

Yukawa bosons in two-dimensional harmonic confinement

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The ground state property of Yukawa Bose fluid confined in a radial harmonic trap is studied. The calculation was carried out using the density functional theory formalism within the Kohn-Sham scheme. The excess-correlation energy for this inhomogeneous fluid is approximated via the local density approximation. A comparison is also made with the Gross-Pitaevskii model. We found that the system of bosons interacting in terms of Yukawa potential in a harmonic trap is energetically favorable compared to the ones interacting via contact delta potential.

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I. YUKAWA BOSE FLUID: AN INTRODUCTION

A system of N Bose particles interacting via the Yukawa potential is called Yukawa Bose fluid (for short, YBF). For three-dimensional space, $D=3$, the Yukawa potential takes the form $V_3(\vec{r})=(\epsilon\sigma/\vec{r})\exp(-\vec{r}/\sigma)$, where ϵ is an energy scale and σ is a length scale having the meaning of a screening length. For the two-dimensional case, however, it is described by $V_2(\vec{r})=\epsilon K_0(\vec{r}/\sigma)$, where $K_0(\vec{x})$ is the modified Bessel function that decays as $\exp(-\vec{x})/\sqrt{\vec{x}}$ at large distance while it behaves in a repulsive manner as $-\ln(\vec{x})$ at short distances. In other words, the Yukawa potential presents a combination of short range with soft-core-type potential.

Early numerical calculation (quantal Monte Carlo simulations) in studying the ground state property of the three-dimensional YBF can be traced back to the work of Ceperley *et al.*^{1,2} There was a spurt of interest in numerical calculation of two-dimensional (2D) ground state property of the 2D-YBF in the 1990s following the idea of Nelson and Seung³ who have shown that the statistical mechanics of the flux-line lattice (FLL) of high- T_c superconductors can be studied through an appropriate mapping onto the 2D-YBF. Magro and Ceperley⁴ have performed diffusion Monte Carlo (DMC) and variational Monte Carlo (VMC) numerical simulations to calibrate the ground state vortex properties and phases (liquid or solid) that correspond to the density and kinetic energy of the system. Similar work related to the first order phase transition of the Abrikosov lattice to liquid of vortices has been reported by Nordborg and Blatter⁵ using the path integral Monte Carlo method. In the late 1990s, other methods such as the STLS model^{6,7} appeared in studying the ground state properties of the 2D-YBF. It has to be noted that all these works were spiralling around the system of homogeneous fluid.

Our work will focus on the harmonically trapped system extending the work based on the quantal Monte Carlo calculations of Magro and Ceperley.⁴ Of particular interest to us is the phase diagram obtained by them for the parameters (ρ, Λ) at transition points displayed in Fig. 1. Here, Λ indicates the De Boer dimensionless parameter defined by $\Lambda^2 = \hbar^2/2m\sigma^2\epsilon$, while ρ and m denote the reduced density and atomic mass, respectively.

Magro and Ceperley⁴ observed that for a particular region $\Lambda > 0.09$, the system is dominated by kinetic energy and

does not crystallize. Below this threshold, however, a peculiar behavior of reentrant liquid has been observed, which means that system is in the liquid phase at very low density as well as at high density. The crystal melts on compression and expansion. It is known that at low density, the system is in liquid phase due to the fact that the screened potential cannot bind to solid phase particles that are, on average, too far apart. For the high density, the crystal is known to melt similar to the mechanism of thermal melting of a Wigner crystal. However, in this work, we are dealing with the liquid phase of Yukawa bosons only. Our calculation rely on the data of the liquid phase near the transition point from the phase diagram (Fig. 1) as an input to the local density approximation (LDA). The use of density functional theory (DFT)-LDA in this work is only a matter of computational convenience primarily due to the availability of the exact Monte Carlo⁴ data of the homogeneous system.

