Order by Disorder in Spin-Orbit Coupled Bose-Einstein Condensates

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Motivated by recent experiments, we investigate the system of isotropically-interacting bosons with Rashba spin-orbit coupling. At the non-interacting level, there is a macroscopic ground-state degeneracy due to the many ways bosons can occupy the Rashba spectrum. Interactions treated at the mean-field level restrict the possible ground-state configurations, but there remains an accidental degeneracy not corresponding to any symmetry of the Hamiltonian, indicating the importance of fluctuations. By finding analytical expressions for the collective excitations in the long-wavelength limit and through numerical solution of the full Bogoliubov-de Gennes equations, we show that the system condenses into a single momentum state of the Rashba spectrum via the mechanism of order by disorder. We show that in 3D the quantum depletion for this system is small, while the thermal depletion has an infrared logarithmic divergence, which is removed for finite-size systems. In 2D, on the other hand, thermal fluctuations destabilize the system.

I. INTRODUCTION AND OVERVIEW

Multicomponent condensates of ultracold atoms offer rich physical systems due to the interplay between superfluidity and internal degrees of freedom [1]. Recently, through the use of synthetic gauge fields, two-component bosons with spin-orbit (SO) coupling have been engineered in the ultracold laboratory [2]. SO coupling in solid-state materials has a long history and is responsible for a variety of interesting physical effects, with notable examples including the spin Hall effect [3] and topological insulators [4]. In addition, SO-coupled materials have diverse applications including spintronics [5]. The newer bosonic counterpart of SO-coupled systems using ultracold atoms have no analog in solid-state systems and are thus expected to exhibit genuinely new physics. SO-coupled cold atomic systems have also received considerable recent theoretical attention [6–21], investigating topics such as spin-striped states [9, 12, 13], fragmentation [8, 19], and the realization of Majorana fermions [7, 15, 16].

Recent experiments [2] have realized a special combination of Rashba [22] and Dresselhaus [23] SO coupling in ultracold atoms. There are also promising proposals to realize more general non-Abelian gauge fields like pure Rashba (c.f. [24]), or even SU(N) gauge fields that provide a toolbox for topological insulators [25]. The conceptually simple system of a Rashba SO-coupled Bose-Einstein Condensate with isotropic interactions (RBEC) has surprisingly rich physics. The non-interacting system has a macroscopic ground state degeneracy as shown in Fig. 1. Interactions at the mean-field level partially remove this degeneracy, but there remains an ‘accidental’ degeneracy not corresponding to any underlying symmetry of the system. Specifically, mean-field theory predicts a superposition of condensates of opposite momenta with their relative amplitudes and phases unspecified.

In this work we show how fluctuations remove this accidental degeneracy and select a unique ground state (up to overall symmetries) through the mechanism of ‘order by disorder’ [20]. Although the phenomenon of order by disorder has been theoretically accepted and discussed within the context of classical spin models [26, 27], quantum magnetism [28, 29] and ultracold atoms [30–33], experimental demonstrations are, at best, scarce [31]. In contrast to the original proposal [20], the degeneracy lifting we find is primarily quantum driven. We determine the fluctuation spectrum by numerically solving the coupled Bogoliubov-de Gennes equations. The resulting modes are integrated over to obtain the free energy as a function of the relative condensate weights and temperature. With this we show that fluctuations select a state with all bosons condensing into a single momentum state in the Rashba spectrum. We estimate the energy splitting per particle due to fluctuations for typical experimental parameters to be on the order of 100 pK. While this splitting is smaller than typical condensate temperatures, it is the total energy which determines the ground state, so this effect should be readily observable provided the RBEC model can be realized.
II. DEFINITION OF HAMILTONIAN AND MEAN-FIELD GROUND STATES

