## Phase separation in the trapped spinor gases with anisotropic spin-spin interaction

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**Abstract.** We investigate the effect of the anisotropic spin-spin interaction on the ground state density distribution of the one dimensional spin-1 bosonic gases within a modified Gross-Pitaevskii theory both in the weakly interaction regime and in the Tonks-Girardeau (TG) regime. We find that for ferromagnetic spinor gas the phase separation occurs even for weak anisotropy of the spin-spin interaction, which becomes more and more obvious and the component of  $m_F = 0$  diminishes as the anisotropy increases. However, no phase separation is found for anti-ferromagnetic spinor gas in both regimes.

**PACS.** 03.75.Mn Multicomponent condensates; spinor condensates – 03.75.Hh Static properties of condensates; thermodynamical, statistical, and structural properties – 67.40.Db Quantum statistical theory; ground state, elementary excitations

Since Bose-Einstein condensates (BECs) of trapped alkali atomic clouds were realized experimentally [1], many new regimes have been investigated extensively. The experimental progress on trapping cold atoms under a highly controllable way has opened the exciting opportunities for studying strongly correlated atomic systems. When BECs are confined in a far-off-resonant optical trap regardless of their hyperfine state, the atomic spin degrees of freedom are liberated and the spinor nature of the condensate can be manifested [2]. It stimulates enormous theoretical and experimental interests in studying a variety of spinrelated properties, such as quantum entanglement of spins, spin domains, etc. [3,4]. Especially, the magnetism of the spinor gas has been studied by many authors [3, 5-7]. A great number of theories and experiments have shown that when the spinor gas realized in a magnetic trap is loaded into an optical trap, the spin domain will form after evolution for a period of time.

Domain formation or phase separation in the multicomponent BECs was also intensively investigated in the past years. The condensate mixture displays a novel phase in which phase separation occurs if there exists a strong repulsive interaction between the species [8]. For the spinor gases, the spin-dependent interaction is much weaker than the contact interaction, and thus the spin-dependent interaction almost has no effect on the total density distribution. Although each component displays a different density profile, no phase separation was found in the case of the isotropic spin-spin interaction [9, 10]. In this paper, we will show that anisotropic spin-spin interaction could result in the formation of the static spin domain in the spinor gases and we mainly focus on one-dimensional (1D) cold atom systems for both the weakly interacting regime and the strongly interacting TG regime.

Recently, there has been tremendous experimental progress towards the realization of trapped 1D cold atom systems [11–14]. An array of 1D quantum gas is obtained by tightly confining the particle motion in two directions to zero point oscillations [15] realized by means of two-dimensional optical lattice potentials. By loading BECs in the optical lattice or changing the trap intensities, and hence the atomic interaction strength, the atoms can be made to act either like a condensate or like a TG gas [16,17]. The important parameter characterizing the different physical regimes of the 1D quantum gas is  $\gamma = mg/\hbar^2 \rho$ , the ratio of the interaction constant, m is the mass of the atom, and  $\rho$  is the density.

Let us consider a repulsively interacting spin-1 Bose condensate trapped by a harmonic potential that does not depend on the atomic internal states  $V(\mathbf{r}) = \frac{m}{2}[\omega_x^2 x^2 + \omega_{\perp}^2(y^2 + z^2)]$ , where *m* is the mass of each boson,  $\omega_x$  is the trapping frequency along the *x* (radial) direction, and  $\omega_y = \omega_z \equiv \omega_{\perp}$  is the trapping frequency along the *y* and *z* (transverse) directions. Assuming the radial confinement  $(\hbar\omega_x)$  much weaker than the transversal one  $(\hbar\omega_{\perp})$  leads to a 1D configuration, in which the motion of the atoms