The motivation behind this work is that we believe that the theory of 2D-YBF can be used in studying the ground state property of the strongly correlated liquid formed at the melted phase of many vortex system in the dilute trapped Bose gas.⁸⁻¹⁰ In the latter system, Bose-Einstein condensate (BEC) is completely depleted by quantum fluctuations, and quantum liquids appear with excitations that can carry fractional statistics. In this situation, vortices can be treated as fundamental objects forming themselves as strongly correlated quantum fluid. This idea has been used in explaining certain features of Hall conductance and magnetization ex-

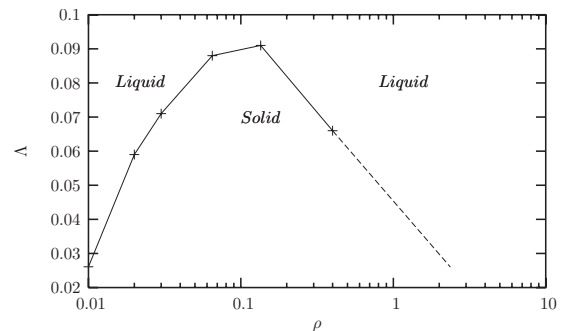


FIG. 1. The phase diagram of Yukawa bosons reproduced from Ref. 4. The pluses are transition points computed with DMC. The dashed line at high densities is the scaling law: $\Lambda \sim 0.04/\sqrt{\rho}$.

periments in high- T_c superconductors.^{5,11,12} On the other hand, the repulsive nature of vortices interacting in the short ranges is well described by the soft-core logarithmic potential. At the edge of the trap, the potential is smoothed out by $\exp(-\tilde{x})/\sqrt{\tilde{x}}$ that decays to zero, making it computationally tractable and ruling out any instability that may occur at the trap boundary. This characteristic makes it plausible for the vortex liquid to be mapped as Yukawa bosons in a similar fashion to one adapted by Nelson and Seung³ for the YBFLL in the high T_c superconductors.

The paper is outlined as follows. In Sec. II, we introduce the density functional theory formalism in showing that by choosing a particular type of auxiliary external trapping potential, the noninteracting system of bosons can be mapped to a real interacting system. We present the numerical calculation the Kohn-Sham equation and Gross-Pitaevskii (GP) in Sec. III. Then, the numerical results will be discussed and concluded.

II. APPLICATION OF DENSITY FUNCTIONAL THEORY IN THE YUKAWA BOSONS SYSTEM

The DFT is originally based on the notion that for a many-electron system, there is a one-to-one mapping between the external potential and the electron density: $v_{ext}(\mathbf{r}) \leftrightarrow \rho(\mathbf{r})$. In other words, the density is uniquely determined given a potential and vice versa. All properties are therefore a functional of the density, because the density determines the potential, which determines the Hamiltonian, which determines the energy and the wave function. Following this train of reasoning, the inhomogeneous dilute system of N interacting bosons can be described within the second quantization language as

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \int d\mathbf{r} \psi^\dagger(\mathbf{r}) V_{ext}(\mathbf{r}) \psi(\mathbf{r}) \\ &+ \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') V(|\mathbf{r} - \mathbf{r}'|) \psi(\mathbf{r}') \psi(\mathbf{r}) \\ &= \hat{H}_0 + \hat{V}_{ext} + \hat{V}_{int}, \end{aligned} \quad (1)$$

where $\hat{H}_0 = \int d\mathbf{r} \psi^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 - \mu \right] \psi(\mathbf{r})$ and $V(|\mathbf{r} - \mathbf{r}'|)$ is the interatomic interaction potential. Here, $V_{ext}(\mathbf{r})$ is the external trapping potential, while m and μ are the atomic mass and the chemical potential, respectively. The annihilation and creation field operators are denoted by $\psi^\dagger(\mathbf{r})$ and $\psi(\mathbf{r})$, respectively, and obey the following Bose-Einstein commutation relations:

$$\begin{aligned} [\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')] &= \delta(\mathbf{r} - \mathbf{r}'), \\ [\psi(\mathbf{r}), \psi(\mathbf{r}')] &= [\psi^\dagger(\mathbf{r}), \psi^\dagger(\mathbf{r}')] = 0. \end{aligned} \quad (2)$$

