Dynamical Instability and Domain Formation in a Spin-1 Bose-Einstein Condensate

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We interpret the recently observed spatial domain formation in spin-1 atomic condensates as a result of dynamical instability. Within the mean field theory, a homogeneous condensate is dynamically unstable (stable) for ferromagnetic (antiferromagnetic) atomic interactions. We find that this dynamical instability naturally leads to spontaneous domain formation as observed in several recent experiments for condensates with rather small numbers of atoms. For trapped condensates, our numerical simulations compare quantitatively to the experimental results, thus largely confirming the physical insight from our analysis of the homogeneous case.

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Spatial domains or pattern formation is a common feature of nonlinear dynamics in extended systems. It has been actively researched in nonlinear optics [1], classical fluids [2], granular materials [3], and recently in atomic Bose-Einstein condensates [4–10]. It is generally understood that the unstable modes of a dynamically unstable system can grow exponentially and eventually lead to the appearance of spatial domain structures that last for a long time.

Many earlier studies have suggested interesting mechanisms for spontaneous domain formation in atomic condensates [4–7]. Most focus on the single- or two-component condensates, where the number(s) of atoms for each component is conserved. The dynamical instability due to attractive atomic interactions is the most prominent among all proposed scenarios for domain formation [4,5,8]. The attractive interaction in a single-component condensate is also believed to be responsible for the formation of a train of solitons, consistent with the fact that it is dynamically unstable [4]. For a two-component condensate, again it is found that an effective attractive interaction is responsible for the dynamical instability and domain formation [5,8,9].

Several groups have also studied three-component, or spin-1, condensates ($F = 1$), which are distinct as the spin mixing interaction [6,10,11] allows for exchanging atoms among spin components $2|m_F = 0\rangle \leftrightarrow |m_F = +1\rangle + |m_F = -1\rangle$ (hereafter as $|0\rangle$, $|+\rangle$, and $|-\rangle$). The number of atoms for each component therefore can change, but the total number of atoms and the system magnetization are conserved. Significant interest now exists for spin-1 condensates because of the recent progress from several experimental groups [12], in particular, the observation of spontaneous domain formation in ^{87}Rb condensates [13]. Robins *et al.* were among the first to study dynamical instability in a spin-1 condensate [10]. They discovered a particular type of stationary state dynamically unstable for ferromagnetic interactions, evidenced by the sudden collapse when propagated with Gross-Pitaevskii (GP) equations, presumably resulting from the amplification of numerical discretization errors. Through extensive numerical simulations, Saito and Ueda also investigated very recently the spontaneous multidomain formation induced by the dynamical instability in a spin-1 condensate with ferromagnetic interactions [11]. A clear picture, however, is still lacking, as indicated by the general lack of comparisons with experimental reports. Our work aims at providing a complete understanding for domain formation in a spin-1 condensate.

To begin with, we consider a homogeneous condensate at an off-equilibrium state initially. For example, a spin-1 condensate in the ground state at a certain nonzero magnetic (B) field for time $t < 0$ will become off-equilibrium when the external B field is changed for $t \geq 0$. This causes the spin-1 condensate to collectively oscillate analogous to a nonrigid pendulum, as we recently showed [13,14]. In addition, we assume the condensate size is much larger than the spin healing length at least in one direction so that domains may be formed. Within our mean field description, the evolution of a spin-1 condensate is described by the coupled GP equations [15]

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\Phi_\pm &= [\mathcal{H} + c_2(n_\pm + n_0 - n_\mp)]\Phi_\pm + c_2\Phi_0^2\Phi_\mp^*,\\
i\hbar\frac{\partial}{\partial t}\Phi_0 &= [\mathcal{H} + c_2(n_+ + n_-)]\Phi_0 + 2c_2\Phi_+\Phi_-\Phi_0^*,
\end{aligned}
\tag{1}
$$

where $\mathcal{H} = -(\hbar^2/2\mathrm{m})\nabla^2 + V_{\rm ext} + c_0 n$, Φ_j is the jth spin component condensate wave function, and $n_j = |\Phi_j|^2$. $c_0 = 4\pi\hbar^2(a_0 + 2a_2)/3\mathrm{m}$ and $c_2 = 4\pi\hbar^2(a_2 - a_0)/3\mathrm{m}$, with a_0 and a_2 the scattering lengths for the two colliding atoms in the symmetric channels of total spin 0 and 2, respectively. The interaction is ferromagnetic (antiferromagnetic) if $c_2 < 0$ (> 0).

