Two-Dimensional Gross-Pitaevskii Equation: Theory of Bose-Einstein Condensation and the Vortex State

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We derive the Gross-Pitaevskii equation in two-dimension from the first principles of two-dimensional scattering theory. Numerical calculation of the condensate wave function shows that atoms in a two-dimensional harmonic trap can be condensed into its ground state. Moreover, the ground state energy and the wave function of two-dimensional vortex state are also obtained. Quantitative comparisons between 2D results and 3D ones are made in detail.

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The recent experimental realization of Bose-Einstein Condensation (BEC) of dilute alkali Bose atoms in magnetic traps \[\frac{2}{3}\] has generated immense interest and activities in theoretical and experimental physics. An interesting, but much less addressed, question is whether such a phase transition due to global coherence exists in two-dimensional (2D) space. It has been known that 2D Bose atoms do not have a long-range order, and consequently BEC of a uniform (untrapped) Bose gas can not occur in 2D at a finite temperature since thermal fluctuations destabilize the condensate \[\frac{3}{3}\].

There has been no direct experimental observation of 2D BEC yet, except the recent related works such as quasi-condensate of atomic hydrogen \[\frac{4}{4}\] and quasi-2D gas of laser cooled atoms \[\frac{5}{5}\]. Nevertheless, recent theoretical studies have suggested a possibility of BEC in 2D in a trapped condition. However, those theoretical approaches so far have been only second-handed. Tempere and Devreese studied harmonically interacting bosons in 2D \[\frac{6}{6}\] and calculated the critical temperature by thermodynamic arguments to show the possible occurrence of 2D BEC. However, it could not provide any information on the 2D-condensate wave function necessary for the atomic density profile.

An analytical approach to interacting bosons in a 2D trap by Gross-Pitaevskii equation (GPE), a nonlinear Schrödinger equation for the macroscopic wave function of weakly interacting bosons, was also attempted by Gonzalez et. al. \[\frac{7}{7}\], but they inevitably faced with a dimensional inconsistency in the relation between coupling constant and scattering length. In other words, the well-known 3D result, \[U_0 = 4\pi\hbar^2a/M\] (interaction strength \[U_0\], s-wave scattering length \[a\], and atomic mass \[M\]) is not directly applicable to 2D GPE. Bayindir and Tanatar recently studied the 2D GPE within the two-fluid model of the mean-field many-body quantum statistical theory and could calculate the condensate fraction \[\frac{8}{8}\]. However, their results were obtained not from the direct solution of the 2D GPE, but from a density estimation. Therefore, the 2D condensate wave function still remains unsolved.

In this Letter, we first derive the “correct” 2D GPE from the first principles of two-dimensional scattering theory and then show the 2D BEC directly by calculating the condensate wave function of trapped atoms. The 2D time-independent Schrödinger equation with the interaction potential \[U(\rho)\] is given by

\[
(\nabla^2 + k^2)\psi_k(\rho) = U(\rho)\psi_k(\rho),
\]

where \[k^2 = 2\mu_mE/\hbar^2\]. Here, \(E\) is the energy and \(\mu_m = (M/2)\) is the reduced mass of two identical particles.

The general solution of Eq. \[\frac{9}{9}\] can be obtained in terms of the 2D Green’s function such that

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

Then, the 2D wave function can be expressed as

\[
\psi_k(\rho) = e^{ik\cdot\rho} + \int d^2\rho' \frac{G_k(\rho, \rho')U(\rho')}{2\sqrt{2\pi\hbar^2}} e^{i(k\cdot\rho'-\frac{\pi}{4})} d^2\rho' U(\rho')e^{i(k'\cdot\rho')},
\]

Here \(H_0\) is the first-kind Hankel function of order zero defined by \(H_0(x) = J_0(x) + iN_0(x)\), where \(J_0\) (\(N_0\)) is the Bessel (Neumann) function of order zero.

For large \(\rho\), it shows the asymptotic behavior of \(H_0(x) \approx \sqrt{2/\pi x}e^{i(x-\pi/4)}\). Note that the Born approximation was used and \(k' = k\hat{p}\).