Let us denote the ground state of the system as $|\Psi_o\rangle$ so the ground state energy is defined as $E_o = \langle \Psi_o | \hat{H} | \Psi_o \rangle$ and the ground state density by $n_o(\mathbf{r}) = \langle \Psi_o | \psi^\dagger \psi | \Psi_o \rangle$. The Hohenberg-Kohn (HK) theorem¹³ guarantees that there exists a unique functional of the density,

$$F[n] = \hat{H}_0[n] + \hat{V}_{int}[n], \quad (3)$$

irrespective of the external potential. The theorem was originally proven for fermions but its generalization also covers bosons. Following HK, we can write the total energy functional of the system as follows:

$$E[n] = F[n] + \int d\mathbf{r} V_{ext}(\mathbf{r}) n(\mathbf{r}). \quad (4)$$

Determination of the ground state energy E_o follows by imposing the stationary conditions

$$\frac{\delta E[n]}{\delta n(\mathbf{r})} = 0, \quad (5)$$

where we will obtain the ground state density $n_o(r)$ that is uniquely determined by the choice of our external potential V_{ext} . In general, the Hohenberg-Kohn theorem does not provide us with a computational scheme to determine the ground state energy. This is provided by the Kohn-Sham (KS) procedure.¹⁴ The idea is to use an auxiliary system (noninteracting reference system) and look for an external potential V_{ext}^s such that the noninteracting system has the same ground state density as the real, interacting system. We write the Hamiltonian of the auxiliary system in the following form:

$$\hat{H}^s = \int d\mathbf{r} \psi^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 - \mu \right] \psi(\mathbf{r}) + \int d\mathbf{r} \psi^\dagger(\mathbf{r}) V_{ext}^s(\mathbf{r}) \psi(\mathbf{r}). \quad (6)$$

Thus, for the ground state $|\Psi_o\rangle$, we can define the unique total ground state energy functional of the auxiliary that can be written as

$$E^s[n_s] = F^s[n_s] + \int d\mathbf{r} n_s(\mathbf{r}) V_{ext}^s(\mathbf{r}). \quad (7)$$

By the KS scheme, we note that $E^s[n_s]$ can be approximated to $E[n]$ or, in other words, the density of the auxiliary system $n_s(\mathbf{r})$ is equivalent to the real system $n(\mathbf{r})$ by choosing a proper choice of auxiliary external potential V_{ext}^s .

Using the above argument and comparing the energy term $F^s[n_s]$ of Eq. (7) with Eq. (3), we can deduce the following functional relation:

$$F[n] = F^s[n] + V_H[n] + F_{xc}[n], \quad (8)$$

where the second term \hat{V}_H is called the Hartree energy defined as

$$\hat{V}_H = \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' V(|\mathbf{r} - \mathbf{r}'|) n(\mathbf{r}) n(\mathbf{r}'). \quad (9)$$

The last term in Eq. (8) represents the exchange-correlation energy $E_{xc}[n(\mathbf{r})]$ that includes all the contributions to the interaction energy beyond the mean field Hartree term. Calculating the variational derivatives in Eq. (5) using Eq. (8), one finds

$$\frac{\delta F^s[n]}{\delta n(\mathbf{r})} + V_H(\mathbf{r}) + \frac{\delta F_{xc}[n]}{\delta n(\mathbf{r})} + V_{ext}(\mathbf{r}) = 0, \quad (10)$$

where the Hartree field reads

$$V_H(\mathbf{r}) = \int d\mathbf{r}' V(|\mathbf{r} - \mathbf{r}'|) n(\mathbf{r}'). \quad (11)$$

Performing a similar variational calculation on Eq. (7), we deduce that the density of the auxiliary system is identical to that of the actual system if

$$V_{ext}^s(\mathbf{r}) = V_{ext}(\mathbf{r}) + V_H(\mathbf{r}) + V_{xc}(\mathbf{r}), \quad (12)$$

where we have introduced in Eq. (12) the exchange-correlation potential $V_{xc} = \delta F_{xc}[n(\mathbf{r})] / \delta n(\mathbf{r})$, which is unknown for most of the systems of interest and thus one has to resort to approximations such as the local density approximation (LDA). This will be dealt with in the following section.