The Hamiltonian describing non-interacting bosons in 3D with SO coupling reads

\[ \mathcal{H}_0 = \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) \left( \frac{p^2}{2m} - \frac{Q}{m} \sigma_\perp \cdot \mathbf{p} \right) \Psi(\mathbf{r}), \]

where \( \Psi(\mathbf{r}) = (\Psi_\uparrow(\mathbf{r}), \Psi_\downarrow(\mathbf{r}))^T \) is a two-component bosonic field operator, \( \mathbf{p} \) is the momentum operator, \( Q \) is the magnitude of the SO coupling, and \( \sigma_\perp \) is a vector composed of Pauli matrices as \( \sigma_\perp = (\sigma_x, \sigma_y, 0) \) (we set \( \hbar = 1 \)). The SO coupling in Eq. (1) is equivalent to the Rashba form [22] through a 90° spin rotation. The single-particle eigenstates of Eq. (1) have spins pointing either parallel or antiparallel to their momenta in the \( xy \) plane, and up to a constant have energies \( E^{(\pm)}_k = \frac{1}{2m} ((k_x \pm Q)^2 + k_z^2) \), where \( k_\perp = (k_x, k_y, 0) \). Clearly, there is a ring in momentum space of degenerate lowest-energy states with \( k_z = 0 \) and \( |k_\perp| = Q \) (Fig. 1). Correspondingly, there is a macroscopic number of ways \( N \) non-interacting bosons can occupy this manifold of states.

For the interacting portion of the Hamiltonian we take the simplest SU(2) invariant form

\[ \mathcal{H}_{\text{int}} = \int d\mathbf{r} \left( \frac{g}{2} [\hat{\rho}(\mathbf{r})]^2 - \mu \hat{\rho}(\mathbf{r}) \right), \]

where \( \hat{\rho}(\mathbf{r}) = \Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r}) \), \( \mu \) is the chemical potential, and \( g = \frac{\hbar \omega}{m} \) where \( \omega \) is an effective scattering length. At the mean-field level one replaces the operators by c-numbers \( \Psi(\mathbf{r}) \to \Psi(\mathbf{r}) \). The states that minimize the kinetic energy, Eq. (1), are in general given by

\[ \Psi(\mathbf{r}) = \sum_{|k_\perp|=Q,k_z=0} A_k e^{ik_\perp r} \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ e^{i\varphi_k} \end{array} \right) \]

where \( A_k \) are arbitrary coefficients and \( \tan(\varphi_k) = k_z/k_y \). Minimizing the interaction energy restricts the mean-field states of Eq. (3) to have a constant density, \( \rho(\mathbf{r}) = \Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r}) \equiv \rho_0 \). Placing this constraint on states in Eq. (3), one finds that \( \Psi(\mathbf{r}) \) can have at most two nonzero coefficients \( A_k \) occurring at opposite momenta. This can be shown by setting each non-zero wavevector component of \( \Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r}) \) to zero. Without loss of generality, we take the momenta to point along the \( x \)-axis and thereby obtain the state

\[ \Psi(\mathbf{r}) = \sqrt{\frac{\rho_0}{2}} \left( \begin{array}{c} ae^{iQx} \left( \begin{array}{c} 1 \\ 1 \end{array} \right) + be^{-iQx} \left( \begin{array}{c} -1 \\ 1 \end{array} \right) \end{array} \right), \]

where \( |a|^2 + |b|^2 = 1 \). We can take \( a \) and \( b \) to be real and parametrized as \( a = \cos \left( \frac{\theta}{2} \right) \) and \( b = \sin \left( \frac{\theta}{2} \right) \) since changing the phases of \( a \) and \( b \) amounts to position displacements and overall phase shifts of \( \Psi(\mathbf{r}) \) in Eq. (4). The selection of \( a, b \) as a result of spin-symmetry breaking interactions (which is resolved at the mean-field level) was worked out in [12]. In contrast, in this work there remains a degeneracy at the mean-field level.

