

## Single-mode approximation in a spinor-1 atomic condensate

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We investigate the validity conditions of the single-mode approximation (SMA) in a spinor-1 atomic condensate when effects due to residual magnetic fields are negligible. For atomic interactions of the ferromagnetic type, the SMA is shown to be exact, with a mode function different from what is commonly used. However, the quantitative deviation is small under current experimental conditions (for <sup>87</sup>Rb atoms). For antiferromagnetic interactions, we find that the SMA becomes invalid in general. The differences among the mean-field mode functions for the three spin components are shown to depend strongly on the system magnetization. Our results can be important for studies of beyond mean-field quantum correlations, such as fragmentation, spin squeezing, and multipartite entanglement.

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Trapped atomic quantum gases have provided a remarkable testing ground for quantum many-body theory [1]. Since the discovery of the first atomic Bose-Einstein condensate [2], mean-field theory has been applied with great success to these systems, arguably because (1) low-energy atom-atom interaction can be simply parametrized by an *s*-wave scattering length  $a_{sc}$  where atoms behave as hard spheres of effective radii  $a_{sc}$ ; and (2) most current atomic gases are dilute with densities  $n$  satisfying  $na_{sc}^3 \ll 1$  [3]. Increasingly, theoretical and experimental attentions are directed towards beyond mean field effects. In this regard, spinor-1 atomic condensates have become a prototype system for many recent studies [4–7]. Several interesting results have already been obtained, e.g., multiparticle and continuous variable-type entanglement [4], spin mixing [5], spinor four-wave mixing [6], and super fragmentation and coherent fragmentation [7]. The single-mode approximation (SMA) is often adopted for these studies when a mean-field approach with a vectorial order parameter becomes inappropriate [8–10]. Beyond mean field quantum effects have been found both when there is no external fields [5,6] and when there is an external magnetic or optical field [11–15]. To justify the use of the SMA, earlier studies often compared with solutions of the coupled Gross-Pitaevskii (GP) equation for the different spin components and enforced an upper limit on the number of atoms [4,11]. While there is not a generally adopted limit, it is typically estimated that  $N$  should be less than  $10^4$ , a rather small number for current experiments.

In this paper we investigate the validity conditions of the SMA in spinor-1 atom condensate [16,17]. Our initial aim was to provide a reliable thermodynamic phase diagram for a trapped spinor-1 atomic gas [18]. Surprisingly, interesting zero temperature results from the coupled GP equations reveal intricate relationships of the mode functions for the three spin components due to the constraint on the system magnetization.

We consider a spinor-1 atomic condensate in the absence of an external magnetic field. As partitioned by Law *et al.* [5], the system Hamiltonian  $H$  separates into a symmetric part (under spin exchange)

$$H_S = \int d\vec{r} \left( \Psi_\alpha^\dagger \mathcal{L}_{\alpha\beta} \Psi_\beta + \frac{c_0}{2} \Psi_\alpha^\dagger \Psi_\beta^\dagger \Psi_\beta \Psi_\alpha \right), \quad (1)$$

with  $\mathcal{L}_{\alpha\beta} = -\hbar^2 \nabla^2 / 2M + V_{\text{ext}}$ , and an asymmetric part

$$H_A = \frac{c_2}{2} \int d\vec{r} \Psi_\alpha^\dagger (F_\eta)_{\alpha\beta} \Psi_\beta \Psi_\mu^\dagger (F_\eta)_{\mu\nu} \Psi_\nu, \quad (2)$$