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is frozen along the transverse directions. In such a situation, the external potential that contributes to the atomic motion reads  $V(x) = \frac{m}{2}\omega_x^2 x^2$ . In second quantization language, the Hamiltonian of our system may be expressed as

$$\mathcal{H} = H_0 + H_{int} + H_{spin} \tag{1}$$

with

$$H_0 = \int dx \hat{\Psi}_i^{\dagger} \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \hat{\Psi}_i,$$
  
$$H_{int} = \frac{c_0}{2} \int dx : \left( \hat{\Psi}_i^{\dagger} \hat{\Psi}_i \right)^2 :,$$

where we are assuming that the interaction between bosons is described by a contact two-body potential, which may be described by a Dirac-delta function. Finally,

$$H_{spin} = \frac{c_2}{2} \int dx \hat{\Psi}_k^{\dagger} \hat{\Psi}_i^{\dagger} [(F_z)_{ij} (F_z)_{kl} + \Delta \left( (F_x)_{ij} (F_x)_{kl} + (F_y)_{ij} (F_y)_{kl} \right)] \hat{\Psi}_j \hat{\Psi}_l$$

describes the spin-spin interaction. In  $H_{spin}$ , the anisotropy parameter  $\Delta$  is introduced phenomenologically to describe the anisotropy of spin-spin interaction, which may arise from the anisotropic magnetic dipole-dipole interaction, whereas  $\Delta = 1$  corresponds to the isotropic model. When  $c_2 < 0$  the system is in a ferromagnetic regime, while for  $c_2 > 0$ , the system is anti-ferromagnetic. We limit our discussion on  $0 \leq \Delta \leq 1$  because only in this regime the phase separation may take place [18]. Here  $\hat{\Psi}_i(x)$   $(\hat{\Psi}_i^{\dagger}(x))$  is the field operator that annihilates (creates) an atom in the ith internal state at location x, i = +, 0, - denotes the atomic hyperfine state  $|F=1, m_F=+1, 0, -1\rangle$ , respectively. Summation is assumed for repeated indices in the above Hamiltonian and the pair of colons denote the normal-order product.  $F_x$ ,  $F_y$ and  $F_z$  are the spin-1 matrices with the quantization axis taken along the z-axis direction. The atomic interaction constants are expressed through the effective 1D interac-tion strength  $U_{0,2}$  with  $c_0 = \frac{U_0 + 2U_2}{3}$  and  $c_2 = \frac{U_2 - U_0}{3}$ , where  $U_{0,2}$  have the following relation

$$U_{0,2} = -\frac{2\hbar^2}{ma_{0,2}^{1D}},$$

$$a_{0,2}^{1D} = -\frac{d_{\perp}^2}{2a_{0,2}} \left(1 - \mathcal{C}\left(a_{0,2}/d_{\perp}\right)\right).$$
(2)

Here  $a_{0,2}$  denotes the *s*-wave scattering lengths between two identical spin-1 bosons in the combined symmetric channel of total spin 0(2) when the cold atoms are trapped intensively in transverse direction with the transverse trapping frequency  $\hbar\omega_{\perp}$  [10,19–21],  $d_{\perp} = \sqrt{\hbar/m\omega_{\perp}}$ and  $C \approx 1.4603$ .

In order to deal with the weakly and strongly interacting regimes on the same footing, we work in a scheme of modified Gross-Pitaevskii theory [10,22–24] in which the energy density  $\epsilon$  ( $\rho$ ) is taken from the exactly solvable problem of a three-component Bose gas [10]. It follows that the properties of a spinor gas are determined by the following spin-dependent energy functional

$$\mathcal{E} = \int dx \left[ \Phi_i^* \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \Phi_i + \rho \epsilon(\rho) \right] + \int dx \frac{c_2}{2} \Phi_k^* \Phi_i^* [(F_z)_{ij} (F_z)_{kl} + \Delta \left( (F_x)_{ij} (F_x)_{kl} + (F_y)_{ij} (F_y)_{kl} \right) ] \Phi_j \Phi_l, \qquad (3)$$

where  $\rho = \sum_{i} \rho_{i} = \sum_{i} |\Phi_{i}|^{2}$  and the energy density [23, 25, 26]

$$\epsilon\left(\rho\right) = \frac{\hbar^2}{2m} \rho e\left(\gamma\right) = \begin{cases} c_0 \rho/2, \, \gamma \ll 1\\ \pi^2 \hbar^2 \rho^2/6m, \, \gamma \gg 1 \end{cases} .$$
(4)

