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Variational Monte Carlo analysis of Bose–Einstein condensation in a two-dimensional trap*

Zheng Rong-Jie(郑荣杰), Jin Jing(金 晶), and Tang Yi(唐 翌)†

Institute of Modern Physics, Xiangtan University, Xiangtan 411105, *China*

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The ground-state properties of a system with a small number of interacting bosons over a wide range of densities are investigated. The system is confined in a two-dimensional isotropic harmonic trap, where the interaction between bosons is treated as a hard-core potential. By using variational Monte Carlo method, we diagonalize the one-body density matrix of the system to obtain the ground-state energy, condensate wavefunction and the condensate fraction. We find that in the dilute limit the depletion of central condensate in the 2D system is larger than in a 3D system for the same interaction strength; however as the density increases, the depletion at the centre of 2D trap will be equal to or even lower than that at the centre of 3D trap, which is in agreement with the anticipated in Thomas–Fermi approximation. In addition, in the 2D system the total condensate depletion is still larger than in a 3D system for the same scattering length.

Keywords: Bose–Einstein condensation, variational Monte Carlo method, two-dimensional trap
PACC: 0530J, 7115Q, 6460

1. Introduction

The realization of Bose–Einstein condensation (BEC) in the gas of alkali-atoms confined in a magnetic trap has attracted considerable experimental and theoretical attention.[1−3] Most of subsequent studies have focused on such issues as the kinetics of condensate,[4] the critical temperature for the occurrence of BEC[5] and coherence phenomena in a three-dimensional (3D) trap.[6,7] Recently, the two-dimensional (2D) BEC has become a hot subject of theoretical and experimental researches, because the 2D boson gas may exhibit unusual features. It was first predicted that BEC could not occur in a low-dimensional uniform boson gas at a finite temperature by Hohenberg's theorem,[8] since thermal fluctuations destabilized the condensate. Later, it is pointed out that this theorem holds true only for homogeneous systems. Quite a lot of theoretical work[9−12] reveals that the effects of thermal fluctuations can be strongly suppressed by the different behaviours exhibited by the density of states in a trap, leading to the occurrence of the true condensate in a low-dimensional trap. Moreover in recent years, the quasi-one-dimensional (quasi-1D)[13,14] and quasi-2D BECs[14] have been realized in experiments by varying the aspect ratio of the condensate and the number of atoms in the condensate. These experiments greatly motivate the theoretical study in 2D BEC, where atomic motion in one axis is frozen completely in the ground state.[15,16] Although the real experiments are not performed in a pure 2D system, they uncover that in the quasi-2D BECs atoms follow the 2D kinematics with 3D interactions.[17,18] So it is generally recognized that the study on the ground-state properties of 2D trapped bosons[19] with 3D interactions is of particular importance to understanding the real behaviours of bosons in a quasi-2D system.

For a 2D dilute Bose gas,[14,20] it is known that the 2D nonlinear Gross–Pitaevskii equation (GPE)[12,21] provides a satisfactory description for the properties of condensate. Calculations using the GPE show that in the dilute limit the dependence of both the ground-state density profile and ground-state energy on the interboson interaction in a 2D system is very similar to that in a 3D system. Many results calculated by other methods[15,22] are also in good agreement with the prediction of the 2D GPE. However, few comparisons have been made between the ground-state properties of bosons in the 2D system and those in the 3D system as the density of system increases, which is instructive for obtaining the quasi-2D BEC in ex-

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†Corresponding author. E-mail: tangyi@xtu.edu.cn

periment. In addition, the GPE is based on mean-field theory that is suitable for describing the characters of dilute systems. Beyond the dilute limit, the mean-field theory does not hold true because of underestimating the depletion of condensate. Fortunately, the properties of condensate can be directly described in terms of the eigenvalues and eigenvectors of the one-body density matrix (OBDM)[23] for an arbitrary condensate density.[24,25] For the 3D case, Dubois *et al* have obtained the ground-state properties of condensate over a wide range of densities by diagonalizing the OBDM for the system with only 128 bosons. In such a system, the interboson interactions are treated as a hard-core potential; that is, the bosons are simulated by the balls, the diameters of which are set to be the value of scattering length of bosons. The density of the system is increased by increasing the s-wave scattering length. In the dilute case, their results are in good agreement with the mean-field results,[26,27] and in the dense limit they can also be used to check the validity of the conclusion that the trapped dense bosons resemble liquid ^{4}He droplets. This means that the variational Monte Carlo (VMC)[28] method combined with the OBDM creates a coherent method of studying the ground-state properties of bosons from the dilute to the dense regime even if the system is small. So in this paper, we will study the properties of a 2D system composed of 64 hard-core bosons with 3D interactions by using the Dubois method.