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

1
where \( F_k \) is the first-order Born scattering-amplitude in 2D with a dimension of \([\text{length}]^{1/2}\). Note that this asymptotic formula is a solution of Eq. (1). Since the scattering cross-section in 2D should have the dimension of \([\text{length}]^2\), we can find

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

where \( j_{in}\) (\( j_{sc}\)) is the incident (scattered) flux density. Note that the total scattering cross-section for small \( k \) becomes \( 2\pi|F_k|^2 \) in 2D instead of \( 4\pi|f_{3D}|^2 \) in 3D (\( f_{3D} \) is the 3D scattering amplitude). Now, if one assumes a delta-function type interaction such that \( U(\rho) = (MU_0/\hbar^2)\delta^2(\rho) \) in Eq. (3), the \( F_k \) can be written as the following complex form

\[
F_k = -\frac{i}{2}\frac{1}{\sqrt{2\pi k}} \frac{MU_0}{\hbar^2}. \tag{6}
\]

The next step is to find the relation between the scattering amplitude and scattering length in 2D. Since the well-known relation \( f_{3D} = -a \), where \( a \) is the s-wave scattering length in 3D, is not directly applicable to 2D, we need to obtain the relation from a partial wave analysis of the two-dimensional collision theory. Outside the range of the potential, the scattered wave has a phase shift \( \delta_m \), and the scattering matrix becomes \( S_m = e^{2i\delta_m} \) (note that \( |S_m| = 1 \) for elastic scattering). Therefore, for large \( \rho \), the solution of Eq. (4) can be written as

\[
\psi_k(\rho) = e^{ik\rho} + \frac{1}{\sqrt{2\pi k\rho}} \sum_{m=-\infty}^{\infty} i^m (S_m - 1) H_m(k\rho)e^{im\theta}
\approx e^{ik\rho} + \frac{1}{\sqrt{2\pi k\rho}} \sum_{m=-\infty}^{\infty} i^m \times (e^{2i\delta_m} - 1)e^{i(k\rho - \frac{m\pi}{2})}e^{im\theta}, \tag{7}
\]

where \( m \) is an integer.

The scattering length is usually defined as the distance for which the two-body wave function is cut off at zero energy. Therefore, the phase shift due to scattering by a potential in 2D can be expressed in terms of the scattering length so that \( (11) \)

\[
\delta_0 = \frac{\pi}{2}\frac{1}{\ln ka}, \tag{8}
\]

where \( 0 < ka \ll 1 \). Note that \( \delta_0 = -ka \) in 3D. Eq. (8) can be easily obtained by the following simple argument. The scattering length is an equivalent hard-disk radius \( a \), imposed by the boundary condition \( \psi_k(a) = 0 \) for the asymptotic wave-function. For \( m = 0 \), the wave function can then be expressed as, at large distance and for small \( k \)

\[
\psi_k(\rho) = J_0(k\rho) - \frac{J_0(ka)}{N_0(ka)} N_0(k\rho)
\]

\[
\sim \frac{2}{\sqrt{2\pi k\rho}} \left[ \cos \left(k\rho - \frac{\pi}{4}\right) - \frac{\pi}{2\ln ka} \sin \left(k\rho - \frac{\pi}{4}\right) \right] \equiv \frac{2}{\sqrt{2\pi k\rho}} \cos \left(k\rho - \frac{\pi}{4} + \delta_0\right). \tag{9}
\]

Note that a 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. (8). Note also that unlike the 3D case where \( a \) can be negative as well, we do not consider the negative scattering length since the centrifugal potential of the lowest partial wave is negative in 2D [see Eq. (14)] so that the extrapolated local wave function cuts the radial axis always above the origin (i.e., \( a > 0 \)).

Now, from Eqs. (5), (6) and (8), we can express the scattering amplitude as a series expansion, and also find that \( m = 0 \) term is a dominant contribution to the 2D system. Therefore, the 2D scattering amplitude becomes a complex form, given by

\[
F_k = \frac{1}{\sqrt{2\pi k}} \frac{1}{\sqrt{2\pi k}} \sum_{m=-\infty}^{\infty} (e^{2i\delta_m} - 1)e^{im\theta}
= \frac{2i\delta_0}{\sqrt{2\pi k}}(1 + i\delta_0 + ...)
\approx \frac{i\pi}{\sqrt{2\pi k}\ln ka}. \tag{10}
\]

Finally, we can obtain the 2D interaction potential \( U_0 \) from Eqs. (3) and (10) as

\[
U_0 = -\frac{2\pi\hbar^2}{M}\frac{1}{\ln ka}. \tag{11}
\]

Here, assuming the system is in the ground state of 2D harmonic potential, we may approximate the small \( k \) to be \( 1/a_{ho} \), where \( a_{ho} = \sqrt{\hbar/M\omega} \) (\( \omega \) is the trap frequency).

