

# Interspecies singlet pairing in a mixture of two spin-1 Bose condensates

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We study the ground-state properties of a mixture formed by two spin-1 condensates in the absence of an external magnetic field. As the collisional symmetry between interspecies bosonic atoms is broken, the interspecies coupling interaction ( $\beta$ ) and interspecies singlet-pairing interaction ( $\gamma$ ) arise. The ground state can be calculated using the angular momentum theory analytically for  $\gamma = 0$ . The full quantum approach of exact diagonalization is adopted numerically to consider the more general case as  $\gamma \neq 0$ . We illustrate the competition between the two interspecies interactions and find that as singlet-pairing interaction dominates (or the total spin vanishes), there are still different types of singlet formations which are well determined by  $\beta$ .

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## I. INTRODUCTION

Since the MIT group succeeded in trapping a  $^{23}\text{Na}$  condensate in an optical potential [1], the spin degrees of freedom are liberated, that give rise to a rich variety phenomena [2] such as spin domains [3], textures [4], spin mixing dynamics [5–7], and fragmentation of condensate [8,10]. The properties of such a three-component spinor condensate were first studied using mean-field theories (MFT) [4,9] and polar and ferromagnetic spinor condensates had been implemented experimentally [11,12]. It was initially predicted that the ground state of  $^{23}\text{Na}$  BEC ( $c_2 > 0$ ) is either polar ( $n_0 = N$ ) or antiferromagnetic ( $n_1 = n_{-1} = N/2$ ) in the mean-field theory. However, the results from many-body theory [5] pointed out that the ground state of  $^{23}\text{Na}$  atoms is a spin singlet with properties drastically different from those of mean-field theories ( $n_1 = n_0 = n_{-1} = N/3$ ). It was shown [8] that the singlet ground state in the zero field is a fragmented condensate with anomalously large number fluctuations ( $\Delta n_\alpha \sim N$ ) and thus has fragile stability. The exact quantum eigenstates in the spin-2 case [13,14] are also found and their magnetic response to a weak magnetic field is compared with their mean-field counterpart [15].

Mixtures of scalar condensates with more than one atomic species or state are actively studied theoretically [16–19]. Experimentally, the Feshbach resonance has exploited to create a double-species condensate with tunable interactions and the dynamics of the superfluid and controllable phase separation are observed [20–23]. By adjusting the two  $s$ -wave scattering lengths  $a_0$  and  $a_2$  through the so-called optical Feshbach resonances [24], the spin-exchange interaction between individual atoms can be precisely tuned. The theoretical studies on mixtures of spinor condensates attracted much attention recently and both mean-field and quantum many-body theories have been applied to this novel system [25–29]. A temporal modulation of spin-exchange interaction, which is tunable with optical Feshbach resonance, was recently proposed to localize the spin mixing dynamics in a  $^{87}\text{Rb}$  condensate [30].

The interspecies scattering parameters between  $^{87}\text{Rb}$  and  $^{23}\text{Na}$  are calculated resorting to the simple approach of the degenerate internal-state approximation (DIA) [31–33] as the low-energy atomic interactions can be mostly attributed

to the ground-state configurations of the two valence electrons. The interspecies scattering lengths for singlet and triplet electronic states are approximately determined already [32,33], given by  $a_S = 109a_0$  and  $a_T = 70a_0$ , where  $a_0$  is the Bohr radius. The interspecies interactions between  $^{87}\text{Rb}$  and  $^{23}\text{Na}$  atoms are then parametrized by three scattering lengths [see Eq. (1) below], each being a linear combination of  $a_S$  and  $a_T$  weighted by the appropriate  $9j$  coefficients for the total combined spins of  $F = 0, 1$ , and  $2$ . Within this approximation, it is found coincidentally that, the parameter for the interspecies singlet-pairing interaction  $\gamma$ , is equal to zero [29].

However, for the more general case of an arbitrary mixture of spin-1 condensate, the hyperfine interaction between nuclear spin and electron spin gives in general non-negligible interspecies pairing and DIA approximation is not applicable [29,31–33]. In this paper, we first study the various quantum phases of the binary mixture of spin-1 condensates in the ground state ignoring the interspecies singlet pairing. Then the situation with competition between intra- and interspecies singlet pairings is considered. Using the full quantum approach of exact diagonalization, we present the detailed phases diagram for the  $\gamma \neq 0$  case.

## II. THE HAMILTONIAN

We take the intracondensate atomic interaction in the form  $V_j(\mathbf{r}) = (\alpha_j + \beta_j \mathbf{F}_j \cdot \mathbf{F}_j) \delta(\mathbf{r})$  with  $j = 1, 2$  for the two species and the interspecies interaction is described as

$$V_{12}(\mathbf{r}) = \frac{1}{2} (g_0^{(12)} P_0 + g_1^{(12)} P_1 + g_2^{(12)} P_2) \delta(\mathbf{r}). \quad (1)$$

In contrast to intracondensate interactions between identical atoms [25,29], the collision between atoms belonging to different species can occur in the total spin  $F = 1$  channel, which makes the mixture more interesting. Here,

$$g_{0,1,2}^{(12)} = 4\pi \hbar^2 a_{0,1,2}^{(12)} / \mu, \quad (2)$$

where  $a_0^{(12)}, a_1^{(12)}, a_2^{(12)}$  are the scattering lengths in the channels of total spin  $F = 0, 1$ , and  $2$ , respectively, and  $\mu = M_1 M_2 / (M_1 + M_2)$  denotes the reduced mass for the pair of atoms, one each from the two different species with masses  $M_1$  and  $M_2$ , respectively.  $P_0, P_1, P_2$  is the corresponding

