Critical fluctuations of an attractive Bose gas in a double-well potential

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received 13 June 2008; accepted in final form 11 August 2008
published online 15 September 2008

PACS 47.20.Ky - Nonlinearity, bifurcation, and symmetry breaking
PACS 68.35.Rh - Phase transitions and critical phenomena
PACS 67.85.Jk - Other Bose-Einstein condensation phenomena

Abstract – We consider a Bose gas with an attractive interaction in a symmetric double-well potential. In the mean-field approximation, the ground-state solution spontaneously breaks the symmetry of the trapping potential above a certain value of the interaction strength. We demonstrate how the Landau-Ginzburg scheme of the second-order phase transition emerges from the quantum model and show the link to the spontaneous symmetry breaking mentioned above. We identify the order parameter, the critical point and analyze quantum fluctuations around it.

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Ultracold atomic gases become ideal systems to investigate many-body physics both theoretically and experimentally [1]. Experimentalists can prepare quantum-degenerate gases in a wide range of trapping potentials and tune strength and even character of particle interactions [2]. The widely used approximation in the study of properties of ultracold dilute bosonic gases is the Gross-Pitaevskii equation [3]. In the most commonly used procedure, the solution of this equation is the starting point for the expansion of the field operator. This enables for calculation of many-body properties of the system in a systematic perturbative way [3,4]. The Gross-Pitaevskii equation is a result of an assumption that all particles are described by the same wave function, often called condensate wave function. Because of interactions between atoms the equation for the condensate wave function is non-linear. This fact can lead to interesting phenomena when the non-linearity exceeds a critical value: spontaneous breaking (bifurcation) of the external trapping potential symmetry may occur even in the ground state of the system [5]. However it is known from the general theorem of the many-body systems that the mean density of the system in the ground state respects the symmetry of the external potential [6]. As the condensate wave function, which is a starting point for perturbative calculus, does not preserve this symmetry, the whole procedure becomes questionable. The authors are not familiar with any systematic perturbative procedure in such case. This fact motivated us to study the many-body properties of such system around the bifurcation point. The simplest system to study is the attractive Bose gas in the symmetric double well in the tight-binding approximation. In this paper we present a useful method for such analysis.

The fact that the spontaneous symmetry breaking takes place in the Gross-Pitaevskii equation reminds us of the Landau-Ginzburg theory of second-order phase transition. Having that in mind, one may expect that the quantum fluctuations of the order parameter will be maximal in the bifurcation point. The study of this fluctuations is the main purpose of this letter.

As it is rich in physical phenomena, the system of ultracold gas in the double-well potential draws the attention of many researchers. Both static and dynamic properties of the repulsive gas were recently studied experimentally [7–12]. However, the effect of spontaneous symmetry breaking has not yet been observed. The symmetry breaking takes place in the double-well system with attractive interactions, but we are aware that its experimental realization might be difficult. A far more promising system is a two-component repulsive gas in the symmetric double-well potential. In this case, spontaneous symmetry breaking occurs in the ground state. Moreover,
spontaneous symmetry breaking occurs also in case of light propagation through non-linear media as well [13], so in principle the results presented here might be of interest for the quantum optics community.

Let us begin our analysis with the introduction of the Bose-Hubbard model in the tight-binding approximation [4,14–16]

\[ \hat{H} = -\frac{\Omega}{2}(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1) + \frac{U}{2}(\hat{a}_1^\dagger \hat{a}_1 \hat{a}_2^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_2 \hat{a}_1^\dagger \hat{a}_1), \]

(1)

where the \( \hat{a}_1 \) (\( \hat{a}_2 \)) operator annihilates an atom in the left (right) well, \( \Omega \) stands for the tunneling rate between the wells and \( U \) is the on-site interaction strength (here we consider attractive interactions hence \( U < 0 \)). Notice that, since the total number of particles \( N \) remains a conserved quantity, we can extract a constant part from the Hamiltonian (1)

\[ \hat{H} = -\frac{\Omega}{2}(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1) + \frac{U}{4}(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2)^2 + \frac{U}{4}(\hat{N}^2 - 2\hat{N}). \]

(2)

The last term will be neglected in the further considerations.