Local density approximation

Before we can actually implement the Kohn-Sham formalism, we have to devise some workable approximations for the exchange-correlation potential $V_{xc}(\mathbf{r})$. The first such approximation to be suggested was the LDA. The idea behind the LDA is very simple; it just ignores the nonlocal aspects of the functional dependence of $V_{xc}(\mathbf{r})$. The true form of $V_{xc}(\mathbf{r})$ will depend not only on the local density $n(\mathbf{r})$ but also on n at all other points \mathbf{r}' , and this functional dependence is, in general, not known. This difficulty is avoided with the assumption that V_{xc} depends only on the local density $n(\mathbf{r})$ and that $E_{xc}[n]$ can thus be written as

$$E_{xc}[n(\mathbf{r})] \approx \int d\mathbf{r} E_{xc}^{hom}[\rho]_{|\rho \rightarrow n(\mathbf{r})}, \quad (13)$$

where $E_{xc}^{hom}[\rho] = \rho \epsilon_{xc}[\rho]$ and $\epsilon_{xc}[\rho]$ is the exchange-correlation energy of a homogeneous system with uniform density ρ . The functional derivatives of the above relation read

$$V_{xc}[n(\mathbf{r})] = \frac{\delta E_{xc}[n(\mathbf{r})]}{\delta n(\mathbf{r})} = \left. \frac{\partial(\rho \epsilon_{xc}[\rho])}{\partial \rho} \right|_{\rho \rightarrow n(\mathbf{r})}. \quad (14)$$

The available numerical data of Magro and Ceperley⁴ and Strepparola *et al.*⁷ permit one to obtain information on the homogeneous excess free energy $f_{ex}[n]$ rather than the homogeneous exchange-correlation energy $f_{xc}[n]$. Thus, it is more convenient to work with excess free energy defined as¹⁵

$$F_{ex}[n(\mathbf{r})] = \hat{V}_H[n(\mathbf{r})] + F_{xc}[n(\mathbf{r})]. \quad (15)$$

In general, the excess-correlation functional energy $F_{ex}[n(\mathbf{r})]$ in a DFT calculation is not known exactly. One can resort to approximations such as the LDA, which reads

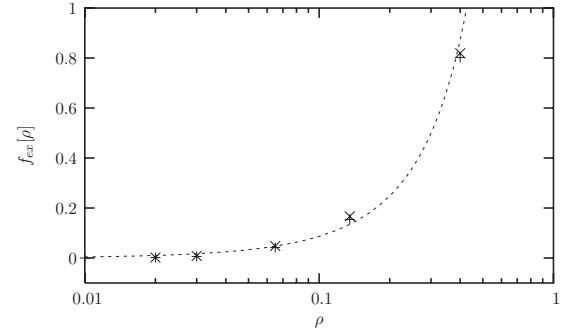


FIG. 2. Homogeneous excess-correlation energy $f_{ex}(\rho)$ versus the dimensionless homogeneous gas density ρ of the VMC data of Magro and Ceperley (Ref. 4) (pluses) and STLS data of Strepparola *et al.* (Ref. 7) (crosses) compared to the fit function [Eq. (18)] (dashed line).