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projection operator with the relationship  $1 = P_2 + P_1 + P_0$  and  $\mathbf{F}_1 \cdot \mathbf{F}_2 = P_2 - P_1 - 2P_0$ , from which we get

$$V_{12}(\mathbf{r}) = \frac{1}{2}(\alpha + \beta \mathbf{F}_1 \cdot \mathbf{F}_2 + \gamma P_0)\delta(\mathbf{r}), \quad (3)$$

with the parameters  $\alpha = (g_1^{(12)} + g_2^{(12)})/2$ ,  $\beta = (-g_1^{(12)} + g_2^{(12)})/2$  and  $\gamma = (2g_0^{(12)} - 3g_1^{(12)} + g_2^{(12)})/2$ .  $P_0$  projects an interspecies pair into a spin singlet state [25]. Furthermore, these parameters can be related to the singlet and triplet scattering lengths by means of a method based on the 9j coefficient [29],

$$\begin{aligned} \alpha &= \frac{\pi \hbar^2}{\mu}(3a_T + a_S), \\ \beta &= \frac{\pi \hbar^2}{4\mu}(a_T - a_S), \\ \gamma &= 0. \end{aligned} \quad (4)$$

Denote the atomic field operators for the spin state  $|1, i\rangle$  as  $\hat{\Psi}_i$  for species 1 and  $\hat{\Phi}_i$  for species 2; the Hamiltonian for the mixture system in the second quantization is represented by

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{12}, \quad (5)$$

$$\begin{aligned} \hat{H}_1 &= \int d\mathbf{r} \left\{ \hat{\Psi}_i^\dagger \left( \frac{\hbar^2}{2M_1} \nabla^2 + U_1 \right) \hat{\Psi}_i + \frac{\alpha_1}{2} \hat{\Psi}_i^\dagger \hat{\Psi}_j^\dagger \hat{\Psi}_j \hat{\Psi}_i \right. \\ &\quad \left. + \frac{\beta_1}{2} \hat{\Psi}_i^\dagger \hat{\Psi}_j^\dagger \mathbf{F}_{1il} \cdot \mathbf{F}_{1jk} \hat{\Psi}_k \hat{\Psi}_l \right\}, \\ \hat{H}_{12} &= \frac{1}{2} \int d\mathbf{r} \left\{ \alpha \hat{\Psi}_i^\dagger \hat{\Phi}_j^\dagger \hat{\Phi}_j \hat{\Psi}_i \right. \\ &\quad \left. + \beta \hat{\Psi}_i^\dagger \hat{\Phi}_j^\dagger \mathbf{F}_{1il} \cdot \mathbf{F}_{2jk} \hat{\Phi}_k \hat{\Psi}_l + \frac{\gamma}{3} \hat{O}^\dagger \hat{O} \right\}. \end{aligned} \quad (6)$$

$H_2$  is the same as  $H_1$  with the substitution of subscript 1 by 2 and  $\hat{\Psi}_i$  by  $\hat{\Phi}_i$  and  $\hat{O} = \hat{\Psi}_1 \hat{\Phi}_{-1} - \hat{\Psi}_0 \hat{\Phi}_0 + \hat{\Psi}_{-1} \hat{\Phi}_1$ .

Through the control of the trapping frequency, we can make the two species sufficiently overlapped and adopt the single spatial-mode approximation (SMA) [5,6,34] for each of the two spinor condensates with modes  $\Psi(\mathbf{r})$  and  $\Phi(\mathbf{r})$ , that is,

$$\hat{\Psi}_i = \hat{a}_i \Psi, \quad \hat{\Phi}_i = \hat{b}_i \Phi, \quad (7)$$

with  $\hat{a}_i$  ( $\hat{b}_i$ ) the annihilation operator for the ferromagnetic (polar) atoms satisfying  $[\hat{a}_i, \hat{a}_j] = 0$  and  $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$  (and the same form of commutations for  $\hat{b}_i$ ). The density-density interaction part is a constant. Hence we only focus on the spin-dependent Hamiltonian,

$$\begin{aligned} \hat{H} &= \frac{c_1 \beta_1}{2} (\hat{\mathbf{F}}_1^2 - 2\hat{N}_1) + \frac{c_2 \beta_2}{2} (\hat{\mathbf{F}}_2^2 - 2\hat{N}_2) \\ &\quad + \frac{c_{12} \beta}{2} \hat{\mathbf{F}}_1 \cdot \hat{\mathbf{F}}_2 + \frac{c_{12} \gamma}{6} \hat{\Theta}_{12}^\dagger \hat{\Theta}_{12}, \end{aligned} \quad (8)$$

with  $\hat{\mathbf{F}}_1 = \hat{a}_i^\dagger \mathbf{F}_{1ij} \hat{a}_j$  ( $\hat{\mathbf{F}}_2 = \hat{b}_i^\dagger \mathbf{F}_{2ij} \hat{b}_j$ ) defined in terms of the  $3 \times 3$  spin-1 matrices  $\mathbf{F}_{1ij}$  ( $\mathbf{F}_{2ij}$ ). The operator,