Let us review briefly the literature dedicated to the systems governed by Bose-Hubbard Hamiltonian. In the case of repulsive interactions \( U > 0 \), the relative number squeezing [16–18] and thermally induced phase fluctuations [19] were predicted and then confirmed in experiment [8,11] and [12]. The a.c. and d.c. Josephson effects were studied experimentally [10]. Time evolution of the relative phase between two Bose-Einstein condensates [7] and the phase evolution during the splitting of the Bose-Einstein condensate into two [9] were measured. For attractive interactions, formation of macroscopic Schrödinger cat states was predicted to occur above the critical value of the interactions [20]. For a critical value of the interactions the ground state exhibits phase squeezing [17]. However, the system with attractive interactions did not attain experimental realization so far.

The Bose-Hubbard Hamiltonian is equivalent to the Lipkin-Meshkov-Glick model which was extensively studied in the context of quantum phase transitions [21]. For instance, a second-order quantum phase transition with the critical exponents of the order parameter given by the mean-field approach was predicted [21,22]. One would expect an enhancement of the fluctuation of the order parameter at the transition point. To our knowledge this was not studied before and it is a main purpose of our study to confirm this prediction.

Let us briefly review the results of the mean-field approach. The foundation of this method is an assumption that all the atoms are in the same quantum state. The most general form of such a state is

\[ \frac{1}{\sqrt{N!}} \left( \sqrt{\frac{1+z}{2}} e^{\frac{z}{2} \varphi} \hat{a}_1^\dagger + \sqrt{\frac{1-z}{2}} e^{-\frac{z}{2} \varphi} \hat{a}_2^\dagger \right)^N |\text{vac}\rangle. \]

(3)

Here, \( z \) is the relative population difference between the wells, \( \varphi \) is a relative phase and \( |\text{vac}\rangle \) denotes the vacuum state. Within the mean-field method we can calculate an expectation value of the Hamiltonian (2) in the state (3).

It reads

\[ \langle \hat{H} \rangle = \frac{\Omega N}{2} \left( \frac{z^2}{2} - \sqrt{1-z^2} \cos \varphi \right), \]

(4)

where the dimensionless parameter,

\[ \gamma = UN/\Omega, \]

(5)

is a ratio of the on-site interaction per atom to the tunneling rate. Notice that the minimum of the expectation value of the Hamiltonian (4) occurs for \( \varphi = 0 \). In case of \( \gamma \geq -1 \), the minimum appears for \( z = 0 \) and for \( \gamma < -1 \) it is shifted to the point \( \pm z_0 \), where \( z_0 = \sqrt{1 - \gamma^2} \). The non-zero value of \( z_0 \) indicates that the solution of the mean-field approximation breaks the symmetry of the trapping potential. We can introduce an order parameter which measures the population imbalance between wells. If we choose it to be \( N|z| \), we can use it to distinguish two "phases" — symmetric and asymmetric states. In order to associate the bifurcation mentioned above with the phenomenon of phase transition, we have to introduce the thermodynamic limit. In our case this limit will consist of \( N \to \infty \) with \( \gamma \) remaining constant. With this limit in mind the mean-field approximation predicts a second-order phase transition in our system.

Now we turn to the quantum model. We introduce a simple method (called a continuum approximation [16,18]) in which the Schrödinger equation obtained from our Bose-Hubbard Hamiltonian reduces to a one-dimensional Schrödinger-like equation of a fictitious particle in an effective potential. Looking at the form of this potential, one can recognize a second-order phase transition in the evolution of the shape of this potential from a parabolic, through quartic, to double well with the change of the interaction strength. It also gives a clear picture of the growth of the fluctuations in the vicinity of the critical point. The short derivation of the continuum approximation is presented below.

As the total number of atoms is conserved, the wave function can be written in a Fock basis of states \( |N-n, n\rangle \) (here \( n \) denotes the number of atoms in the right potential well), as

\[ |\Psi\rangle = \sum_{n=0}^{N} \psi_n |N-n, n\rangle. \]

(6)

Then the stationary Schrödinger equation obtained from Hamiltonian (2) reads

\[ \sum_{n} \left( \Omega \frac{\psi_{n+1}}{2} \sqrt{(N-n)(n+1)} + \psi_{n-1} \sqrt{(N-n+1)n} \right) - \frac{U}{4} \psi_n (N-2n)^2 + \frac{\Omega}{4} \psi_{n+1} \psi_{n-1} |N-n, n\rangle = 0. \]

(7)

