Two-dimensional Yukawa Bose liquid: A Singwi-Tosi-Land-Sjölander study

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We study the ground-state properties of a two-dimensional Yukawa boson liquid within the self-consistent scheme of Singwi *et al.* [Phys. Rev. **176**, 589 (1968)]. The interaction potential being short ranged and having a soft core is the screened Coulomb interaction in two dimensions. We calculate the static structure factor and local-field corrections describing the short-range correlation effects, and compare our results with the Monte Carlo simulations. [S0163-1829(98)02323-6]

I. INTRODUCTION

The many-body problem of a collection of particles obeying Bose statistics and a given interparticle interaction is a paradigm for understanding various physical properties of realistic systems such as liquid helium and neutron matter. The fluid of charged bosons embedded in a uniform neutralizing background is another model with possible relevance and application to superconductivity. Bosons interacting with the Yukawa potential [i.e., $V\sim \exp(-r)/r$ in three dimensions] has been used to determine the crystallization of systems with soft-core potentials.[1]

In this work, we study the ground-state properties of a two-dimensional Yukawa Bose liquid (2D-YBL) within the self-consistent-field method. There are several motivating reasons for our investigation. In two dimensions, the Yukawa bosons interact via the potential $K_0(r/\sigma)$, which may be regarded as the screened Coulomb potential with σ being the screening length. The celebrated self-consistent-field method of Singwi, Tosi, Land, and Sjölander[2] (STLS) has been applied to a variety of bosonic systems to determine the ground-state correlations. These include charged bosons interacting via the long-range Coulomb forces,[3] systems with short-range interactions,[4] and systems with hard-core interactions.[5] Results are often compared to the available Monte Carlo (MC) simulations which provide accurate ground-state energies. The STLS approach enjoys reasonable success, especially in the weak to moderate coupling regime. The 2D Yukawa potential can be termed as short ranged with a soft core. Recent calculations on the charged bosons interacting via a $\ln(r)$ potential[6] showed qualitative agreement with the MC simulations[7] on the same system in the fluid phase. Thus, it seems timely to apply the STLS method to the 2D-YBL problem to obtain some complementary results to the current MC simulations.[8,9] Another impetus for studying the 2D-YBL comes from the suggestion of Nelson[10] that the classical statistical mechanics of flux-line liquids as occur in high-T_c superconductors can be mapped onto a 2D quantum system. The observation of the melting of the vortex lattices in high-T_c materials[11] such as $YBa_2Cu_3O_{7-\delta}$ and $Bi_2Sr_2CaCu_2O_{8+x}$ in transport, magnetization, and neutron-diffraction-type experiments have revealed a rich phase diagram. Theoretical calculations studying this melting transition range from quantum and classical MC simulations,[8,9,12,13] to density-functional theory approaches,[14] and perturbation expansion techniques.[15] The flux-line liquid model proposed by Nelson[10] assumes that London limit is applicable (the ratio of the penetration depth to coherence length is very large, which holds true for high-T_c materials), and the angular dependence of the vortex interaction is neglected.

Our primary aim is to see how well the STLS approach models the ground-state static and dynamic properties of 2D Yukawa bosons. To this end, we calculate the static structure factor, the pair-correlation function, and the dispersion of the collective modes to compare with available MC simulations. Both the zero-temperature quantum MC simulations of Magro and Ceperley[8] and the path-integral MC calculations of Nordborg and Blatter[9] indicate a first-order transition at about the same critical parameters. In our calculations we are limited to studying the fluid phase of the Yukawa boson model, thus little can be said about the possible freezing transition into the crystal phase. However, various ground-state correlation functions can signal the approach to the transition, as in the case of Bose Coulomb liquid.[6,7]

The rest of this paper is organized as follows. In Sec. II, we provide self-consistent-field equations for 2D-YBL. Section III contains the results of our calculations. We conclude with a brief summary in Sec. IV.

II. THEORY

The bare interparticle interaction for the Yukawa bosons in two dimensions is given by $U^0(r)=\epsilon\ K_0(r/\sigma)$, where K_0 is the zero-order modified Bessel function of the second kind, and ϵ and σ are, respectively, the fundamental energy and length scales; in relation to the type-II high- T_c superconductivity, they are matched to the material parameters.[10]