$$\hat{\Theta}_{12}^\dagger = \hat{a}_0^\dagger \hat{b}_0^\dagger - \hat{a}_1^\dagger \hat{b}_{-1}^\dagger - \hat{a}_{-1}^\dagger \hat{b}_1^\dagger, \quad (9)$$

creates a singlet pair with one atom each from the two species, in much the same way that the operators,

$$\hat{A}^\dagger = (\hat{a}_0^\dagger)^2 - 2\hat{a}_1^\dagger \hat{a}_{-1}^\dagger, \quad \hat{B}^\dagger = (\hat{b}_0^\dagger)^2 - 2\hat{b}_1^\dagger \hat{b}_{-1}^\dagger, \quad (10)$$

create pairs with two atoms from the same species [8,13]. The interaction coefficients are  $c_1 = \int d\mathbf{r} |\Psi(r)|^4$ ,  $c_2 = \int d\mathbf{r} |\Phi(r)|^4$ , and  $c_{12} = \int d\mathbf{r} |\Psi(r)|^2 |\Phi(r)|^2$ .

In the following we perform all analysis in the single-mode regime in the absence of external fields. As learned from previous studies [34], SMA is shown to be exact for atomic interaction of the ferromagnetic type. For polar interaction, if the magnetization  $M = 0$ , the SMA wave function is still exact and becomes invalid only if  $M$  is large. In our mixture, we can safely apply the SMA to the wave function of both polar and ferromagnetic atoms in the absence of an external magnetic field. The ground state for polar atoms is a fragile fragmented state with  $M = 0$ . Small external fields or spatial dependence drive the system to symmetry broken states which are better captured by mean-field theory. Very recently the symmetry broken phase has been found in this binary mixture in the presence of a weak magnetic field [28].

In our previous study [27] we report the anomalous fluctuations for the numbers of atoms in the mixture of  $^{23}\text{Na}$  (polar) and  $^{87}\text{Rb}$  (ferromagnetic) condensates in their  $F = 1$  manifold. DIA has been adopted to ignore the  $\gamma$  term. The ferromagnetic  $^{87}\text{Rb}$  condensate provides a smooth background where the quantum many-body states are hardly affected by the fluctuation, while the fragile polar atoms  $^{23}\text{Na}$  are easier influenced. Especially in the ground state of the AA phase, the interspecies antiferromagnetic spin exchange is large enough to polarize both species and a maximally entangled state is realized between two species with total spin  $F = 0$ .

### III. THE SITUATION OF $\gamma = 0$

In this section, we consider the simple situation of  $\gamma = 0$  with the Hamiltonian,

$$\hat{H}_A = \frac{c_1 \beta_1}{2} \hat{\mathbf{F}}_1^2 + \frac{c_2 \beta_2}{2} \hat{\mathbf{F}}_2^2 + \frac{c_{12} \beta}{2} \hat{\mathbf{F}}_1 \cdot \hat{\mathbf{F}}_2. \quad (11)$$

or in an alternative form,

$$\hat{H} = a \hat{\mathbf{F}}_1^2 + b \hat{\mathbf{F}}_2^2 + c \hat{\mathbf{F}}^2, \quad (12)$$

where  $a = c_1 \beta_1 / 2 - c_{12} \beta / 4$ ,  $b = c_2 \beta_2 / 2 - c_{12} \beta / 4$ ,  $c = c_{12} \beta / 4$ , and  $\hat{\mathbf{F}} = \hat{\mathbf{F}}_1 + \hat{\mathbf{F}}_2$  is the total angular momentum operator. A constant energy shift of  $c_j \beta_j N_j$  has been trivially eliminated. The results may serve as reference states for the complete ground-state phases.

The eigenstates of the Hamiltonian (12) are then simply the common eigenstates of the commutative operators  $\hat{\mathbf{F}}_1^2$ ,  $\hat{\mathbf{F}}_2^2$ ,  $\hat{\mathbf{F}}^2$ , and  $\hat{F}_z$ , denoted by

$$|F_1, F_2, F, m\rangle = \sum_{m_1 m_2} C_{F_1, m_1; F_2, m_2}^{F, m} |F_1, m_1\rangle |F_2, m_2\rangle, \quad (13)$$

where the states in uncoupled representation,

$$\begin{aligned} |F_1, m_1\rangle &= Z_1^{-\frac{1}{2}} (\hat{F}_{1-})^{F_1 - m_1} (\hat{a}_1^\dagger)^{F_1} (\hat{A}^\dagger)^{(N_1 - F_1)/2} |0\rangle, \\ |F_2, m_2\rangle &= Z_2^{-\frac{1}{2}} (\hat{F}_{2-})^{F_2 - m_2} (\hat{b}_1^\dagger)^{F_2} (\hat{B}^\dagger)^{(N_2 - F_2)/2} |0\rangle, \end{aligned}$$

span a Hilbert space of dimension  $(N_{1,2} + 1)(N_{1,2} + 2)/2$ , respectively [13]. Here  $C$ 's are the Clebsch-Gordon coefficients,  $Z_{1,2}$  are the normalization constants, and  $\hat{F}_{1-}$  ( $\hat{F}_{2-}$ ) is the

lowering operator for  $m_1(m_2)$ . Minimizing the corresponding eigenenergies of the Hamiltonian,