Let $\Phi_j = \sqrt{n_j}e^{i\theta_j}$ and define a relative phase $\theta = \theta_+ + \theta_- - 2\theta_0$; Eq. (1) simplifies to the following [14]:

$$
\begin{aligned}
\dot{n}_0 &= \frac{2c_2}{\hbar}n_0\sqrt{(n-n_0)^2 - m^2}\sin\theta,\\
\dot{\theta} &= \frac{2c_2}{\hbar}\left[(n-2n_0) + \frac{(n-n_0)(n-2n_0) - m^2}{\sqrt{(n-n_0)^2-m^2}}\cos\theta\right],
\end{aligned}
\tag{2}
$$

due to the conservation of atomic density ($n = n_+ + n_0 + n_-$) and the magnetization ($m = n_+ - n_-$). Equations (2) defines an energy conserving dynamics, with the effective energy per unit of volume given by

$$\begin{aligned}\mathcal{E} &= \frac{E}{V}\\ &= \frac{1}{2}c_0 n^2 + \frac{1}{2}c_2[m^2 + 2n_0(n - n_0)\\ &\quad + 2n_0\sqrt{(n-n_0)^2 - m^2}\cos\theta].\end{aligned} \tag{3}$$

We note that Eq. (2) for a homogeneous condensate differs from a trapped one even under single spatial mode approximation despite sharing the same dynamical Eq. (2).

Within the mean field approximation, the average spin of a condensate $\vec{f} = f_x\hat{x} + f_y\hat{y} + m\hat{z}$, where $f_j = \langle F_j\rangle$ with $F_{x,y,z}$ being the spin-1 matrices, is also conserved in addition to the conservations of n and m [16]. The energy functional Eq. (3) thus becomes $\mathcal{E} = \frac{1}{2}c_0 n^2 + \frac{1}{2}c_2 f^2$, if $f^2 \equiv f_x^2 + f_y^2 + m^2$. We note that the mean field theory model cannot be applied to extreme cases such as $N_0 = 0$ and $N_0 = N$, where quantum effects are important.

We adopt three approaches to study dynamical stability of the off-equilibrium collective oscillations of a condensate: the effective potential method, the Bogoliubov method, and direct numerical simulations. By going into a rotating frame, an entire orbit reduces to a stationary point in the phase space [14]. The effective potential then becomes $\mathcal{F} = (c_0/2)n^2 + (c_2/2)(m^2 + f_x^2 + f_y^2) - \mu n - \eta m - \delta_x f_x - \delta_y f_y$, where parameters $\{\mu, \eta, \delta_x, \delta_y\} = \{c_0 n, c_2 m, c_2 f_x, c_2 f_y\}$ define the rotating frame and are obtained through

$$\frac{\partial\mathcal{F}}{\partial n} = 0, \qquad \frac{\partial\mathcal{F}}{\partial m} = 0, \qquad \frac{\partial\mathcal{F}}{\partial f_x} = 0, \qquad \frac{\partial\mathcal{F}}{\partial f_y} = 0.$$

Our system is dynamically stable if its Hessian matrix of $\mathcal{F}$ with respect to $\{n, m, f_x, f_y\}$ is positive definite and dynamically unstable if the Hessian matrix has any negative eigenvalue. It is easy to check that the eigenvalues of the Hessian matrix are $\{c_0, c_2, c_2, c_2\}$. Thus, an antiferromagnetically interacting spin-1 condensate is dynamically stable, while a ferromagnetically interacting one is dynamically unstable since $c_2 < 0$.

We next employ the Bogoliubov transformation to find out the corresponding unstable modes. Starting from the stationary point in the rotating frame as found above, the equation of motion for collective excitations can be cast in a matrix form [17] as $\mathcal{M}\cdot\vec{x} = \hbar\omega\vec{x}$, with a vector $\vec{x} = (\delta\Psi_+, \delta\Psi_0, \delta\Psi_-, \delta\Psi_+^*, \delta\Psi_0^*, \delta\Psi_-^*)^T$. $\delta\Psi_j$ and $\delta\Psi_j^*$ denote the deviations from the stationary point, and the associated matrix is

$$\mathcal{M} = \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B}^* & -\mathcal{A}^* \end{pmatrix},$$

