Bose-Einstein condensation in a two-dimensional trap

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The theory of Bose-Einstein condensation in a two-dimensional(2D) harmonic trap is developed from 2D Gross-Pitaevskii equation. The 2D interaction strength is obtained from a 2D collision theory. We show the realization of 2D condensation of trapped Bose atoms directly by obtaining the stable solutions for the condensate wave function from the 2D Gross-Pitaevskii equation. We calculate the ground-state energy of the 2D system, and also the wave function of the 2D vortex state. In particular, the 2D energy state becomes less stable than the 3D case with the number of trapped atoms. The results of the 2D Bose condensation are also compared with those of the well-known 3D case.

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I. INTRODUCTION

The recent experimental realization of Bose-Einstein Condensation(BEC) of alkali atoms in magnetic traps has generated much interest and activity in theoretical and experimental physics. An interesting, but less addressed, question is whether such a phase transition due to global coherence exists in two-dimensional(2D) space. Even though it has been known that 2D BEC of a uniform(untrapped) Bose gas cannot occur in 2D at a finite temperature since thermal fluctuations destabilize the condensate, it has been suggested that spatially-varying potentials which break the uniform distribution may create BEC in 2D inhomogeneous systems. In the presence of trapping potential, the effect of thermal fluctuations are strongly quenched due to the different behavior exhibited by the density of states.

At zero temperature, the 2D condensation can be described by the 2D Gross-Pitaevskii equation(GPE), a mean-field approximation for the macroscopic wave function of weakly interacting bosons. The GPE is obtained from mean-field many-body quantum-statistical theory and has been proven to explain the condensate state of dilute Bose system satisfactorily. Although no direct experimental observation of 2D BEC has been reported yet, recent theoretical works suggest a possibility of 2D BEC in a trapped condition. However, most of the theoretical approaches for 2D BEC have been rather indirect and sometimes even faced with several difficulties.

Tempere and Devreese studied harmonically-interacting bosons in 2D. They calculated the critical temperature from a grand-partition function to show the occurrence of 2D BEC, but without any knowledge of the 2D condensate wave function for the density profile. Jackson et al. studied the 2D vortex state by direct substitution of the 3D interaction strength into the 2D GPE, which resulted in a dimensional inconsistency. Bayindir et al. solved the 2D GPE using the two-fluid model a density estimation and obtained the temperature dependence of the internal energy and condensate fraction, where the 2D interaction strength was still treated just as a free variable. Haugset et al. calculated the density profile and ground state energy for a finite number of 2D Bose particles by diagonalizing the Hamiltonian numerically, where a modified 2D interaction strength was used to solve the dimensional inconsistency. Analytical approach of interacting Bosons in 2D trap by 2D nonlinear GPE was attempted by Gonzalez et. al., and they studied the ground-state energy density by applying the Haugset et al.’s modified form of the 2D interaction strength to the 2D GPE.

Previous 2D researches are based on the size-independent concepts: if the atomic motion in any one axis is frozen completely in the ground state, the system is considered as two-dimension. Moreover, most of the studies considered the 2D trap as an extremely anisotropic 3D trap and still far from the pure 2D system. On the other hand, we will focus on the 2D system which is confined by a 2D harmonic trap in (x,y)-direction and by ideal rigid walls in z-direction. In this system, the 2D interaction strength has a logarithmic form which will be derived using a 2D scattering theory in the next section. Quasi-2D atomic systems, where atoms follow the 2D kinematics with the 3D interactions, have been recently realized for spin-polarized atomic hydrogen adsorbed on the surface of liquid helium and quasi-condensation has been indirectly demonstrated. Although no pure 2D BEC has been studied experimentally yet, the 2D GPE is quite valid even in quasi-2D at low temperatures. Moreover it will provide us a guide to a better understanding of the 2D statistical properties of the quasi-2D system.

In this paper, we will solve the 2D GPE numerically and show the existence of the 2D BEC directly by obtaining the stable condensate wave functions and the 2D ground state energy density of the trapped Bose atoms. Possible vortex states in 2D are also discussed. The re-
sults of the 2D Bose condensation are then compared with those of the well-known 3D cases.

