Fate of a Bose-Einstein Condensate in the Presence of Spin-Orbit Coupling

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Intensive theoretical studies have recently predicted that a Bose-Einstein condensate will exhibit a variety of novel properties if spin-orbit coupling is present. However, an unambiguous fact has also been pointed out: Rashba coupling destroys a condensate of noninteracting bosons even in high dimensions. Therefore, a conceptually important question arises as to whether or not a condensate exists in the presence of interaction and a general type of spin-orbit coupling. Here we show that interaction qualitatively changes the ground state of bosons under Rashba spin-orbit coupling. Any infinitesimal repulsion forces bosons either to condense at one or two momentum states or to form a superfragmented state that is a superposition of infinite numbers of fragmented condensates. The superfragmented state is unstable against the anisotropy of spin-orbit coupling in systems with large numbers of particles, leading to the revival of a condensate in current experiments.

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Spin-orbit coupling (SOC) is the underlying mechanism for many fundamental quantum phenomena, ranging from the atomic fine structure to the newly discovered novel properties of topological insulators [1,2]. The recent realization of synthetic SOC for neutral alkali atoms in laboratories provides physicists with a new platform to study the effects of SOC in many-body systems, in which a wide range of parameters can be well controlled in experiments [3–6]. In particular, spin-orbit coupled bosons offer physicists a unique opportunity to explore how SOC may manifest itself at the macroscopic level. As it is known as a textbook result that bosons naturally form a condensate at the ground state in three and two dimensions, intensive theoretical effort has predicted a number of macroscopic quantum phenomena exhibited by a Bose-Einstein condensate in the presence of SOC [7–16].

On the other hand, a significant effect of SOC on noninteracting bosons has also been realized recently. It was pointed out that some types of SOC may completely destroy a noninteracting condensate at zero or any finite temperatures even in high dimensions [17–19]. To see this effect, one can start from the single-particle Hamiltonian for spin-orbit coupled bosons, which can be written as

$$\mathcal{K} = \sum_{\sigma}\int d^D r \hat{\Psi}^{\dagger}_{\sigma}(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2M}\right)\hat{\Psi}_{\sigma}(\mathbf{r}) + H_{\rm SOC}, \quad (1)$$

where D is the dimension, $\sigma = \uparrow, \downarrow$, $\hat{\Psi}^{\dagger}_{\sigma}(\mathbf{r})$ ($\hat{\Psi}_{\sigma}(\mathbf{r})$) is the creation (annihilation) operator at $\mathbf{r}$, and M is the mass. The part of SOC in the Hamiltonian is described by

$$H_{\rm SOC} = -i\int d^D r \hat{\Psi}^{\dagger}_{\uparrow}(\mathbf{r})(\lambda_x\partial_x - i\lambda_y\partial_y)\Psi_{\downarrow}(\mathbf{r}) + \text{c.c.}, \quad (2)$$

where $\lambda_{x,y}$ is the coupling strength. For $D = 3$ the low energy part of the single-particle spectrum can be written as

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2}{2M}(|\mathbf{k}_{\perp}|^2 + k_z^2) - \sqrt{\lambda_x^2 k_x^2 + \lambda_y k_y^2}, \quad (3)$$

where $\mathbf{k} = (k_x, k_y, k_z)$ is the momentum and $\mathbf{k}_{\perp} = (k_x, k_y)$. For $D = 2$, one can simply set $k_z = 0$ in Eq. (3). Among all the configurations of SOC, Rashba coupling corresponding to $\lambda_x = \lambda_y = \lambda$ is of particular interest. For both $D = 2$ and $D = 3$, the kinetic energy minimum under Rashba coupling becomes a circle in the x-y plane with radius $|\mathbf{k}_{\perp}| = k_0 \equiv M\lambda/\hbar^2$, which means an infinite degeneracy of the single-particle ground state. Correspondingly, the low-energy density of states becomes that in $(D-1)$ dimension in the absence of SOC. Therefore, a noninteracting condensate is completely destroyed at zero temperature for $D = 2$ [19] and at any finite temperature for $D = 3$ [17,18].

