Quantum information approach to a Bose–Einstein condensate in a tilted double-well system

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Received 1 December 2011, in final form 9 January 2012
Published 14 February 2012
Online at stacks.iop.org/JPhysB/45/055301

Abstract
We study the ground-state properties of bosons in a tilted double-well system. We use fidelity susceptibility to identify the possible ground-state transitions under different tilt values. For a very small tilt (for example $10^{-10}$), two transitions are found. For a moderate tilt (for example $10^{-3}$), only one transition is found. For a large tilt (for example $10^{-1}$), no transition is found. We explain this by analysing the spectrum of the ground state. The quantum discord and total correlation of the ground state under different tilts are also calculated to indicate those transitions. In the transition region, both quantities have peaks decaying exponentially with the particle number $N$. This means that for a finite-size system the transition region cannot be explained by the mean-field theory, but in the large-$N$ limit it can be.

1. Introduction

The many-body quantum states in ultracold gases have been studied with a high interest, because there are many parameters that can be adjusted in experiments to control the static state as well as the dynamics of the system. As a paradigm model, a Bose–Einstein condensate (BEC) in a double-well system provides a useful setup to tackle the properties of quantum systems. By loading ultracold atoms in double wells, one can study fundamental quantum mechanical effects and many important quantum many-body phenomena, for example, interferometry [1], quantum information processing [2], quantum phase transition [3], quantum superposition state [4], Josephson oscillations and nonlinear self-trapping form of dynamics [5].

Recently, it was found that in some ultracold gas systems (such as rotating BEC and BEC in double wells with a very small tilt), the ground-state transition cannot be described by the mean-field theory, although the ground states before and after transition are very consistent with the mean-field description [6–10]. This is because in the transition region, the ground state is no longer a product of single-particle states but a strongly correlated entangled state. How to characterize such states is under intensive study. Moreover, in [6–10], the system sizes under study are not too large. The property of quantum correlation in the transition region for a larger system is an interesting problem.

The appearance of quantum correlation in the ground state in the transition region makes it reasonable to use some tools borrowed from quantum information theory to investigate the transition. In this paper, our goal is to use fidelity susceptibility and quantum correlation to study the ground-state transition of BEC in double wells with an arbitrary tilt. In section 2, we introduce the model and give the prediction of the ground-state transition according to the semi-classical picture. In section 3, we calculate the fidelity susceptibility which can precisely locate the critical point of a possibly unknown quantum transition [11]. Different behaviours of the fidelity susceptibility under different tilts are found. In section 4, enlightened by the fact that entanglement can also show a rather interesting behaviour at the critical point of a quantum transition [12], we calculate two quantities of quantum correlation: total correlation and quantum discord, both of which can exhibit signatures of the quantum transitions [13]. Moreover, quantum discord can appear even when entanglement is absent [14–17] so it is a more suitable quantity than entanglement to characterize the quantumness of the correlation. We find that both total correlation and
quantum discord are non-zero in the transition region, but their values decrease with the particle number. By doing a finite-size analysis, an exponential decay of them with the particle number is found. This means that although for a small system the transition is dominated by the quantum correlation, for a very large system no quantum correlation exists during the transition. A brief summary is given in section 5.

2. Model

The single-level Bose–Hubbard Hamiltonian for \( N \) atoms in a double-well system can be written as

\[
\mathcal{H} = -J(\hat{a}_L^\dagger \hat{a}_R + \hat{a}_R^\dagger \hat{a}_L) - U(\hat{n}_L(\hat{n}_L - 1) + \hat{n}_R(\hat{n}_R - 1)) - V_0(\hat{n}_L - \hat{n}_R),
\]