with

$$\mathcal{A} = \begin{pmatrix} \varepsilon_k + (c_0+c_2)n_+ + c_2 n_0 & c_0\Phi_0^*\Phi_+ + c_2\Phi_0\Phi_-^* & (c_0-c_2)\Phi_-^*\Phi_+ \\ c_0\Phi_0\Phi_+^* + c_2\Phi_0^*\Phi_- & \varepsilon_k + c_0 n_0 + c_2(n_+ + n_-) & c_0\Phi_0\Phi_-^* + c_2\Phi_0^*\Phi_+ \\ (c_0-c_2)\Phi_-\Phi_+^* & c_0\Phi_0^*\Phi_- + c_2\Phi_0\Phi_+^* & \varepsilon_k + (c_0+c_2)n_- + c_2 n_0 \end{pmatrix}$$

and

$$\mathcal{B} = \begin{pmatrix} (c_0+c_2)\Phi_+^2 & (c_0+c_2)\Phi_0\Phi_+ & c_2\Phi_0^2 + (c_0-c_2)\Phi_-\Phi_+ \\ (c_0+c_2)\Phi_0\Phi_+ & c_0\Phi_0^2 + 2c_2\Phi_-\Phi_+ & (c_0+c_2)\Phi_0\Phi_- \\ c_2\Phi_0^2 + (c_0-c_2)\Phi_-\Phi_+ & (c_0+c_2)\Phi_0\Phi_- & (c_0+c_2)\Phi_-^2 \end{pmatrix}.$$

$\varepsilon_k = \hbar^2k^2/2\mathsf{m}$ is kinetic energy of the collective excitation mode with wave vector k.

The eigenfrequencies of the Bogoliubov excitations are obtained from the characteristic equation $\det(\mathcal{M} - \hbar\omega I) = 0$, explicitly given by

$$[2c_s\varepsilon_k + \varepsilon_k^2 + c_s^2\mathsf{f}^2 - (\hbar\omega)^2][(\varepsilon_k^2 - (\hbar\omega)^2)(2c_s\varepsilon_k + \varepsilon_k^2 - (\hbar\omega)^2) + 2c_n\varepsilon_k(\varepsilon_k^2 + 2c_s\varepsilon_k(1-\mathsf{f}^2) - (\hbar\omega)^2)] = 0, \tag{4}$$

with $c_n = c_0 n$, $c_s = c_2 n$, and $\mathsf{f} = f/n$. The frequencies are then given by

$$\begin{aligned}(\hbar\omega)_{1,2}^2 &= \varepsilon_k[(c_n + c_s + \varepsilon_k) + \sqrt{(c_n - c_s)^2 + 4c_n c_s\mathsf{f}^2}],\\ (\hbar\omega)_{3,4}^2 &= \varepsilon_k[(c_n + c_s + \varepsilon_k) - \sqrt{(c_n - c_s)^2 + 4c_n c_s\mathsf{f}^2}],\\ (\hbar\omega)_{5,6}^2 &= (\varepsilon_k + c_s)^2 - c_s^2(1-\mathsf{f}^2).\end{aligned} \tag{5}$$

The corresponding modes are termed as density modes (solid lines), spin modes (dotted lines), and quadrupolar spin modes (dashed lines as in Fig. 1) by Ho [15]. Figures 1(a) and 1(b) show the real and imaginary parts of the typical dispersion relation for a ^{87}Rb spin-1 condensate [18], respectively. All frequencies are real for an antiferromagnetically interacting (e.g., ^{23}Na) condensate.

Our analysis here parallels that of Refs. [8,9] for a two-component condensate. We find two interesting features in Fig. 1(b). One of them at k_- is the most unstable mode at the maximum imaginary frequency; it determines short time behavior such as the time scale for domains to emerge. The other is the largest wave vector k_m with an (infinitesimal) imaginary frequency which determines the long time behavior such as the final domain size. From Eq. (5), we find the time scale for the emergence of a

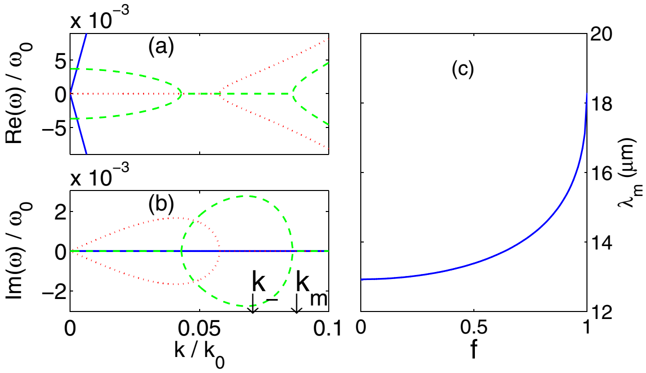

FIG. 1 (color online). Real part (a) and imaginary part (b) of a typical Bogoliubov spectrum for a spin-1 condensate with ferromagnetic interaction. Panel (c) shows the smallest wavelength of a homogeneous spin-1 ^{87}Rb condensate at $n = 1.9 \times 10^{14}$ cm^{-3}.