III. CALCULATION OF COLLECTIVE EXCITATIONS

The degeneracy with respect to \( \theta \) is accidental, i.e. it does not correspond to any symmetry of the Hamiltonian \( \mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}} \). We thus expect quantum fluctuations about the mean-field state Eq. (4) to remove this degeneracy and to select a unique ground state through the order-by-disorder mechanism. To this end, we write \( \Psi(\mathbf{r}) = \Psi(\mathbf{r}) + \psi(\mathbf{r}) \) and perform a Bogoliubov expansion of \( \mathcal{H} \) to quadratic order in \( \psi(\mathbf{r}) \). Up to a constant the interaction Hamiltonian becomes \( \mathcal{H}_{\text{int}} = \frac{\delta}{2} \int d\mathbf{r} [\delta\hat{\rho}(\mathbf{r})]^2 \)

where \( \delta\rho(\mathbf{r}) = \Psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) + \psi^\dagger(\mathbf{r}) \Psi(\mathbf{r}) \). It proves useful to transform to the variables \( \hat{\chi}(\mathbf{r}) = (\chi_\uparrow(\mathbf{r}), \chi_\downarrow(\mathbf{r}))^T \) where \( \chi(\mathbf{r}) = e^{i\sigma_y \frac{\tau}{2} - i\sigma_x Q x} e^{i\sigma_y \frac{\tau}{2}} \psi(\mathbf{r}) \) for which the interaction Hamiltonian takes the simple form \( \mathcal{H}_{\text{int}} = \frac{\delta}{2} \int d\mathbf{r} \left( \chi_\uparrow(\mathbf{r}) + \chi_\downarrow(\mathbf{r}) \right)^2 \).

The full Bogoliubov Hamiltonian, \( \mathcal{H}_{\text{Bog}} \), can be written compactly in matrix form if we introduce the four-component vector

\[ \hat{\Phi}(\mathbf{r}) = \left( \hat{\chi}^T(\mathbf{r}), \hat{\chi}_\downarrow(\mathbf{r}) \right)^T. \]

Then up to a constant independent of \( \theta \) we find that \( \mathcal{H}_{\text{Bog}} = \frac{\delta}{2} \int d\mathbf{r} \hat{\Phi}^\dagger(\mathbf{r}) \mathbf{M}(\mathbf{r}, p) \hat{\Phi}(\mathbf{r}) \), where

\[ \mathbf{M}(\mathbf{r}, p) = 1 \otimes \left( \frac{p^2}{2m} + \frac{g\rho_0}{2} (1 + \sigma_x) \otimes (1 + \sigma_z) \right. \]

\[ - \left. \frac{Qp_y}{m} (1 \otimes \sigma_y \cos(2Qx) - \sigma_z \otimes \sigma_y \sin(2Qx)) \right). \]

In this expression, all \( \theta \)-dependence is included in \( \sigma_\theta \equiv \cos(\theta) \sigma_x + \sin(\theta) \sigma_z \) and \( \sigma_\theta \) is the Knöcker product. This Hamiltonian can be diagonalized using a symplectic transformation [35,36], which amounts to solving the Bogoliubov-de Gennes equations,

\[ \eta \mathbf{M}(\mathbf{r}, p) \mathbf{v}_{kn}(\mathbf{r}) = \epsilon_{kn} \mathbf{v}_{kn}(\mathbf{r}), \]

for positive eigenvalues \( \epsilon_{kn} \), where \( \eta = \sigma_z \otimes 1 \) and \( \mathbf{v}_{kn}(\mathbf{r}) \) is a four-component function. Because of the translational symmetries of \( \mathbf{M}(\mathbf{r}, p) \), the eigenvalues are labelled with band index \( n \) and momentum \( \mathbf{k} \) in the Brillouin zone (BZ) defined as \( -\infty < k_y, k_z < \infty \) and \( -Q \leq k_x \leq Q \). As usual, the eigenvectors are normalized as \( \langle \mathbf{v}_{kn} | \eta | \mathbf{v}_{kn'} \rangle \equiv \int d\mathbf{r} \mathbf{v}_{kn}^\dagger(\mathbf{r}) \eta \mathbf{v}_{kn'}(\mathbf{r}) = \delta_{kn} \delta_{nn'} \delta_{\eta} \). In practice, Eq. (7) is simplest to solve in momentum space. Since the momentum space representation of \( \mathbf{M}(\mathbf{r}, p) \) is an infinite matrix, in numerical calculations it must be truncated at high momentum and the eigenvalues of interest must be checked to be independent of the cutoff.