The rest of this paper is organized as follow. In Section 2, we introduce the Dubois method, i.e. the VMC method combined with OBDM. In Section 3, we obtain the ground-state properties of 64 bosons confined in a 2D harmonic trap by using the above method, and we compare the core condensate density in the 2D system with that in a 3D system for the same scattering length. The difference between the results calculated by the VMC method and the analytical results in the Thomas–Fermi (TF) approximation is also shown. Finally, we draw some conclusions in Section 4.

2. Method

We consider a system in which N bosons are confined in a 2D trapping potential with the Hamiltonian

$$H = \sum_{i=1}^{N} [-\frac{\hbar^2}{2m}\nabla_i^2 + V_{\rm ext}(r_i)] + \sum_{i<j}^{N} V_{\rm int}(|r_i - r_j|). \quad (1)$$

Here, $Y_{\rm ext}(r_i)$ is the potential of an external harmonic trap, satisfying

$$V_{\rm ext}(r) = \frac{1}{2} m\omega_{\rm ho}^2 r^2 \,, \quad (2)$$

where $\omega_{\rm ho}$ determines the trap frequency. $V_{\rm int}(|r_i - r_j|)$ represents the interboson interaction being a hard-core potential in the following form:

$$V_{\rm int}(r) = \begin{cases} \infty & r \le a_0 \,, \\ 0 & r > a_0 \,, \end{cases} \quad (3)$$

where a_0 is the hard-core diameter of bosons. If the scattering length $a_{\rm Rb}$ of the atom ^{87}Rb is taken as the characteristic length of the hard-core potential, $a_{\rm ho} = (\hbar/m\omega_{\rm ho})^{1/2}$ as the characteristic trap length, then there exists a universal relation $a_{\rm Rb}/a_{\rm ho} = 4.33 \times 10^{-3}$. To describe the ground state properties of bosons in the above system, we introduce a variational trial wavefunction which is similar to that used by Dubois. The wavefunction is a production of a single-particle function $\varphi(\alpha, r)$ and a paired Jastrow function[29] $f(|r_i - r_j|)$,

$$\psi(r_1, \ldots, r_N, \alpha) = \prod_i \varphi(\alpha, r_i) \prod_{i<j} f(a_0, |r_i - r_j|) \,, \quad (4)$$

where

$$\varphi(\alpha, r) = \exp[-\alpha(x^2 + y^2)] \,, \quad (5)$$

is in the form of a Gaussian function with a variational parameter α, and

$$f(a_0, r) = \begin{cases} 1 - a_0/r \,, & r > a_0 \,, \\ 0 & r \le a_0 \,, \end{cases} \quad (6)$$

is a paired Jastrow wavefunction. By minimizing the energy of the system, i.e. the expectation value of the Hamiltonian defined as

$$\langle \hat{H} \rangle = \frac{\int {\rm d}r_1 \ldots {\rm d}r_N \psi^* \psi \left(\dfrac{\hat{H}\psi}{\psi} \right)}{\int {\rm d}r_1 \ldots {\rm d}r_N \psi^* \psi} \,, \quad (7)$$

with Monte Carlo method, we obtain an optimal trail wavefunction ψ_0.

With the obtained ψ_0, we can proceed to calculate the OBDM

$$\rho_{\rm B}(r, r') = \langle \hat{\psi}^+(r') \hat{\psi}(r) \rangle \quad (8)$$

as discussed in Ref.[24]. Then, the natural orbitals (NO) $\phi_i(r)$ and their occupation number N_i will be obtained by diagonalizing $\rho_{\rm B}(r, r')$. The NO with the highest occupation number corresponds to the condensate orbital $\phi_0(r)$. The condensate fraction is defined as $n_0 = N_0/N$.