domain is $\sim 1/|\omega(k_-)| = h/(|c_s|\sqrt{1-\mathsf{f}^2})$ and the domain width is about $\lambda_m = 2\pi/k_m = h/\sqrt{2m|c_s|(1+\sqrt{1-\mathsf{f}^2})}$. It is typically of the order of spin healing length. Figure 1(c) displays the f dependence of λ_m at $n = 1.9 \times 10^{14}$ cm^{-3} for a homogeneous ^{87}Rb spin-1 condensate. For the domains to form, a condensate has to be larger than λ_m, at least in one direction.

We note that the spin domain formation as discussed here is different from striation patterns as observed in (antiferromagnetic) ^{23}Na condensates. The stripe patterns arise from interplay of an external B field, a field gradient, and immiscibility among different spin components [6]. No domains were observed in Stenger *et al.*'s experiment [6] at negligible B fields where the $|+\rangle$ and $|-\rangle$ components coexist. At finite values of B fields, phase separation between the $|0\rangle$ and the $|\pm\rangle$ components occurs [19]. In Miesner *et al.* and Stamper-Kurn *et al.*'s experiments [6], only two spin components were involved due to the relatively large bias B field (~ 15 G).

Our analysis shows that the formation of spin domains is a direct consequence of dynamic instability for a condensate with ferromagnetic interactions. To provide a clearer physical picture for domain formation, we now work in the lab frame. We focus on $d\mathcal{E}/dm$, which in fact calibrates the formation of the spin domain. We find

$$\frac{d\mathcal{E}}{dm} = c_2 m\left[1 - \frac{n_0\cos\theta}{\sqrt{(n-n_0)^2 - m^2}}\right]. \qquad (6)$$

Figure 2 shows the surfaces where the above first order derivative is zero. The region below the saddle surface in Fig. 2 of an orbit is unstable if $c_2 < 0$. Here the meaning of "unstable" is generalized, referring to the dynamical property where the local magnetization tends to deviate further from $m = 0$. For example, in the lower right allowed region of $d\mathcal{E}/dm < 0$, $\Delta m > 0$ is required to lower the local energy $\mathcal{E} \approx \mathcal{E}(m) + (d\mathcal{E}/dm)\Delta m$. Thus, m tends to increase. Similarly, the lower left allowed region would

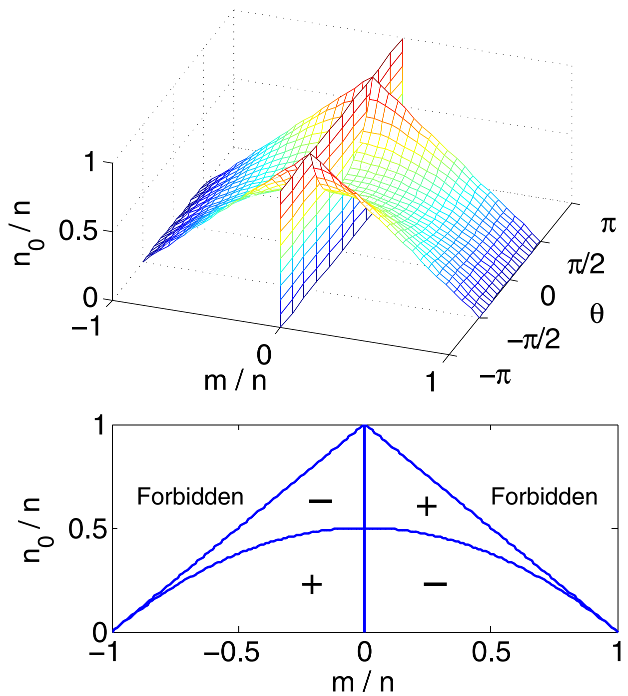

FIG. 2 (color online). Surfaces of $d\mathcal{E}/dm = 0$ (top) and the cross section at $\theta = 0$ (bottom). The plus signs denote $d\mathcal{E}/dm > 0$ and the minus signs denote $d\mathcal{E}/dm < 0$.

make m decrease. The combined effect is dynamically unstable orbits, separation of $|+\rangle$ and $|-\rangle$ components, and the eventual formation of spin domains.