$$F_{ex}[n(\mathbf{r})] \approx \int d\mathbf{r} F_{ex}^{hom}[n]_{|n \rightarrow n(\mathbf{r})}, \quad (16)$$

where $F_{ex}^{hom}[n] = n f_{ex}^{hom}[n]$. The functional derivatives (excess-correlation potential) of the above relation can be written as

$$V_{ex}(\mathbf{r}, n(\mathbf{r})) = \frac{\delta F_{ex}[n(\mathbf{r})]}{\delta n(\mathbf{r})} = \left. \frac{\partial(n f_{ex}[n])}{\partial n} \right|_{n \rightarrow n(\mathbf{r})}. \quad (17)$$

Information on the homogeneous excess-correlation energy $f_{ex}[n]$ can be obtained by subtracting the kinetic energy from the total ground state energy of a homogeneous system with N boson. In Fig. 2, plots of the DMC data of Magro and Ceperley⁴ and the STLS data of Strepparola *et al.*⁷ are depicted along with the following fit:

$$f_{ex}[\rho] = -\frac{2\rho}{\log(\rho)}. \quad (18)$$

III. NUMERICAL CALCULATION FOR THE KOHN-SHAM EQUATION

We summarize here the algorithm in our numerical calculations which are commonly used in the literature to minimize energy functional $E[\Psi, \Psi^*] = \langle \Psi | H_o + V_{ext}^s | \Psi \rangle$, where $\Psi = \sqrt{n(r)} \exp(i\phi)$ in which the phase ϕ fixes the velocity of the fluid through the relation $v = \nabla \phi / m$. We minimize $E[\Psi, \Psi^*]$ by assuming the normalization condition $\int dr \Psi^* \Psi = N$ to obtain the following nonlinear the time independent Kohn-Sham equation:

$$\left[-\nabla^2 + x^2 - \frac{2n(x)}{\log[n(x)]} \right] \Psi(x) = \mu \Psi(x). \quad (19)$$

In the above equation, we have incorporated the auxiliary external potential based on Eqs. (12) and (15)–(18) using an isotropic planar trapping external potential $V_{ext} = (1/2)m\omega^2 r^2$, with ω as the radial frequency. We have scaled all lengths and energies by harmonic oscillator unit $a_{ho} = \sqrt{\hbar/m\omega}$ and $\hbar\omega/2$, respectively. We obtained the ground state solution of the system by numerical iteration method by

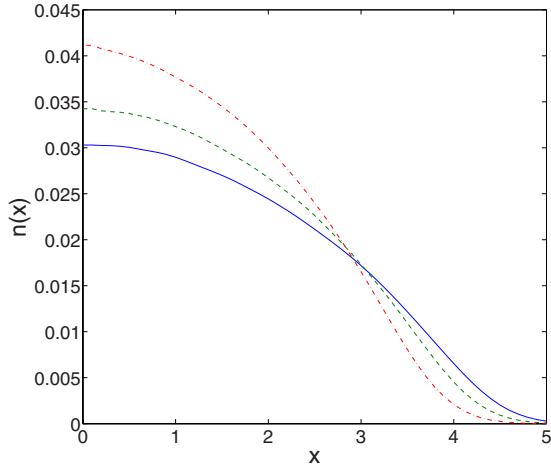


FIG. 3. (Color online) Top panel: Density profiles of the YBF $n(x)$ (in arbitrary units) as a function of x (in $\sqrt{\hbar}/m\omega$ units) for various number of atoms $N=200$ (solid line), 150 (dashed line), and 100 (dashed-dotted line).

using a two-step Crank-Nicholson discretization technique.

The density profiles as a function of N are shown in Fig. 3. The profile shows a maximum at the center of trap and it decreases monotonically with x . To make a quantitative measurement, we fix the solution for Eq. (19) for $N=100$ (n_1) as a standard and compare the differences in density for the other two values at the trap center [$\Delta n = n_2(0) - n_1(0)$ and $\Delta \tilde{n} = n_3(0) - n_1(0)$]. Here, $n_2(0)$ and $n_3(0)$ correspond to the solution of Eq. (19) for $N=150$ and $N=200$, respectively, at the center of trap. We found that the differences Δn and $\Delta \tilde{n}$ decrease with $\Delta n/n_1$ and $\Delta \tilde{n}/n_1$ by as large as 17%–26%. The explanation of these results is quite straightforward. The areal integral of the density $n(r)$ yields the total number of atoms in the system. Hence, larger number of atoms produced a much profound profile. The central density of the cloud decreases rapidly with increasing N , but the density distribution is flattened due to stronger repulsion between particles.