Eq. (11) is a key result of this Letter, and there will be no dimensional inconsistency in deriving the 2D GPE. Now, the 2D condensate wave function can be obtained from the 2D GPE such that (12)

\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{ext}(\rho) + NU_0\phi^2(\rho) \right] \phi(\rho) = \mu\phi(\rho), \tag{12}
\]

where \( \int d^2\rho \phi^2(\rho) = 1 \) and \( N \) is the number of condensate particles. We assume a 2D isotropic, harmonic trap potential \( V_{ext}(\rho) = \frac{1}{2}M\omega^2\rho^2 \). Then we can simplify Eq. (13) for numerical calculation by introducing the dimensionless variables \( (\rho \to a_{ho}\rho, \mu \to \hbar\omega\mu \) and \( \phi \to a_{ho}^3\phi \) and the dimensionless interaction of \( N \) atoms, \( \bar{U}(N) = 4\pi N/|\ln(a/a_{ho})| \), as

\[
\left[ -\nabla^2 + \rho^2 - 2\mu + \bar{U}\phi^2(\rho) \right] \phi(\rho) = 0, \tag{13}
\]

or
\[- \frac{d^2u}{d\rho^2} + \left[ \rho^2 - \frac{1}{4\rho^2} - 2u + \tilde{U}(\rho) \right] u(\rho) = 0 \, , \tag{14} \]

where \( \phi(\rho) = u(\rho)/\sqrt{\rho} \). Here the 2D chemical potential \( \mu \) can be obtained from the normalization condition. Note that the scattering length \( a \) is the only atomic parameter that contributes to the condensate state.

The procedure to solve Eq. (13) or Eq. (14) is very similar to the case of 3D [13]. For the non-interacting case, the solution is still Gaussian with \( \phi(\rho) = \pi^{-1/2} e^{-\rho^2/2} \). In the strongly repulsive limit (Thomas-Fermi limit), we obtain the parabolic solution \( \phi^2(\rho) = (2\mu - \rho^2)/\tilde{U} \). With a typical value of \( ka \sim a/a_{\text{ho}} = 10^{-3} \) in Eq. (11), we have plotted the 2D condensate wave function versus \( \rho \) and \( N \) in FIG. 1. Note that although the 2D condensate wave functions show the overall behaviors similar to those of the 3D case, they approach the parabolic limit more rapidly with increasing the number of atoms. In other words, the effect of atomic interaction potential becomes more prominent in 2D. Note also that the 2D condensation is not very sensitive to the scattering length due to its logarithmic dependence. This implies that each bosonic alkali atom with positive scattering length may exhibit similar condensate characteristics in 2D. Refer to TABLE 1 for more detailed comparisons between our 2D results and well-known 3D ones.

The ground-state energy of the 2D system can be obtained from the energy functional \( E \) as [12]

\[ E[\phi] = \int d^2 \rho \left[ \frac{\hbar^2}{2M} |\nabla \phi|^2 + \frac{1}{2} M \omega^2 \rho^2 |\phi|^2 + \frac{U_0}{2} |\phi|^4 \right] . \]

With the Gaussian trial function \( \phi(x) = \sqrt{N/(\pi a^2)} e^{-x^2/2a^2} \), Eq. (15) satisfies the following relation

\[ E \geq \frac{\hbar^2}{M} \sqrt{1 + \frac{N}{|\ln ka|}} \hbar \omega . \]  

\[ \tag{16} \]

The ground-state energy per particle of Eq. (16) is plotted in FIG. 2 with the same parameter \( ka \sim a/a_{\text{ho}} = 10^{-3} \) and is compared with the well-known 3D result of \(^{87}\text{Rb} \). It is interesting to note that as the number of atom is increased, the 2D system becomes much unstable in contrast to the 3D case.

Now, let us consider the vortex states in 2D in connection with superfluidity of the hydrodynamic theory. The 2D system may rotate around the 2D trap center, resulting in a quantized circulation of atoms. An angular momentum quantum number \( \kappa \) can be then assigned to the quantum winding of the 2D vortex state, which can be written as \( \phi(\rho) = \psi(\rho) e^{iS(\rho)} \), where \( \psi(\rho) = \sqrt{n(\rho)} \) is the modulus. When the phase \( S \) is chosen as \( \kappa \theta \) (\( \kappa \) is an integer), one finds vortex states with a tangential velocity \( v = \kappa \hbar/M \rho \). As a result of the quantum circulation, the angular momentum of the system with respect to the \( \rho = 0 \) axis becomes \( L = N \kappa \hbar \). Including the vortex term in Eq. (12), we now obtain the 2D GPE with vortex states as

\[ \left[ -\nabla^2 + \frac{\kappa^2}{\rho^2} + \rho^2 - 2\mu + \tilde{U}(\rho) \right] \psi(\rho) = 0 . \]

The wave functions for \( \kappa = 1 \) vortex state are plotted in FIG. 3. We observe, in particular, that the overall shape and the \( N \)-dependence of the vortex-state wave functions are qualitatively similar to those of 3D [12]. Note that 2D BEC transition looks analogous to the Kosterlitz-Thouless (KT) vortex-state transition. However, the phase transition of 2D BEC does not necessarily involve any interaction between atoms and this is the fundamental difference between the two transitions in 2D.

