Quantum tri-criticality and phase transitions in spin-orbit coupled Bose-Einstein condensates

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We consider a spin-orbit coupled configuration of spin-1/2 interacting bosons with equal Rashba and Dresselhaus couplings. The phase diagram of the system is discussed with special emphasis to the role of the interaction treated in the mean-field approximation. For a critical value of the density and of the Raman coupling we predict the occurrence of a characteristic tri-critical point separating the spin mixed, the phase separated and the single minimum states of the Bose gas. The corresponding quantum phases are investigated analyzing the momentum distribution, the longitudinal and transverse spin-polarization and the emergence of density fringes. The effect of harmonic trapping as well as the role of the breaking of spin symmetry in the interaction Hamiltonian are also discussed.

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A large number of papers has been recently devoted to the theoretical study of artificial gauge fields in ultracold atomic gases (for a recent review see, for example, [1]). First experimental realizations of these novel configurations have been already become available [2,3]. This field of research looks very promising from both the theoretical and experimental point of view, due to the possibility of realizing exotic configurations of non trivial topology [1], with the emergence of new quantum phases in both bosonic [4] and fermionic [5] gases, and the possibility to simulate electronic phenomena of solid state physics. In the case of Bose gases a key feature of these new systems is the possibility of revealing Bose-Einstein condensation in single-particle states with non-zero momentum.

In the paper [3] it was possible to realize spin-orbit coupling in Bose-Einstein condensates, and to identify experimentally a quantum phase transition from a spatially spin mixed state to a phase-separated configuration by tuning the Raman coupling between two hyperfine states of $^{87}$Rb atoms. Important features of the resulting phases were anticipated in the paper by Ho and Zhang [6] and discussed in detail in the same experimental paper [3]. The purpose of this letter is to provide a theoretical description of the phase diagram corresponding to the spin-orbit coupled Hamiltonian employed in [3]. We point out the occurrence of an important density dependence in the phase diagram which shows up in the appearance of a tri-critical point that, to our knowledge, has never been predicted for such systems.

We will consider the mean-field energy functional (for simplicity we set $\hbar = m = 1$)

$$E(\psi_a, \psi_b) = \int d^3r \left[ (\psi_a^* \psi_a^0 h_0 (\psi_a^0 \psi_b^0) + g_{aa} |\psi_a|^4 \right. \right.$$

$$\left. + \frac{g_{bb}}{2} |\psi_b|^4 + g_{ab} |\psi_a|^2 |\psi_b|^2 \right]$$

(1)

describing an interacting spin-1/2 Bose-Einstein condensate, where $\psi_a$ and $\psi_b$ are the condensate wave functions relative to the two spin components interacting with the coupling constants $g_{ij} = 4\pi a_{ij}$, with $a_{ij}$ the corresponding s-wave scattering lengths, and

$$h_0 = \frac{1}{2} \left[ p_x^2 + p_z^2 \right] + \frac{\Omega}{2} \sigma_x + \frac{\delta}{2} \sigma_z + V_{\text{ext}}$$

(2)

is the single-particle Hamiltonian characterized by equal contributions of Rashba $\hbar\Omega$ and Dresselhaus $\hbar\delta$ spin-orbit couplings and a uniform magnetic field in the $x$-$z$ plane. In Eq. (2) $\Omega$ is the Raman coupling constant accounting for the transition between the two spin states, $k_0$ is the strength associated with the spin-orbit coupling fixed by the momentum transfer of the two Raman lasers, $\delta$ fixes the energy difference between the two single-particle spin states, $\sigma_i$ are the usual $2 \times 2$ Pauli matrices, while $V_{\text{ext}}$ is the external trapping potential.