where \( \hat{a}_i^\dagger (\hat{a}_i) \) creates (annihilates) a boson in the \( i \)th well \((i = L, R)\), \( \hat{n}_i = \hat{a}_i^\dagger \hat{a}_i \). \( J \) is the tunnelling energy and \( U \) is the on-site interaction (a positive (negative) \( U \) corresponds to attractive (repulsive) atom–atom interaction). \( V_0 \) is the tilt which can destroy the left–right symmetry and is non-zero in real experiments. We set \( J = 1 \) for convenience and only consider \( U > 0 \) in this paper. The above Hamiltonian can be diagonalized in the \((N + 1)\)-dimensional Fock space spanned by \( |n_L, n_R = N - n_L\rangle \). The dynamics of the system is controlled by the parameter \( \lambda \equiv NU/J \). As \( \lambda \) passes from the weak region to the fermionization limit, the dynamics of these atoms, which are initially prepared mostly in one well, will change from Josephson oscillation (simply tunneling back and forth between two potential wells) to self-trapping above a critical interaction strength [5]. Moreover, the static properties of the system, such as the ground state, are also closely related to \( \lambda \).

We can replace the operators \( \hat{a}_i \) with numbers \( a_i = \sqrt{ni} e^{i\phi} \) in equation (1) to obtain a semi-classical Hamiltonian

\[
\frac{\mathcal{H}}{N} = - \sqrt{1 - \frac{z^2}{4}} \cos \phi - \frac{\lambda}{4N} (Nz^2 + N - 2) - V_0z, \tag{2}
\]

where \( \phi = \phi_L - \phi_R \) and \( z = (n_L - n_R)/N \) characterize the imbalance. To minimize the energy, it is obvious that \( \phi \) should be zero. Then, for each \( V_0 \) and \( \lambda \), we can find the position \( z_{\text{min}} \) of the local minimum of equation (2) by solving \( \frac{d}{dz} \frac{\mathcal{H}}{N} \big|_{\phi=0} = 0 \).

For \( V_0 \lesssim 10^{-3} \), at a critical \( \lambda \approx 2 \), \( z_{\text{min}} \) increases from 0 abruptly, giving a hint of quantum transition of the ground state.

3. Fidelity susceptibility

In this section, by diagonalizing the Hamiltonian (1), we use fidelity susceptibility to show the quantum transition of the ground state predicted by the semi-classical Hamiltonian (2). The ground-state fidelity susceptibility is defined as

\[
\chi(\lambda) = - \lim_{\delta \lambda \to 0} \frac{2 \ln F}{\delta \lambda^2} = \sum_{n=0}^{N} \left| \langle \Psi_0(\lambda) | \frac{\partial^2}{\partial \lambda^2} | \Psi_0(\lambda) \rangle \right|^2 \left[ E_0(\lambda) - E_0(\lambda) \right],
\]

where \( \Psi_0(\lambda) [\Psi_\eta(\lambda)] \) is the ground (excited) state of \( \mathcal{H}, E_\eta(\lambda) [E_0(\lambda)] \) is the corresponding ground (excited) energy. Here we suppose that \( \mathcal{H} \) has a non-degenerate ground state. In our system, \( \frac{\partial^2 \mathcal{H}}{\partial \lambda^2} = - \frac{1}{N} \hat{n}_L(\hat{n}_L - 1) + \hat{n}_R(\hat{n}_R - 1) \). When \( V_0 = 0 \), the ground states are degenerate for some values of \( \lambda \). To break this degeneracy, we add a non-zero tilt and then we can use fidelity susceptibility to study the quantum transition of the ground state.

In figure 1, we fix the particle number \( N \) to show the relation between \( \chi(\lambda) \) and \( V_0 \). We find that under a small \( V_0 \), \( \chi(\lambda) \) has two peaks. With the increase of \( V_0 \), the position of the left peak does not change, but the right peak moves left towards smaller \( \lambda \). When \( V_0 \) is moderate (for example, when \( V_0 = 10^{-10} \)), only one peak remains and continues moving left. When \( V_0 \) is large enough (for example, when \( V_0 = 10^{-3} \)), no peak remains.

