Modulational instability of spinor condensates

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We demonstrate, analytically and numerically, that the ferromagnetic phase of the spinor Bose-Einstein condensate may experience modulational instability of the ground state leading to a fragmentation of the spin domains. Together with other nonlinear effects in the atomic optics of ultracold gases (such as coherent photoassociation and four-wave mixing) this effect provides one more analogy between coherent matter waves and light waves in nonlinear optics.

Recent experimental studies of Bose-Einstein condensation (BEC) in an optical trap have opened a new direction in the research of ultracold atomic clouds associated with their spin degree of freedom, or spinor BEC. An optical trap does not force atoms to align along the orientation of the strong confining magnetic field, as happens in the case of a magnetic trap, allowing the study of atoms confined in all hyperfine states. Several recent theoretical studies have predicted a variety of novel phenomena that may occur in the spinor BEC, such as the propagation of spin waves and the existence of topological states -skyrmions, vortex states without a core. In the case of spin-1 bosons such as $^{23}$Na, $^{39}$K and $^{87}$Rb, the dynamics of the spinor BEC is described by the three spin degrees of freedom ($m_F = 1, 0, -1$ of the $F = 1$ atomic hyperfine state) which are coupled parametrically. Depending on the parameters, such as scattering lengths, in an optical trap the ground state of the spinor BEC can be either ferromagnetic or antiferromagnetic ("polar").

In this paper, we demonstrate that the parametric coupling between the spin degrees of freedom provides a physical mechanism for the modulational instability of the ferromagnetic ground state, for large enough densities of spinor BEC. In contrast, the antiferromagnetic state is always modulationally stable. This effect is reminiscent of the quasiparticle instabilities in two-component homogeneous condensates that are known to occur only for certain ratios of the inter- and intra-component interaction strengths. It also suggests one more example of a deep analogy between the coherent matter waves and light waves in nonlinear optics, along with the already studied cases of four-wave mixing and atomic-molecular photoassociation.

Model. We consider an atomic spinor BEC in an optical trap in the magnetic-field-free case. The Hamiltonian for the spinor BEC in the optical trap has the form:

$$H = \int \! d\mathbf{r} \left( \sum_{m_F} \frac{c_0}{2} S_{m_F,m_F'} + \frac{c_2}{2} S_{m_F,m_F',m_F''} \right),$$

where $S_{m_F,m_F'} = \sum_{\mathbf{r}} \psi_{m_F}^\dagger(\mathbf{r}) h_{m_F}(\mathbf{r}) \psi_{m_F'}(\mathbf{r})$, $S_{m_F,m_F',m_F''} = \sum_{\mathbf{r}} \sum_{m_F''} \sum_{m_F'''} \sum_{m_F''''} \psi_{m_F}^\dagger(\mathbf{r}) \psi_{m_F'}(\mathbf{r}) \psi_{m_F'''}^\dagger(\mathbf{r}) h_{m_F''''}(\mathbf{r}) \psi_{m_F''''}(\mathbf{r})$. In the equations above $h_{m_F}(\mathbf{r}) = -\hbar^2 \nabla^2/2m + V_T(\mathbf{r})$ is the single-atom Hamiltonian, and $V_T(\mathbf{r})$ is the trapping potential created by an optical field. Without loss of generality, we restrict ourselves to the case of hyperfine atomic state $F = 1$ with the corresponding sub-levels: $m_F = -1, 0, 1$.

The nonlinear interaction between different spin components of the condensate is governed by the spin-independent and spin-dependent interaction strengths, $c_0 = 4\pi \hbar^2 (2a_2 + a_0)/3m$ and $c_2 = 4\pi \hbar^2 (a_2 - a_0)/3m$, respectively. Here $a_0$ and $a_2$ are the s-wave scattering lengths for two colliding atoms with total angular momentum $F_{\text{tot}} = 0$ and $F_{\text{tot}} = 2$. The coefficient $c_2$ is calculated to be positive for the polar spinor condensate (e.g., $^{23}$Na) and negative for a ferromagnetic condensate (e.g., $^{87}$Rb) (see, e.g., \cite{2}). Whether the spinor condensate is ferromagnetic or antiferromagnetic arises from the fundamental gauge symmetry of the system, which in turn is dependent on the sign of the coefficient $c_2$ ($c_0$ is always positive for condensates with repulsive interactions, such as the $^{23}$Na and $^{87}$Rb considered here).