where  $\Psi_\alpha$  ( $\alpha=0, \pm$ ) denotes the annihilation field operator for the  $\alpha$ th component.  $F_{\eta=x,y,z}$  are the spin-1 matrix representation, and a summation over repeated indices is assumed in Eqs. (1) and (2). The external trapping potential  $V_{\text{ext}}(\vec{r})$  is spin independent as in a far off-resonant optical dipole force trap (FORT) which makes atomic spinor degrees of freedom completely accessible. The pair interaction coefficients are  $c_0 = 4\pi\hbar^2(a_0 + 2a_2)/3M$  and  $c_2 = 4\pi\hbar^2(a_2 - a_0)/3M$ , with  $a_0$  ( $a_2$ ) the *s*-wave scattering length for two spin-1 atoms in the combined symmetric channel of total spin 0 (2). The only state changing collision in Eq. (2) occurs through the coupling  $\Psi_0^\dagger \Psi_0^\dagger \Psi_+ \Psi_- + \text{H.c.}$ , which conserves the system magnetization  $\mathcal{M} = \int d\vec{r} \langle F_z \rangle = \int d\vec{r} [\Psi_+^\dagger \Psi_+ - \Psi_-^\dagger \Psi_-]$ .  $\mathcal{M}$ -changing inelastic (“bad”) collisions occur at a much longer time scale as compared with a condensate’s typical lifetime, and therefore are excluded here as in all previous studies. Although the real-time dynamics governed by  $H_S + H_A$  conserves the total atom number  $N = \int d\vec{r} [\Psi_+^\dagger \Psi_+ + \Psi_0^\dagger \Psi_0 + \Psi_-^\dagger \Psi_-]$  and  $\mathcal{M}$ , the ground state obtained from a global minimization of  $H_S + H_A$  is not automatically guaranteed to have the same  $N$  and  $\mathcal{M}$ . We therefore introduce separate Lagrange multipliers  $\mathcal{B}$  to guarantee the conservation of  $\mathcal{M}$  and the chemical potential  $\mu$  to conserve  $N$ . The ground state is then determined by a minimization of the free-energy functional  $\mathcal{F} = H_S + H_A - \mu N - \mathcal{B}\mathcal{M}$ . Mathematically, this task turns out to be highly nontrivial. In fact, most previous discussions on spinor-1 condensates did not minimize  $H$  under the constraint of a conserved  $\mathcal{M}$ . Therefore, their resulting ground states are the global ground states that can only be reached if the system can coherently adjust its initial  $\mathcal{M}$  value. Such a situation is inconsistent with current experiments.

One of the strongest physics support for the SMA comes from the fact that  $a_0 \sim a_2$  for a spinor-1 ( $^{87}\text{Rb}$ ) condensate. This gives rise to  $|c_2| \ll |c_0|$  [5,9]. Thus  $H_A$  is much smaller as compared with  $H_S$ , and can be considered as a perturbation by assuming the SMA

$$\Psi_\alpha(\vec{r}) = a_\alpha \phi_{\text{SMA}}(\vec{r}), \quad \alpha = 0, \pm, \quad (3)$$

i.e., with a common mode function  $\phi_{\text{SMA}}(\vec{r})$  (normalized to 1). The Fock state boson operators  $a_\alpha$  satisfy  $[a_\alpha, a_\gamma^\dagger] = \delta_{\alpha\gamma}$ ,  $[a_\alpha, a_\gamma] = 0$ .  $\phi_{\text{SMA}}(\vec{r})$  is determined from  $H_S$  alone (without  $H_A$ ) according to [5]

$$\left[ -\frac{\hbar^2 \nabla^2}{2M} + V_{\text{ext}} + c_0 N |\phi_{\text{SMA}}|^2 \right] \phi_{\text{SMA}}(\vec{r}) = \mu \phi_{\text{SMA}}(\vec{r}). \quad (4)$$

It shares similar physics of the often used spin-charge separation in condensate matter systems. Since its introduction, the SMA has been used frequently [4–7,19]. A notable exception is the work by Ueda [20], who went beyond the SMA by studying a translational invariant system with the use of a plane-wave basis. Correlations between spatial and spinor degrees of freedom were then shown to lead to effects associated with density waves and spin waves. For a trapped system as studied here, the use of a plane-wave basis becomes inappropriate.

The same SMA is sometimes also used in a spin-1/2 system by assuming  $\phi_0(\vec{r}) = \phi_1(\vec{r})$  [21–24]. This is less critical as the resulting Hamiltonian proportional to  $J_z^2$  remains in the same symmetry group in the Schwinger boson representation, although with a different coefficient and the presence of additional linear terms in  $J_\mu$ . The validity of the SMA in this case has been tested recently using the rigorous positive- $P$  approach [23,24].