The first line of energy functional (3) is made up of three contributions: the first one derives from the usual kinetic energy operator, the second one represents the additional term related to the inhomogeneity due to the external confinement V(x) [27], and the last one corresponds to the energy density in the homogeneous system. In the second and third lines, the contribution deriving from spinspin interaction is involved; in particular, the term in the square brackets has the explicit form

$$\Delta \left( 2\rho_0 \rho_- + 2\rho_+ \rho_0 + 2\Phi_0^{*2} \Phi_+ \Phi_- + 2\Phi_0^2 \Phi_-^* \Phi_+^* \right) + \rho_+^2 + \rho_-^2 - 2\rho_+ \rho_-.$$
(5)

At this point, we stress that, generally, the spin-spin interaction coupling  $(c_2)$  constant is much smaller than the *s*-wave interaction one  $(c_0)$ , i.e.  $c_2 \ll c_0$ . If we assume that there is no spin-spin interaction  $(c_2 = 0)$  and no external trapping (V(x) = 0), then the system described by Hamiltonian (1) is integrable [26]; its ground-state energy density has the same form as that of Lieb-Liniger problem [25].

In the system both the total atom number and the magnetization  $\mathcal{M} = \int dx \langle F \rangle = \int dx \left[ \Phi_+^* \Phi_+ - \Phi_-^* \Phi_- \right]$  are conserved [9,28]. In order to obtain the ground state from a global minimization of  $\mathcal{E}$  with the constraints on both N and  $\mathcal{M}$ , we introduce separately Lagrange multiplier B to conserve M and the chemical potential  $\mu$  to conserve N. The ground state is then determined by a minimization of the free-energy functional  $\mathcal{F} = \mathcal{E} - \mu N - B\mathcal{M}$ . The dynamics of  $\Phi_i$  is governed by the coupled GPEs

$$i\hbar \frac{\partial \Phi_{+}}{\partial t} = [H - B + c_{2} (\rho_{+} + \Delta \rho_{0} - \rho_{-})] \Phi_{+} + c_{2} \Delta \Phi_{0}^{2} \Phi_{-}^{*},$$
  

$$i\hbar \frac{\partial \Phi_{0}}{\partial t} = [H + c_{2} (\rho_{+} + \rho_{-})] \Phi_{0} + 2c_{2} \Delta \Phi_{+} \Phi_{-} \Phi_{0}^{*},$$
  

$$i\hbar \frac{\partial \Phi_{-}}{\partial t} = [H + B + c_{2} (\rho_{-} + \Delta \rho_{0} - \rho_{+})] \Phi_{-} + c_{2} \Delta \Phi_{0}^{2} \Phi_{+}^{*},$$
  
(6)

with

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) + \tilde{F}(\rho)$$
(7)



and

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$$\tilde{F}(\rho) = \frac{\partial}{\partial \rho} \left[ \rho \epsilon \left( \rho \right) \right] = \begin{cases} c_0 \rho, \quad \gamma \ll 1\\ \pi^2 \hbar^2 \rho^2 / 2m, \, \gamma \gg 1 \end{cases} .$$
(8)

We obtain the ground state of spin-1 BECs by propagating the coupled GPEs equation (6) in imaginary time. In each propagating step, the wave function  $\Phi_i$  is normalized to conserve the atomic number and by adjusting the Lagrange multiplier *B* the conservation of magnetization  $\mathcal{M}$  is assured. In our procedure the Crank-Nicholson scheme is used. We will determine the ground state for the 1D spinor Bose gases trapped in the harmonic trap  $V(x) = \frac{1}{2}m\omega_x^2 x^2$  both in the weakly interacting regime and in the TG regime.