$$E = aF_1(F_1 + 1) + bF_2(F_2 + 1) + cF(F + 1), \quad (14)$$

we can get the ground-state energy determined by different parameters  $c_1\beta_1$ ,  $c_2\beta_2$ , and  $c_{12}\beta$ . In Fig. 1, using the full quantum approach of exact diagonalization we calculate ground-state order parameters  $\langle \hat{F}_1^2 \rangle$ ,  $\langle \hat{F}_2^2 \rangle$ , and  $\langle \hat{F}_1 \cdot \hat{F}_2 \rangle$  to illustrate the different phases as  $c_{12}\beta$  changes. The results are presented for three typical cases (a)  $c_1\beta_1 = -1, c_2\beta_2 = -2$ , (b)  $c_1\beta_1 = 1, c_2\beta_2 = 2$ , and (c)  $c_1\beta_1 = -1, c_2\beta_2 = 2$  with equal atomic numbers in two species (i.e.,  $N_1 = N_2 = N = 100$ ). We see that the results agree fairly well with the simulated annealing approach in the mean-field theory [25] except for some small deviations originated from pure quantum effect. For instance, the maximum and minimum values are  $N(N + 1) = 10100$  and 0 for  $\langle \hat{F}_1^2 \rangle$  and  $\langle \hat{F}_2^2 \rangle$ , but they are  $N^2 = 10000$  and  $-N(N + 1) = -10100$  for  $\langle \hat{F}_1 \cdot \hat{F}_2 \rangle$ .

### A. The case $c_1\beta_1 < 0, c_2\beta_2 < 0$

For the mixture of two ferromagnetic condensates, there are generally two phases FF and AA separated by the critical point 0 as shown in Fig. 1(a). The FF phase is described by a set of degenerate states generated by repeatedly applying

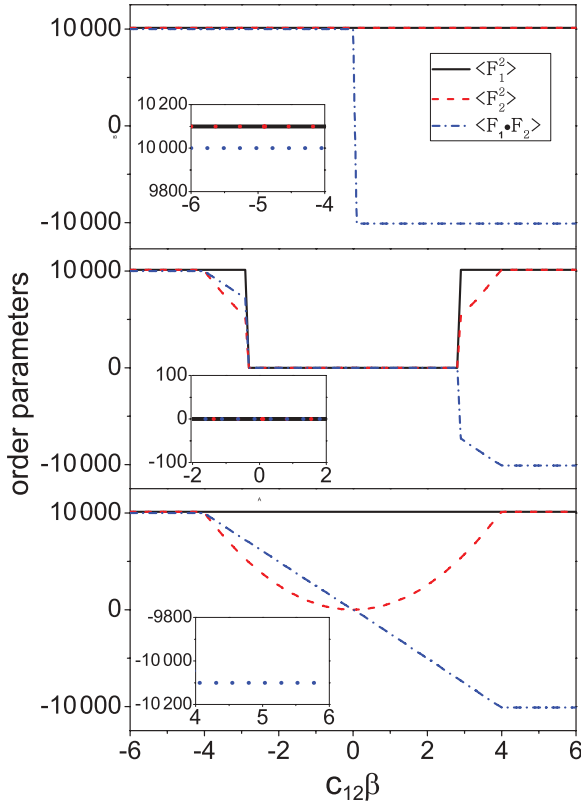


FIG. 1. (Color online) The dependence of ground-state order parameters on  $c_{12}\beta$  at fixed values of (a)  $c_1\beta_1 = -1, c_2\beta_2 = -2$ ; (b)  $c_1\beta_1 = 1, c_2\beta_2 = 2$ ; (c)  $c_1\beta_1 = -1, c_2\beta_2 = 2$ ; and  $c_{12}\beta = 0$  (all in units of  $|c_1\beta_1|$ ). Black solid lines, red dashed lines, and blue dot-dashed lines denote, respectively, the order parameters  $\langle \hat{F}_1^2 \rangle$ ,  $\langle \hat{F}_2^2 \rangle$ , and  $\langle \hat{F}_1 \cdot \hat{F}_2 \rangle$ .

the lowering operators  $(\hat{F}_{1-} + \hat{F}_{2-})$  on the extreme states for  $(F - m)$  times,

$$|F_1, F_2, F, m\rangle = (\hat{F}_{1-} + \hat{F}_{2-})^{F-m} |F_1, F_2, F, F\rangle, \quad (15)$$

with  $m = 0, \pm 1, \dots, \pm F$ . The extreme states,

$$|F_1, F_2, F, F\rangle = C_{N,N;N,N}^{2N,2N} |N, N\rangle |N, N\rangle, \quad (16)$$

can be simply described as  $Z^{1/2}(\hat{a}_1^\dagger)^N(\hat{b}_1^\dagger)^N|0\rangle$ . The AA phase is a singlet  $|N, N, 0, 0\rangle$  with all states obeying the condition  $m_1 + m_2 = 0$ . All channels of total spin zero have to be taken into account and we have

$$|N, N, 0, 0\rangle = \sum_{m_1=-N}^N C_{N,m_1;N,-m_1}^{0,0} |N, m_1\rangle |N, -m_1\rangle. \quad (17)$$

### B. The case $c_1\beta_1 > 0, c_2\beta_2 > 0$

The mixture of two polar condensates allows for five distinct phases FF, MM<sub>-</sub>, PP, MM<sub>+</sub>, and AA separated by four critical points  $-(2N - 1)c_2\beta_2/N$ ,  $-c_1\beta_1 - c_2\beta_2$ ,  $c_1\beta_1 + c_2\beta_2$  and  $(2N - 1)c_2\beta_2/(N + 1)$  corresponding to  $c_{12}\beta \simeq -4, -3, 3$ , and 4 in Fig. 1(b).