The behaviour of \( \chi(\lambda) \) can be understood from the analysis of the ground state. The ground state can be expanded as \( |\Psi_0\rangle = \sum_{n=0}^{N} \epsilon_k |k, N - k\rangle \), where \( n_L = k \) and \( n_R = N - k \). Through studying the spectrum \( |c_k|^2 \) as a function of \( k \), we can know the configuration of particles in the two wells. Figure 2 shows the spectra under different tilts \( V_0 = 10^{-10}, 10^{-3} \) and \( 10^{-1} \). Under \( V_0 = 10^{-10} \) (figure 2(a)), when \( \lambda \lesssim 2.06 \), \( |c_k|^2 \) is symmetric and has a peak at \( k = N/2 \), which is consistent with the knowledge that the ground state is a binomial state \( |\Psi_0\rangle \equiv \frac{1}{\sqrt{n!}} \sum_{n=0}^{N} \sqrt{n!} |k, N - k\rangle \) at \( \lambda = 0 \) under \( V_0 = 0 \).

When \( 2.06 \lesssim \lambda \lesssim 2.22 \), \( |c_k|^2 \) is still symmetric but has two peaks. This means that the ground state becomes a cat-like state. When \( \lambda \gtrsim 2.22 \), \( |c_k|^2 \) only has one peak which moves towards \( k = N \), meaning all particles tend to locate in one well and self-trapping occurs. Therefore, at a small enough tilt, there are three phases, reflected by two peaks of fidelity susceptibility. If we increase the tilt, the cat-like region becomes smaller and finally vanishes after the tilt is increased to an appropriate value, for example \( V_0 = 10^{-3} \) in figure 2(b). At this value of the tilt, the ground state will change from the binomial configuration to the self-trapping directly at some critical \( \lambda \), reflected by the single peak of \( \chi(\lambda) \). For a very large tilt, \( |c_k|^2 \) is not symmetric in the whole region (figure 2(c)) and no ground-state transition appears.

So far our discussion is based on a fixed particle number \( N \). Now we need to fix the tilt and enlarge \( N \) to see what happens in the large-\( N \) limit. The heights of peaks in both

![Figure 1](image_url)

**Figure 1.** The fidelity susceptibility \( \chi(\lambda) \) for \( N = 800 \) under tilt \( V_0 = 10^{-10}, 10^{-3}, 10^{-4}, 10^{-5} \). One can see a clear transition from double peaks to a single peak around \( V_0 = 10^{-5} \).

![Figure 2](image_url)

**Figure 2.** The spectra under different tilts \( V_0 = 10^{-10}, 10^{-3}, 10^{-1} \) for \( N = 800 \). (a) \( \lambda \approx 2.06 \), \( |c_k|^2 \) is symmetric and has a peak at \( k = N/2 \). (b) \( 2.06 \lesssim \lambda \lesssim 2.22 \), \( |c_k|^2 \) is still symmetric but has two peaks. (c) \( \lambda \gtrsim 2.22 \), \( |c_k|^2 \) only has one peak which moves towards \( k = N \).
double- and single-peak regions diverge with $N$ exponentially, as predicted by the fidelity susceptibility theory (figure 3(c)). In the double-peak region (figure 3(a)), when we increase $N$, the distance between the two peaks becomes smaller. A finite-size analysis of the positions $\lambda_{\text{max}}$ of both peaks shows that $|\lambda_{\text{max}} - 2| \propto N^{-d_p}$ with $d_p \approx 0.6799$ for the left peak and $d_p \approx 0.738$ for the right peak. Therefore, $\lambda_{\text{max}}$ of both peaks will tend to 2 when $N \to \infty$, being consistent with the prediction of equation (2). Similarly, in the single-peak region (figure 3(b)), $|\lambda_{\text{max}} - 2|$ is also proportional to $N^{-d_p}$ with $d_p \approx 0.8941$. We can know from these results that in the thermodynamic limit there is only one direct quantum phase transition from the binomial state to the self-trapping state. The double transition from the binomial state to the cat state then to the self-trapping state under a small tilt and for moderate $N$ is actually a crossover. Our results confirm that the fidelity susceptibility is useful for detecting not only quantum phase transitions but also crossovers [18].