For a spinor-1 condensate, however, complications arise when spin component mode functions are taken to be different. The effective Hamiltonian thus obtained contains no angular momentum symmetry at all in its corresponding Schwinger boson representation. This naturally calls for a critical investigation of the SMA. To check the validity of the SMA, we start with the mean field and find separate spin component mode functions  $\langle \Psi_\alpha \rangle = \Phi_\alpha$  (at zero temperature). The dynamics of  $\Phi_\alpha$  for the ground state is governed by  $H_S + H_A$ , which obeys the following coupled GP equation:

$$\begin{aligned} i\hbar \dot{\Phi}_+ &= [\mathcal{H} - \mathcal{B} + c_2(n_+ + n_0 - n_-)]\Phi_+ + c_2 \Phi_0^2 \Phi_-^*, \\ i\hbar \dot{\Phi}_0 &= [\mathcal{H} + c_2(n_+ + n_-)]\Phi_0 + 2c_2 \Phi_0^* \Phi_+ \Phi_-, \\ i\hbar \dot{\Phi}_- &= [\mathcal{H} + \mathcal{B} + c_2(n_- + n_0 - n_+)]\Phi_- + c_2 \Phi_0^2 \Phi_+^*, \end{aligned} \quad (5)$$

with  $\mathcal{H} = -\hbar^2 \nabla^2 / 2M + V_{\text{ext}} + c_0 n$ ,  $n_\alpha = |\Phi_\alpha|^2$ , and  $n = n_+ + n_0 + n_-$ . We have developed a reliable numerical algorithm based on propagating Eq. (5) in imaginary time ( $it$ ) that converges to the ground state while maintaining the conservation of both  $N$  and  $\mathcal{M}$ . We take the initial wave function to be a complex Gaussian with a constant velocity, i.e.,

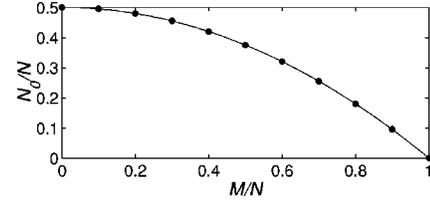


FIG. 1. The  $\mathcal{M}$  dependence of  $N_0$  in the ferromagnetic case. The solid line shows  $N_0/N = (1 - \mathcal{M}^2/N^2)/2$ , while the dots are numerical results. The agreement is remarkable.

$e^{-(x^2/2q_x^2 + y^2/2q_y^2 + z^2/2q_z^2)} e^{-i\vec{k} \cdot \vec{r}}$ , where  $q_x$ ,  $q_y$ ,  $q_z$ , and  $\vec{k}$  are adjustable parameters that shall not affect the final converged solution. In the simplest case for the ground state, we assume  $\Phi_\alpha(\vec{r}) = |\Phi_\alpha(\vec{r})| e^{i\theta_\alpha}$  with  $\theta_\alpha$  a global phase independent of  $\vec{r}$ . Then only the relative phase  $\Delta = 2\theta_0 - \theta_+ - \theta_-$  shows up in  $\mathcal{F}$  with a term proportional to  $c_2 |\Phi_+ \Phi_- \Phi_0^2| \cos \Delta$ . This gives  $\Delta = 0$  (for  $c_2 < 0$ ) or  $\pi$  (for  $c_2 > 0$ ) when  $\mathcal{F}$  is minimized [25], a conclusion also verified by numerical calculations. As first stated by Ho [9], the spinor-1 condensate Hamiltonian  $H = H_S + H_A$  is invariant under gauge transformation  $e^{i\theta}$  and spin rotations  $\mathcal{U}(\alpha, \beta, \tau) = e^{-iF_z \alpha} e^{-iF_y \beta} e^{-iF_z \tau}$ . For the ground state that conserves  $\mathcal{M}$ , however, the spin rotation symmetry is reduced to the subgroup  $\text{SO}(2)$  generated by  $e^{-iF_z \alpha}$ . Thus irrespective of the signs of  $c_2$ , a transformation of the form  $e^{-i\theta_0} e^{-iF_z(\theta_+ - \theta_-)/2}$  can always reduce a complex solution to a real one [25].