In Fig. 2 we show the two gapless (Goldstone) modes for several values of \( \theta \), found numerically from Eq. (7). In experiments of [2], \( \varepsilon_Q = \frac{Q^2}{2m} \simeq g\rho_0 \), so we set these quantities to be equal. The dispersion is plotted along
The average of the spin and density modes is selected from fluctuations. Noting this, in the right panel we plot the average (arithmetic mean) of the density and spin modes. In both plots we have fixed $g\rho = \frac{Q^2}{2m}$.

$k_y$ since, as can be seen from Eq. (7), the spectrum $\varepsilon_{kn}$ has no $\theta$-dependence when $k_y = 0$. We refer to the dispersions as ‘density’ and ‘spin’ modes since they reduce to the known expressions $\varepsilon_{kd} = \sqrt{\varepsilon_k (\varepsilon_k + 2g\rho_0)}$ and $\varepsilon_{ks} = \varepsilon_k$ in the limiting case of $Q = 0$, where $\varepsilon_k = \frac{k^2}{2m}$ is the free particle dispersion. One sees that upon increasing $\theta$ from zero to $\pi/2$, the spin mode decreases in energy while the density mode increases. This gives, in a sense, a competing effect in terms of which $(a,b)$ configuration is selected from fluctuations. Noting this, in the right panel we plot the average of the spin and density modes for each value of $\theta$. One sees that the average is always lowest in energy for $\theta = 0$. This indicates that the zero-point fluctuations from the Goldstone modes will select $\theta = 0$ state though things become more subtle for $T > 0$. Such a state, as can be seen from Eq. (4), corresponds to all bosons condensing into a single momentum state of the RBEC system. The order-by-disorder mechanism will be considered more quantitatively below.

Analytical expressions for the dispersions and eigenvectors of Eq. (7) can be found perturbatively in the long-wavelength limit $\varepsilon_k \ll \varepsilon_Q, g\rho_0$. In this limit one finds $\varepsilon_{kd} = \sqrt{2g\rho_0 (\varepsilon_{kzz} + \lambda\varepsilon_{ky} \sin^2(\theta))}$ and $\varepsilon_{ks} = \sqrt{\varepsilon_{kzz} (\varepsilon_{kzz} + \lambda\varepsilon_{ky} \sin^2(\theta))^2}$ for the density and spin modes respectively where $\lambda = g\rho_0/(4\varepsilon_Q + 2g\rho_0)$ and $k_{zz} = \sqrt{k_x^2 + k_y^2}$. These agree well with the numerical results shown in Fig. [2] for small $k$ except for two special cases which require more careful analysis. In particular, for $\theta = 0$, the density mode disperses quadratically along $k_y$ while for $0 < \theta \leq \pi/2$ the spin mode disperses as $k_y^3$ along $k_y$. Otherwise the density and spin mode have respectively linear and quadratic dispersions about their minima. It is interesting to compare these to the noninteracting energies shown in Fig. 1 which have quadratic and quartic dispersions about their minima.

IV. QUANTUM AND THERMAL ORDER BY DISORDER

Let us now consider the free energy due to quantum and thermal fluctuations described by $\mathcal{H}_{\text{Bog}}$. It is useful to separate out the contribution from zero-point fluctuations and write $F(\theta) = F_q(\theta) + F_t(\theta)$ where

$$F_q(\theta) = \frac{1}{2} \sum_{\mathbf{k} \in \text{BZ}, n} \varepsilon_{kn}(\theta),$$

$$F_t(\theta) = k_B T \sum_{\mathbf{k} \in \text{BZ}, n} \ln \left(1 - e^{-\beta \varepsilon_{kn}(\theta)}\right),$$

and $\beta = 1/k_B T$ is inverse temperature. Reminiscent of the zero-point photon contribution to the Casimir-Polder force [37], the purely quantum contribution $F_q(\theta)$ written as it is diverges. This divergence can be regularized by subtracting the free energy for a particular mean-field configuration which we take to have $\theta = 0$: $\Delta F_q(\theta) = F_q(\theta) - F_q(0)$. This regularized expression converges [38], and no renormalization of the effective range of interactions is needed. The zero-point contribution to the free energy numerically computed as a function of $\theta$ is shown in Fig. 3(a) where the summation is performed over 26 bands (we emphasize that in order to obtain quantitatively correct results, including only the gapless modes is insufficient). One sees, indeed, that the $\theta = 0$ state has the lowest energy and at $T = 0$ such a state is unambiguously selected.