II. TWO-DIMENSIONAL SCATTERING THEORY

The relation between interaction strength, $g$, and the s-wave scattering length, $a$, is well-known in 3D as $g = 4\pi \hbar^2 a/m$. However, the 3D result is not applicable to a 2D GPE: substitution of the 3D relation into the 2D GPE results in dimensional inconsistency. As a first step to obtain the correct 2D GPE, the interaction strength in 2D is derived from the following 2D scattering theory [17–20]. We begin with the 2D time-independent Schrödinger equation with the interaction $\phi \psi$, given by

\[
(\nabla_{\rho}^2 + k^2)\psi_k(\rho) = U(\rho)\psi_k(\rho),
\]

where $k^2 = 2\mu m E/\hbar^2$, $\mu m$ is the reduced mass of two particles (m/2). One can find the general solution of Eq. (1) with the help of the 2D Green’s function

\[
(\nabla_{\rho}^2 + k^2)G_k(\rho, \rho') = \delta^2(\rho - \rho').
\]

The general solution of the 2D Green’s function is the Hankel function [21,22]. Therefore the 2D wave function can be expressed as

\[
\psi_k(\rho) = e^{ik\rho} + \int d^2\rho' G_k(\rho, \rho')U(\rho')\psi(\rho') = e^{ik\rho} - \frac{i}{\sqrt{2\pi k\rho}} \int d^2\rho' U(\rho') e^{i(k-k')\rho'}. \tag{3}
\]

Here $H_0$ is the first kind Hankel function of order zero defined by $H_0(\rho) = J_0(\rho) + i N_0(\rho)$, where $J_0$ and $N_0$ are Bessel and Neumann function of order zero. For large $\rho$, it has the asymptotic behavior $H_l(\rho) \sim \sqrt{2/\pi \rho} \rho^{l/2} e^{i(l/2 - 1/2 - \pi/4)}$, where $l$ is an integer. The Born approximation is applied to the last step, and $k' = k\rho$.

In 2D, for large $\rho$, the scattered wave function should have the form

\[
\psi_k(\rho) \approx e^{ik\rho} + F_k e^{i(k\rho - \frac{\pi}{4})}, \tag{4}
\]

where $F_k$ is the first-order Born scattering amplitude in 2D which has a dimension of $\text{(length)}^{1/2}$. This asymptotic formula should be a solution of the time independent Schrödinger equation (1), and satisfy $\rho \rightarrow \infty$ limit of the Green’s function solution. The scattering cross-section in 2D now has the dimension of length given by

\[
\frac{d\sigma_{2D}}{d\theta} = |J_{sc}|^2 = |F_k|^2, \tag{5}
\]

where $J_{sc}$ and $J_{inc}$ are incident and scattered flux densities. We note that the total scattering cross-section for small $k$ should be $2\pi |F_k|^2$ in 2D instead of $4\pi |f_{3D}|^2$ in 3D. If one assumes the delta-function type interaction $U(\rho) = (mg/\hbar^2)\delta^2(\rho)$, the 2D scattering amplitude $F_k$ is obtained in the complex form from Eqs. (3) and (4) as

\[
F_k = \frac{i}{2} \frac{1}{\sqrt{2\pi k\hbar^2}} \frac{mg}{k}. \tag{6}
\]

The next step is to find the relation between the scattering amplitude and the scattering length in 2D. The well-known relation $f_{3D} = -a$, where $f_{3D}$ is the 3D scattering amplitude and $a$ is the s-wave scattering length in 3D, is not directly applicable in 2D. In general, the s-wave scattering length in 2D, $b$, is different from the one in 3D, $a$, and the s-wave scattering length in 2D is not known yet from experiment.