4. Quantum discord

It is usually stated that the quantum transition of the ground state can be indicated by some quantum information quantity, such as entanglement of the ground state. Here we revisit this problem by studying the correlation in the transition region of our system. Before we discuss this, we first introduce two quantities we use to describe the correlation: the total correlation and quantum discord.

Suppose that we have a system $AB$ composed of two subsystems $A$ and $B$. Then we can use three density matrices $\rho_{AB}$, $\rho_A$ and $\rho_B$ to describe the states of the whole system and the two subsystems, respectively, where $\rho_{AB} = \text{Tr}_B(\rho_{AB})$. The joint entropy of the whole system is defined as the von Neumann entropy of $\rho_{AB}$: $S(\rho_{AB}) = -\text{Tr}(\rho_{AB} \ln \rho_{AB})$. Similarly, we can also calculate the von Neumann entropy $S(\rho_{AB})$ of $\rho_{AB}$. If $\rho_{AB}$ is a pure state, $S(\rho_{AB}) = -\text{Tr}(\rho_{AB} \ln \rho_{AB})$ is called as the entanglement entropy and used to quantify the quantum entanglement between $A$ and $B$. However, if $\rho_{AB}$ is a mixed state (like the two-body reduced density matrix in our system), $S(\rho_{AB})$ is not a good measure of entanglement. The total correlation (the quantum mutual information) between $A$ and $B$ is given by $I_{AB} = S(\rho_A) - S(\rho_A | \rho_B)$, where $S(\rho_A | \rho_B) = S(\rho_{AB}) - S(\rho_B)$. Generally speaking, a bipartite quantum state $\rho_{AB}$ is a hybrid object with both classical and quantum characteristics. So the total correlation $I_{AB}$ could also be split into two parts: the quantum part and the classical part.
The classical part is defined as the maximum information about one subsystem that can be obtained by performing measurements on the other subsystem. Let us consider a measurement performed only on subsystem B. This measurement can be described by a complete set of projectors \( \{M_k\} \), where \( M_k \geq 0 \) and \( \sum_k M_k = 1_B \). The state of system AB after the application of \( M_k \) becomes

\[
\rho^{A}_{AB} = \frac{1}{(\text{tr} M_k)^2} (I_A \otimes M_k) \rho_{AB} (I_A \otimes M_k),
\]

with \( p_k = \text{Tr}[(I_A \otimes M_k) \rho_{AB} (I_A \otimes M_k)] \). According to the definition, the classical correlation can be obtained as \( C_{AB} = S(\rho_A) - \text{min}_{k \in \{M_k\}} \text{tr}(\rho_k S(\rho_A^k)) \), where \( \rho_A = \text{Tr}_B \rho_{AB} \) and \( \rho_A^k = \text{Tr}_B \rho_{AB}^k \). In this scenario, a quantity that provides information on the quantum component of the correlation between two systems can be introduced as the difference between the total correlation and the classical correlation. This quantity is what we call quantum discord \( D_{AB} = I_{AB} - C_{AB} \). Interestingly, the quantum discord includes quantum correlation that can be present in states that are not entangled, revealing that all the entanglement quantities such as concurrence, entanglement entropy, etc., do not capture the whole of quantum correlation between two mixed separate systems. For pure states, the discord reduces exactly to the entanglement entropy.