To characterize the 2D-YBL system, we employ the wave-number-space (q-space) formalism, there the 2D bare Yukawa interaction becomes $U^0(q)=2\pi\epsilon\sigma^2/(1+\sigma^2q^2)$, which is well behaved at the origin and short ranged, the consequences of which will be displayed in the following sections. For the dielectric formulation[16] of this many-body system, beyond the random-phase approximation (RPA), the self-consistent local-field correction scheme of STLS is implemented. The expression for the local-field correction (LFC), that incorporates the corrections to the RPA mean field, becomes

$$G(q_n)=\frac{1}{2\pi\rho}\int_0^\infty dp_n p_n[1-S(p_n)]\;\; I(p_n,q_n), \qquad (1)$$

where

$$I(p_n,q_n)=-\frac{1+q_n^2}{2q_n^2}\,\frac{1+p_n^2-q_n^2-\sqrt{(1+p_n^2+q_n^2)^2-4p_n^2q_n^2}}{\sqrt{(1+p_n^2+q_n^2)^2-4p_n^2q_n^2}}. \qquad (2)$$

In the above expressions and throughout the text we use normalized variables, denoted by the subscript n; using σ as the unit for length and ϵ for the energy, $\rho=n\sigma^2$ also represents the normalized density with n being the density. Unlike the case with the long-range interactions as in electron liquids,[2] the short-range nature of the Yukawa potential reflects itself with a nonzero value for the $q\to0$ limit of the LFC, given by

$$G(q_n=0)=\frac{1}{2\pi\rho}\int_0^\infty dp_n\frac{p_n}{(1+p_n^2)^2}[1-S(p_n)]. \qquad (3)$$

The static structure factor of the 2D-YBL depends on the LFC through

$$S(q_n)=\frac{1}{\left(1+\dfrac{4\pi\rho}{(1+q_n^2)\Lambda^{*2}q_n^2}[1-G(q_n)]\right)^{1/2}}, \qquad (4)$$

where $\Lambda^*=[\hbar^2/2m\sigma^2\epsilon]^{1/2}$ is the de Boer parameter. Equations (1) and (4) are solved iteratively, until a self-consistent solution is reached within a predetermined tolerance value. In arriving at Eq. (4), one major simplification is made, by assuming total Bose-Einstein condensation for the *noninteracting* 2D bosons, which is actually known to be impossible in two dimensions.[17] The outcomes of this simplification are assessed in Sec. III by comparing our results, with the formally exact, quantum Monte Carlo (QMC) method. So the noninteracting density response function in condensate approximation of the the 2D bosons, along the imaginary frequency axis $i\omega$, becomes

$$\chi^0(q,i\omega)=\frac{-2n\epsilon_q}{(\hbar\omega)^2+\epsilon_q^2}, \qquad (5)$$

where n is the density and $\epsilon_q=\hbar^2q^2/2m$. The corresponding interacting density response function is given as

$$\chi(q,i\omega)=\frac{\chi^0(q,i\omega)}{1-U^0(q)[1-G(q)]\chi^0(q,i\omega)}. \qquad (6)$$

Equation (4) is obtained by applying the fluctuation-dissipation theorem[16] along the rotated —imaginary— frequency axis[18] as

$$S(q)=-\frac{\hbar}{n\pi}\int_0^\infty d\omega\;\chi(q,i\omega); \qquad (7)$$

performing the frequency integral yields Eq. (4).

For the organization of our presentation, we list the remaining expressions for the quantities needed in characterizing the 2D-YBL. The pair-correlation function becomes

$$g(r_n)=1+\frac{1}{2\pi\rho}\int_0^\infty dq_nq_nJ_0(q_nr_n)[S(q_n)-1], \qquad (8)$$

where $r_n=r/\sigma$ is the normalized 2D radial distance and $J_0(x)$ is the zero-order Bessel function of the first kind. Collective excitations of the 2D-YBL can be characterized both by the dispersion relation and the density of these collective excitations. The former occurs at the normalized —to ϵ— energies

$$E_{n,c}(q_n)=\Lambda^*q_n\sqrt{\Lambda^{*2}q_n^2+\frac{4\pi\rho}{1+q_n^2}[1-G(q_n)]}. \qquad (9)$$

The density of collective excitations is defined as $D_c(E)=\Sigma_{\mathbf{q}}\delta[E-E_c(q)]$, which reduces to

$$D_c(E)=\frac{A}{2\pi}\sum_i\frac{1}{\left|\dfrac{dE_c(q_i)}{dq_i}\right|}, \qquad (10)$$

where q_i is the ith root of the equation $E_c(q)=E$; in our results, we take the area A to be unity, or equivalently, we refer to density of collective excitations per unit area.