Whereas the disappearance of a noninteracting condensate under Rashba coupling is rather clear, a few fundamental questions remain unanswered so far. (i) What is the ground state of interacting bosons? Is it a trivial uncondensed state, an ordinary condensate, or an exotic many-body state with novel correlations? (ii) If it is a condensate or an exotic state, how does the uncondensed state of noninteracting bosons change to these states when interaction is turned on? (iii) What is the effect of anisotropy in spin-orbit coupling? In this Letter, we shall present answers to all of the above questions (i)–(iii).

We first note that the infinite degeneracy of single-particle ground states makes interaction effects highly nonperturbative. To determine the many-body ground state amounts to selecting the state with the lowest interaction energy from an infinitely degenerate subspace, which is known to be a challenging problem, for instance, two-dimensional electrons in quantum Hall regions [20]. For studies of spin-orbit coupled bosons in the literature, a mean field approach has been adopted to compare energies of a special class of states that can be described by condensate wave functions [8–14]. However, with the observation that SOC may completely destroy a condensate, one naturally has concerns about the validity of mean field approach. In particular, it is unclear whether interaction will lead to an exotic many-body ground state other than an ordinary condensate.

To explore the exact many-body ground state, we expand the interaction between two-component bosons

$$\hat{\mathcal{U}} = \Omega \int d^D r (g_1 \hat{n}_\uparrow^2(\mathbf{r}) + g_2 \hat{n}_\downarrow^2(\mathbf{r}) + g_{12}\hat{n}_\uparrow(\mathbf{r})\hat{n}_\downarrow(\mathbf{r})) \quad (4)$$

in the basis of single-particle eigenstates, where $\hat{n}_\sigma(\mathbf{r}) = \hat{\Psi}_\sigma^\dagger(\mathbf{r})\hat{\Psi}_\sigma(\mathbf{r})$ is the density operator, Ω is the volume of the system, and $g_{i=1,2} > 0$, $g_{12} > 0$ are the intra- and interspin repulsion. In this basis, the effective interaction can be formulated as

$$\hat{\mathcal{U}}_L = \sum_{\phi_1,\phi_2,\phi_3,\phi_4} U_{\phi_1,\phi_2}^{\phi_3,\phi_4} \hat{L}_{\phi_1}^\dagger \hat{L}_{\phi_2}^\dagger \hat{L}_{\phi_3} \hat{L}_{\phi_4}/4, \qquad (5)$$

where

$$U_{\phi_1,\phi_2}^{\phi_3,\phi_4} = g_{12} e^{i(\phi_1-\phi_4)} + g_2 + g_1 e^{i(\phi_1+\phi_2-\phi_3-\phi_4)}, \qquad (6)$$

$\hat{L}_\phi^\dagger$ ($\hat{L}_\phi$) is the creation (annihilation) operator in the subspace $\mathcal{L}$ composed of all single-particle ground states, and ϕ is the polar angle on the circle $|\mathbf{k}_\perp| = k_0$ [19].

Before presenting the details of our analysis, we first summarize our main results here. (1) Any infinitesimal repulsion forces bosons to form a single-particle condensate or a fragmented condensate, distinct from noninteracting systems where a condensate is absent. (2) Interaction inevitably builds up a superposition of fragmented condensates with an even particle number, and the exact ground state becomes a superfragmented state beyond the prediction of mean field theory. (3) Superfragmented states collapse in systems with large numbers of particles if a finite anisotropy exists in SOC, leading to the revival of a condensate in current experiments. The results (1)–(3) answer the questions (i)–(iii) raised above.