Now we consider quantum discord and the total correlation between two particles in our double-well system (see [19] for the discussion of the entanglement between identical particles). Because all particles are identical qubits, we have \( I_{AB} = 2S_1 - S_2 \), where \( S_1(S_2) \) is the von Neumann entropy of one- (two-) particle reduced density matrix. Here the one-particle and two-particle reduced density matrices are defined as \( \rho_{1,i,j} = \frac{1}{N} | (a_i^\dagger a_j) \rangle \langle (a_i^\dagger a_j) | \) and \( \rho_{2,i,j,k,l} = \frac{1}{N(N-1)} | (a_i^\dagger a_j a_k^\dagger a_l) \rangle \langle (a_i^\dagger a_j a_k^\dagger a_l) | \) respectively, where \( i, j, k, l \in \{L, R\} \) and the average is made under the ground state. For qubits, each complete set of projectors contains two elements labelled by two parameters \( \theta \in [0, \pi] \) and \( \phi \in [0, 2\pi] \), such that

\[
M_1(\theta, \phi) = \begin{pmatrix} \cos \frac{\theta}{2} & \sin \frac{\theta}{2} \cos \phi e^{i\psi} \\ \sin \frac{\theta}{2} \cos \phi e^{i\psi} & \sin \frac{\theta}{2} \end{pmatrix},
\]

\[
M_2(\theta, \phi) = \begin{pmatrix} \sin^2 \frac{\theta}{2} & -\sin \frac{\theta}{2} \cos \phi e^{i\psi} \\ -\sin \frac{\theta}{2} \cos \phi e^{i\psi} & \cos^2 \frac{\theta}{2} \end{pmatrix}.
\]

One can note that actually we can write \( M_i(\theta, \phi) = |\Phi_i(\theta, \phi)\rangle \langle \Phi_i(\theta, \phi)| \) and \( \Phi_i(\theta, \phi) = (-\sin \frac{\theta}{2} \cos \phi, e^{i\psi}) \). Then the quantum discord can be expressed as

\[
D_{AB} = I_1 - S_2 + \min_{\{\theta, \phi\}} \sum_{i=1}^{2} p_i(\theta, \phi) S[\rho_i^A(\theta, \phi)],
\]

where \( p_i(\theta, \phi) = \text{Tr}[(I_A \otimes M_i(\theta, \phi)) \rho_{AB} (I_A \otimes M_i(\theta, \phi))] \) and \( \rho_A^A(\theta, \phi) = \frac{1}{p_i(\theta, \phi)} (I_A \otimes M_i(\theta, \phi) \rho_{AB} (I_A \otimes M_i(\theta, \phi))) \). Although in some cases one can obtain an analytical expression for \( D_{AB} \) [17], we have to do a numerical calculation here. We divide the domains of \( \theta ([0, \pi]) \) and \( \phi ([0, 2\pi]) \) into 100 equal intervals, respectively, and search the minimization.

Similar to what we did in section 3, we first fix the particle number \( N \) to study the relation between correlations and \( V_0 \) (figure 4). We find that \( D_{AB} \) and \( I_{AB} \) have similar behaviours. Under a small tilt \( V_0 = 10^{-10} \), each correlation in the transition

![Figure 4](imageurl)

**Figure 4.** The quantum discord \( D_{AB} \) and total correlation \( I_{AB} \) for \( N = 800 \) under different tilts \( V_0 = 10^{-10}, 10^{-3} \) and \( 10^{-1} \). One can see that with the increase of \( V_0 \), both \( D_{AB} \) and \( I_{AB} \) decrease.