In the first part of the paper we will consider uniform configurations, neglecting the effect of the trapping potential ($V_{\text{ext}} = 0$) and assume a spin symmetric interaction with $g_{aa} = g_{bb} \equiv g$ and $\delta = 0$. The ground state condensate wave function will be determined using a variational procedure based on the following ansatz for the spinor wave function:

$$\left( \begin{array}{c} \psi_a \\ \psi_b \end{array} \right) = \frac{1}{\sqrt{N/V}} \left[ C_1 \left( \cos \theta \right) e^{ik_{1z}z} + C_2 \left( -\cos \theta \right) e^{-ik_{1z}z} \right]$$

(3)

where $N$ is the total number of atoms, $V$ is the volume of the system. For a given value of the average density $n = N/V$, the variational parameters are then $C_1$, $C_2$, $k_1$ and $\theta$. Their values are determined by minimizing the energy (1) with the normalization constraint $\sum_{i=a,b} \int d^3r |\psi_i|^2 = N$ (i.e. $|C_1|^2 + |C_2|^2 = 1$). Minimization with respect to $\theta$ yields the general relationship $\theta = \arccos(k_1/k_0)/2$ ($0 \leq \theta \leq \pi/4$), fixed by the single-particle Hamiltonian (2). Once the other variational parameters are determined, one can calculate key physical quantities like, for example, the momentum distribution accounted for by the parameter $k_1$, the longitudinal and
transverse spin polarization of the gas
\[
\langle \sigma_z \rangle = \frac{k_1}{k_0} \left( |C_1|^2 - |C_2|^2 \right), \quad \langle \sigma_x \rangle = -\frac{\sqrt{k_0^2 - k_1^2}}{k_0}
\]
and the density
\[
n(x) = n \left[ 1 + 2|C_1C_2| \sqrt{\frac{k_0^2 - k_1^2}{k_0}} \cos(2k_1 x + \phi) \right].
\]
where \( \phi \) is the relative phase between \( C_1 \) and \( C_2 \). The ansatz \( 3 \) describes exactly the ground state of the single-particle Hamiltonian \( h_0 \) (ideal Bose gas). In this case, for \( \Omega \leq 2k_0^2 \), the energy, as a function of \( k_1 \), exhibits two minima located at the values \( \pm k_0 \sqrt{1 - \Omega^2/4k_0^2} \) and the ground state is degenerate of the actual values of \( C_1 \) and \( C_2 \). For \( \Omega > 2k_0^2 \) the two minima disappear and all the atoms condense into the zero momentum state \( k_1 = 0 \).

The same ansatz is well suited to discuss the role of interactions. By inserting \( 3 \) into \( 1 \), we find that the energy per particle \( \varepsilon = E/N \) takes the form
\[
\varepsilon = \frac{k_0^2}{2} - \frac{\Omega}{2k_0} \sqrt{k_0^2 - k_1^2} - F(\beta) \frac{k_1^2}{2k_0^2} + G_1 (1 + 2\beta)
\]
where we have defined the dimensionless parameter \( \beta = |C_1|^2 |C_2|^2 \) \((0 \leq \beta \leq 1/4)\), and the function
\[
F(\beta) = (k_0^2 - 2G_2) + 4(G_1 + 2G_2) \beta
\]
with the interaction parameters \( G_1 = n \left( g + g_{ab} \right) /4 \), \( G_2 = n \left( g - g_{ab} \right) /4 \). The variational parameters to minimize the energy are then \( k_1 \) and \( \beta \).

Let us first consider minimization with respect to \( k_1 \). If \( \Omega > 2F(\beta) \) the energy \( 9 \) is an increasing function of \( k_1 \) and the minimum takes place at \( k_1 = 0 \). If instead \( \Omega < 2F(\beta) \) one finds that \( \varepsilon \) is minimized by the choice
\[
k_1(\beta) = k_0 \sqrt{1 - \frac{\Omega^2}{4[F(\beta)]^2}}, \quad (8)
\]
which generalizes the ideal gas result \( F(\beta) = k_0^2 \). Eqs.\((7)-(8)\) explicitly show that the momentum distribution is modified by the interactions. We find the following result for the energy per particle
\[
\varepsilon = -\frac{\Omega^2}{8F(\beta)} + G_1 + G_2 (1 - 4\beta), \quad (9)
\]
The ground state of the system can be found by looking for the minimum of \( 9 \) with respect to \( \beta \). One can easily prove that the second order derivative of \( 9 \) with respect to \( \beta \) is negative. The ground state is then compatible with the following three phases:

(I) The spin mixed or “stripe” phase with \( k_1 \neq 0, \beta = 1/4 \) and hence \( \langle \sigma_z \rangle = 0 \). In this phase the atoms condense in a superposition of two plane wave states with wave vector \( \pm k_1 \) and the density \( 5 \) exhibits fringes. This configuration is characterized by a degeneracy associated with the relative phase between the coefficients \( C_1 \) and \( C_2 \) which fixes the actual spatial position of stripes.