When  $\mathcal{B} = 0$  as for ferromagnetic interactions with any values of magnetization  $\mathcal{M} \leq N$  or for antiferromagnetic interactions with  $\mathcal{M} = 0$ , we find  $|\phi_+| = |\phi_-|$  from the symmetry of Eq. (5). We then rescale the wave function  $\phi_\alpha = \Phi_\alpha / \sqrt{N_\alpha}$  such that  $\phi_\alpha$  is normalized to 1 [ $\int d\vec{r} |\Phi_\mu(\vec{r})|^2 = N_\mu$ , the number of atoms in the  $\mu$ th component], the asymmetric interaction energy then becomes

$$\begin{aligned} E_A &= \frac{c_2}{2} \int d\vec{r} [(N_+ |\phi_+|^2 - N_- |\phi_-|^2)^2 \\ &\quad + 2N_+ N_0 |\phi_+|^2 |\phi_0|^2 + 2N_- N_0 |\phi_-|^2 |\phi_0|^2 \\ &\quad + 4N_0 (N_+ N_-)^{1/2} |\phi_0|^2 |\phi_+| |\phi_-| \cos \Delta]. \end{aligned} \quad (6)$$

For ferromagnetic interactions ( $c_2 < 0$  and  $\Delta = 0$ ), we thus prove in general that  $E_A$  is minimized when

$$|\phi_+| = |\phi_0| = |\phi_-| = |\phi|, \quad (7)$$

and  $N_0/N = (1 - \mathcal{M}^2/N^2)/2$ . The latter result (independent of all other parameters) was first obtained in Ref. [11] assuming the SMA, i.e., essentially assuming Eq. (7). Our numerical solutions closely follow this as shown in Fig. 1. For antiferromagnetic interactions ( $c_2 > 0$ ),  $\mathcal{B} = 0$  holds only when  $\mathcal{M} = 0$ . In this case, using  $\Delta = \pi$ , we prove in general that  $E_A$  is minimized to zero under Eq. (7), while  $N_0$  can be any value  $\leq N$  [11].

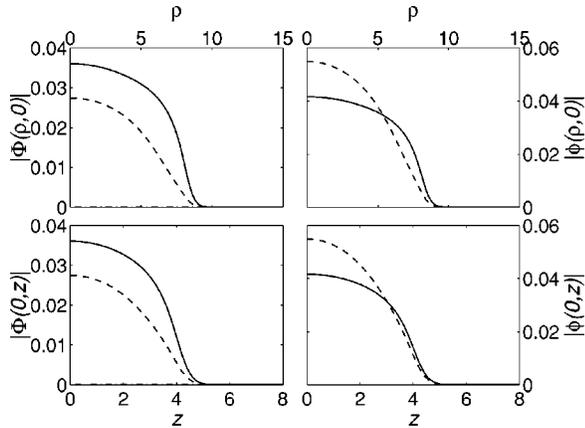


FIG. 2. The original (left column) and the renormalized (right column) wave functions along radial (upper panel) and axial (lower panel) directions for the + (solid line) and the - (dashed line) spin components. Other parameters are  $N=3.16 \times 10^5$ ,  $\mathcal{M}/N=0.5$ , and  $\lambda=2$ . All lengths are in units of  $\sqrt{\hbar/m\omega_r}$ .

For antiferromagnetic interactions ( $\mathcal{M} \neq 0$ ), we find that mode functions for the three spin components are different (see Fig. 2). Further analysis show that  $E_A$  is minimized if  $N_0=0$  [11].

We now discuss the relationship of Eq. (7) to the SMA Eq. (4). We note that the validity of Eq. (7) (including  $H_A$ ) is in fact not equivalent to the validity of the SMA (excluding  $H_A$ ). For ferromagnetic interactions, with Eq. (7) and the relation between  $N_0$  and  $\mathcal{M}$ , Eq. (5) simplifies to

$$\left[ -\frac{\hbar^2 \nabla^2}{2M} + V_{\text{ext}} + (c_0 + c_2)N|\phi|^2 \right] \phi(\vec{r}) = \mu \phi(\vec{r}). \quad (8)$$

This shows that  $\phi(\vec{r})$  is independent of  $\mathcal{M}$ , and its deviation from  $\phi_{\text{SMA}}$  comes only from the  $c_2$  term. This result can in fact be easily understood. Since  $c_0 + c_2 = 4\pi\hbar^2 a_2/M$ ,  $\phi(\vec{r})$  of Eq. (8) is simply the ground state of the GP equation for an atomic scattering length of  $a_2$ . In a ferromagnetic state, atomic spins are aligned locally. Two such atoms ( $F_{1,2}=1$ ) only collide in the symmetric total spin  $F=2$  channel. For quantitative results, we compared  $|\langle \phi | \phi_{\text{SMA}} \rangle|$  for  $^{87}\text{Rb}$  atoms with  $a_0=101.8a_B$  and  $a_2=100.4a_B$  [26] ( $a_B$  is the Bohr radius). Other assumptions are the typical radial trap frequency  $\omega_r=2\pi \times 10^3$  (Hz), the axial trap frequency  $\omega_z = \lambda\omega_r$ , and  $\lambda=0.1, 1$ , and  $10$ . We also took  $N=3.16 \times 10^5$  and varied the total magnetization  $\mathcal{M}/N$  from 0 to 1.