III. RESULTS AND DISCUSSION

The two dimensionless parameters controlling the underlying physics of the 2D-YBL are the normalized density ρ and the de Boer parameter Λ^*, the latter being inversely related to the mass of the bosons. Using as a guideline the phase diagram of this system obtained by Magro and Ceperley,[8] we perform computations at the values $\Lambda^*=0.1$, 0.0645, and 0.05, for ρ ranging between 2 and 0.01. The path-integral Monte Carlo (PIMC) calculations of Nordborg and Blatter[9] place the liquid-solid transition to $\Lambda^*\approx0.062$ in agreement with Ref. 8. Even though we are content with the liquid phase, the indications of the liquid-solid phase transition exist in several quantities. We first display the LFC curves in the range of the ρ-Λ^* plane mentioned above; it can be noted from Fig. 1 that, as $\rho\to0$, $G(q)\to1$. Thus, in essence for very low densities, the LFC cancels the mean-field established by the RPA, suggesting there the use of the Hartree-Fock approach. The static structure factor curves in Fig. 2 show a tendency toward a structure formation as the density decreases. Furthermore, the peak value of $S(q)$ data is then seen to diminish beyond some density, in agreement

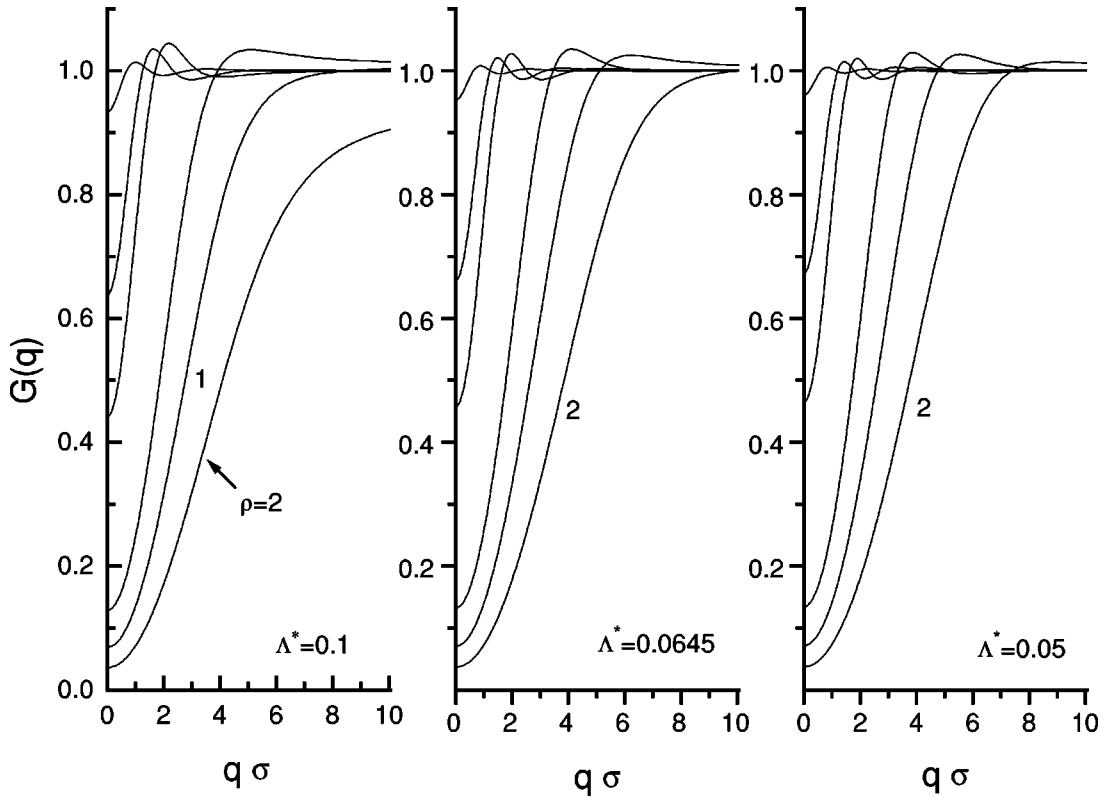

FIG. 1. Local-field correction of the 2D-YBL for $\Lambda^*=0.1$, 0.0645, and 0.05. At each Λ^* value, $\rho=2$, 1, 0.5, 0.1, 0.05, and 0.01 curves are plotted, ordered sequentially with the $\rho=2$ ones being indicated.

