Orbital elementary excitations as probes of entanglement and quantum phase transitions of collective spins in an entangled Bose-Einstein condensate

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A mixture of two species of pseudospin-1/2 Bose gases exhibits interesting interplay between spin and orbital degrees of freedom. Expectation values of various quantities of the collective spins of the two species play crucial roles in the Gross-Pitaevskii-like equations governing the four orbital wave functions in which Bose-Einstein condensation occurs. Consequently, the elementary excitations of these orbital wave functions reflect properties of the collective spins. When the coupling between the two collective spins is isotropic, the energy gap of the gapped orbital excitation peaks, while there is a quantum phase transition in the ground state of the effective Hamiltonian of the two collective spins, which have previously been found to be maximally entangled.

PACS numbers: 03.75.Mn, 03.75Gg, 05.30.Rt

I. INTRODUCTION

A current trend in condensed matter physics is the interplay between spin and orbital degrees of freedom. It is interesting to explore this topic in the realms of Bose-Einstein condensation (BEC), as physical effects on single-particle levels are often enhanced by Bose statistics. A possible avenue is spinor Bose gases. The perspective is more broadened if we consider a mixture of two distinct species of spinor Bose gases, where there are several coupling strengths for the collective spins of the two species, which depend upon the orbital wave functions. This situation leads to coupling between spin and orbital degrees of freedom. For simplicity, let us focus on a mixture of two species of pseudospin-1/2 Bose gases with both intraspecies and interspecies spin-exchange interactions. Interspecies spin-exchange causes interspecies entanglement and the so-called entangled Bose-Einstein condensation (EBEC), which is different from a mixture of two species of spinless atoms, where the two species are disentangled and individually undergoes BEC. EBEC amplifies quantum entanglement from individual particles to macroscopic condensates. This ground state bears some analogies with the lowest energy state of a single species of pseudospin-1/2 atoms in a double well, but there are also differences due to the fact that two atoms of distinct species are distinguishable and thus the numbers of atoms are respectively conserved.

It has been shown that the interspecies entanglement in the ground state is maximal at the isotropic parameter point of the effective Heisenberg coupling of the two collective spins, and that the larger the particle numbers of the two species, the steeper the entanglement peak. In this brief report, after elucidating that the entanglement peak is indeed located at a quantum phase transition point, we study how the ground state of the collective spins affects the elementary excitations of the orbital wave functions in which EBEC occurs. Furthermore, we find that in the vicinity of this quantum phase transition, the energy gap of the gapped orbital elementary excitation is strikingly different from those of disentangled ground states. Away from the quantum phase transition point, the elementary excitations tend to approach those of a disentangled ground state.

II. THE MODEL

Consider a dilute gas of two distinct species of atoms. Each atom has an internal degree of freedom represented as a pseudospin-1/2, with \(z\)-component basis states \(\uparrow\) and \(\downarrow\). For a single species of pseudospin-1/2 gas, it was argued that the conservation of a small total spin in the cooling process invalidates the single orbital mode approximation. In our system, in contrast, under the single orbital mode approximation, the total spin of the mixture can still be arbitrarily small due to the distinguishability of the two species. Therefore, there is no reason against the usual single orbital mode approximation, which works well in most of the BEC systems. Moreover, a field theoretical approach without using single orbital mode approximation confirms its validation. Therefore, for each atom of species \(\alpha (\alpha = a, b)\) and pseudospin \(\sigma (\sigma = \uparrow, \downarrow)\), we can safely assume that only the single-particle orbital ground state \(\phi_{\alpha \sigma}(\mathbf{r})\) is occupied. Then the many-body Hamiltonian can be written as

\[
\mathcal{H} = \sum_{\alpha, \sigma} f_{\alpha \sigma} N_{\alpha \sigma} + \frac{1}{2} \sum_{\alpha, \sigma, \sigma'} K_{\sigma \sigma'}^{\alpha \alpha} N_{\alpha \sigma} N_{\alpha \sigma'} + \sum_{\sigma} K_{\sigma \sigma}^{ab} N_{\sigma \sigma} N_{\sigma \sigma} + K_{c} (a_{\uparrow} a_{\downarrow} b_{\uparrow} b_{\downarrow} + a_{\downarrow} a_{\uparrow} b_{\downarrow} b_{\uparrow}),
\]