The relation is obtained from partial wave analysis of collision theory. The incident wave can be written as an expansion of plane wave in cylindrical coordinate [22]

\[
e^{ik\rho \cos \theta} = \frac{1}{2} \sum_{l=-\infty}^{\infty} i^l (H_l(k\rho) + H_{-l}^*(k\rho)) e^{il\theta}, \tag{7}
\]

where $l$ is an integer. Away from the range of potential, the scattered wave has a phase shift $\delta_l$, and the scattering matrix is obtained as $S_l = e^{2i\delta_l}$ since $|S_l| = 1$ for elastic scattering. Therefore, for large $\rho$, the solution of Eq. (3) is written as

\[
\psi_k(\rho) = e^{ik\rho} + \frac{1}{2} \sum_{l=-\infty}^{\infty} i^l (S_l - 1) H_l(k\rho) e^{il\theta}
\approx e^{ik\rho} + \frac{1}{\sqrt{2\pi k\rho}} \sum_{l=-\infty}^{\infty} i^l (e^{2i\delta_l} - 1) e^{i(k\rho - \frac{\pi}{4})} e^{il\theta}. \tag{8}
\]

Scattering length is defined as the distance where the two-body wave function vanishes for zero energy. The phase shift due to potential scattering is given as a function of the scattering length, and it is well-known as $\delta_{0,2D} = -\pi a$ in 3D, whereas

\[
\delta_0 = \frac{\pi}{2} \frac{1}{\ln kb} \left[ 1 + O\left( \frac{1}{\ln kb} \right) \right], \tag{9}
\]

in 2D [19]. Note that it is effective only in the low energy scattering limit, $kb << 1$. It can be easily checked as follows. The scattering length is just the intercept of the radial wave function satisfying the boundary condition $\psi_k(b) = 0$. Therefore, for $l = 0$, the wave function at large distance and small $k$ is expressed as

\[
\psi_k(\rho) = J_0(k \rho) - \frac{J_1(k \rho)}{N_0(k \rho)} N_0(k \rho)
\approx \frac{2}{\sqrt{2\pi k\rho}} \left[ \cos \left( k \rho - \frac{\pi}{4} \right) - \frac{\pi}{2\ln kb} \sin \left( k \rho - \frac{\pi}{4} \right) \right]
= \frac{2}{\sqrt{2\pi k\rho}} \cos \left( k \rho - \frac{\pi}{4} + \delta_0 \right). \tag{10}
\]
The necessary condition for the validity of the Born approximation is that the phase shift $\delta_0$ be very small for small $k$, which can be easily confirmed from Eq. (1). Note that unlike the 3D case where $a$ can be negative, we do not consider the negative scattering length here since the centrifugal potential of the lowest partial wave is negative in 2D so that the extrapolated local wave function cuts the radial axis always above the origin [19].

Comparing Eq. (8) with Eq. (6), the scattering amplitude is written as a series expansion, and the $l = 0$ state contributes to the 2D system. Therefore, the 2D scattering amplitude becomes

$$F_k = \frac{1}{\sqrt{2\pi}k} \sum_{l=-\infty}^{\infty} (e^{2i\delta_0} - 1) e^{il\theta}$$

$$= \frac{2i\delta_0}{\sqrt{2\pi}k} (1 + i\delta_0 + ...)$$

$$\simeq \frac{i\pi}{\sqrt{2\pi}k} \frac{1}{\ln kb}.$$  

(11)

Finally, we obtain the 2D interaction $g$ from Eqs. (3) and (11) as

$$g = -\frac{2\pi\hbar^2}{m} \frac{1}{\ln kb}.$$  

(12)

In general the 2D interaction strength is given as [17]

$$g = \frac{4\pi\hbar^2\xi}{m}.$$  

(13)

Here $\xi$ is a dimensionless atomic parameter given by

$$\xi = -\frac{1}{2} \frac{1}{\ln kb}.$$  

(14)

where $\xi$ is positive since $kb \ll 1$. Note that the logarithmic dependence of the interaction term suggests similar condensate characteristics in 2D for most bosonic alkali atoms with positive scattering length.