From Eq. (1) we can derive three coupled field equations for the case under consideration:

$$i\hbar \frac{\partial \psi_1}{\partial t} = \mathcal{L} \psi_1 + c_2 (\psi_1^\dagger \psi_0^\dagger + \psi_0^\dagger \psi_0) \psi_1 + c_2 \psi_1 \psi_0^\dagger \psi_0^\dagger,$$

$$i\hbar \frac{\partial \psi_{-1}}{\partial t} = \mathcal{L} \psi_{-1} + c_2 (\psi_{-1}^\dagger \psi_{-1} + \psi_{-1}^\dagger \psi_{-1}) \psi_{-1} + c_2 \psi_{-1} \psi_{-1}^\dagger \psi_{-1}^\dagger,$$

$$i\hbar \frac{\partial \psi_0}{\partial t} = \mathcal{L} \psi_0 + c_2 (\psi_1^\dagger \psi_1 + \psi_{-1}^\dagger \psi_{-1}) \psi_0 + 2c_2 \psi_0^\dagger \psi_1^\dagger \psi_{-1}.$$
where \( \mathcal{L} \equiv \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_T(r) \right] + c_0(x_j^1 \psi_{j-1} + \psi_j^1 \psi_0 + \psi_j^1 \psi_1) \). Next, we introduce the following linear field transformation for the quantum-field components, and treat the components as the corresponding mean fields:

\[
\phi_+ \equiv \frac{1}{\sqrt{2}}(\psi_1 + \psi_{-1}), \\
\phi_- \equiv \frac{1}{\sqrt{2}}(\psi_1 - \psi_{-1}), \\
\phi_0 \equiv \psi_0.
\]

As will become clear below, the advantage of this basis is that the stationary solutions for all three spinor components can be described by a single equation.

The coupled dynamical equations in the new basis have the following form:

\[
i \frac{\partial \phi_+}{\partial t} = \mathcal{L}\phi_+ + c_2 \left( (|\phi_-|^2 + |\phi_0|^2)\phi_+ + (\phi_+^2 + \phi_0^2)\phi_+^* \right), \\
i \frac{\partial \phi_-}{\partial t} = \mathcal{L}\phi_- + c_2 \left( (|\phi_+|^2 + |\phi_0|^2)\phi_- + (\phi_2^2 - \phi_0^2)\phi_-^* \right), \\
i \frac{\partial \phi_0}{\partial t} = \mathcal{L}\phi_0 + c_2 \left( (|\phi_+|^2 + |\phi_-|^2)\phi_0 + (\phi_+^2 - \phi_-^2)\phi_0^* \right),
\]

where this time \( \mathcal{L} \equiv \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_T(r) \right] + c_0(x_j^2 + |\phi_0|^2 + |\phi_-|^2). \) The wave functions, time, spatial coordinates, and interaction strengths are measured in the units of \((\hbar/m\omega)^{-3/4}\), \(\omega^{-1}\), \((\hbar/m\omega)^{1/2}\), and \((\hbar\omega)^{-1}(\hbar/m\omega)^{-3/2}\), respectively, where \( \omega \) is the axial trapping frequency.

**Stationary states.** The dynamics of the spinor condensate described by Eqs. (4) is, in general, spin mixing. However, any stable stationary solution of the system (3) represents a non-spin-mixing, or spin-polarized state of the system. Such stationary states have a constant population of each spin component and can be found by introducing the following ansatz:

\[
\phi_j = \sqrt{n_j(r)} e^{-i\mu_j t} e^{i\theta_j},
\]

where \( j = (+, -) \), \( \theta_j \) are the relative phases of each component with respect to \( \phi_0(\theta_0 \equiv 0) \), and \( \mu_j \) are the respective chemical potentials. Finally, \( n_+ + n_0 + n_- = n \) is the total density of the spinor condensate.

Upon substitution of the ansatz (5) into Eqs. (4), it becomes apparent that the stationary solutions can exist in this dynamical system only under the condition \( \mu_+ = \mu_- = \mu_0 \equiv \mu \). Another condition is that the spin components of the condensate are **locked in phase**. For a stationary state to exist, the variables \( 2\theta_- \) and \( 2\theta_+ \) can take only two distinct values, 0 or \( \pi \). In such a stationary state, the spinor eigenfunctions \( \sqrt{n_j} \) are eigenmodes of the same effective potential created both by the optical trap and by the nonlinear interaction of all spin components. Moreover, all three eigenmodes correspond to the same eigenvalue, \( \mu \). This means that these eigenfunctions are proportional to each other and therefore can be presented in the form: \( n_j(r) = r_n(r) \), where constant coefficients \( r_n \) represent the population of each spin component in a steady state, with \( r_+ + r_- + r_0 = 1 \). The spatial profiles of all three stationary spinor components obey the same time-independent equation:

\[
\left( -\frac{1}{2}\nabla^2 - \mu + V_T(r) \right) \sqrt{n(r)} + \chi n(r) \sqrt{n(r)} = 0. \quad (6)
\]