![Figure 5](imageurl)

**Figure 5.** (a) The quantum discord \( D_{AB} \) and the total correlation \( I_{AB} \) for different particle numbers \( N = 800, 1000 \) and 1200 under a small tilt \( V_0 = 10^{-10} \). One can find that with the increase of \( N \), both \( D_{AB} \) and \( I_{AB} \) decrease. (b) The quantum discord \( D_{AB} \) and the total correlation \( I_{AB} \) for different particle numbers \( N = 800, 1000 \) and 1200 under a moderate tilt \( V_0 = 10^{-3} \). One can also find that with the increase of \( N \), both \( D_{AB} \) and \( I_{AB} \) decrease. (c) The finite-size scaling analysis of the peak values of both \( D_{AB} \) and \( I_{AB} \) under the small tilt \( V_0 = 10^{-10} \) from \( N = 3000 \) to 9000. One can see that \( D_{AB}(N) \) and \( I_{AB}(N) \) show a negative slope, where \( D_{AB}(N) \) is the peak value of \( D_{AB}(I_{AB}) \). This means both of them decay to zero in the large-\( N \) limit. A similar analysis (not shown here) demonstrates that under a moderate \( V_0 = 10^{-3} \), the peak values of both \( D_{AB} \) and \( I_{AB} \) also decay to zero in the large-\( N \) limit.
region is remarkably larger than that out of the transition region, which means that this transition cannot be described by the mean-field theory for this system size. However, for each correlation we only observe one peak, whose position is near the position of the right peak of $\chi(\lambda)$ (figure 3(a)). If we increase the tilt to $V_0 = 10^{-3}$, both $D_{AB}$ and $I_{AB}$ become smaller. However, a peak still exists, whose position is near the position of the single peak of $\chi(\lambda)$ (figure 3(b)). If the tilt is further increased, both $D_{AB}$ and $I_{AB}$ are almost zero, meaning the ground state is almost a product state for any $\lambda$.

Then, we want to know whether we can have a non-zero correlation in the large-$N$ limit. After fixing $V_0$, we find both $D_{AB}$ and $I_{AB}$ decrease with $N$ (figures 5(a) and (b)). Through a finite-size analysis for the tilt $V_0 = 10^{-10}$, we find the peak values of the correlations decay exponentially as $N^{-d}$ ($d_c \approx 0.6661$ for quantum discord and $d_i \approx 0.7426$ for the total correlation). This means that in the $N \to \infty$ limit, there will not be correlation in the transition region and this transition can be described by the mean-field theory. For $V_0 = 10^{-3}$, a similar conclusion can also be obtained.

5. Summary

In this paper, we analyse the quantum transition of the ground state for the single-level Bose–Hubbard model in a double-well system with an arbitrary tilt. A semi-classical Hamiltonian predicts that for a not too large tilt, this transition occurs at $NU/J = 2$. We use fidelity susceptibility $\chi(\lambda)$ to identify this transition. We find that for a small tilt, $\chi(\lambda)$ has two peaks which are at the same position in the $N \to \infty$ limit. One peak corresponds to the transition from a binomial state to a cat-like state and the other peak corresponds to the transition from a cat-like state to the self-trapping state. While for a moderate tilt, only one peak of $\chi(\lambda)$ is observed, which corresponds to the direct transition from a binomial state to self-trapping. For a large tilt, no transition is observed in $\chi(\lambda)$.

We also use two quantities describing correlation, quantum discord and the total correlation to indicate the ground-state transition. For a finite system size, each correlation has a peak in the transition region (either for a small tilt or a moderate tilt), meaning that the transition cannot be described by the mean-field theory. However, by doing a finite-size analysis, we find that in the $N \to \infty$ limit, both correlations decay exponentially with the particle number to zero. It is an interesting generalization to check the behaviour of quantum correlation with system size in other systems where a ground-state transition that cannot be described by the mean-field theory exists, such as the rotating BEC.

Acknowledgments

Zhuo Liu thanks the financial support from the MPG–CAS Joint Doctoral Promotion Programme (DPP) and Max–Planck Institute of Quantum Optics. Hongli Guo thanks the financial support from the MPG–CAS Joint Doctoral Promotion Programme (DPP) and Max–Planck Institute for the Physics of Complex Systems. Heng Fan is supported by ‘973’ program (grant no. 2010CB922904).

Note added. Zhuo Liu and Hongli Guo equally contributed to this work. Hongli Guo is the corresponding author of this paper.

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