In addition to the 2D scattering length, $b$, we do not have any reliable value of the wave-vector, $k$, in 2D. An approximation that the wave-vector $k$ be the inverse of the largest distance available in the perpendicular direction may not be correct. However, the experimental results provide the value of the product $kb$ as described in the next section. Note that in an extremely anisotropic 3D system, the dimensionless atomic parameter is given as $\xi_c = (1/\sqrt{2\pi})a/a_z$, where $a_z = \hbar/m\omega_z$, and moreover $\xi_c < \xi$ in general.

**III. THE CONDENSATE STATE AND ITS ENERGY STATE**

Now the 2D condensate wave function of trapped dilute Bose atoms of mass $m$ can be obtained from the 2D GPE

$$-\frac{\hbar^2}{2m} \frac{\nabla^2}{\rho} + V_{ext}(\rho) + N g \psi^2(\rho) \psi(\rho) = \mu \psi(\rho),$$  

(15)

where $\int d\rho \psi^2(\rho) = 1$, and $N$ is the number of condensate particles. Here, we assume a 2D isotropic, harmonic trap $V_{ext}(\rho) = \frac{1}{2} m \omega^2 \rho^2$ where $\omega$ is the trap frequency. Then we can simplify Eq. (13) for numerical calculation by introducing dimensionless variables ($\rho \to a_h \rho$, $\mu \to \hbar \omega \mu$, and $\psi \to a_h \psi$)

$$[-\nabla^2 + \rho^2 - 2\mu + 8\pi N \psi^2(\rho)] \psi(\rho) = 0,$$  

(16)

where $a_h = \sqrt{\hbar/m\omega}$ is the 2D harmonic oscillator length, and $\mu$ is the 2D chemical potential which is obtained from the normalization condition. Note that the product of incident wave-vector and scattering length, $kb$, is the only atomic parameter that contributes to the condensate states.

In the numerical calculation of the GPE, we need the value of the atomic parameter $\xi$ in Eq. (13) which is a function of $k$ and $b$. Although they are not known separately, we are able to deduce their product $kb$ from experimental data, which appears together in the 2D GPE. It is certain that different Bose atoms have different 2D scattering lengths, but the logarithmic dependence makes the difference less sensitive. A recent experiment of the hydrogen on helium surface by Safonov et al. [18] has reported $\xi = 1/7$ which indicates $kb = 3 \times 10^{-2}$. Although their system actually satisfies a quasi-2D condition, one can still take this value in the 2D GPE as an effective interaction potential. Since it is well known that the 2D GPE is valid even in quasi-2D at low temperatures [16], and moreover it hints the 2D atomic characteristics in the quasi-2D system, it is useful to quantify the criterion for the quasi-2D, or the effective thickness of the 3D system to exhibit the 2D statistical properties. The criteria of the effective thickness of the trapped 2D Bose system may by obtained [19].

The next procedure to solve Eq. (16) is almost similar to those of 3D [20][21]. We have plotted the 2D condensate wave functions versus $\rho$ for several values of atom number $N$ in Fig. 1. It corresponds to the $z = 0$ cut of the anisotropic contour plot of the ground states in 3D. The spatial distribution of the condensate in 2D is much broader than that in 3D, and the condensate wave functions approach the parabolic limit more rapidly with the increase of the number of atoms. In other words, the effect of atomic interaction potential becomes more prominent in 2D.

In the non-interacting case, the solution is still Gaussian with $\psi(\rho) = \pi^{-1/2} e^{-\rho^2/2}$. In the strongly repulsive limit or Thomas-Fermi limit, it has the parabolic solution of $\psi^2(\rho) = (2\mu - \rho^2)/8\pi N$. The overall shape of the condensate wave functions are similar with that of 3D, but it approaches the parabolic limit more quickly with the number of atoms [24]. Therefore, the peak of the density profile decreases much faster in 2D. The 2D
healing length that balances between the quantum pressure and the interaction energy of the condensate is also different from that of 3D. Refer to TABLE 1 for detailed comparison.