Depending on the relative phases, there exist **four different phase-locked steady state solutions** of Eqs. (3) with different populations in each spin component and different values of the coefficient \( \chi \) in Eq. (3):

**Case 1.** \( e^{i\theta_-} = 1, e^{i\theta_+} = i \), \( r_0 \) and \( r_\pm \) are constrained by \( r_+ + r_- + r_0 = 1 \), and \( \chi = c_0 + c_2 \).

**Case 2.** \( e^{i\theta_-} = 1, e^{i\theta_+} = i \); \( r_+ = r_0 + r_- = 1/2 \), and \( \chi = c_0 + c_2 \).

**Case 3.** \( e^{i\theta_-} = i, e^{i\theta_+} = i \); \( r_- = r_0 + r_+ = 1/2 \), and \( \chi = c_0 + c_2 \).

**Case 4.** \( e^{i\theta_-} = i, e^{i\theta_+} = i \); \( r_0 = r_- + r_+ = 1/2 \), and \( \chi = c_0 + c_2 \).

**Modulational stability analysis.** The stationary solutions described above may correspond to different metastable states of the spinor condensate, provided that they are linearly stable. Linear instability, i.e. exponential growth of the modulation of the stationary homogeneous condensate, was previously hinted to be responsible for complex spatial modulations of the condensate in a trap, that ultimately lead to the destruction of the non-spin-mixing state (3). However, no stability analysis of the spinor BEC has been carried out previously. Similar phenomenon occurring due to the nonlinear interaction of light beams (and pulses) in optical media is called **modulational instability** (MI) and is well studied in the context of nonlinear optical fibers.

To perform the MI analysis for the spinor BEC, we first note that the stationary homogeneous (or constant density) solutions corresponding to the phase relations in the cases 1-4 above have the form: \( n^h(r) = \mu/\chi \). Next, we add a small (generally complex) perturbation to the homogeneous solutions, taking the functions \( \phi_0 \) and \( \phi_\pm \) in the form:

\[
\phi_j(r, t) = (\sqrt{n_j^h} + \delta \phi_j) e^{i\theta_j - i\mu t}
\]

Substituting Eqs. (3) into Eqs. (3), omitting the terms containing \( V_T \), and linearizing around the homogeneous solutions, we obtain the dynamical equations for the perturbations \( \delta \phi_j(r, t) \), which can be used to analyze the stability of the homogeneous solutions in the cases 1-4 against the growth of periodic perturbations. If the perturbations are taken in the form \( \delta \phi_j = (u_j + iv_j) e^{i\omega t} \), where \( k = (k_x, k_y, k_z) \), these equations become: \( \delta A \Omega T = 0 \), where \( \Omega = (u_+, v_+, u_0, v_0, u_-, v_-) \). The matrix \( A \) being too cumbersome to write out here. If the characteristic equation, det \( A = 0 \), resolved with respect to the perturbation
frequency $\omega$, has a real or complex root for some real positive $k^2$, the spinor condensate is modulationally unstable. In general, such an equation is of the sixth order in $\omega$. For simplicity, we can assume one of the populations $r_j$ equal to zero, and the other two equal to each other. Then for case 1, all possible eigenvalues are given by:

$$
\omega_1^2 = -\frac{k^2}{2} \left( \frac{k^2}{2} + \mu \frac{c_2}{c_0} \right),
$$
$$
\omega_2^2,3 = -\frac{k^4}{4} - \mu \frac{k^2}{2} \left( 1 + \frac{c_2}{c_0} \pm \sqrt{1 + \frac{c_2}{c_0}} \right).
$$

From these expressions, and keeping in mind that $|c_2/c_0| < 1$, one can see that the real positive values of $\omega^2$, and hence the MI of this solution, can occur only for the ferromagnetic state, i.e. when $c_2/c_0 < 0$.