We also compare the YBF model with the conventional GP equation. This can be done by taking a contact potential $g\delta(|r-r'|)$ in Eq. (11), where $g = (4\pi\hbar^2/m)\log[2\hbar^2/(m\mu a^2)]$ is the coupling parameter for the two-dimensional BEC^{16–18} incorporating the s -wave scattering length a . We assumed a negligible exchange correlation between the atoms ($V_{xc}=0$) and would like to stress here that the condensate density is approximated to the total density $n_{GP}(r)$ at absolute zero temperature (neglecting quantum fluctuation). Based on the similar arguments in obtaining Eq. (19), we obtain the time independent Gross-Pitaevskii equation

$$[-\nabla^2 + x^2 + \tilde{g}n_{GP}(x)]\Psi(x) = \mu\Psi(x), \quad (20)$$

where \tilde{g} is the dimensionless scaled coupling parameter. We have also calculated the total energy of YBF and GP model as a function of the number of atoms, and the result is shown in Fig. 4. Increasing N , we observe an increase of both in-

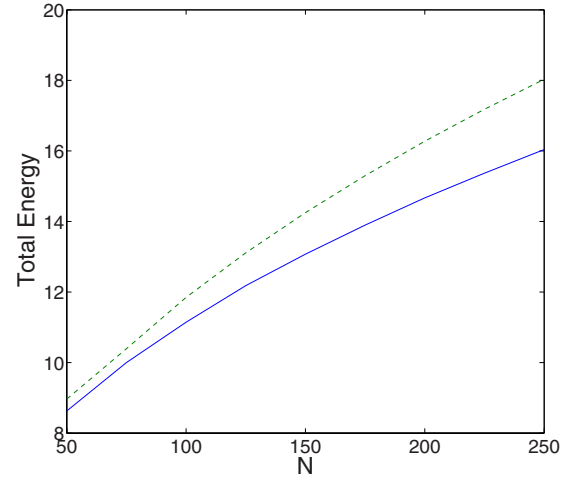


FIG. 4. (Color online) Total energies (in $\hbar\omega/2$ units) as a function of N .

teraction and harmonic oscillator potential energy for both GP and YBF models. The latter effect follows from the expansion of the cloud. On the contrary, the kinetic energy per particle decreases because the density profile is flattened. The GP energy curve (dashed line) remains well above the YBF curve (solid line) for all ranges of N . The energetic superiority of GP solution demonstrates the strongly repulsive nature of delta potential compared to the soft-core nature of the Yukawa potential as the number of atoms increases in the system.

In summary, we have studied the system of N Yukawa bosons in a 2D harmonic trap at absolute zero temperature. The central issue of this work is the use of density functional theory formalism within the Kohn-Sham scheme in reproducing the result of Monte Carlo simulation of Magro and Ceperley⁴ for the liquid phase in a harmonic trap. Physically sensible result through the local density approximation is obtained for the trapped system by knowing the homogeneous exchange-correlation energy. The ground state properties (density profiles and total energies) have been obtained by solving the nonlinear equations Eqs. (19) and (20). Our results show that bosons interacting with the Yukawa potential are energetically favorable compared to the contact delta potential for all ranges of N considered in this work. The results have, so far, not been verified. In light of the above, we trust that the YBF model through an appropriate mapping (boson-vortex) can be efficiently used to study strongly correlated liquid formed at the melted phase of vortices in a harmonically trapped rotating Bose gases.

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