3. Results

Firstly, in Fig.1, we give the density profiles of 2D and 3D ideal boson gases, which are confined in the 2D and 3D harmonic traps respectively. Obviously, in the 2D system the density of condensate decreases more rapidly than in the 3D system as r increases. That is, a larger proportion of bosons are confined near the centre of trap in the 2D system than in the 3D system. So, it is expected that the dependence of important measurable quantity on interboson interaction is enhanced more dramatically in the 2D system than in the 3D system as the interboson interaction strength increases. For instance, it is known that the condensate will be depleted significantly because of interactions between bosons. Then, one expects the depletion of core condensate in the 2D system will be larger than in the 3D system for the same interboson interaction strength.

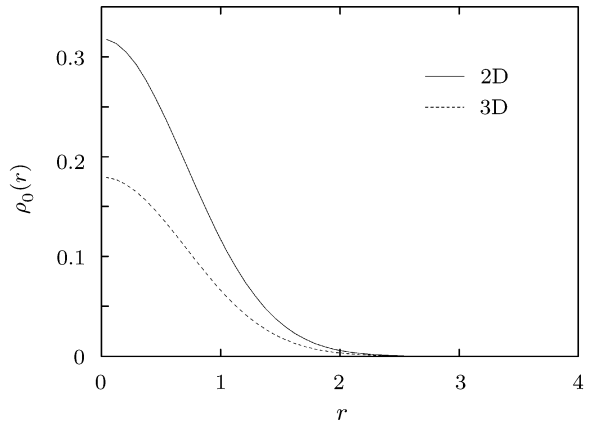


Fig.1. The solid line and dash line correspond to the density profiles of 2D and 3D ideal boson gases, which are confined in the 2D and in 3D harmonic traps respectively. All lengths are in units of the trap length $a_{\rm ho} = \sqrt{\hbar/m\omega_{\rm ho}}$.

In order to investigate the dependences of depletion on the interboson interaction in different dimensions, the ratio of central condensate density in the TF approximation to that in an ideal boson gas is shown as a function of interboson interaction strength in the 2D and 3D traps respectively. It is known that in the TF approximation the interatomic interaction is so large that the kinetic energy can be neglected. Using dimensionless units, analytical expression of the density profile can be written as

$$\rho_{\rm TF}(r) = |\psi(r)|^2 = g^{-1}[\mu - V_{\rm ext}(r)]\,, \qquad (9)$$

where g describes the interboson interaction strength, μ is the chemical potential. For different g, the chemical potential μ is obtained with the condensation normalized by $\rho_{\rm TF}(r)$. Then, the ratio $\lambda = \rho_{\rm TF}(0)/\rho_{\rm ideal}(0)$ is calculated as a function of g in Fig.2. The result shows that the density of core condensate in the 2D system decreases more rapidly than in 3D system as interaction strength increases in the region $0 < g < 180$, that is, the depletion of central condensate in the 2D system increases more rapidly than in the 3D traps as g increases, which is in agreement with the anticipated in Fig.1. However, when g is larger than 180, the density of core condensate in the 2D system decreases more slowly than in the 3D system, which is abnormal as g increases. We believe that this abnormality arises because of the especial distribution of condensate in the dense limit.

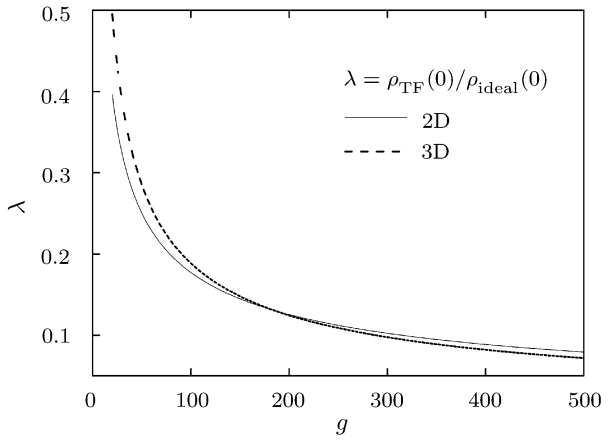


Fig.2. The solid line and dash line correspond to the ratios of central condensate density in the TF approximation to that in an ideal boson gas in the centres of 2D trap and in 3D trap respectively. The coupling constant g describes the interboson interaction strength, in units of $\hbar^2 a_{\rm ho}/m$.