We now turn to the finite-temperature contribution to the free energy. Interestingly, one finds that the sign of the thermal contribution $\Delta F_t(\theta) = F_t(\theta) - F_t(0)$ is negative and opposite to that of $\Delta F_q(\theta)$. Furthermore, the magnitude of the thermal contribution is always smaller than the contribution from zero-point fluctuations, in contrast to typical situations where thermal fluctuations enhance the degeneracy lifting and are larger in magnitude for modest temperatures (see, e.g. [30]). Another instance of where quantum and thermal fluctuations select different states is in Ref. [33]. The sign of $\Delta F_t$ at low $T$ can be understood by noting that the spin mode has the lowest energy for $\theta = \pi/2$ (Fig. 2).

As seen in Fig. 3(b), the magnitude of $\Delta F_t(\theta)$ approaches $\Delta F_q(\theta)$ at high $T$, so that $\Delta F(\theta) = \Delta F_q(\theta) + \Delta F_t(\theta) = 0$ ($T^{-1} \to 0$) in this limit. This behavior can be understood through a high $T$ expansion of the free energy

$$F_t(\theta) \approx k_B T \sum_{\mathbf{k} \in \text{BZ}, n} \ln (\beta \varepsilon_{kn}(\theta)) - \frac{1}{2} \sum_{\mathbf{k} \in \text{BZ}, n} \varepsilon_{kn}(\theta).$$

As the second term cancels the quantum contribution,
we focus on the larger first term which can be written as
\[
k_B T \sum_{\mathbf{k} \in \text{BZ}',n} \ln \left| \beta \mathcal{E}_{\mathbf{k}n}(\theta) \right| = \frac{1}{2} k_B T \ln |\text{det}(\beta \mathbf{H}(r, p))| = k_B T \sum_{\mathbf{k} \in \text{BZ}',n} \ln |\beta \lambda_{\mathbf{k}n}|
\]
where \( \lambda_{\mathbf{k}n} \) are the eigenvalues of \( \mathbf{M}(r, p) \) and we have used \( |\text{det}(\eta)| = 1 \). The second summation above is over the reduced Brillouin zone BZ' which is restricted to positive values of \( k_x \). The eigenvalues \( \lambda_{\mathbf{k}n} \) are independent of the condensate configuration given by \( \theta \). This can be seen by noting that the \( \theta \)-dependence of \( \mathbf{M}(r, p) \) can be removed through the unitary transformation \( \mathbf{M}(r, p) \rightarrow \mathbf{U} \mathbf{M}(r, p) \mathbf{U}^\dagger \) where \( \mathbf{U} = \frac{1}{2} (1 + \sigma_x) \otimes 1 + \frac{1}{2} (1 - \sigma_x) \otimes e^{\beta \sigma_y} \). Thus to this order we find that \( \Delta F(\theta) = -\Delta F_{\bar{q}}(\theta) \).

The next-order term in the high-temperature expansion has \( 1/T \) dependence which is evident in the numerical results shown in Fig. 3(b).

V. CONDENSATE DEPLETION

Having established using the Bogoliubov expansion that fluctuations select \( \theta = 0 \), we now investigate the self-consistency of this approach. This is determined by the depletion or the number of particles excited out of the condensate \( N_{\text{ex}} \) as a fraction of the total particle number \( N \). Consistency of course requires that this be finite, while neglecting of terms beyond quadratic order in \( \mathcal{H}_{\text{Bog}} \) is quantitatively reliable only if \( N_{\text{ex}} \ll N \). The quantum and thermal contributions to \( N_{\text{ex}} = N_q + N_t \) are, respectively, \( N_q = \frac{1}{2} \sum_{\mathbf{k} \in \text{BZ},n} \langle \mathbf{v}_{\mathbf{k}n} | (1 - \eta) | \mathbf{v}_{\mathbf{k}n} \rangle \) and \( N_t = \sum_{\mathbf{k} \in \text{BZ},n} \langle \mathbf{v}_{\mathbf{k}n} | f(\mathcal{E}_{\mathbf{k}n}) \rangle \), where \( f(x) = (e^{\beta x} - 1)^{-1} \) is the Bose-Einstein distribution function. The only possible divergences of these expressions are in the infrared, and so can be studied analytically using the small-\( k \) expansion.