To investigate the effect of an isotropy parameter  $\Delta$ . we evaluate the density profile of the ground state of 1D spinor gases for the <sup>87</sup>Rb (ferromagnetic) with  $a_0 = 102a_B$ and  $a_2 = 100 a_B$  ( $a_B$  is the Bohr radius) in the harmonic trap for different anisotropy parameters. By properly tuning the parameters, the system may be either in the weakly interacting regime or in the TG regime. Let us first consider the specific system with the typical parameters of the trap  $\omega_x = 0.5$  kHz,  $\omega_{\perp} = 50$  kHz and the atomic number N = 2000, in which case the effective interaction strength  $\gamma \sim 0.008$  indicating that the system is in the weakly interacting regime. Figure 1 displays the density profiles in unites of N/a with  $a = \sqrt{\hbar/m\omega_x}$  for different anisotropy parameter  $\varDelta$  in the weakly interaction regime with  $m = \frac{M}{N} = 0.2$ . When the spin-spin interaction is isotropic, i.e.  $\Delta = 1.0$ , the three different components superpose each other and they have similar distributions. In the case of weak anisotropy, for instance  $\Delta = 0.9$  here, the distribution has changed explicitly. Therefore the ground state configurations have positive magnetization in some region but negative in another. Also the 0 component (dashed line) diminishes as the anisotropy increases. As the anisotropy becomes more and more clear, the components tend to separate and coincide only at the boundary between them. The components always try to avoid

Fig. 1. The density profile of ground state of a spin-1 <sup>87</sup>Rb condensates for the + (solid line) component, 0 (dashed line) component and - (dash-dot lines) component in the weakly interaction regime with m = 0.2. (a)  $\Delta = 1.0$ ; (b)  $\Delta = 0.9$ ; (c)  $\Delta = 0.8$ ; (d)  $\Delta = 0.5$ ; (e)  $\Delta = 0.2$ ; (f)  $\Delta = 0.0$ . In this figure the length is in the unit of  $a = 1.2 \,\mu$ m.

each other. It is shown that when  $\Delta = 0.2$  the 0 component disappears completely and the density profiles of + component (solid line) and – component (dash-dot lines) exhibit in the form of phase separation. The corresponding density profiles in the TG regime are plotted in Figure 2 with m = 0.2. In this regime the parameters are tuned to  $\omega_x = 10$  Hz,  $\omega_{\perp} = 500$  kHz, the atomic number N = 50 and the effective interaction strength  $\gamma \sim 15$ . In this case, the similar density distributions occur. Comparing the Figure 1a and the Figure 2a we see that the density profiles in the TG regime behave like that of Fermions. According to Figure 2b, with the very weak anisotropy, obvious phase separation has occurred in the Tonks regime. Figure 3 displays the density profiles for different magnetization but with the same anisotropy parameter, which indicates that the magnetization only influences on the ratio of the atomic numbers between the + component and – component. It turns out that although the spinspin interaction is much small, its property affects greatly the density distribution of each component of the spinor gas and the phase separation occurs more easily in the TG regime than in the weakly interacting regime. The 1D spinor gas in the TG regime might provide us a good platform to investigate the magnetism of the cold atoms.

For further studying the effect of anisotropy on the anti-ferromagnetic system, we consider a condensate of <sup>23</sup>Na in the weakly interacting regime with  $a_0 = 50a_B$  and  $a_2 = 55.1a_B$ . The trap frequencies are chosen as  $\omega_x = 50$  Hz,  $\omega_\perp = 10$  kHz and N = 1000 so that  $\gamma \sim 0.001$ . The density profiles are shown in Figure 4 with m = 0.2 for anisotropic and isotropic case. It is shown that no phase separation occurs even for very large anisotropy and the same distribution as the case of isotropic spin-spin interaction displays [10]. From the above results, it is obvious that the density distributions of every component strongly depends on its' anisotropy and the ferromagnetic or the anti-ferromagnetic properties of the relatively weak spin interactions, whereas the total density is almost not affected by the weak spin interactions.