Figure 3 shows the condensate orbitals for the 64 bosons in a 2D harmonic trap, with hard-core diameter a increasing from zero to $64a_{\rm Rb}$. Here, our goal is to check the difference in condensate density distribution between the 2D and 3D systems, as the scattering length of bosons increases. At $a = a_{\rm Rb}$, the system corresponds to $N = 64$ Rb atoms in the 2D harmonic trap. It is very clear that the condensate orbital spreads out, that is, the density of condensate at the centre of the trap decreases as scattering length increases. At $a = 64a_{\rm Rb}$, the condensate density is effectively constant nearly $3.5a_{\rm ho}$ off the centre of trap in the 2D trap, which corresponds to $3a_{\rm ho}$ in 3D trap.[24] It is noticeable that in the dense limit the conden-

sate distribution has a significant deviation from that in the dilute limit. So, we expect that the depletion of central condensate in the 2D and 3D systems will be significantly affected by the abnormal condensate distribution.

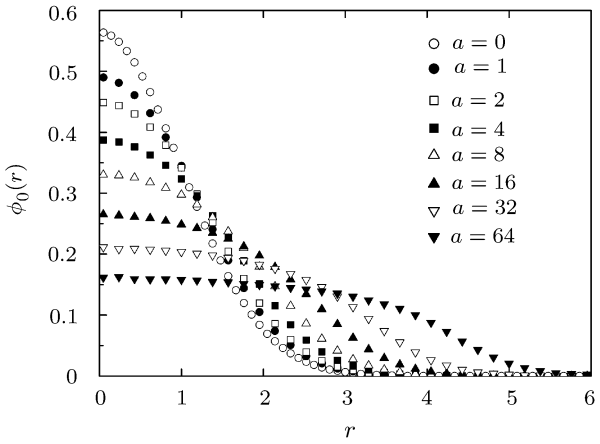


Fig.3. Condensate wavefunctions for 64 hard-core bosons confined in a 2D harmonic trap with scattering lengths $a = 0, 1, \ldots, 64a_{\mathrm{Rb}}$. All lengths are in units of the trap length of $a_{\mathrm{ho}} = \sqrt{\hbar/m\omega_{\mathrm{ho}}}$.

In Fig.4, we show the dependences of ratio $\gamma = \rho_{\mathrm{VMC}}(0)/\rho_{\mathrm{ideal}}(0)$ on the scattering length for 64 bosons confined in the 2D and in 3D traps respectively. In the region $0 < a < 32a_{\mathrm{ho}}$, the density of condensate in the centre of 2D trap decreases more rapidly than in the 3D trap: that is, the depletion of condensate in the centre of 2D trap increases more rapidly than in the centre of 3D trap as a increases. This is also in good agreement with the expected in the dilute limit. As the density of the system increases, one can see that the condensate densities become effectively constant. On the other hand, the depletion of condensate more depends on the density of system than on the interboson interaction in a homogeneous system. So, it appears that the trapping potential plays a dominant role in the distribution of condensate in the dense limit. Therefore, the depletion of central condensate in the 3D system is abnormally larger than in the 2D system in the dense limit. The above results show the character similar to that in the TF approximation.

The condensate fraction n_0 is given in Fig.5 for 64 hard-core bosons confined in the 2D and in 3D traps. The condensate fraction decreases more rapidly in the 2D system than in the 3D system, as scattering length increases. We attribute this outcome to the fact that in the dense limit the condensate in the 3D system covers a larger fraction of trap than in the 2D system. Therefore, although the density of central condensate is higher in the 2D system than in the 3D system in the dense limit, the condensate fraction in the 2D system is still lower than in 3D system for the same scattering length.

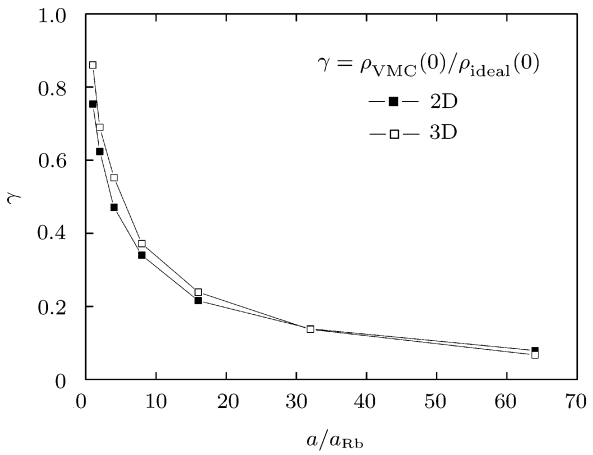


Fig.4. The ratio $\gamma = \rho_{\mathrm{VMC}}(0)/\rho_{\mathrm{ideal}}(0)$ for 64 hard-core bosons, which are confined in the 2D and in 3D traps, with the scattering lengths $a = 0, 1, \ldots, 64a_{\mathrm{Rb}}$.