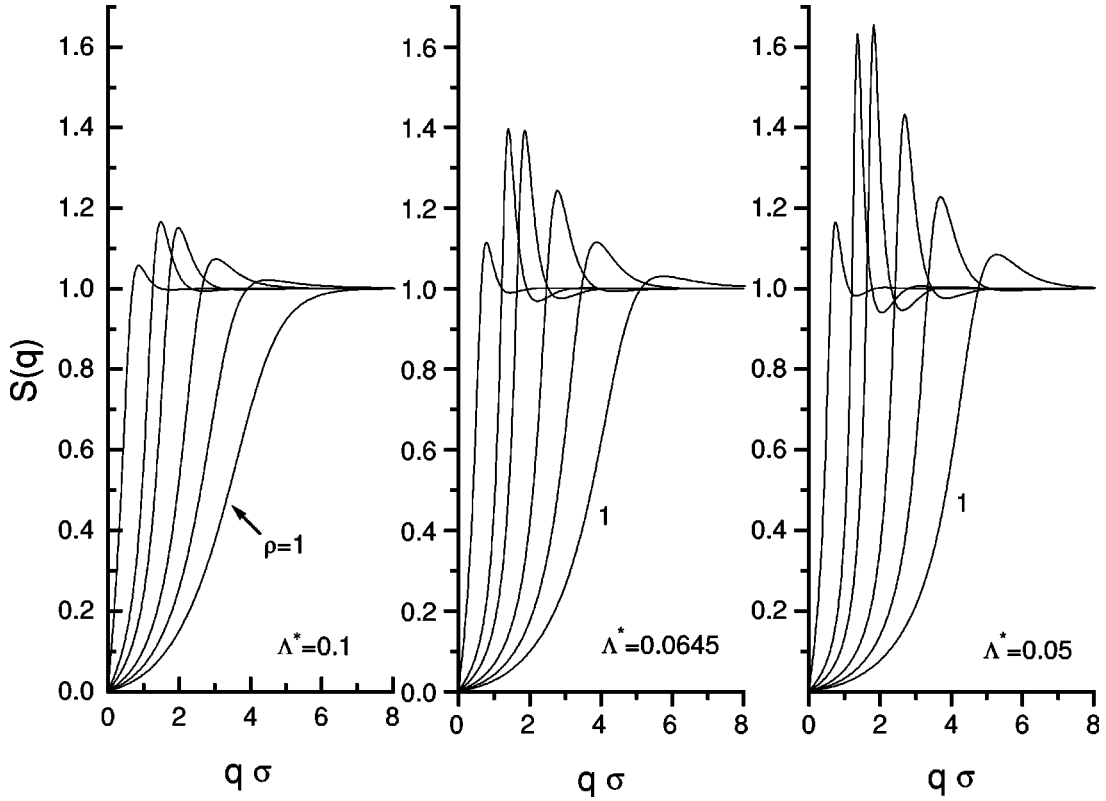

FIG. 2. Static structure factor of the 2D-YBL for $\Lambda^*=0.1$, 0.0645, and 0.05. At each Λ^* value, $\rho=1$, 0.5, 0.25, 0.1, 0.05, and 0.01 curves are plotted, ordered sequentially with the $\rho=1$ ones being indicated.