In 3D at \( T = 0 \), \( N_q \) is finite and so can be sufficiently small provided weak-enough interactions. Our numerical results in fact demonstrate that the depletion is small even for moderately strong interactions, including in the region of experimental relevance. For \( T > 0 \), the thermal contribution is instead found to have a logarithmic divergence in 3D. This divergence (similar to that occurring in quasi-2D scalar condensates) is naturally removed for finite-sized systems and the condensate will thereby satisfy the stability criterion. For 2D condensates with isotropic SO coupling, the situation is different. Here, the quantum depletion again converges, but the thermal depletion diverges as \( 1/k \) for small \( k \). Thus, at \( T > 0 \) our theory is unstable in 2D, which is consistent with work suggesting fragmentation \([8, 19]\). Our conclusions on the stability of the condensate are, remarkably, identical to those based on the simple application of the Einstein criterion to the noninteracting spectrum. This is particularly surprising since the low-\( k \) region is strongly modified by the interactions, giving quasiparticle modes that disperse with different powers than in the noninteracting case.

VI. EXPERIMENTAL FEASIBILITY

We now comment on the experimental feasibility of observing order by disorder in RBEC. We first consider the magnitude of the degeneracy lifting. As a prototypical example we take spin one \(^{87}\text{Rb}\). For a typical density of \( \rho_0 = 2 \times 10^{14} \text{cm}^{-3} \) and \( \rho_B = \frac{\hbar^2}{2m} \), we find (for the appropriate scattering lengths) that at zero temperature the free energy splitting per particle due to fluctuations is \( \Delta F(\pi/2)/k_B N = 110 \text{pK} \). One should note that this number should not be directly compared with the condensate temperature since the total energy determines the ground state. It is this energy which will determine experimental timescales for the relaxation to the ground state. Spin-one atoms also possess a spin-dependent interaction term which we have neglected. For \(^{87}\text{Rb}\), however, this spin-dependent interaction is relatively small (5% of that of the spin-independent) and as a result the degeneracy lifting from fluctuations is typically larger. Alternatively, one could use fermionic homonuclear molecules that have a singlet ground state. More importantly, schemes to create SO coupling in bosonic systems typically rely on utilizing dressed states \([2, 18, 24]\) which can induce anisotropic interactions. The magnitude of such terms and their effect on the order-by-disorder mechanism will be left to future work when it becomes clear which of the several possible schemes is most promising to realize Rashba coupling.

Another entity of experimental relevance is the harmonic confining potential. The results of the current manuscript will hold if the conditions for the local den-
sity approximation (LDA) are satisfied. For our system this requires that the energy splitting of the single-particle states as recently found in [20, 21] be small compared to the interaction energy. This energy splitting becomes small for weak trapping and/or strong SO coupling, resulting in a large quasi-degenerate manifold of single-particle states. Conversely, in the weakly interacting limit (where LDA is inapplicable) recent work [20, 21] has shown the ground states of the RBEC system in a trap can form vortex lattices.

VII. CONCLUSION

In conclusion we have investigated the system of Rashba SO-coupled bosons with isotropic interactions (RBEC). In general bosons with SO coupling offer a genuinely new class of systems which has not been addressed in the vast solid state literature on spintronics [5]. In particular, we have established that fluctuations select the RBEC system to condense into a single momentum state. We have argued that such a configuration is stable in 3D but destabilized when $T > 0$ in 2D. We expect bosons with Rashba SO coupling to be realized in the near future for which the predicted configuration will be observable in Stern-Gerlach experiments. In future studies it will be interesting to investigate more general combinations of Rashba and Dresselhaus SO coupling. Such systems also possess accidental mean-field degeneracies and thus fluctuations are expected to play an important role in determining their ground states. In addition it will be interesting to investigate RBEC systems in two dimensions.

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