where \(\alpha_{\sigma}\) denoted annihilation operator associated with \(\phi_{\alpha \sigma}(\mathbf{r})\) of species \(\alpha\), \(N_{\alpha \sigma} = \alpha_{\sigma}^{\dagger} \alpha_{\sigma}\) is the corresponding number of atoms. For each species \(\alpha\), the total particle number \(N_{\alpha} = N_{\alpha \uparrow} + N_{\alpha \downarrow}\) is a constant.

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The coefficients $K's$ are shorthand for $K_{αβ}^{α′β′} = g_{ασα′σ′}^αg_{βσβ′σ′}^β \int f^α_{σα′}f^{β}_{σβ′}\phi_{ασ}\phi_{βσ}\,d^3r$, where $g_{ασα′σ′}^α = 2\pi^2\epsilon_{ασα′σ′} / m_{αβ}$, with $\epsilon_{ασα′σ′}$ being the scattering length for the scattering in which an $α$-atom flips its pseudospin from $σ_1$ to $σ_1$ while a $β$-atom flips its pseudospin from $σ_1$ to $σ_2$, $μ_{αβ} = m_αm_β / (m_α + m_β)$ is the reduced mass. For intraspecies scattering, $K_{ασα′} = K_{ασα′}^σ$, $K_{ασ′β} ≡ K_{ασ′β}^σ$ is the single-particle energy. For interspecies scattering, $K_{ασα′}^σ ≡ K_{ασα′}^σ$, $K_α ≡ K_α^{σω}$, $f_σ ≡ ε_σ - K_α^{α′} / 2$, where $ε_σ = \int f^α_{σα′}(-\hbar^2\nabla^2 / 2m_α + U_α)\phi_{ασ}\,d^3r$ is the single-particle energy.

For simplicity, we assume that the scattering lengths satisfy $g_{ασα′σ′}^α = g_{ασα′σ′}^β = g_α$, $g_{ασβ′σ′}^α = g_β$, $g_{ασσ′σ′}^α = g_d$, $g_{α′σ′σ′}^α = g_0$. Moreover, we focus on the uniform case $φ_α = 1 / \sqrt{Ω}$, where $Ω$ is the volume of the system. The total spin operator of species $α$ is $S_α = \sum_{σ′} s_{ασ′} a_{σ'}$, where $s_{ασ′}$ is the single spin operator. In terms of $S_α$, the Hamiltonian can be transformed into that of two coupled giant spins $S_a = N_a / 2$ and $S_b = N_b / 2$.

\[ H = J_⊥ (S_a S_b + S_{αy} S_{βy}) + J_z S_a S_b + E_0 \]

where $J_⊥ = g_0 N_α N_β / (2m) \cal{g}_a + N_α N_β (g_α + g_β)$ and $\cal{g}_a = (g_α + g_β)$. Without loss of generality, let $S_a ≥ S_b$. We focus on antiferromagnetic couplings $g_a > 0$ and $g_b > g_d > 0$.

### III. Quantum Phase Transition

There is a quantum phase transition at the parameter point $g_d = g_a - g_d$. The ground states are qualitatively different in the limits of $g_a \gg g_d$ and $g_a \ll g_d$.

In a mean-field approximation, the ground state is disentangled into the two species, and can be written as $|G⟩_{MF} = (e^{-iϕ_α} e^{iϕ_β} \cos \frac{π}{4} ω) |α⟩_a + e^{iϕ_α} 2sin \frac{π}{4} ω |β⟩_b \otimes (e^{-iϕ_β} 2sin \frac{π}{4} ω |α⟩_b + e^{iϕ_β} \sin \frac{π}{4} ω |β⟩_a) N_b \otimes N_a$, with mean-field energy $E_{MF} = 2g_0 (⟨S_{αx}⟩⟨S_{βx}⟩ + ⟨S_{αy}⟩⟨S_{βy}⟩) + \frac{2g_0 (g_α - g_β)}{\Omega} ⟨S_{αz}⟩⟨S_{βz}⟩$, a constant is neglected, $⟨S_{αz}⟩ = N_a \sinθ_α \sinϕ_α$, $⟨S_{βz}⟩ = N_b \cosθ_α$, $(α = a, b$).