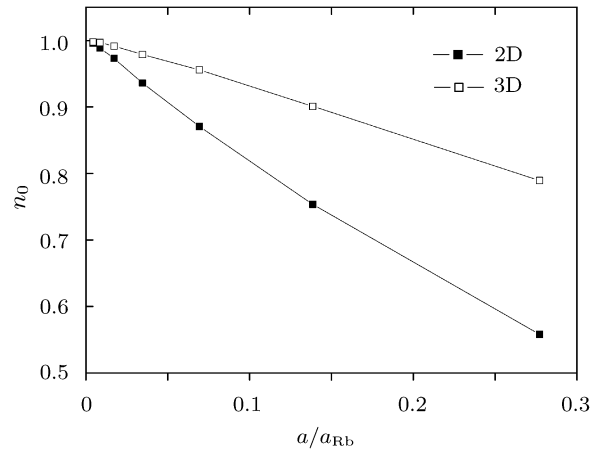


Fig.5. Condensate fraction n_0 as a function of the ratio of interacting hard-core diameter a to the trap length a_{ho}, for 64 bosons confined in the 2D and in 3D traps.

Finally, in Fig.6, we obtain the ground state energy per particle in the 2D and 3D systems for $1 < a < 64a_{\mathrm{Rb}}$ respectively. It is very clear that the energy increases more rapidly in the 2D system than in the 3D system. In the insert, we calculate the ratio $\eta = (E_{\mathrm{TF}} - E_{\mathrm{ideal}})/E_{\mathrm{ideal}}$, which can make the situation clearer. It is noticeable that the ground-state energy is more dependent on the interboson interaction than the depletion of condensate, which has been

proved in the 3D case.

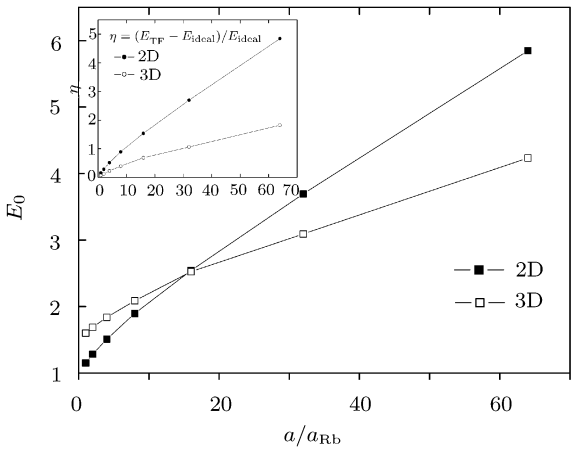


Fig.6. Ground-state energies as a function of the ratio $a/a_{\rm Rb}$, in units of $\hbar\omega_{\rm ho}$, for 64 hard-core bosons confined in the 2D and in 3D harmonic traps with scattering lengths $a = 0, 1, \ldots, 64a_{\rm Rb}$. In the insert, the ratio $\eta = (E_{\rm TF} - E_{\rm ideal})/E_{\rm ideal}$ is also calculated.

4. Discussion and summary

In this paper, we have calculated the ground-state properties of bosons, which are confined in a 2D harmonic trap, over a wide range of densities by using the VMC method combined with OBDM. It is obvious that in the dilute limit the condensate density profile spreads out as scattering length increases, which is similar to the result calculated by GP equation.[21] This means that in the dilute limit the depletion of central condensate in the 2D trap is larger than in the 3D trap. As the density of system increases, the depletion of central condensate in the 3D trap abnormally exceeds that in 2D trap. This result is also in good agreement with the outcome in the TF approximation. However, we also find that the total depletion of condensate in the 2D system is still higher than in 3D system for the same scattering length, which can be seen as a proof that we must decrease the density of bosons in a trap to realize the quasi-2D BEC in experiment. In addition, it is shown that the ground-state energy is more dependent on interboson interaction than the depletions of condensate, which has been proved in the 3D system.

The studies of a two-body hard-core potential with a positive scattering length a are performed. It will be interesting to extend these studies to a two-body potential with a negative a,[30] or to other potential forms such as soft-core potential.[16] In the future, we will be studying these problems.

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