We start from the two-body problem that can be solved exactly to illuminate the underlying physics. The Fock states can be written as either $|\phi,\theta\rangle = \hat{L}_\phi^\dagger \hat{L}_{\phi+\theta}^\dagger|0\rangle$ for $\theta \neq 0$ or $|\phi,0\rangle = \hat{L}_\phi^\dagger \hat{L}_\phi^\dagger|0\rangle/\sqrt{2}$. θ is the relative angle between the two bosons on the circle. The diagonal term of the interaction matrix element, i.e., the Hartree-Fock energy $E_{\rm HF}^{[2]} = \langle\phi,\theta|\hat{\mathcal{U}}_L|\phi,\theta\rangle$, where the superscript $[N]$ denotes an N-body system, can be written as

$$E_{\rm HF}^{[2]} = \begin{cases} g_{12}(1+\cos\theta)/2 + g_1 + g_2, & \theta \neq 0, \\ (g_{12} + g_1 + g_2)/2, & \theta = 0. \end{cases} \qquad (7)$$

Equation (7) shows that $|\phi,0\rangle$ and $|\phi,\pi\rangle$ minimize $E_{\rm HF}^{[2]}$ for $\gamma < 1$ and $\gamma > 1$, respectively, where $\gamma = g_{12}/(g_1+g_2)$. States with $\theta \neq 0$, π always have higher energies. For $\gamma > 1$, two bosons occupy two opposite points on the circle; i.e., fragmentation occurs. Without SOC, it is well known that fragmentation is energetically unfavorable due to the cost of Fock energy when bosons occupy different momentum states [21]. The presence of Rashba coupling suppresses the term in Fock energy that is proportional to g_{12} by a factor of $\cos\theta$. Therefore, fragmentation may occur at large enough g_{12}.

We now consider the off-diagonal term of the interaction matrix elements. Note that for $\theta \neq \pi$, each Fock state is characterized by a unique finite momentum and cannot be coupled by interaction which conserves the total momentum. Therefore, they are eigenstates in the manifold of the kinetic energy minimum. However, all states with $\theta = \pi$ carry zero total momentum and can be coupled by interaction. The Hamiltonian within the zero momentum subspace can be written as

$$H^{[2]} = E_\pi \int_0^\pi d\phi \hat{P}_\phi^\dagger \hat{P}_\phi + \int_0^\pi d\phi d\phi' \mathcal{V}_{\phi,\phi'}^{[2]} \hat{P}_{\phi'}^\dagger \hat{P}_\phi (1-\delta_{\phi,\phi'}), \qquad (8)$$

where $E_\pi = g_1 + g_2$ is the Hartree-Fock energy for $\theta = \pi$, $P_\phi^\dagger = \hat{L}_\phi^\dagger \hat{L}_{\phi+\pi}^\dagger$ is the pair creation operator, and $\mathcal{V}_{\phi,\phi'}^{[2]} = (g_2 + g_1 e^{2i(\phi'-\phi)})$. Equation (8) is equivalent to to a one-dimensional ring with an "infinite-range" tunneling [22]. The ground states are infinitely degenerate and can be written as

$$|SF_\nu^{[2]}\rangle = \frac{1}{\sqrt{\pi}} \int_0^\pi d\phi e^{i2\nu\phi} \hat{P}_\phi^\dagger|0\rangle, \qquad (9)$$

where ν is an arbitrary integer other than 0 and 1.

The wave function in Eq. (9) describes a small superfragmented state composed by the superposition of small fragmented condensates. It is straightforward to derive that the corresponding ground state energy is exactly zero, in spite of the repulsive interaction. As the eigenenergy of any state with a finite total momentum is positive, we conclude that the ground state for the two-body problem is always a small superfragmented state, regardless of the ratio between g_{12} and $g_1 + g_2$. The underlying physics is that the superposition of zero momentum states on the circle completely cancels the positive Hartree-Fock energy. This is consistent with the result obtained from a different approach of renormalizing the interaction, which found that the renormalized interaction between two particles with zero momentum on the circle is reduced to zero [23,24].