1Strictly speaking, the term \( z^2 \gamma/2 \) should be multiplied by \( (N-1)/N \). However, as we are in the large-\( N \) limit, we set this prefactor to be equal to unity.
Let $z_n$ denote the variable related to the relative population difference
\[ z_n = \frac{(N - n) - n}{N} = 1 - \frac{2n}{N}. \tag{8} \]

Using this variable, eq. (7) transforms into
\begin{align*}
\frac{\Omega N}{2} \left[-\psi_{n+1} + \frac{1 + z_n}{2} \frac{1 - z_n}{2} + \frac{1}{N} \right] - \psi_{n-1} \left[1 + \frac{1 + z_n}{2} \frac{1 - z_n}{2} + \frac{U N^2}{4} \right] \psi_n z_n^2 &= E \psi_n. \tag{9}
\end{align*}

For a large number of particles the $\frac{1}{N}$ terms can be dropped\(^2\). Also in this limit the variable $z_n$ may be treated as a continuous variable (i.e. $z_n \to z$) and we approximate the finite differences by a second-order differential operator
\begin{align*}
\frac{\psi_{n+1} + \psi_{n-1} - 2\psi_n}{(2/N)^2} \simeq \frac{d^2}{dz^2} \psi(z). \tag{10}
\end{align*}

Upon completing this procedure, we reduce eq. (9) to the following form:
\begin{align*}
\frac{\Omega N}{2} \left[\frac{2}{N^2} \sqrt{1 - z^2} \frac{d^2}{dz^2} + V(z) \right] \psi(z) &= E \psi(z), \tag{11}
\end{align*}
where we introduced the effective dimensionless potential $V(z)$
\[ V(z) = -\sqrt{1 - z^2} + \frac{\gamma}{2} z^2, \tag{12} \]
with $\gamma$ defined above. Notice that the operator on the left-hand side of eq. (11) is non-Hermitian\(^3\). However, our starting eq. (9) is a result of an action of a Hermitian operator (2) on the wave function (6). In principle, we could obtain the continuous limit in a way conserving hermiticity, but the derivation would require much more sophisticated expansion and would lose its illustrative character. Instead, we present an alternative derivation and we argue that the corrections required to restore hermiticity in eq. (11) are negligible in the large $N$ limit. To follow this derivation, let us start with the Hamiltonian
\[ H = -\frac{\Omega}{2} \left[ \alpha_1^\dagger \alpha_2 + \alpha_2^\dagger \alpha_1 \right] + \frac{U}{2} \left[ |\alpha_1|^4 + |\alpha_2|^4 \right]. \tag{13} \]

Notice that the second quantization procedure of (13) leads to (1). Here $\alpha_1$ are mode amplitudes, which in
\footnote{It is justified as along as $\psi_n$ is close to zero for $z_n \simeq \pm 1$. Numerical solutions of eq. (9) show that this condition is satisfied except for the region $\gamma \ll -1$, when the strong condensate splitting occurs.}

\footnote{The derivation of the continuum approximation presented in [16,18] neglected the term $\sqrt{1 - z^2}$ in front of the second derivative. In this case the Hamiltonian operator is Hermitian. This approximation is well justified in the case of repulsive interactions, where the average $(z^2) \ll 1$. In the attractive case studied here it is true only for $\gamma > -1$.}

the second quantization are replaced with annihilation operators. Additionally, the quantity $|\alpha_1|^2 + |\alpha_2|^2 = N$ remains constant during the evolution governed by (13). Next we introduce the new variables $z$ and $\varphi$:
\begin{align*}
\alpha_1 &= \sqrt{N} \sqrt{1 + \frac{z}{2}} e^{i\varphi_1}, & \alpha_2 &= \sqrt{N} \sqrt{1 - \frac{z}{2}} e^{i\varphi_2}, \tag{14}
\end{align*}
and obtain
\begin{align*}
H &= \frac{\Omega N}{2} \left[ \frac{1}{2} \sqrt{1 - z^2} (1 - \cos \varphi) 
+ \frac{1}{2} (1 - \cos \varphi) \sqrt{1 - z^2} + V(z) \right] + \frac{U}{4} N^2, \tag{15}
\end{align*}
where $V(z)$ is defined by eq. (12) and $\varphi = \varphi_1 - \varphi_2$ (the constant term $U N^2$ will be neglected in the further considerations). Mind that the Hamiltonian (15) is given by the same formula as (4) (see footnote 4), and that the variable $z$ has the same meaning as that of the continuum approximation variable, defined by eq. (8).