For antiferromagnetic interactions ($c_2 > 0$), θ usually oscillates around π. Thus, $d\mathcal{E}/dm > 0$ for $m > 0$ and $d\mathcal{E}/dm < 0$ for $m < 0$. So the magnetization always oscillates around zero, and no domain forms. This coincides with the findings of the dynamical stability analysis for an antiferromagnetically interacting condensate.

Finally, we perform numerical simulations of Eq. (1) to confirm the mechanism of dynamical instability-induced spin domain formation. The initial conditions are as in the experiment [13], with ^{87}Rb condensates [$N_0(0)/N = 0.744$, $\theta(0) = 0$, for the ground state of $N = 2.0 \times 10^5$ at $B = 0.3$ G and $M = 0$], in a trap $V_{\rm ext}(\vec{r}) = (\mathsf{m}/2)(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$, with $\omega_x = \omega_y = (2\pi)240$ Hz and $\omega_z = (2\pi)24$ Hz. In one of the simulations, we intentionally include additive small white noise ($\sim 1.0 \times 10^{-5}$), although still much larger than numerical errors [20] during the propagation. We find that it takes a shorter time for the $|+\rangle$ and $|-\rangle$ components to separate when white noise is included. Figure 3 shows the evolution of axial density distributions. Phase separation between the $|+\rangle$ and $|-\rangle$ components is seen, accompanied by the formation of domains. This proves again that dynamical instability causes the formation of domains. The domain width (an upper limit), as estimated from $\lambda_m = h/\sqrt{2\mathsf{m}|c_2|\langle n\rangle(1+\sqrt{1-\mathsf{f}^2})} \approx 15\ \mu$m, is consistent with both simulations and experimental observations [13].

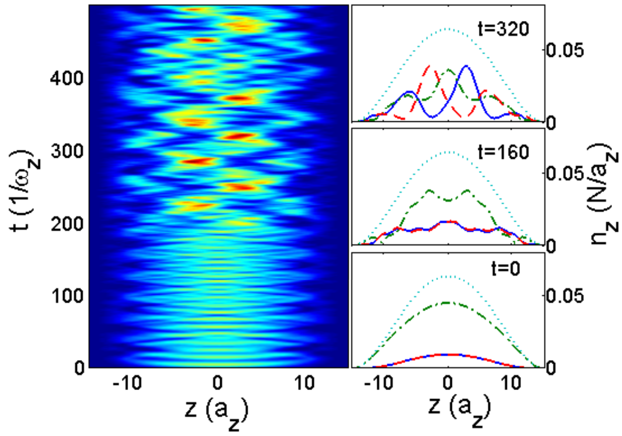

FIG. 3 (color online). Typical evolutions for spin domain formation in a ^{87}Rb condensate. The initial state is the ground state at $B = 0.3$ G. The B field is then set to zero and small white noises are added throughout the evolution. The left contour plot is for the $|+\rangle$ component. The right column shows the density distribution of all three components at times $t = 0, 160, 320$ $(1/\omega_z)$. Solid, dashed-dotted, and dashed lines denote, respectively, the $|+\rangle$, $|0\rangle$, and $|-\rangle$ components. Dotted lines are for the total density. The axial density is $n_z \equiv \int \sum_j |\Phi_j|^2 2\pi r dr$. $a_z = \sqrt{\hbar/m\omega_z} \simeq 2.2$ μm and the average condensate density is $\sim 1.9 \times 10^{14}$ cm^{-3}.

In a spinor condensate, spin wave excitations normally refer to dynamically stable (or relatively more stable) collective modes. Once excited, they lead to coherent cyclic dynamics in both spatial and temporal dimensions. Spin domains, on the other hand, refer to unstable modes, with a fixed pattern in the long time limit.

In conclusion, we have presented a systematic study of dynamical stability and the accompanied mechanism for domain formation in a spin-1 condensate. Our results affirm that a ferromagnetically interacting condensate is dynamically unstable and evolves spontaneously into multidomain structures, contrary to dynamically stable antiferromagnetic condensates. Our work provides a clear physical picture for recently observed spontaneous domain formations in spin-1 condensates [13].

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