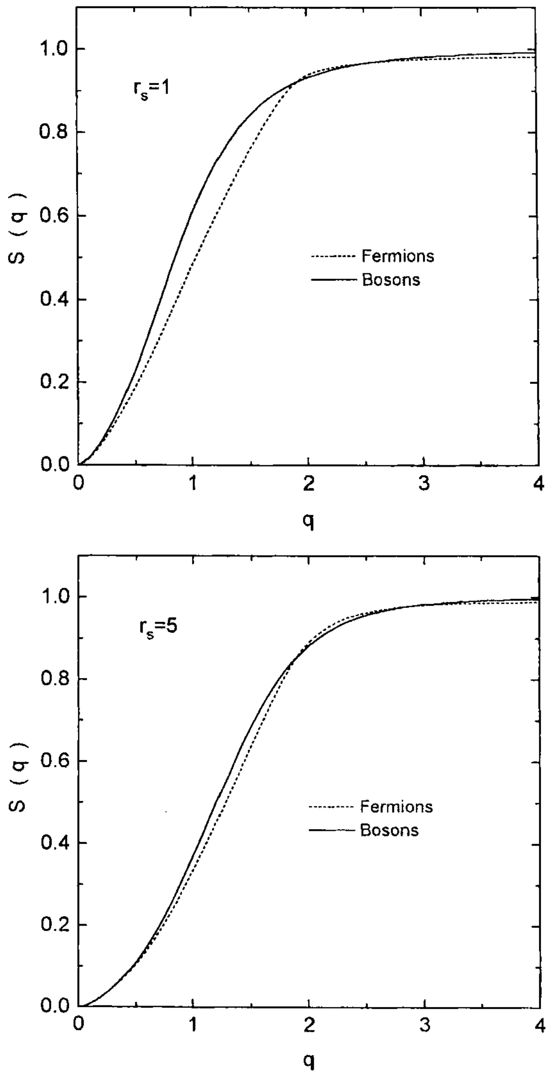

FIGURE 5 The static structure factor $S(q)$ vs q for bosons and fermions in STLS at $r_s = 1$ and 5.

plasmon excitation has infinite life-time at $q = 0$. However, at finite q, this has both dispersion and damping and meets the electron-hole pair continuum at a critical value of q. The dispersion curves for the plasmon excitation (in units of plasmon frequency $\omega_p(q)$) in the case of electron fluid are shown in Figure 6 at different r_s. In contrast with the Bose fluid (Fig. 3), the dispersion curve for the fermion fluid exhibits a minimum only when $r_s \geq 2$. This difference in the excitation spectrum of two fluids clearly demonstrates the importance of correlation effects in the Bose fluid even in the high density limit. Chiofalo, Conti, and Tosi [17] have drawn a similar comparison between electron and charged Bose fluids in 3D. On cross examining the results, we find that the qualitative nature of the difference in the behavior of two fluids does remain same while going from 3D to 2D.

5. CONCLUSIONS

We have studied the ground state of a two-dimensional charged Bose fluid within the self-consistent mean-field approximation. The

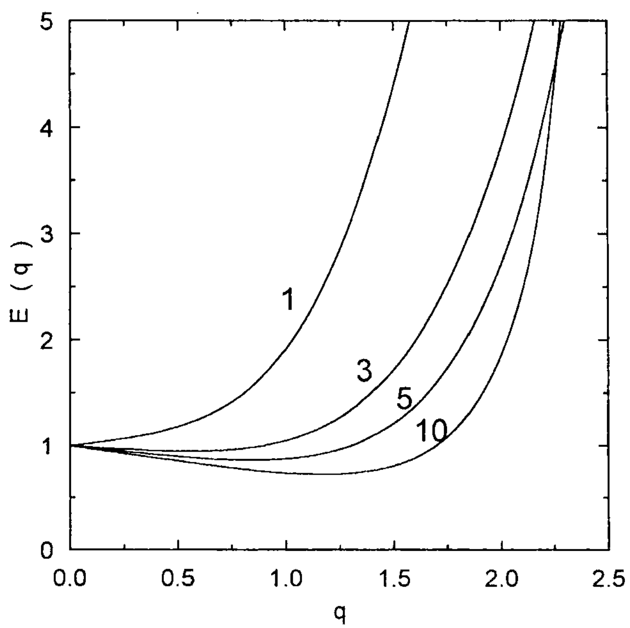

FIGURE 6 The collective density excitation spectrum $E(q)$ (in units of plasmon frequency $\omega_p(q)$) vs q for fermions in STLS at various values of r_s.

correlation effects are incorporated by satisfying in an approximate way the third-frequency moment sum rule of the density response function. The ground-state properties thus obtained are found to be in reasonable agreement with the diffusion Monte Carlo calculation provided the density is sufficiently high ($r_s \leq 2$). The reason underlying the relatively poor quality of PV results for $r_s > 2$ has its probable origin in the neglect of correlational kinetic energy term in the expression for the local-field correction factor (Eq. (14)). In view of recent DMC calculation of the boson distribution function in 3D, the PV approximation (namely, setting $\langle KE \rangle = 0$) seems reliable only in the high density limit. The DMC study reveals that the interacting Bose distribution function shows difference from its ideal behavior and this effect becomes more pronounced with increasing r_s. This, in turn, implies a depletion of the condensate phase which we have presently assumed. Thus, an increase in r_s contributes towards an increase in correlational kinetic energy and consequently, the PV approximation becomes less valid. The inclusion of effects related with the depletion of condensate phase desires further study of the problem.

We have also presented a comparison between the results of electron and charged Bose fluids. The comparison reveals that the statistics effects play an important role in determining the properties of the fluid at least in the intermediate fluid density range. However, at sufficiently large r_s, it seems that the correlations are essentially determined by the Coulomb correlations.

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