The above discussion can be directly generalized to an N-body system. For systems with an even particle number, a single-particle condensate $|C^{[N]}\rangle_\phi = \hat{L}_\phi^{\dagger N}|0\rangle/\sqrt{N!}$ and a fragmented condensate $|F^{[N]}\rangle_\phi = \hat{L}_\phi^{\dagger N/2}\hat{L}_{\phi+\pi}^{\dagger N/2}|0\rangle/(N/2)!$ minimize $E_{\rm HF}^{[N]}$ for $\gamma > 1$ and $\gamma < 1$, respectively, where ϕ is an arbitrary phase reflecting the rotation symmetry in the momentum space. For an odd particle number $N = 2n + 1$ ($n = 1, 2, \ldots$), the fragmented condensate is simply given by $|F^{[2n+1]}\rangle_\phi = \hat{L}_\phi^{\dagger n} \hat{L}_{\phi+\pi}^{\dagger n+1}|0\rangle/\sqrt{n!(n+1)!}$. Any other Fock state in $\mathcal{L}$ costs additional Hartree-Fock energy proportional to the total particle number, as shown in Fig. 1. Therefore, all bosons condense at one or two momentum states to minimize $E_{\rm HF}^{[N]}$, distinct from noninteracting systems where bosons can distribute on the circle $|\mathbf{k}_\perp| = k_0$ arbitrarily.

Among all the above states that minimize Hartree-Fork energy, $|C^{[N]}\rangle_\phi$ or $|F^{[2n+1]}\rangle_\phi$ with different values of ϕ cannot be mixed with each other, due to the constraint of total momentum conservation. However, such a constraint is absent for $|F^{[2n]}\rangle_\phi$, as all of them have zero total momentum and any two of them are inevitably coupled by a series of scattering, as demonstrated in Fig. 1. This type of tunneling is known to be crucial in the presence of degenerate ground states, and produces macroscopic or mesoscopic quantum coherence in various systems [25–28]. In our case, it fundamentally changes the ground state structure when fragmentation occurs with an even particle number.

We derive an effective Hamiltonian in the subspace composed of all fragmented condensates (see the Supplemental Material [29]),

$$H_{\rm eff}^{[2n]} = \int_0^\pi d\phi \mathcal{E}_F^{[2n]} \hat{O}_\phi^\dagger \hat{O}_\phi + \int_0^\pi d\phi d\phi' \mathcal{V}_{\phi,\phi'} \hat{O}_{\phi'}^\dagger \hat{O}_\phi (1 - \delta_{\phi,\phi'}), \quad (10)$$

where $\hat{O}_\phi^\dagger = \hat{L}_\phi^{\dagger n} \hat{L}_{\phi+\pi}^{\dagger n}/n!$ is the creation operator for a fragmented condensate, and

$$\mathcal{V}_{\phi,\phi'} = (-1)^{n-1} \frac{(g_2 + g_1 e^{i2(\phi'-\phi)})^n}{(g_1 + g_2 + g_{12})^{n-1}} n^2. \quad (11)$$

The diagonal term $\mathcal{E}_F^{[2n]} = E_{\rm HF}^{[2n]} - \mathcal{E}'$, where $E_{\rm HF}^{[2n]}$ is the Hartree-Fock energy and $\mathcal{E}'$ is the diagonal part of the correction to the energy due to the coupling between $|F^{[2n]}\rangle_\phi$ and high energy states (see the Supplemental Material [29]). As $\mathcal{E}'$ is independent of ϕ, it does not affect the structure of the ground state wave function.

Similarly to $H^{[2]}$ discussed above, $H_{\rm eff}^{[2n]}$ is also analytically solvable (see the Supplemental Material [29]). For the simplest case with $g_1 = 0$, with an "infinite-range" constant tunneling $t = (-1)^{n-1} g_2^n n^2/(g_2 + g_{12})^{n-1}$ [22], the eigenstates can be written as

$$|SF_\nu^{[2n]}\rangle = \frac{1}{\sqrt{\pi}} \int_0^\pi d\phi e^{i2\nu\phi} \hat{O}_\phi^\dagger |0\rangle, \quad (12)$$

where ν is an integer, with the corresponding eigenenergy

$$E_\nu^{[2n]} = \mathcal{E}_F^{[2n]} + (-1)^{n-1} \frac{g_2^n n^2}{(g_2 + g_{12})^{n-1}} (\pi\delta_{\nu,0} - 1). \quad (13)$$