The ground-state energy for 2D condensate bosons can be calculated in a similar way. With the dimensionless variables defined before, we obtain the dimensionless energy density as

$$\varepsilon = \int \left[ \frac{1}{2} \left| \nabla \psi \right|^2 + \frac{1}{2} \rho^2 \left| \psi \right|^2 + 2\pi \xi N \left| \psi \right|^4 \right] d^2 \rho. \quad (17)$$

Using a Gaussian trial function, we easily find the ground-state energy density satisfies

$$\varepsilon \geq \sqrt{1 + 2\xi N}. \quad (18)$$

The ground-state energy per particle in Eq. (18) is plotted in Fig. 2, and compared with the well-known 3D results of $^{87}$Rb. The 2D system becomes more excited for a given $N$ and less stable as $N$ is increased with respect to the 3D case. We have summarized the fundamental differences between our 2D results and the well-known 3D ones in TABLE 1.

### IV. THE VORTEX STATE

Now let us consider the vortex states of the 2D system. The hydrodynamic theory connected to superfluidity is understood by vortex. The 2D system can be rotating about the center of the 2D trap to give quantized circulation of atomic motion. The angular momentum quantum number $\kappa$ gives the quantum winding of the 2D vortex state. A vortex state with winding number $\kappa$ is written as $\psi(\rho) = \phi(\rho)e^{i\kappa S}$. Here $\phi(\rho) = \sqrt{n(\rho)}$ is the modulus. The phase $S$ is chosen as $\kappa \theta$ where $\kappa$ is an integer. An angular momentum quantum number $\kappa$ can be then assigned to the quantum winding of the 2D vortex state, and one finds the vortex states with a tangential velocity $v = \kappa \theta / m \rho$. As a result of the quantum circulation, the angular momentum of the system with respect to the $\rho = 0$ axis becomes $L = N \kappa \hbar$.

Adding the vortex term of $\kappa^2 / \rho^2$, Eq. (13) is directly converted into the vortex state

$$\left[ -\nabla^2 + \frac{\kappa^2}{\rho^2} + \rho^2 - 2\mu + 8\pi \xi N \phi^2(\rho) \right] \phi(\rho) = 0. \quad (19)$$

The wave function for $\kappa = 1$ vortex state is plotted in Fig. 3. The overall shape and $N$ dependence of the vortex-state wave function are similar with those of 3D [24]. As expected, the vortex state also corresponds to the $z = 0$ cut of the anisotropic contour plot of vortex state in 3D. We also observe that the 2D vortex has a larger radius than the 3D one.

The critical angular velocity or the energy difference between the vortex state of $\kappa = 1$ and the ground state $\kappa = 0$ in Eq. (13) is obtained analytically as

$$\varepsilon_{\kappa=1} - \varepsilon_{\kappa=0} = 2\sqrt{1 + \frac{\xi N}{2}} - 1 + 2\xi N. \quad (20)$$

For $\varepsilon_{\kappa=1}$, the trial function of $\phi \sim \rho e^{-\rho^2}$ type was employed. With the increase of the number of particles, the vortex-excitation energy in 2D is much smaller than the 3D one, which indicates that vortices are expected to be produced more easily in 2D than 3D.

Although there are fundamental differences between the 2D and the 3D results as summarized in TABLE 1, it will be interesting to compare with the quasi-2D scheme considered as a limiting case of 3D. For comparison of the 2D trap with an extremely squeezed 3D trap, we take the 3D external potential given by $V_{ext}(\rho, z) = (1/2)m \omega^2 (\rho^2 + \lambda^2 z^2)$. Here $\lambda$ is the anisotropy parameter and much larger than 1 for the quasi-2D system, whereas $\lambda \rightarrow \infty$ for the 2D trap. With a fixed number of atoms, we plot the condensate wave functions versus $\lambda$, from the 3D GPE in Fig. 4. We find the 3D wave functions merge very slowly with $\lambda$, but does not reach the pure 2D limit at all.