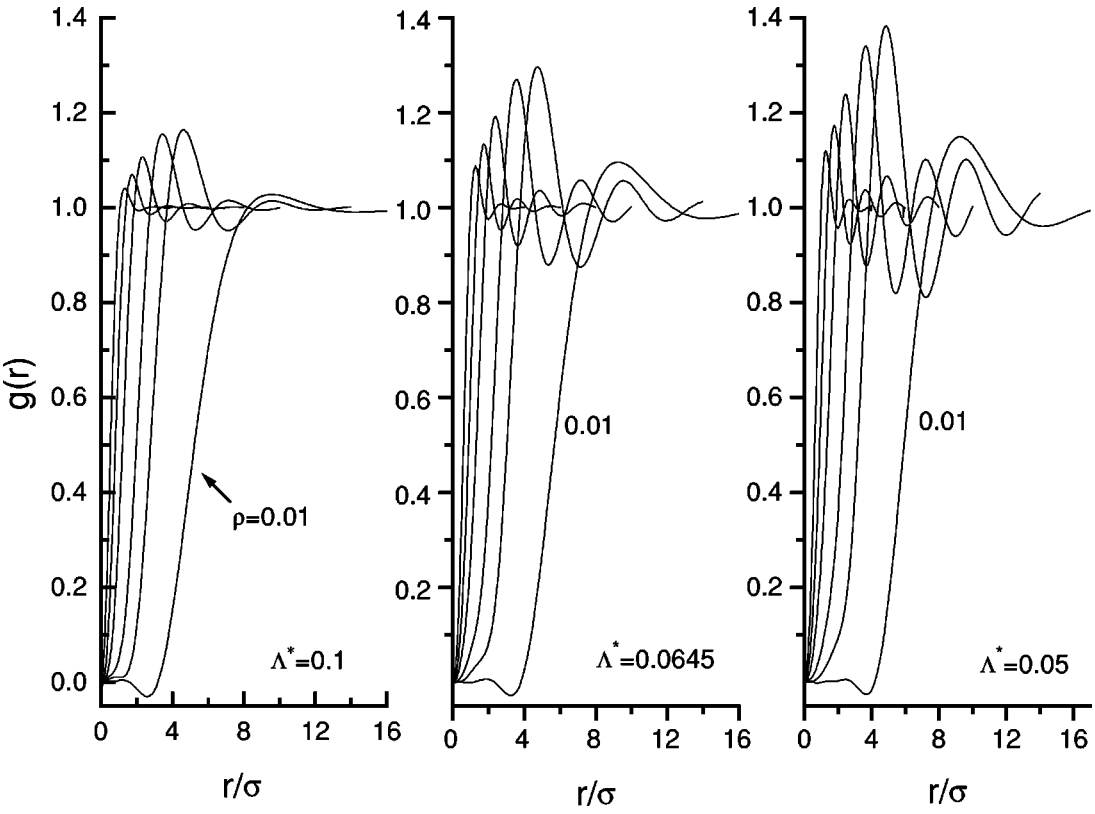

FIG. 3. Pair-correlation function of the 2D-YBL for $\Lambda^*=0.1$, 0.0645, and 0.05. At each Λ^* value, $\rho=1$, 0.5, 0.25, 0.1, 0.05, and 0.01 curves are plotted, ordered sequentially with the $\rho=0.01$ ones being indicated.

with the crossing of a solid-liquid phase boundary interpretation. Similar conclusions can be drawn from the pair-correlation function analysis, illustrated in Fig. 3. As a matter of fact, the phase diagram obtained by Magro and Ceperley[8] shows a reentrant behavior along the ρ direction for a constant Λ^* value, so that liquid-to-solid and solid-to-liquid transitions occur at two distinct ρ values. Our $g(r)$ and $S(q)$ results signal the presence of the phase boundary belonging to the low-ρ branch only, bringing the possibility of the other high-ρ branch being a higher-order transition. An energy-based consideration is required for the exact location of the phase boundary, as our estimates from these plots are rough. In Fig. 4, we compare our (STLS) $g(r)$ results at $\rho=0.02$ and $\Lambda^*=0.0645$, with the MC data of Magro and Ceperley.[8] The STLS results agree very well with the variational Monte Carlo results; however, the diffusion Monte Carlo technique shows more pronounced structure than these two. It is conceivable that a more refined integral-equation based theory such as the hypernetted-chain (HNC) approximation may capture the information contained in MC simulations. Recent application of the HNC method to charged bosons has been very successful in this regard.[19]

The collective excitation dispersion shows the maxon-roton structure as displayed in Fig. 5, gradually disappearing toward low densities. The low-density limiting behavior can be obtained from Eq. (9) using $G(q)\rightarrow 1$ as $E_{n,c}(q_n) \rightarrow \Lambda^{*2} q_n^2$. There is no gap in the long-wavelength excitation energy for 2D-YBL, in contrast to the case of Bose Coulomb liquid interaction via $\ln(r)$ potential.[6,7] Our results are qualitatively similar to the recent PIMC simulation results of Nordborg and Blatter.[9] In fact, the critical parameters ρ_c and Λ_c^{*2}, at which the roton energy vanishes, are usually interpreted as the transition to the solid phase. The zero of the excitation spectrum may be considered as a *soft mode*, and the wave vector q_c associated with it indicates the periodicity of the lattice. The q values where roton minima occur, can be matched —but not exactly— to those q values where $S(q)$ attains a peak. We can obtain the roton effective mass m^* from the curvature of the dispersion curve at the wave number q_{n0} corresponding to the roton minimum as, $m/m^* = E''_{n,c}(q_{n0})/(2\Lambda^{*2})$, where m is the free boson mass. In

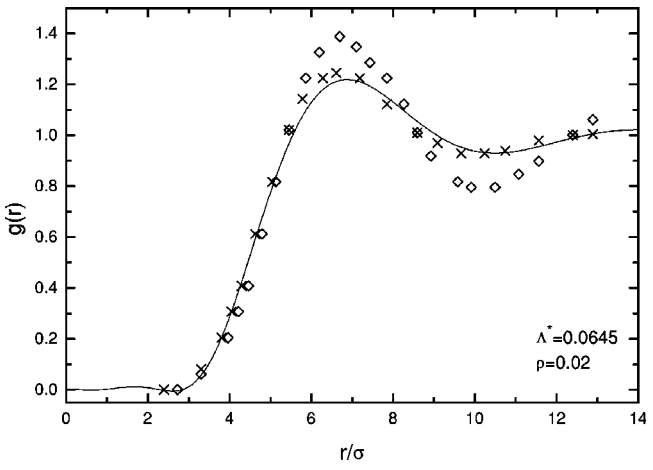

FIG. 4. Comparison of the pair-correlation functions of the STLS (solid line), diffusion Monte Carlo (diamonds), and the variational Monte Carlo (crosses) methods. The Monte Carlo data are extracted from the plot in Ref. 8.