For $g_a < g_d$, $E_{MF}$ is minimal when $θ_α = θ_β = θ = π/2$ while $ϕ_α = ϕ_β = π$, that is, the two spins are antiparallel and are on $x - y$ plane.

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One can also use the so-called fidelity susceptibility to analyze the QPT [14, 15]. For a Hamiltonian $H(η) = H_0 + η H_1$, where $η$ is a driving parameter, the ground state fidelity is defined as $F = |⟨ψ_0(η + δη)|ψ_0(η)⟩|$. For a nondegenerate ground state, the fidelity susceptibility is $χ(η) ≡ -\lim_{δη \to 0} \frac{2Im F}{δη} = \sum_α |ψ_α(η)|^2 |H_0| |ψ_α(η)|^2$, where $|ψ_0(η)⟩$ and $|ψ_0(η)⟩$ are the ground and excited states of $H(η)$, respectively. In our Hamiltonian, $H_0 = J_z S_a S_b$, $H_1 = J_z (S_a S_b + S_{αy} S_{βy})$, $η ≡ g_0 / (g_a - g_d)$.

### IV. Elementary Excitations of the Orbital Wave Functions

Now we show how the spectra of the elementary excitations of the orbital wave functions vary with the many-body ground state. These single-particle wave functions are governed by the the generalized time-dependent Gross-Pitaevskii-like equations, which are determined by minimizing the energy, i.e. the expectation of the Hamiltonian under the many-body ground state, as a functional of the many-body wave functions [16]. Previous calculations have been focused on the many-body singlet ground state [7], here we make a more general consideration.

From the Hamiltonian, we obtain the Gross-Pitaevskii...
equations

\[ \langle N_\alpha \rangle \frac{\partial}{\partial \beta} \phi_{\alpha \sigma} = \{ \langle N_\alpha \rangle \} \left[ -\frac{\hbar^2}{2m_\alpha} \nabla^2 + U_\alpha(\mathbf{r}) \right] + \langle N_\alpha^2 - N_\alpha \rangle g_\alpha \phi_{\alpha \sigma}^2 \]

\[ + \langle N_\alpha N_\beta \rangle g_\alpha \phi_{\alpha \sigma}^2 + \langle N_\alpha N_\beta \rangle g_\alpha \phi_{\alpha \sigma}^2 \]

\[ + \langle N_\alpha N_\beta \rangle g_\alpha \phi_{\alpha \sigma}^2 \phi_{\alpha \sigma} \]

\[ + \langle \alpha \alpha \beta \sigma \phi_{\alpha \sigma} \phi_{\alpha \sigma} \phi_{\alpha \sigma} \phi_{\alpha \sigma} \alpha \rangle \]

where \( \beta \neq \alpha, \) \( \bar{\sigma} \neq \sigma, \) \( \langle O \rangle \) represents the expectation value of the operator \( O \) in the many-body ground state.

The particle number operators whose expectation values appear in the Gross-Pitaevskii-like equations can be represented in terms of collective spins of the two species, because of the relations \( N_\alpha = N_\alpha / 2 + \eta_\alpha S_{\alpha z}, \) with \( \eta_\alpha = 1 \) and \( \eta_\beta = -1, \)

\[ \langle \alpha \alpha \beta \sigma \phi_{\alpha \sigma} \phi_{\alpha \sigma} \phi_{\alpha \sigma} \phi_{\alpha \sigma} \alpha \rangle \]

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With these spin quantities as the coefficients, the Gross-Pitaevskii-like equations reflect coupling between spin and orbital degrees of freedom. As the ground state varies with the parameters, so are the expectation values of these spin quantities.