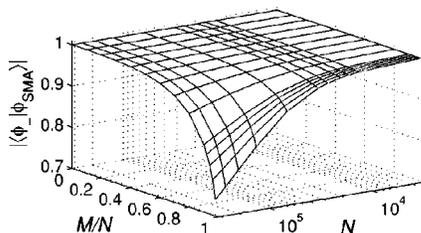


FIG. 3.  $\mathcal{M}$  and  $N$  dependence of the overlap integral  $|\langle \phi_- | \phi_{\text{SMA}} \rangle|$  for  $^{23}\text{Na}$  atoms ( $\lambda=1$ ).  $|\langle \phi_+ | \phi_{\text{SMA}} \rangle|$  is essentially 1 to within  $\pm 0.001$  in the same region.

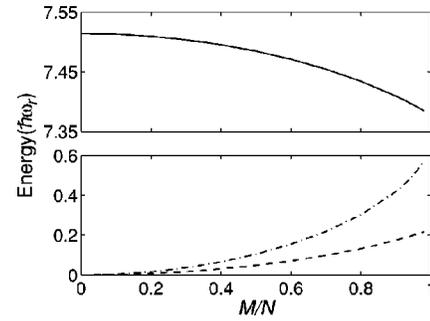


FIG. 4. The  $\mathcal{M}$  dependence of energy components (in units of  $\hbar\omega_r$ )  $E_{c_0}$  (solid line),  $E_A$  (dashed line), and  $\mathcal{B}\mathcal{M}$  (dash-dotted line) for the  $^{23}\text{Na}$  atom at  $\lambda=1$  and  $N=3.16 \times 10^5$ .

Under these conditions, we find uniformly that  $|\langle \phi | \phi_{\text{SMA}} \rangle| \approx 1$  essentially because  $|c_2| \ll |c_0|$ .

For antiferromagnetic interactions ( $c_2 > 0$ ), the following two special cases arise: (1) when  $\mathcal{M}=0$ , using Eq. (5), we prove that  $|\phi_a| = |\phi_{\text{SMA}}|$ , which means the SMA is exact in this case; (2) when  $\mathcal{M}=N$ ,  $\phi_+$  satisfies the same equation as Eq. (8), so its derivation from the SMA only originates from the  $c_2$  term. For  $^{23}\text{Na}$  atoms, we use  $a_0=50a_B$  and  $a_2=55a_B$  [27] as an example in this case. Other parameters used are the same as in the ferromagnetic case. Since  $N_0=0$ , we consider only the  $\pm$  components. Figure 2 shows the original and renormalized wave function for  $N=3.16 \times 10^5$ ,  $\mathcal{M}/N=0.5$ , and  $\lambda=2$ . We see clearly that  $\phi_+$  and  $\phi_-$  are different. Figure 3 shows the magnetization and atom number dependence of  $|\langle \phi_- | \phi_{\text{SMA}} \rangle|$  for a spherical trap. Since the + component contains the majority number of atoms, it is natural to find  $|\langle \phi_+ | \phi_{\text{SMA}} \rangle| \approx 1$ . The value of  $|\langle \phi_+ | \phi_{\text{SMA}} \rangle|$  at  $\mathcal{M} \approx N$  also indicates that the deviation contributed by  $c_2$  alone is also small for  $^{23}\text{Na}$  atoms. While for  $|\langle \phi_- | \phi_{\text{SMA}} \rangle|$  we see it becomes as low as 0.75 when  $N=3.16 \times 10^5$  and when  $\mathcal{M}$  approaches  $N$ . To distinguish the different sources of deviations, we plot  $E_{c_0} = (c_0/2) \int d\vec{r} n^2$ ,  $E_A$ , and  $\mathcal{B}\mathcal{M}$  in Fig. 4. We see that the  $\mathcal{B}\mathcal{M}$  term contributes the most. In Fig. 5 the overlap integral is shown to also depend on the trap aspect ratio  $\lambda$ .