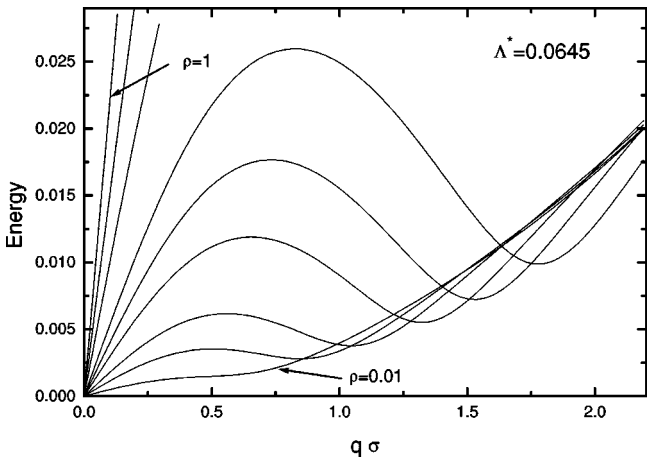

FIG. 5. Collective excitation dispersion of the 2D-YBL for $\Lambda^*=0.0645$. Energies are normalized to ϵ. $\rho=1$, 0.5, 0.25, 0.1, 0.07, 0.05, 0.03, 0.02, and 0.01 curves are shown, ordered sequentially with the $\rho=1$ and 0.01 curves being indicated.

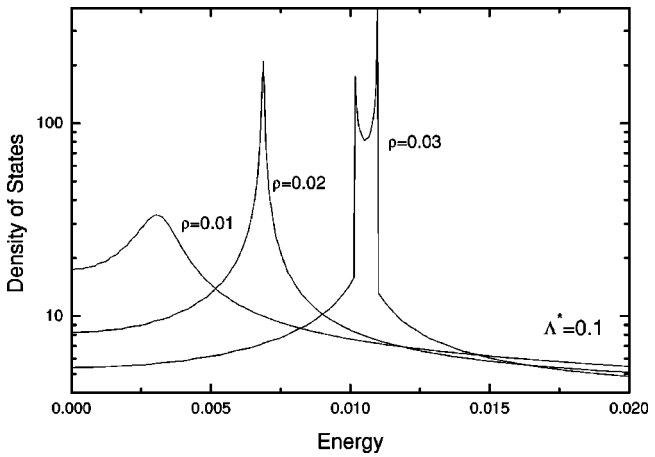

FIG. 6. Density of collective excitations (per unit area) of the 2D-YBL with respect to normalized energy for $\Lambda^*=0.1$.

Table I, we tabulate m/m^* values for the curves displayed in Fig. 5. In this table we also include the estimate obtained by expanding the energy spectrum around q_{n0} to yield $m/m^*=[2/S(q_{n0})-q_{n0}^2S''(q_{n0})/S(q_{n0})^2]/2$, under the approximation that $S'(q_{n0})$ vanishes, which is responsible from the slight deviation from the curvature calculation. The observation is that, among the densities considered, m/m^* has its largest value at the $\rho=0.1$.

The density of collective excitations presents the information contained in the dispersion curves in an alternative way, and is likely to be observed experimentally. It has been found useful to study the plasmon density of states in interpreting the photoelectron spectra in layered materials, particularly high-T_c superconductors.[20] A double-peak —in our case divergence— behavior is indicative of the maxon-roton structure. As the density is lowered these peaks merge and then diminish, as seen in Fig. 6.

Our treatment focuses on the zero-temperature properties of the liquid state of the 2D Yukawa bosons. Therefore, it seems as if little can be said about the solid-liquid phase transition boundary. However, recent freezing theories developed by Senatore and co-workers,[21,22] and Denton, Nielaba, and Ashcroft[23] aim to predict the phase-transition point using as input, the structural information of the liquid phase. Particularly, using both the second-order functional expansion theory and weighted-density approximations, they arrived at the conclusion that,[22] the freezing of the liquid state requires $G(\mathbf{G})>1$, for some reciprocal-lattice vector $\mathbf{G}$. According to this finding and our results in Fig. 1, we can simply conjecture that at $\Lambda^*=0.1$ value for $\rho=2$ and 1, crystalline phase is not favorable. Moroni and Senatore[22] applied their second-order theory to the crystallization of ^{4}He at zero temperature, which bares some resemblance with the YBL due to common Bose statistics and similar short-ranged interactions. A key quantity in their formalism is the so-called quantum direct correlation function $K(q)$, given as