(II) The separated phase with \( k_1 \neq 0, \beta = 0 \) and hence \( \langle \sigma_z \rangle \neq 0 \), where the atoms condense into a single plane wave state with wave vector either \( k_1 \) \((C_2 = 0)\) or \(-k_1 \) \((C_1 = 0)\), the actual value being determined by a mechanism of spontaneous spin symmetry breaking.

(III) The single minimum or “zero momentum” phase with \( k_1 = 0 \) and \( \langle \sigma_z \rangle = 0 \) where the atoms condense in the zero momentum state.

We first notice that the spin mixed phase is compatible only with positive values of the interaction parameter \( G_2 \), favoring anti-ferromagnetic configurations. In fact in the opposite case \( G_2 < 0 \), the first order derivative \( \partial \varepsilon / \partial \beta \) is always positive and the ground state is always in the phase separated configuration (II) or in the “zero momentum” phase (III).

In the most interesting \( G_2 > 0 \) case, the system will be always in the phase (I) for small values of the Raman coupling constant \( \Omega \). If the condition
\[
k_0^2 > 4G_2 + \frac{4G_2^2}{G_1} \quad (10)
\]
is satisfied, the systems will exhibit a phase transition (I) to (II) at the frequency
\[
\Omega_{I-II}^{(1)} = 2 \left[ (k_0^2 + G_1) \left( k_0^2 - 2G_2 \right) \frac{2G_2}{G_1 + 2G_2} \right]^{1/2} \quad (11)
\]
This generalizes the result derived in [11], which corresponds to the low density (or weak coupling) limit of [11], i.e. \( G_1, G_2 \ll k_0^2 \). The transition frequency in this limit approaches the density independent value
\[
\Omega_{I-II}^{(1-III)} = 2k_0^2 \gamma / (1 + 2\gamma) \quad (12)
\]
where we have introduced the dimensionless interaction parameter \( \gamma = G_2 / G_1 = (g - g_{ab}) / (g + g_{ab}) \). By further increasing \( \Omega \), the system will enter the phase (III) at the frequency
\[
\Omega_{II-III}^{(1)} = 2 (k_0^2 - 2G_2) \quad (13)
\]
If instead the condition [10] is not satisfied, the transition will occur directly from the phase (I) to (III) at the frequency
\[
\Omega_{I-III}^{(1)} = 2 (k_0^2 + G_1) - 2 \left[ (k_0^2 + G_1) G_1 \right]^{1/2} \quad (14)
\]
In the strong coupling limit \( G_1 \gg k_0^2 \) [14] approaches the constant value \( k_0^2 \).

The critical point where the phase (II) disappears is fixed (see Eq.\((11)\)) by the condition \( G_1^{(c)} = k_0^2 / 4\gamma (1 + \gamma) \), corresponding to the critical value
\[
n^{(c)} = k_0^2 / (2\gamma g) \quad (15)
\]
for the density. If $n < n^{(c)}$, one has two transitions (I-II and II-III), while if $n > n^{(c)}$, only one phase transition (I-III) can take place.

In Fig. 1 we plot the momentum $k_1$, the energy per particle $E/N$, the transverse and longitudinal spin polarizations $\langle \sigma_z \rangle$ and $\langle |\sigma_z| \rangle$ as a function of $\Omega$. Red solid lines: “stripe phase” $k_1 \neq 0$ and $\beta = 1/4$; blue solid lines: “separated phase” $k_1 \neq 0$ and $\beta = 0$; green solid lines: “zero momentum phase” $k_1 = 0$; open circles: ground state. The parameters: $G_1/k_0^2 = 0.2$, $G_2/k_0^2 = 0.05$ (a)-(d), $G_2/k_0^2 = 0.16$ (e)-(h).

In Fig. 2 we show the phase diagram for three different phases. The value of the spin polarization $\langle |\sigma_z| \rangle$ and $k_1$ are reported in (a) and (b) respectively. The transition lines separating different phases merge at a tri-critical point at $n = n^{(c)}$. The value of $\langle |\sigma_z| \rangle$ always vanishes for $n > n^{(c)}$. However the phase transition (I-III) is well identified by the behavior of the momentum $k_1$. The parameters employed in Fig. 2 correspond to rather large values of the critical density. More accessible values of $n^{(c)}$ can be obtained employing smaller values of $k_0$. Experimentally this can be achieved by playing with the angle between the two Raman lasers. Reducing the value of $k_0$ has also the advantage of increasing the spatial separation between the fringes in the “stripe phase” (I), thereby making their experimental detection easier.