As the reduced single-particle density matrix $\langle \hat{L}_\phi^\dagger \hat{L}_{\phi'} \rangle$ of $|SF_\nu^{[2n]}\rangle$ is zero, and the reduced $2n$-particle density matrix $\langle \hat{L}_\phi^{\dagger n} \hat{L}_{\phi+\pi}^{\dagger n} \hat{L}_{\phi'}^n \hat{L}_{\phi'+\pi}^n \rangle$ has a unique macroscopic eigenvalue $(n!/\pi)^2$, $|SF_\nu^{[2n]}\rangle$ is a superfragmented state [27]. The superfragmented state we find here has two exotic features that are absent in previous studies [25–28]. First, it is

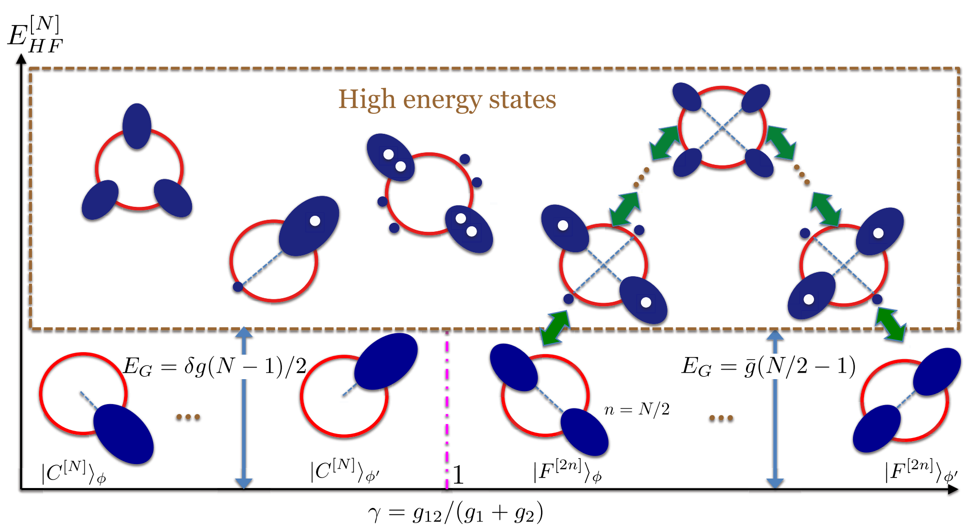

FIG. 1 (color online). Hartree-Fock energy $E_{\rm HF}^{[N]}$ of N particles. Red circles represent the kinetic energy minimum, and blue ellipses represent a large number of bosons occupying the same momentum state. Blue and white dots represent a single boson and a hole in the condensate, respectively. The single-particle and fragmented condensate minimize $E_{\rm HF}^{[N]}$ for $\gamma < 1$ and $\gamma > 1$. They are separated from high energy states by an energy gap $E_G = \bar{g} + N\delta g/2$ or $E_G = \bar{g}(N/2 - 1)$, where $\bar{g} = (g_1 + g_2 + g_{12})$ and $\delta g = g_1 + g_2 - g_{12}$. Any two fragmented condensates with even particle numbers $N = 2n$ are coupled through a sequence of tunneling induced by n steps of scattering, as shown by the green arrows.

composed of an infinite number of macroscopically occupied states other than just a few. Second, each of them is characterized by a winding number ν. In other words, bosons first form a fragmented condensate and then the condensate "rotates" in the momentum space acquiring a complex phase in the superposition. We note that both features originate from the intriguing interplay between Rashba SOC and interaction, which gives rise to an angular-dependent effective interaction as shown in Eq. (6). We have verified the superfragmented state as the ground state for a four-body problem using numerical simulations.