Now we can perform quantization by replacing the conjugate variables $z$ and $\varphi$ with operators $\hat{z}$ and $\hat{\varphi}$ obeying the commutation relation $[\hat{z}, \hat{\varphi}] = i \frac{\pi}{\Omega}$ [4,19].

- In the case of repulsive interactions, the phase fluctuations are dominant over fluctuations of population imbalance $z$. In this case it is convenient to choose phase representation, i.e. replace $\hat{z}$ with $\frac{\hat{z}}{N} \frac{d}{d\hat{z}}$ [19].

- On the other hand, in the case of attractive interactions the phase fluctuations are small, $\cos \hat{\varphi} \simeq 1 - \frac{1}{2} \hat{z}^2$, and it is more convenient to choose z representation; $\hat{\varphi} = \frac{\hat{z}}{N} \frac{d}{d\hat{z}}$.

In the case of attractive interactions, we obtain
\[ H = \frac{\Omega N}{2} \left[ -\frac{1}{N^2} \sqrt{1 - z^2} \frac{d^2}{dz^2} - \frac{1}{N^2} \sqrt{1 - z^2} + V(z) \right]. \tag{16} \]

The Schrödinger equation takes the form
\begin{align*}
- \frac{1}{N^2} \left[ \sqrt{1 - z^2} \frac{d^2}{dz^2} + \frac{d^2}{dz^2} \sqrt{1 - z^2} \right] \psi(z) + V(z) \psi(z) &= \frac{2E}{N \Omega} \psi(z). \tag{17}
\end{align*}

This is again a one-dimensional Schrödinger-like equation for a particle in the potential $V(z)$, where the coefficient $2/N$ plays the role of $\hbar$. One can compare eq. (11) and eq. (17); the difference consists of two terms
\[ \frac{1}{N^2} \frac{z}{\sqrt{1 - z^2}} \frac{d}{dz^2} \psi(z) - \frac{1}{N^2} \left[ \frac{d^2}{dz^2} \sqrt{1 - z^2} \right] \psi(z). \tag{18} \]

\[^4\text{The Hamiltonian (15) can be obtained from the Hamiltonian (1) as the expectation value of the coherent state $|\alpha_1 \rangle \otimes |\alpha_2 \rangle$ with $|\alpha_1|^2 + |\alpha_2|^2 = N$. The equation (4) is the expectation value of the same Hamiltonian (1) but calculated on the two-mode coherent state (3). The important difference between the two-mode coherent state (3) and the tensor product of two one-mode coherent states $|\alpha_1 \rangle \otimes |\alpha_2 \rangle$ is that the second one does not conserve the number of particles. This leads to the differences of the order $1/N$ which we neglect.}\]
Fig. 1: (Color online) Comparison of the probability density $|\psi(z_n)|^2$ obtained by diagonalization of the exact Hamiltonian (2) (solid black lines) and by solution of eq. (17) (dashed red lines) at the critical point, i.e. for $\gamma = -1$. Panels (a) and (b) correspond to ground states while (c) and (d) to the ninth excited states. Results for $N = 200$ are presented in (a) and (c) and for $N = 10^4$ in (b) and (d).

To estimate the first term, we notice that the characteristic width of the wave function $\psi$ scales like a certain positive power of $1/N$ (since $2/N$ plays the role of $\hbar$). Hence each derivative over $z$ generates a factor of the order of positive power of $N$, and so the first derivative is much smaller than the second one. The second term contributes to the potential and contains a factor of $1/N^2$. In conclusion, for large $N$ both these terms can be neglected.

Note that eq. (17) turns out to generate accurate results even for a relatively low number of atoms. In order to evaluate the quality of the continuum approximation, we compare the eigenstates (fig. 1) and the energy level diagrams (fig. 2) obtained by solving eq. (17) and by numerical diagonalization of the Hamiltonian (2) for 200 and $10^4$ particles. Already at the level of few hundred particles, the results obtained within the continuum approximation seems to be indiscernible from the exact ones. It is worth noticing that there is an exact mapping between the Schrödinger equation (7) and effective one-dimensional Schrödinger equation (see ref. [22]). However, the continuous variable used in [22], contrary to our approach, does not possess a clear interpretation of the relative population difference.