In the region  $c_{12}\beta \in [-(2N - 1)c_2\beta_2/N, -c_1\beta_1 - c_2\beta_2]$ , the MM<sub>-</sub> phase takes the same form as Eq. (15), with extreme states represented by

$$|F_1, F_2, F, F\rangle = C_{N,N;F_2,F_2}^{N+F_2,N+F_2} |N, N\rangle |F_2, F_2\rangle, \quad (18)$$

or  $Z^{1/2}(\hat{a}_1^\dagger)^N(\hat{b}_1^\dagger)^{F_2}(\hat{B}^\dagger)^{(N-F_2)/2}|0\rangle$ . In the MM<sub>-</sub> phase the atoms in species 1 are totally polarized in one direction and form a “steady magnetic field” (black solid line), and those in species 2 are partially polarized in the same direction. Increasing the strength of the coupling interaction ( $|c_{12}\beta|$ ) breaks singlet pairs in species 2 one by one, and results in the increase of the total spin.

In the region  $c_{12}\beta \in (-c_1\beta_1 - c_2\beta_2, c_1\beta_1 + c_2\beta_2)$ , the two species are essentially independent for a weak interspecies spin-exchange interaction. The PP phase is a total spin singlet described by the direct product of the well-known polar ground state  $Z^{-1/2}(\hat{A}^\dagger)^{N/2}(\hat{B}^\dagger)^{N/2}|0\rangle$  [8,13], giving rise to  $\langle \hat{F}_1^2 \rangle = 0$ ,  $\langle \hat{F}_2^2 \rangle = 0$ , and  $\langle \hat{F}_1 \cdot \hat{F}_2 \rangle = 0$ .

In the region of  $c_{12}\beta \in [c_1\beta_1 + c_2\beta_2, (2N - 1)c_2\beta_2/(N + 1)]$ , however, the MM<sub>+</sub> phase favors that the atoms in species 2 are polarizing to the opposite direction of those in species 1 and the total spin gradually decreases. This situation is much more complicated because all states that satisfy the condition  $m_1 + m_2 = N - F_2$  are involved and the summation index runs over all possible Clebsch-Gordon coefficients, giving rise to the following extreme state,

$$|F_1, F_2, F, F\rangle = \sum_{m_1, m_2} C_{N, m_1; F_2, m_2}^{N-F_2, N-F_2} |N, m_1\rangle |F_2, m_2\rangle. \quad (19)$$

### C. The case $c_1\beta_1 < 0, c_2\beta_2 > 0$

In the case of a mixture of a ferromagnetic and a polar condensate, four possible phases FF, MM<sub>-</sub>, MM<sub>+</sub>, and AA are separated by three critical points  $-(2N - 1)c_2\beta_2/N, 0$  and  $(2N - 1)c_2\beta_2/(N + 1)$  corresponding to  $c_{12}\beta = -4, 0, 4$  in Fig. 1(c).

It has been shown that the ground state of polar atoms ( $c_2\beta_2 > 0$ ) only is a fragmented condensate with anomalously large number fluctuations and fragile stability [8], which can be described as  $(\hat{B}^\dagger)^{N/2}|0\rangle$ . The  $\hat{B}^\dagger$  and  $\hat{B}$  are invariant under any rotation of the system, and commute with  $\hat{F}_2$  and  $\hat{F}_{2z}$ . However, for a ferromagnetic condensate ( $c_1\beta_1 < 0$ ) the ground state favors that all atoms are aligned in the same direction [i.e.,  $(\hat{a}_1^\dagger)^N|0\rangle$ ] and much more stable. So when these two kinds of atoms are mixed together, the polar atoms are more easier to be influenced, but their back action on to the stable ferromagnetic atoms is negligible. This can be seen from the constant black solid line in Fig. 1(c).

An interesting observation is that for large and negative (positive) value of parameter  $c_{12}\beta$  the system enters the same phase FF (AA), no matter how the atoms interact inside each species. Detailed calculations show that in the FF phase all atoms are polarized in the same direction and the total spin reaches its maximum value. The ground state is highly degenerate with degeneracy  $2F + 1$ . Take the state  $|F_1, F_2, F, m = 0\rangle$  as an example; the atomic populations are

$$\begin{aligned} \langle n_0^{(j)} \rangle &= \frac{2N^2}{4N - 1}, \\ \langle n_{\pm 1}^{(j)} \rangle &= \frac{N^2 - N/2}{4N - 1}, \end{aligned} \quad (20)$$

which reduces to  $(N/4, N/2, N/4)$  for each species for large  $N$ . The number fluctuations,

$$\begin{aligned} \langle \Delta n_0^{(j)} \rangle &= \frac{2N}{4N - 1} \sqrt{\frac{4N^2 - 9N/2 + 1}{4N - 3}}, \\ \langle \Delta n_{\pm 1}^{(j)} \rangle &= \frac{N/2}{4N - 1} \sqrt{\frac{32N^2 - 34N + 7}{4N - 3}}, \end{aligned} \quad (21)$$