$$K(q)=\frac{1}{\chi^0(q,0)}-\frac{1}{\chi(q,0)}. \tag{11}$$

Using Eq. (6), this function can be put into the form

$$\frac{nK(q_n)}{\epsilon}=\frac{2\pi\rho}{1+q_n^2}[1-G(q_n)]. \tag{12}$$

Moroni and Senatore observed that[22] the use of Feynman approximation to this expression, given by

$$\frac{nK_F(q_n)}{\epsilon}=\frac{\Lambda^{*2}q_n^2}{2}\left[\frac{1}{S^2(q_n)}-1\right], \tag{13}$$

leads to appreciable deviations from the experimentally obtained quantum direct correlation function, with the Feynman approximation having larger oscillations around zero. In Fig. 7, we plot the direct correlation function $K(q)$ calculated from Eq. (12) [or Eq. (13), as they are the same within our Bogoliubov-Feynman type-approximation] for the 2D-YBL system. The interesting observation is that use of Feynman approximation for 2D Yukawa bosons does not lead to large oscillations as in the ^{4}He problem. The systematic application of density-functional freezing theories to the 2D Yukawa Bose system seems to be beneficial for both assessing these freezing theories and validating the phase diagram obtained by the QMC or PIMC techniques.[8,9]

In the dielectric formulation of the interacting bosons, we have used the response function, assuming that all the par-

TABLE I. Wave numbers (q_{n0}) corresponding to roton minima and normalized reciprocal roton effective masses (m/m^*) at $\Lambda^*=0.0645$. For m/m^*, both curvature results and estimates using expansion in terms of static structure factor —see text— are given.

ρ	q_{n0}	m/m^* (curvature)	m/m^* (expansion)
0.02	0.85	5.4	5.5
0.03	1.05	9.2	9.3
0.05	1.32	13.7	13.8
0.07	1.53	15.8	16.0
0.1	1.78	16.9	17.0
0.25	2.60	14.5	14.7
0.5	3.46	10.3	10.4
1.0	4.54	6.6	6.7

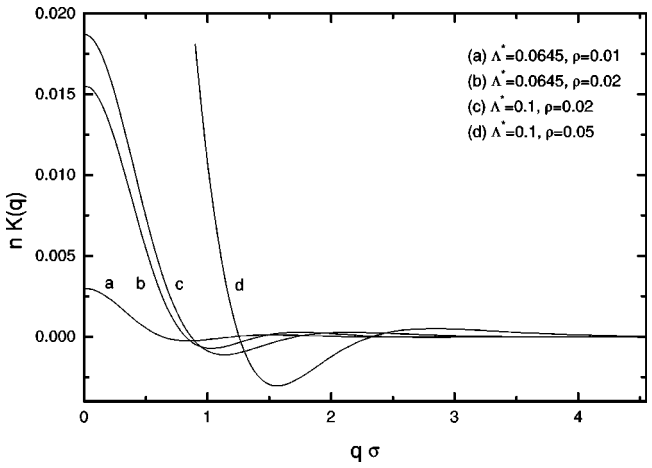

FIG. 7. nK normalized to ϵ vs the normalized wave number, where n is the density of 2D-YBL, and K is the quantum direct correlation function. Several ρ and Λ^* combinations are considered.

ticles are in the condensate. In general, the interaction effects would deplete the condensate, which we have not accounted for in a self-consistent manner. The condensate depletion should have the effect of decreasing the static structure factor $S(q)$, lowering the collective-mode excitation energies, and thus reducing the the sound velocity associated with the long-wavelength phonons. The MC simulations[7–9] strongly indicate that there is no condensate in the 2D Coulomb Bose liquid and YBL, but a superfluid phase exists. Our attempt to estimate the number of particles out of the condensate through the formula

$$N-N_0=\frac{1}{2}\sum_q \left(\frac{\epsilon_q-N_0U^0(q)}{E_c(q)}-1\right), \tag{14}$$

which is based on the Bogoliubov approximation, shows that the condensate depletion is rather sizable, especially in the strong coupling limit. From the surprisingly good agreement between the MC simulations and our results for the various correlation functions and the excitation spectrum, we may conclude that the present formulation models the ground-state properties reasonably well. A possible way of taking the non-condensed bosons into account, within the present formalism, would be to employ a model momentum distribution n_k for particles with $k\neq 0$. The response function $\chi(q,\omega)$ could be calculated with the model n_k, and the condensate fraction may be treated as a parameter. It would also be interesting to compare the static dielectric function calculated from $1/\varepsilon(q,0)=1+U^0(q)\chi(q,0)$ [i.e., the $\omega=0$ limit of the full dielectric function $\varepsilon(q,\omega)$] with the direct MC evaluation of the same quantity. Our calculations (not shown) indicate that as q approaches the reciprocal-lattice vector associated with the crystal phase, the magnitude of $1/\varepsilon(q,0)$ becomes very large, pointing towards the formation of a localized structure.