Let us now discuss the effect of the trap. In order to simplify the analysis we have considered harmonic trapping with frequency $\omega_0$ only along the $x$-axis. Without interaction, one can calculate the ground state using a similar variation ansatz, replacing the plane waves in (3) by the functions $e^{\pm ik_1 x}e^{-\omega_0 x^2/2}$, corresponding, in the absence of the gauge field, to the usual harmonic oscillator Gaussians. The energy per particle is easily calculated and reads:

$$
\varepsilon = \frac{\omega_0}{2} + \frac{k_0^2 - k_1^2}{2} - \frac{\Omega}{2k_0} \sqrt{k_0^2 - k_1^2} - (C_1^* C_2 + C_2^* C_1) \frac{k_1^2}{2k_0} e^{-k_1^2/\omega_0}
$$

(16)
The ground state can be found by minimizing $\varepsilon$ with respect to $k_1$, $C_1$ and $C_2$ with the normalization constraint. The first term in (10) is just the zero point energy due to the presence of the trap. The following two terms are the same as for the uniform case without interactions, i.e. (6) with $G_1 = G_2 = 0$. The last term shows the effect of the trap, fixing the relative phase between the coefficients $C_1$ and $C_2$ in the ground state. Consequently the degeneracy occurring in the uniform case will be lifted even in the absence of interactions (where $\phi = 0$). Physically this is the consequence of the non-orthogonality of the two Gaussians states centered in $\pm k_1$. According to (10), for $k_1 \neq 0$, the system prefers to stay in the spin mixed phase, and exhibits density modulation in space even without interactions. On the other hand the interaction is crucial for the appearance of the phase separated configuration. Since the last term of (10) scales exponentially, the effect of the trap is weak for $k_1^2 \gg \omega_0$, and becomes more and more important when $k_1^2$ is comparable to $\omega_0$.

To describe the role of the interaction we implement the mean-field approximation by solving numerically the Gross-Pitaevskii equation for the condensate wave function. We find that the properties discussed in the first part of the work for the uniform system almost hold conditions. We find that the properties discussed in the first part of the work almost hold if $\omega_0$ is large enough.

FIG. 3: (Color online) Spin polarization $|\langle \sigma_z \rangle|$ as a function of $\Omega$ for the trapped case (red solid line), and for the uniform case using the density in the center of the trap (blue dashed line). The parameters are chosen as follows: $\omega_0 = 2\pi \times 20\text{ Hz}$, $k_0/\omega_0 = 4$, $g_{aa} = g_{bb} = 101.20 \text{ a}_B$, $g_{ab} = 100.99 \text{ a}_B$, where $\text{ a}_B$ is Bohr radius. The density in the center of the trap corresponds to $n \approx 3.9 \times 10^{13} \text{ cm}^{-3}$.

The correction (17) to the mean-field approximation by solving numerically the Gross-Pitaevskii equation for the condensate wave function is given by

$$\varepsilon = \left( G_3 + \frac{\delta}{2} \right) \frac{k_1}{\omega_0} \left( |C_1|^2 - |C_2|^2 \right)$$

where we have considered the low density (weak coupling) limit. By choosing $\delta = -2G_3$ the correction (17) identically vanishes and the transition frequency (12) is not consequently affected by the inclusion of the new terms in the Hamiltonian. Using the $^{87}\text{Rb}$ parameters introduced above we then find the value $\Omega^{(1)}_{1LD} = 0.19 E_L$ ($E_L = k_0^2/2$) in agreement with the findings of (3) corresponding to $n/n^{(c)} \ll 1$. For higher densities, the value of $\delta$ should be instead taken $\Omega$ dependent in order to ensure exact compensation.

In conclusion, we have investigated the phase diagram of a spin-orbit coupled two-component Bose-Einstein condensates using a variation ansatz based on the mean-field approximation. We predict a rich phase diagram characterized by the occurrence of three different quantum phases, and by a characteristic tri-critical point where the three phases merge at a critical value of the density and of the Raman frequency.

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