are in order of  $\sqrt{N}$  for large  $N$ . On the other hand, in the AA phase, atoms in species 1 and 2 are fully polarized, however, in opposite directions and the total spin vanishes [27]. The singlet ground state is a fragmented condensate [8,27] and the single-particle density matrix is diagonal with atoms equally populated  $\langle n_{0,\pm 1}^{(j)} \rangle = N/3$  or  $(N/3, N/3, N/3)$  for each species. The fluctuations,

$$\begin{aligned} \langle \Delta n_0^{(j)} \rangle &= \frac{\sqrt{N^2 + 9N}}{3\sqrt{5}}, \\ \langle \Delta n_{\pm 1}^{(j)} \rangle &= \frac{2\sqrt{N^2 + 3N/2}}{3\sqrt{5}}, \end{aligned} \quad (22)$$

are anomalously large (in order of  $N$ ), thus the fragmented condensate is fragile.

#### IV. THE SITUATION OF $\gamma \neq 0$

The last term  $c_{12}\gamma$  in Hamiltonian (8) is related to the interspecies singlet pairing. Although  $[\hat{\mathbf{F}}^2, \hat{\Theta}_{12}^\dagger \hat{\Theta}_{12}] = 0$ , we notice that  $[\hat{\mathbf{F}}_1^2, \hat{\Theta}_{12}^\dagger \hat{\Theta}_{12}] \neq 0$ , and  $[\hat{\mathbf{F}}_2^2, \hat{\Theta}_{12}^\dagger \hat{\Theta}_{12}] \neq 0$ . Thus, in general, they do not belong to a set of commutative operators and the system is not solvable. In the special case of  $c_1\beta_1 = c_2\beta_2 = \frac{1}{2}c_{12}\beta$ , we found that the spin-dependent Hamiltonian reduces to a sum of commutative operators.

The eigenstates can be constructed by several building blocks [13,14,26,35] which can be found via generating function method. To see more clearly the role played by the  $\gamma$  term, we focus on a special case in which  $c_{12}\gamma$  is much larger than the other parts of the Hamiltonian and  $c_1\beta_1 < 0, c_2\beta_2 > 0$ . We know that the  $\gamma$  term encourages pairing two different types of atoms into singlets when  $\gamma < 0$ . In this case the interspecies singlet-pairing interaction dominates the system and the total spin vanishes, namely  $\langle \hat{\mathbf{F}}^2 \rangle = \langle (\hat{\mathbf{F}}_1 + \hat{\mathbf{F}}_2)^2 \rangle = 0$ . There are two typical cases obeying the above condition. In one case we have  $\langle \hat{\mathbf{F}}_1^2 \rangle = 0, \langle \hat{\mathbf{F}}_2^2 \rangle = 0$ , and  $\langle \hat{\mathbf{F}}_1 \cdot \hat{\mathbf{F}}_2 \rangle = 0$ , which means the singlet formation occurs inside each species, and the atoms in the same species are all paired with no net spin left. In the other case we have  $-2\langle \hat{\mathbf{F}}_1 \cdot \hat{\mathbf{F}}_2 \rangle = \langle \hat{\mathbf{F}}_1^2 \rangle + \langle \hat{\mathbf{F}}_2^2 \rangle \neq 0$ , which means some intraspecies pairs are broken, meanwhile singlet formation occurs between different species. Under the condition  $N_1 = N_2 = 100$ , numerical results show that the above two cases indeed exist and are well determined by the parameter  $c_{12}\beta$ .

We consider the direct product of the Fock states of the two species  $|n_1^{(1)}, n_0^{(1)}, n_{-1}^{(1)}\rangle \otimes |n_1^{(2)}, n_0^{(2)}, n_{-1}^{(2)}\rangle$ , which may be equivalently defined as

$$\begin{aligned} \hat{h}_\alpha^{(1,2)} |n_0^{(1)}, m_1, n_0^{(2)}, m_2; m\rangle \\ = n_\alpha^{(1,2)} |n_0^{(1)}, m_1, n_0^{(2)}, m_2; m\rangle. \end{aligned} \quad (23)$$

Here  $m_{1,2}$  are the corresponding magnetization specified as  $m_{1,2} = n_1^{(1,2)} - n_{-1}^{(1,2)}$  and  $m = m_1 + m_2$  is the total magnetization. For simplification, we restrict ourselves into the subspace that the total magnetization is conserved  $m = 0$ , in which case all states are nondegenerate. The Hamiltonian (8) is then represented in a sparse matrix and with the approach of exact diagonalization we numerically get the ground state of the system, on which the order parameters are calculated.

Figure 2 shows the dependence of the four order parameters on  $c_{12}\beta$  at fixed values of  $c_1\beta_1 = -1, c_2\beta_2 = 2$ , and  $c_{12}\gamma = -20$ . We find that in the region of  $c_{12}\beta < 0$ ,  $\langle \hat{\mathbf{F}}_1^2 \rangle, \langle \hat{\mathbf{F}}_2^2 \rangle$ , and  $\langle \hat{\mathbf{F}}_1 \cdot \hat{\mathbf{F}}_2 \rangle$  are all approximately equal to zero, corresponding to the first case of vanishing total spin. However, for positive  $c_{12}\beta$ , atoms in each species begin to polarize and are fully polarized for  $c_{12}\beta \geq 2$ , with the negative value of  $\langle \hat{\mathbf{F}}_1 \cdot \hat{\mathbf{F}}_2 \rangle$  showing that they are polarized to the opposite directions. During the whole process the three order parameters always obey the condition  $-2\langle \hat{\mathbf{F}}_1 \cdot \hat{\mathbf{F}}_2 \rangle = \langle \hat{\mathbf{F}}_1^2 \rangle + \langle \hat{\mathbf{F}}_2^2 \rangle$ . The distinction in the envelope of  $\langle \hat{\mathbf{F}}_1^2 \rangle$  and  $\langle \hat{\mathbf{F}}_2^2 \rangle$  in the region  $0 < c_{12}\beta < 2$  lies in the choice of  $c_1\beta_1 = -1, c_2\beta_2 = 2$ .