An important issue is the relation between the continuum approximation and the result of the quantization procedure of the Hamiltonian (15). Both these resulting Schrödinger equations (11) and (17) have a common root which is the Hamiltonian (13). This Hamiltonian can either be second-quantized using canonical quantization, leading to Hamiltonian (1). Then, using the continuum approximation, we obtain the Schrödinger equation (11). On the other hand, it can be second-quantized using the relative phase operator. This directly leads to the Schrödinger equation (17). The thus-obtained Schrödinger equations yield wave functions $\psi(z)$ which have the same interpretation $-|\psi(z)|^2$ is the probability density for the system having relative population imbalance $z$. Moreover, both these approximations lead to equations which almost do not differ. We want to add that these approximations are independent and we do not know any formal relation between them.

In our opinion the real value of the continuum approximation is that one can predict the properties of the system by simply analyzing a form of the effective potential. Figure 3 presents the shape of the potential for three crucial regions: before ($\gamma > -1$), at ($\gamma = -1$), and beyond ($\gamma < -1$) the critical point. In the first region the potential has typically a quadratic form, while at $\gamma = -1$ it broadens substantially and becomes quartic. In the last region it has a form of a double well with the minima at $z = \pm z_0$. This analysis paints a picture of the second-order quantum phase transition, with the critical point at $\gamma = -1$. In
order to see that, we have to recall the order parameter introduced above.

We have chosen the order parameter to be $N|z|$, (see footnote 5) already, upon discussing the mean-field approximation. Within the mean-field approximation, we are dealing with the average value of $N|z|$. The same variable can be defined in the quantum model (2). Hence the order parameter can be expressed in terms of creation and annihilation operators

$$ \hat{B} = |\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2|, $$

(19)

The quantum average $\langle \hat{B} \rangle/N$ tends towards the mean-field value of $|z|$. The shape of the potential determines the shape of the ground-state wave function, which is always symmetric. For $\gamma \geq -1$ it is bell shaped and centered around $z = 0$, and when $\gamma < -1$ the wave function has a double-hump structure, centered around $\pm z_0$. Since the effective $\hbar$ is $2/N$, the width of the wave function decreases with increasing $N$. The wave function will be centered around the minima of the potential $V(z)$, which, as we mentioned above, is given by the mean-field approximation. This shows that the mean value of $\langle \hat{B} \rangle/N$ indeed will approach the mean-field value. This fact was noticed in ref. [21].

Now we want to investigate the most important issue of our paper, the fluctuations of the order parameter. The key observation is that since the potential is of Landau-Ginzburg type, it is clear that the fluctuations of the order parameter will be maximal at the critical point. The more quantitative analysis of this issue can be made using the continuum approximation and the full quantum model. The variance of $\hat{B}$ in the ground state of the double-well system vs. $\gamma$ is shown in fig. 4 for two different numbers of particles. It indicates that the fluctuations are maximal around the critical point. With increasing value of $N$ the width of the variance decreases and the position of the maximum tends to $\gamma = -1$.

In conclusion, we have analyzed the behavior of the ground state of the Bose gas with attractive interactions in a symmetric double-well potential. This system experiences second-order quantum phase transition which is revealed within the description called continuum approximation. This approximation allows for reduction of the many-body system in the two-mode approximation (Bose-Hubbard model) to a problem of a fictitious quantum particle in an effective potential. Transformation of the effective potential from quadratic through quartic to double well with the increase of the interactions strength fits well to the Landau-Ginzburg scenario and allows for identification of the order parameter and the critical point. The presence of the critical point manifests itself by a sudden increase of the fluctuations of the order parameter (the so-called critical fluctuations), which we confirm numerically.

In our opinion, the two main advantages of the continuum approximation are the following: First, it gives a clear picture of the dynamical and static properties of the system. Second, it is useful when the number of particles in the system gets large and the exact calculations are very difficult. In the case of ultracold gases the quantum fluctuations might be dominated by temperature effects. These effects can be included in our method and it will be demonstrated in the future paper.

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We acknowledge insightful discussions with M. NAPIÓRKOWSKI. The work of BO was supported by the Polish Government scientific funds (2008-2010) as a research project. KS was partly supported by the Polish Government scientific funds (2008-2011) and Marie Curie ToK project COCOS (MTKD-CT-2004-517186). PZ and JCh acknowledge the support of the Polish Government scientific grant (2007-2010) and MT of the Polish Government scientific grant (2006-2009). The research was conducted within LFPPi network.

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