### V. DISCUSSIONS

The 2D nonlinear Schrödinger equation (GPE) is not a simple extension of the 3D case but is connected into a totally different 2D collision theory which requires different approach. We have developed the theory of the 2D GPE for trapped neutral Bose atoms in a 2D harmonic trap. Applying the quasi-2D experimental value of $\xi = 1/7$ to the effective interaction strength, one can solve the 2D GPE numerically without detailed knowledge of $k$ and $b$ separately.

We have obtained the stable solutions of the 2D GPE, which predicts possible existence of 2D BEC. The ground-state energy of the condensate particle is also calculated and it is found that the 2D system becomes less stable as the number of trapped atoms is increased, compared with the 3D case. We also have obtained the wave functions of the 2D vortex state numerically and its critical angular velocity.

The 2D BEC transition may look similar to the Kosterlitz-Thouless (KT) [24] vortex-state transition, but the phase transition of 2D BEC does not need any strong interaction between atoms. That is the fundamental difference between the two transitions.

The logarithmic dependence of the interaction potential on the scattering length makes the 2D system less sensitive to the species of the atoms used for condensation. That will make every alkali atoms of positive scattering length show similar condensate wave patterns in 2D. The comparison between our 2D and well-known 3D results are summarized in TABLE 1.

The quasi-2D scheme can be interpreted as a limiting case of the 3D one. By varying the trapping field,
it is possible to separate the single-particle states in the oscillation into well-defined bands. To compare the situation of 2D trap with an extremely squeezed 3D trap, we take the external potential for 3D as $V_{\text{ext}}(r_\perp, z) = (1/2)m\omega^2(r_\perp^2 + \lambda^2 z^2)$, where $\lambda \gg 1$. The case of negative scattering length in 2D will be discussed later.

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TABLE I. The comparison of the 3D and the 2D BEC. The dimensionless atomic variable $\xi$ is defined by $\xi = -1/(2 \ln kb)$.
| Parameter                              | $D = 3$                                      | $D = 2$                                      |
|----------------------------------------|----------------------------------------------|----------------------------------------------|
| Scattering amplitude                   | $f_{3D} = -a$                                | $F_{2D} = -i\sqrt{\frac{2\pi}{k}}\xi$      |
| Interaction strength                   | $g_{3D} = \frac{4\pi\hbar^2 a}{m}$           | $g_{2D} = \frac{4\pi\hbar^2 \xi}{m}$        |
| Healing length                         | $\xi_{3D} = (8\pi n_{3D} a)^{-1/2}$          | $\xi_{2D} = (8\pi \xi n_{2D})^{-1/2}$       |
| Chemical potential                     |                                              |                                              |
| (noninteracting)                       | $\mu_{3D} = 1.5 \hbar \omega$               | $\mu_{2D} = \hbar \omega$                   |
| (strongly interacting)                 | $\mu_{3D} = \frac{1}{2} \left( \frac{15a N}{a_{h.o}} \right)^{2/5} \hbar \omega$ | $\mu_{2D} = (4\xi N)^{1/2} \hbar \omega$   |
| Radius of condensation                 | $r_c = \left( \frac{15a N}{a_{h.o}} \right)^{1/5}$ | $\rho_c = (16\xi N)^{1/4}$                  |
| Ground state energy                    | $E_{3D} = \frac{5}{2} \mu_{3D} N \propto N^{7/5}$ | $E_{2D} = \frac{2}{7} \mu_{2D} N \propto N^{3/2}$ |
| Center lowering of density profile     | $|\phi_{3D}(0)|^2 \propto N^{-3/5}$           | $|\phi_{2D}(0)|^2 \propto N^{-1/2}$          |
$\varepsilon(E/N)$

$\log N$

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2D (\(^1\)H)

3D (\(^{87}\)Rb)
\[ \phi(\rho) \]

For different values of \( N \):
- \( N = 1 \)
- \( N = 10 \)
- \( N = 100 \)
- \( N = 1000 \)
$\phi(\rho)$ vs $\rho$

- **3D**
- **2D**