For simplicity, we focus on the uniform case in absence of external field \( U, \) the lowest energy wave functions are thus \( \phi^0_{\alpha \sigma} = e^{-i \omega_{\alpha \sigma} \tau / \hbar}, \) where \( \omega_{\alpha \sigma} \) is the chemical potential determined by substituting \( \phi^0_{\alpha \sigma} \) in

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where \( \beta \neq \alpha, \) \( \bar{\sigma} \neq \sigma, \) \( \langle O \rangle \) represents the expectation value of the operator \( O \) in the many-body ground state.
and $g_s - g_d$. It is easy to write down

$$
\Delta = \frac{1}{\sqrt{3}} \sqrt{\Gamma_3 + \sqrt{\Gamma_3^2 + \Gamma_4^2}} \\
= \rho \sqrt{2g_e \lambda_z} \{(g_e + g_e + g_s + g_d)\lambda_z + g_e \lambda_\perp + g_d - g_s\} \\
(9)
$$

Obviously $\Delta \neq 0$ only if $g_e \neq 0$. Hence interspecies spin exchange is necessary for opening a gap in an orbital excitation.

We have numerical calculated $\lambda_z$ and $\lambda_\perp$ for various values of $g_e$ and $g_s - g_d$, and then obtained $\Delta$ by using (9). It is found that when $N \to \infty$,

$$
ger_e < g_s - g_d : \lambda_z \to 1, \lambda_\perp \to 0, \text{ hence } \Delta \to 0, \\
ger_e = g_s - g_d : \lambda_z \to 1/3, \lambda_\perp \to 2/3, \\
ger_e > g_s - g_d : \lambda_z \to 0, \lambda_\perp \to 1. (10)
$$

It can be seen that the numerical result at $g_e = g_s - g_d$ is the same as the exact result. $\lambda_\perp \to 0$ implies that the effect of spin exchange diminishes, consequently $\omega_3 \to \omega_1$, $\omega_4 \to \omega_2$, the excitations become two doubly degenerate ones. Note that this is under the condition that each scattering strength is symmetric for the two pseudospin states of each species.

As shown in Fig. 2 the larger the numbers of atoms of the two species, the closer is the gap to that under the disentangled ansatz, except in the vicinity the critical point, where the gap varies rapidly with $g_e/(g_s - g_d)$. At critical point, as the atom numbers increase, the gap quickly saturates to a non-zero value.

Under a disentangled mean-field ground state, one has $\lambda_z = 1$ and $\lambda_\perp = 0$ for $g_e < g_s - g_d$, and $\lambda_z = 0$ and $\lambda_\perp = 1$ for $g_e > g_s - g_d$. Therefore, far away from the critical point $g_e = g_s - g_d$, $\lambda_z$ and $\lambda_\perp$, and thus the actual elementary excitations, are close to those under the disentangled mean-field states. But the disentangled ansatz clearly fails in the vicinity of the critical point $g_e = g_s - g_d$, as it tells that $\lambda_z$ and $\lambda_\perp$ are arbitrary non-negative values satisfying $\lambda + \lambda_\perp = 1$.

V. SUMMARY

A mixture of two pseudospin-1/2 Bose gases with interspecies spin exchange displays interesting interplay between spin and orbital degrees of freedom. The many-body Hamiltonian is simplified to an anisotropic Heisenberg coupling between the two collective spins of the two species, hence the particle numbers and correlations and fluctuations are equivalent to the corresponding quantities of the collective spins. These quantities enter the general Gross-Pitaevskii-like equations governing the four orbital wave functions, in which BEC occurs. Consequently, the elementary excitations of the orbital wave functions depend on the nature of collective spins in the many-body ground state, and thus serve as probes of entanglement and quantum phase transitions in the latter. Especially, we have shown that the gap of one of the excitations peaks at the antiferromagnetic isotropic parameter point of the effective Heisenberg coupling, which is critical point of quantum phase transition, where the interspecies entanglement and fidelity susceptibility also peak. These properties should be carried over to a spin-1 mixture [10].

Acknowledgments

We thank Li Ge and Shi-Jian Gu for useful discussion. This work was supported by the National Science Foundation of China (Grant No. 11074048), the Shuguang Project (Grant No. 07S402) and the Ministry of Science and Technology of China (Grant No. 2009CB929204).

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