IV. SUMMARY

We have performed calculations on some static and dynamic properties of a 2D Yukawa Bose liquid using the self-consistent field method of Singwi *et al.*[2] The Yukawa bosons in two dimensions interact via the $K_0(r)$ potential, in contrast to the $\ln(r)$ potential of the Coulomb Bose liquid. We have studied the static structure factor, local-field factor, pair-correlation function, and dispersion of the collective modes for the 2D-YBL, and found reasonably good agreement with the available MC simulations. Our calculations for the liquid state signal the freezing transition at around the same critical parameters deduced from MC results.

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[1] D. Ceperley, G. V. Chester, and M. H. Kalos, Phys. Rev. B **17**, 1070 (1978); D. Ceperley, M. H. Kalos, and G. V. Chester, Phys. Rev. D **13**, 3208 (1976).
[2] K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968); K. S. Singwi and M. P. Tosi, Solid State Phys. **36**, 177 (1981).
[3] S. Conti, M. L. Chiofalo, and M. P. Tosi, J. Phys. (Paris) **6**, 8795 (1994); M. L. Chiofalo, S. Conti, and M. P. Tosi, Mod. Phys. Lett. B **8**, 1207 (1994).
[4] R. Lobo, Phys. Rev. B **2**, 2640 (1975).
[5] J.-P. Rino and N. Studart, Mod. Phys. Lett. B **10**, 1507 (1996).
[6] R. K. Moudgil, P. K. Ahluwalia, K. Tankeshwar, and K. N. Pathak, Phys. Rev. B **55**, 544 (1997); N. Mutluay and B. Tanatar (unpublished).
[7] W. R. Magro and D. M. Ceperley, Phys. Rev. Lett. **73**, 826 (1994).
[8] W. R. Magro and D. M. Ceperley, Phys. Rev. B **48**, 411 (1993).
[9] H. Nordborg and G. Blatter, Phys. Rev. Lett. **79**, 1925 (1997).
[10] D. R. Nelson, Phys. Rev. Lett. **60**, 1973 (1988); D. R. Nelson and H. S. Seung, Phys. Rev. B **39**, 9153 (1989); D. R. Nelson, J. Stat. Phys. **57**, 511 (1989).
[11] For a review, see P. H. Kes, H. Pastoriza, T. W. Li, R. Cubitt, E. M. Forgan, S. L. Lee, M. Konczykowski, B. Khaykovich, D. Majer, D. T. Fuchs, and E. Zeldov, J. Phys. I **6**, 2327 (1996).
[12] L. Xing and Z. Tešanović, Phys. Rev. Lett. **65**, 794 (1990).
[13] S.-T. Chui, Europhys. Lett. **20**, 535 (1992); H. R. Ma and S.-T. Chui, Phys. Rev. Lett. **67**, 505 (1991).
[14] S. Sengupta, C. Dasgupta, H. R. Krishnamurthy, G. I. Menon, and T. V. Ramakrishnan, Phys. Rev. Lett. **67**, 3444 (1991); G. I. Menon, C. Dasgupta, H. R. Krishnamurthy, T. V. Ramakrishnan, and S. Sengupta, Phys. Rev. B **54**, 16 192 (1996).
[15] E. Brézin, A. Fujita, and S. Hikami, Phys. Rev. Lett. **65**, 1949 (1990); S. Hikami, A. Fujita, and A. I. Larkin, Phys. Rev. B **44**, 10 400 (1991).
[16] D. Pines and P. Nozières, *The Theory of Quantum Liquids* (Benjamin, New York, 1966).

[17] P. C. Hohenberg, Phys. Rev. **158**, 383 (1967).
[18] D. Pines, *Elementary Excitations in Solids* (Benjamin, New York, 1963).
[19] V. Apaja, J. Halinen, V. Halonen, E. Krotscheck, and M. Saarela, Phys. Rev. B **55**, 12 925 (1997).
[20] H. Morawitz, I. Bozovic, V. Z. Kresin, G. Rietveld, and D. van der Marel, Z. Phys. B **90**, 277 (1993).
[21] G. Senatore and G. Pastore, Phys. Rev. Lett. **64**, 303 (1989).
[22] S. Moroni and G. Senatore, Europhys. Lett. **16**, 373 (1991); Phys. Rev. B **44**, 9864 (1991); C. N. Likos, S. Moroni, and G. Senatore, *ibid.* **55**, 8867 (1997).
[23] A. R. Denton, P. Nielaba, and N. W. Ashcroft, J. Phys. (Paris) **9**, 4061 (1997).