The fourth order parameter  $\langle \hat{\Theta}_{12}^\dagger \hat{\Theta}_{12} \rangle / 3$  reflects the feature of the total spin  $F$  of the system. It takes a constant value, which is actually the maximum value, in the entire region of  $c_{12}\beta$  in Fig. 2 (see the green line), while the total spin reaches its minimum value 0. In order to see more clearly the competition between the interspecies coupling and singlet-pairing interactions, in Fig. 3 we illustrate four order parameters for different values of  $c_{12}\gamma$ . An obvious variation can be easily seen from, for example, Fig. 3(d), where the black solid line ( $\gamma = 0$ ) gradually changes to the purple dashed line ( $\gamma = -20$ ). We find that when  $\gamma = 0$  the order parameters  $\langle \hat{\Theta}_{12}^\dagger \hat{\Theta}_{12} \rangle / 3$  become zero in the FF phase, implying that the total spin  $F$  gets to its maximum [Fig. 3(a)], while in the

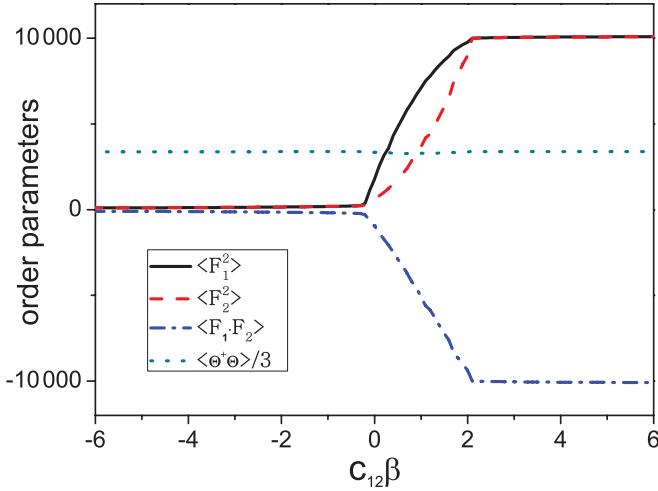


FIG. 2. (Color online) The dependence of ground-state order parameters on  $c_{12}\beta$  at fixed values of  $c_1\beta_1 = -1$ ,  $c_2\beta_2 = 2$ , and  $c_{12}\gamma = -20$  (in the unit of  $|c_1\beta_1|$ ). Black solid lines, red dashed lines, blue dot-dashed lines, and green dotted lines denote, respectively, the order parameters  $\langle \hat{F}_1^2 \rangle$ ,  $\langle \hat{F}_2^2 \rangle$ ,  $\langle \hat{F}_1 \cdot \hat{F}_2 \rangle$ , and  $\langle \hat{\Theta}_{12}^\dagger \hat{\Theta}_{12} \rangle / 3$ .

AA phase it equals to a constant value and the total spin  $F$  vanishes. In between the two limits “0” and “constant,” the intermediate value of the order parameters  $\langle \hat{\Theta}_{12}^\dagger \hat{\Theta}_{12} \rangle / 3$  indicates that the system is a mixture with both singlet pairs and nonzero net magnetization. This feature can be well understood for the special case when  $\gamma = 0$  and  $\beta = 0$ , marked as a small dip in the black solid line in Fig. 3(a). We find that  $\langle \hat{\Theta}_{12}^\dagger \hat{\Theta}_{12} \rangle / 3 = 10000/9$ , which can be obtained analytically. In fact, the state at this point can be simply expressed as a direct product of two well-known states (ferromagnetic and polar),  $(\hat{a}_1^\dagger)^N |0\rangle \otimes (\hat{B}^\dagger)^{N/2} |0\rangle$ , and we find that on this state,

$$\begin{aligned} \frac{1}{3} \langle \hat{\Theta}_{12}^\dagger \hat{\Theta}_{12} \rangle &= \frac{1}{3} \langle \hat{a}_1^\dagger \hat{a}_1 \hat{b}_{-1}^\dagger \hat{b}_{-1} - \hat{a}_0^\dagger \hat{a}_1 \hat{b}_0^\dagger \hat{b}_{-1} + \hat{a}_{-1}^\dagger \hat{a}_1 \hat{b}_1^\dagger \hat{b}_{-1} \\ &\quad - \hat{a}_1^\dagger \hat{a}_0 \hat{b}_{-1}^\dagger \hat{b}_0 + \hat{a}_0^\dagger \hat{a}_0 \hat{b}_0^\dagger \hat{b}_0 - \hat{a}_{-1}^\dagger \hat{a}_0 \hat{b}_1^\dagger \hat{b}_0 \\ &\quad + \hat{a}_1^\dagger \hat{a}_{-1} \hat{b}_{-1}^\dagger \hat{b}_1 - \hat{a}_0^\dagger \hat{a}_{-1} \hat{b}_0^\dagger \hat{b}_1 + \hat{a}_{-1}^\dagger \hat{a}_{-1} \hat{b}_1^\dagger \hat{b}_1 \rangle \\ &= \frac{1}{3} \langle \hat{a}_1^\dagger \hat{a}_1 \hat{b}_{-1}^\dagger \hat{b}_{-1} \rangle \\ &= \frac{1}{3} N \frac{N}{3} = N^2/9, \end{aligned}$$

which agrees with the numerical result. We notice that the system is a mixture with  $N/2$  polar pairs and net magnetization  $F = F_1 = N$ .