Carrying out an identical analysis for the cases 2-4, we find the following possible eigenvalues:

$$
\omega_1^2 = -\frac{k^2}{2},
$$
$$
\omega_2^2 = -2 \left( \frac{k^2}{2} - 2\mu \frac{c_2}{c_0 + c_2} \right)^2,
$$
$$
\omega_3^2 = -2 \left( \frac{k^2}{2} + 2\mu \right).
$$

Here all $\omega^2$ are negative and therefore, MI does not occur in any of the cases 2-4, neither for a ferromagnetic nor for a polar state.

It is possible to show that the conclusions of the MI analysis above hold in the most general case, when none of the populations $r_j$ are zero. Thus homogeneous solutions in the polar state never experience MI.

**Numerical simulations.** The MI analysis for the homogeneous condensate does not, strictly speaking, apply to the trapped condensate. However, it can serve as an indication of the spinor condensate behavior since the instability of the homogeneous condensate is bound to trigger the formation of the complex patterns in the trapped condensate cloud if the characteristic spatial extend of the condensate, $l$ (in dimensionless units), is larger than the largest length scale of the spatial patterns due to the MI, $L = k_{\text{min}}^{-1}$. For the only case when the MI of the spinor system does occur, this condition becomes $l > (\mu|c_2/c_0|)^{-1/2}$.

To test the results of our stability analysis and to demonstrate the effect of the MI on the trapped spinor condensate, we carry out numerical simulations of the dynamical equations (8). Because of the anisotropic nature of the optical trapping potential, the cigar shaped BEC is assumed to be quasi-one-dimensional and hence we use the ansatz $\phi_j(x, t) = \Psi(x, y) \phi_j(z, t)$, where $z$ is the direction of weak confinement, and $\Psi(x, y)$ is the wavefunction of the two-dimensional harmonic oscillator. This leads us to the one-dimensional (1D) dynamical spinor system for $\phi_j(z, t)$ which is identical to the system (8) with $L = \frac{1}{2} (-\partial^2/\partial z^2 + z^2) + \chi_0(|\phi_+|^2 + |\phi_0|^2 + |\phi_-|^2)$. The dimensionless interaction coefficients are $\chi_{0,2} = c_{0,2} \alpha$, and $\alpha = \int |\Psi(x, y)|^4 dx dy / \int |\Psi(x, y)|^2 dx dy$ is the transverse structure factor. Using the initial conditions specified by:

$$
\phi_j(z) = \sqrt{r_j n(z)e^{i\theta_j}},
$$

where $n(z)$ is the 1D spatial profile determined from Eq. (8), we solve the 1D equivalent of Eqs. (8) numerically for the cases 1-4 of the stationary phase-locked solutions.
In agreement with the analytical results, we only observe MI for the ferromagnetic state \((c_2/c_0 < 0)\) in the case 1. The results of a representative calculation for the ferromagnetic state (corresponding to \(^{87}\text{Rb}\)) are shown in Figs. 1 and 2. In all other cases the spinor BEC remains stable to periodic modulation of its components.

Our results show that the effect of the MI on the trapped spinor BEC is twofold. First, the instability destroys the non-spin-mixing stationary state, leading to population transfer between the spin components, as shown in Fig. 1. Second, the MI causes periodic spatial modulation of the condensate which, being confined by the trap, grows to be chaotic with time (see Fig. 2). In the short term, MI causes the spatial fragmentation of the spin domains shown in Fig. 3 for the original spinor components, \(\psi_j\).

Finally, to check that our results are dimensionally independent we have also numerically analyzed the spinor system in two dimensions, and again found that the MI only occurs in the ferromagnetic state for the stationary solution of case 1, as shown in Fig. 4.

In conclusion, we have predicted analytically and demonstrated numerically the possibility of MI of the ferromagnetic ground state of the spinor BEC. This effect resembles the parametric MI in birefringent optical fibers with the Kerr nonlinearity, and it provides one more direct analogy between matter wave, and nonlinear, optics.

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![FIG. 3. Spatial intensity profiles of the original spinor components, \(\psi_j\), demonstrating spin domain fragmentation. \(\psi_-\)(z) (dots), \(\psi_+\)(z) (dashed), \(\psi_0\)(z) (dot-dashed) and the total density (solid). Parameters are as in Fig. 1.](image)

![FIG. 4. Development of MI in the 2D case, shown for the spatial intensity profile of the \(\phi_+\) spin component. Initial conditions are calculated from Eq. (6). Parameters are as Fig. 1 with the structure factor \(\alpha_{2D} = 1\).](image)

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