Although there are fundamental differences between our purely 2D results and 3D ones as summarized in TABLE 1, it will be interesting to consider the quasi-2D or \((2+1)\)D scheme as a limiting case of 3D, in the sense that the atoms obey 2D statistics while their interactions are 3D. To compare the situation of 2D trap with an extremely squeezed 3D trap, we take the 3D external potential as \( V_{\text{ext}}(r, z) = (1/2)M \omega^2 (r^2 + \lambda^2 z^2) \). Fixing the number of atoms and increasing the \( \lambda \), (note that as \( \lambda \to \infty \), \( V_{\text{ext}} \) approaches 2D trap). Solving the 3D GPE with fixed number of atoms, we have presented how the condensate wave functions behave with \( \lambda \) in FIG. 4. We can observe the 3D wave functions merge to the 2D limit but slowly as \( \lambda \) is increased.

In summary, we have developed the 2D collision theory to obtain the 2D scattering length and the interaction strength. We then derived the 2D nonlinear Schrödinger equation (GPE) for trapped neutral Bose atoms with and without vortex state. The 2D condensate and vortex state wave functions are calculated numerically from the 2D GPE. Despite the apparent differences, we observe the qualitative behaviors similar to the 3D BEC, but do not expect 2D BEC for negative scattering length. The ground state energy per particle is calculated and compared with that of the well-known 3D traps. We also have considered the practical quasi-2D case as an extreme of very thin 3D trap.

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| Dimension                  | $D = 3$                                                                 | $D = 2$                                                                 |
|----------------------------|------------------------------------------------------------------------|------------------------------------------------------------------------|
| Interaction strength       | $U_{3D} = \frac{4\pi\hbar^2 a}{M}$                                    | $U_{2D} = \frac{2\pi\hbar^2}{M} \left(\frac{1}{\ln km}\right)$       |
| Healing length             | $(8\pi\hbar a_{3D})^{-1/2}$                                            | $(\frac{4\pi\hbar a_{2D}}{\ln km})^{-1/2}$                           |
| Chem. potential (noninteracting) | $\frac{1.5}{\rho} \left(\frac{15\alpha N}{\rho\omega}\right)^{2/5} \hbar \omega$ | $\frac{1}{\rho} \left(\frac{2N}{\ln km}\right)^{1/2} \hbar \omega$ |
| Chem. potential (interacting) | $\frac{1.5}{\rho} \left(\frac{15\alpha N}{\rho\omega}\right)^{2/5} \hbar \omega$ | $\frac{1}{\rho} \left(\frac{2N}{\ln km}\right)^{1/2} \hbar \omega$ |
| Radius of cond.            | $r_c = \left(\frac{15\alpha N}{\rho\omega}\right)^{1/5}$             | $\rho_c = \left(\frac{8N}{\ln km}\right)^{1/4}$                      |
| Cond. energy               | $\frac{2}{\pi} \mu_{3D} N \propto N^{1/5}$                           | $\frac{2}{\pi} \mu_{2D} N \propto N^{3/2}$                           |
| Center lowering           | $|\phi(0)|_{3D}^2 \propto N^{-3/5}$                                    | $|\phi(0)|_{2D}^2 \propto N^{-1/2}$                                   |
FIG. 1. The 2D condensate wave functions for a typical value of $k\alpha = 10^{-3}$.

FIG. 2. The ground-state energy per particle of Eq. (16). The unit of y-axis is $\hbar\omega$. 
FIG. 3. The 2D wave functions of vortex state for a quantum circulation $\kappa = 1$ and a typical value of $ka = 10^{-3}$.

FIG. 4. The behavior of asymmetric 3D condensate wave functions for fixed $N = 100$. From the top left $\lambda = 10, 100, 300, 1000$. The dotted line is the 2D condensate wave function of the same $N$. Note that $
abla_{3D} = \left[ \int dz |\phi_{3D}(r, z)|^2 \right]^{1/2}$. 