0.00



Fig. 4. The density profile of ground state of a spin-1 <sup>23</sup>Na condensates for the + (solid line) component, 0 (dashed line) component and – (dash-dot lines) component in the weakly interaction regime with m = 0.2. (a)  $\Delta = 0.5$ ; (b)  $\Delta = 1.0$ . In this figure the length is in the unit of  $a = 7.4 \,\mu\text{m}$ .

8

6

0.00

C

6

4 X

Finally, we discuss the possible experimental realization of anisotropic spin interaction in spinor gases. It is well known that magnetic dipolar interactions are anisotropic despite the fact that dipolar interactions are rather weak comparing to the spin interactions. The relative strength of the dipolar and the spin exchange interactions is estimated to be  $10^{-1}$  for <sup>87</sup>Rb and  $10^{-3}$ for <sup>23</sup>Na [29]. Since the magnetic dipole-dipole interaction is irrelevant to the *s*-wave scattering length, we may tune the *s*-wave scattering length experimentally by the Feshbach resonance so that the strength of isotropic spinspin interaction  $c_2$  is comparable to that of dipole-dipole interaction, and thus the anisotropic interaction becomes

Fig. 2. The density profile of ground state of a spin-1 <sup>87</sup>Rb condensates for the + (solid line) component, 0 (dashed line) component and – (dash-dot lines) component in the Tonks regime with m = 0.2. (a)  $\Delta = 1.0$ ; (b)  $\Delta = 0.9$ ; (c)  $\Delta = 0.8$ ; (d)  $\Delta = 0.5$ ; (e)  $\Delta = 0.2$ ; (f)  $\Delta = 0.0$ . In this figure the length is in the unit of  $a = 8.5 \,\mu$ m.

Fig. 3. The density profile of ground state of a spin-1 <sup>87</sup>Rb condensates for the + (solid line) component, 0 (dashed line) component and – (dash-dot lines) component in the weakly interaction regime with  $\Delta = 0.2$ . (a) m = 0.0; (b) m = 0.5; (c) m = 0.8. In this figure the length is in the unit of  $a = 1.2 \,\mu$ m.

obvious. Although a condensate of strongly anisotropic spinor gases remains to be realized, experimentalists in reference [30] have already successfully demonstrated the effect of the dipole-dipole interaction. With the present rapid development in the experimental manipulation of cold atoms, the goal of making a condensate of spinor gases with anisotropic spin interaction does not seem to be far-fetched. It is worth indicating that our approach can be directly applied to deal with the three-dimensional (3D) problem for which the mean-field theory corresponds to our weakly interacting theory. It follows that a 3D spinor gas with anisotropic spin interactions also displays phase separation. However, the result for the strongly interacting regime can not be extended to the higher-dimensional case in which no TG gas can be realized. Our work is helpful to understand the properties of the spinor condensates and deepen our understanding of formation of spin domains in spinor gases.

In summary, we have studied the density profile of the ground states of 1D spin-1 Bose gases for different anisotropy parameter  $\Delta$ . The distributions of the ferromagnetic spinor gas are affected tremendously by  $\Delta$  although the  $c_2$  term is very small compared with  $c_0$  term in equation (1). Even if the anisotropy is weak, the distributions show obvious difference from that of the isotropic case. In the large anisotropy the component of  $m_F = 0$  disappears and obvious phase separation occurs both in the weakly interaction regime and in the Tonks regime. And the effect of anisotropy in the TG regime can display more obviously with weaker anisotropy than the former case. However, when the spinor gas is anti-ferromagnetic, the distribution is no longer being affected by the anisotropy parameter.

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