Finally, we discuss the implications of our result on the macroscopic alignment of the total spin of a spinor condensate. For ferromagnetic interactions, the spatial distribution of the total spin  $\langle \vec{F}(r) \rangle \equiv \sum_{\alpha\beta} \Phi_{\alpha}^*(r) \vec{F}_{\alpha\beta} \Phi_{\beta}(r)$  is found to

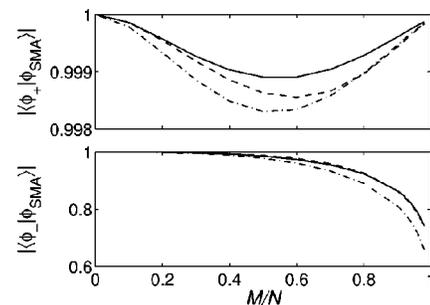


FIG. 5. The overlap  $|\langle \phi_{\pm} | \phi_{\text{SMA}} \rangle|$  for  $\lambda=0.1$  (solid line), 1 (dashed line), and 10 (dash-dotted line).

be pointed along the same direction, i.e., independent of the spatial coordinates. Using  $\Delta=0$ ,  $N_0=N(1-\mathcal{M}^2/N^2)/2$ , and  $N_{\pm}=N(1\pm\mathcal{M}/N)^{2/4}$ , it can be expressed as

$$\langle \vec{F}(\vec{r}) \rangle = |\phi(\vec{r})|^2 \begin{pmatrix} \sqrt{N^2 - \mathcal{M}^2} \cos(\theta_+ - \theta_0) \\ -\sqrt{N^2 - \mathcal{M}^2} \sin(\theta_+ - \theta_0) \\ \mathcal{M} \end{pmatrix}. \quad (9)$$

For antiferromagnetic interactions, we find

$$\langle \vec{F}(\vec{r}) \rangle = \begin{pmatrix} 0 \\ 0 \\ N_+ |\phi_+(\vec{r})|^2 - N_- |\phi_-(\vec{r})|^2 \end{pmatrix}, \quad (10)$$

a state with all spins aligned in the  $\pm z$  direction. It reduces to  $\langle \vec{F}(\vec{r}) \rangle = \vec{0}$  for  $\mathcal{M}=0$ .

To conclude, we presented both analytic and numerical studies of the validity of the SMA. We find that deviations of the ground state solution from the  $\phi_{\text{SMA}}(\vec{r})$  come from two sources: the  $c_2$  or the  $\mathcal{B}$  (due to conservation of  $\mathcal{M}$ ) term. For ferromagnetic interactions, the only source is the  $c_2$  term, which is negligible for  $^{87}\text{Rb}$  atoms. One can therefore safely use the SMA. For antiferromagnetic interactions, if  $\mathcal{M}=0$ ,  $\phi_{\text{SMA}}$  becomes the exact ground-state wave function. For  $\mathcal{M}>0$ , however, one can still use the  $\phi_{\text{SMA}}$  for  $\phi_+$ , but

$\phi_-$  differs significantly if both  $N$  and  $\mathcal{M}$  are large. In this case the  $\mathcal{B}\mathcal{M}$  term contributes the most to the deviation. Our conclusions from this study apply to the ground states of a spinor condensate. For dynamic problems Ref. [11], the SMA may become worse. Our study suggests that instead of making the SMA as in Eq. (3), an improved SMA could consist of  $\Psi_{\mu} = a_{\mu} \phi_{\mu}(\vec{r})$ , where the mean-field solution  $\Phi_{\mu}(\vec{r})$  and its associated effective spin mode function  $\phi_{\mu} = \Phi_{\mu}(\vec{r})/\sqrt{N_{\mu}}$  are obtained under the constraints of conserved  $N$  and  $\mathcal{M}$ . Such an approach can be important in studying beyond mean-field quantum correlations. In a forthcoming paper, we will report some results on condensate fragmentation.

In summary, we have presented a detailed investigation of the SMA for a spinor-1 condensate and pointed out interesting structures of its ground state for both ferromagnetic and antiferromagnetic interactions.

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