It is known that the superfragmented state is fragile in systems with large numbers of particles. In our case, Eq. (13) shows that the energy difference between the superfragmented state and the fragmented condensate can be characterized by $\eta = 1 - E_\nu^{[2n]}/\mathcal{E}_F^{[2n]}$. For a small total particle number $N = 2n$, η takes a large value. For example, one estimates that $\eta \approx 0.61, 0.11, 0.1$ for $N = 4, 6, 8$, and $g_2/g_{12} = 0.9$, which means a large energy is gained by forming a superfragmented state. While this fact strikingly changes the properties of a few-body system, one notes that η decreases exponentially with increasing particle number $N = 2n$, i.e., $\eta \sim (1 + \frac{g_{12}}{g_2})^{-n+1}$. This is a typical feature of a high order process that requires multiple steps of two-body scattering to couple two degenerate states. When $N \to \infty$, η vanishes, which means a fragmented condensate becomes degenerate with the exact many-body ground state in the thermodynamic limit. In current experiments, $N \sim 10^5$–10^6, one can easily see that η is a negligible number.

The tiny η for a large value of N indicates that a big superfragmented state is unstable against external perturbation. For our discussions, the anisotropy of SOC, which always exists in practice, is naturally such a perturbation. Assuming $\lambda_x > \lambda_y$, Eq. (3) shows that kinetic energy minimums are located at two separate points $\mathbf{k} = \pm k_{x0} = \pm M\lambda_x/\hbar^2$. We define the circle $|\mathbf{k}_\perp| = k_{x0}$ as $\mathcal{L}'$, on which the expression for interaction energy is identical to that in Eq. (10), with ϕ replaced by $\varphi = \arg\{\lambda_x k_x, \lambda_y k_y\}$ [19]. The kinetic energy in $\mathcal{L}'$ is now a function of ϕ,

$$K(\phi) = \frac{\hbar^2}{2M}k_{x0}^2 - k_{x0}\lambda_x\sqrt{1 - \alpha(2-\alpha)\sin^2\phi}, \qquad (14)$$

where $\alpha \equiv (\lambda_x - \lambda_y)/\lambda_x$ characterizes the anisotropy of SOC, and leads to an offset of kinetic energy $\Delta(\alpha) = (K(\pi/2) - K(0))N = \alpha N M\lambda_x^2/\hbar^2$ in $\mathcal{L}'$.

For single-particle condensates and fragmented condensates with odd particle numbers, any infinitesimal α picks up $|C^{[N]}\rangle_{\phi=0}$ or $|F^{[N]}\rangle_{\phi=0}$ as the ground state, which favors the kinetic energy with no cost of interaction energy. For superfragmented states, we define a characteristic anisotropy

$$\alpha^* = \frac{\hbar^2}{2M\lambda_x^2}\left(\frac{g_2}{g_2 + g_{12}}\right)^{n-1} g_2 n, \qquad (15)$$

by setting the kinetic energy offset equal to the strength of off-diagonal coupling induced by interaction, i.e., $\Delta(\alpha^*) = t$. For small anisotropy $\alpha \ll \alpha^*$, the interaction energy is dominant and a superfragmented state forms. For $\alpha \gg \alpha^*$, forming a superposition of fragmented condensates costs too much kinetic energy, and a single fragmented condensate $|F^{[N]}\rangle_{\phi=0}$ becomes the ground state. A more quantitative analysis is given in the Supplemental Material [29]. Using Eq. (15), one estimates that $\alpha^* = 9\%, 4\%, 2\%$ for $N = 4, 6, 8$, $g_2/g_{12} = 0.9$ and $g_2 n\hbar^2/(2M\lambda_x^2) = 0.2$. This means a small superfragmented state is stable in a finite range of anisotropy. With increasing N, α^* decreases exponentially. One can verify that for $N \sim 10^5$–10^6, the typical particle number in current experiments, α^* is essentially zero. Therefore, one concludes that a superfragmented state collapses to a fragmented condensate. An additional external potential that breaks the translation invariance will further change the fragmented condensate to a stripe condensate (see the Supplemental Material [29]).

Whereas we have answered fundamental questions about whether, when, and why a condensate exists in the presence of SOC, our work also demonstrates that the coupling between Hartree-Fock energy minimums becomes particularly important in a spin-orbit coupled few-body system. Evidence for this type of coupling has been found in a recent numerical calculation [30]. Provided that significant progress is made on manipulating a few atoms in current experiments [31,32] as well as in producing a uniform trap [33], we hope that our work will stimulate more studies on SOC induced novel ground states of mesoscopic cold atomic systems.

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