In our system there exist three states, on which the average of total spin amounts to zero. Although we have  $\hat{F}^2 (\hat{A}^\dagger)^{N/2} (\hat{B}^\dagger)^{N/2} |0\rangle = 0$ ,  $\hat{F}^2 |N, N, 0, 0\rangle = 0$ , and  $\hat{F}^2 (\hat{\Theta}_{12}^\dagger)^N |0\rangle = 0$ , the difference between these states can be easily seen from an example  $N_1 = N_2 = N = 2$ . We find that

$$\begin{aligned} |2, 2, 0, 0\rangle &= Z^{1/2} \sum_{m_1, m_2} C_{F_1, m_1; F_2, m_2}^{F=0, m=0} |2, m_1\rangle |2, m_2\rangle \\ &= \frac{1}{48} \{ C_{2,0;2,0}^{0,0} (\hat{F}_{1-})^2 (\hat{F}_{2-})^2 (\hat{a}_1^\dagger)^2 (\hat{b}_1^\dagger)^2 |0\rangle \\ &\quad + C_{2,1;2,-1}^{0,0} (\hat{F}_{1-})^2 (\hat{F}_{2-})^2 (\hat{a}_1^\dagger)^2 (\hat{b}_1^\dagger)^2 |0\rangle \} \end{aligned}$$

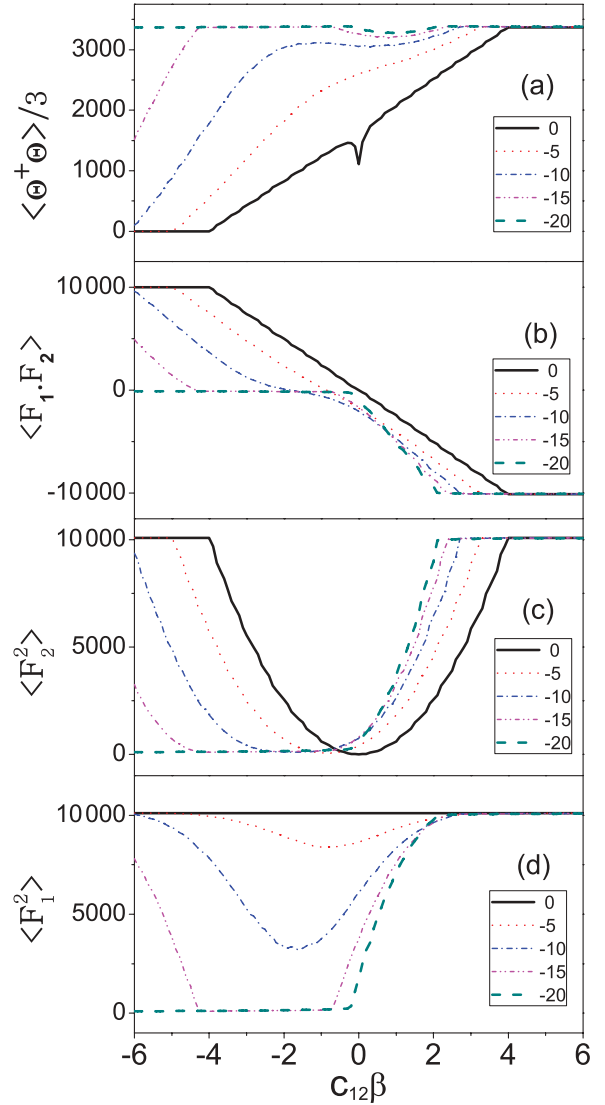


FIG. 3. (Color online) The dependence of the four order parameters on the parameter  $c_{12}\beta$  for different interspecies pairing interaction parameter  $c_{12}\gamma = 0, -5, -10, -15, -20$ .

$$\begin{aligned} &+ C_{2,2;2,-2}^{0,0} (\hat{F}_{1-})^2 (\hat{F}_{2-})^2 (\hat{a}_1^\dagger)^2 (\hat{b}_1^\dagger)^2 |0\rangle \\ &+ C_{2,-1;2,1}^{0,0} (\hat{F}_{1-})^2 (\hat{F}_{2-})^2 (\hat{a}_1^\dagger)^2 (\hat{b}_1^\dagger)^2 |0\rangle \\ &+ C_{2,-2;2,2}^{0,0} (\hat{F}_{1-})^2 (\hat{F}_{2-})^2 (\hat{a}_1^\dagger)^2 (\hat{b}_1^\dagger)^2 |0\rangle \} \\ &= \frac{1}{2\sqrt{5}} ((\hat{\Theta}_{12}^\dagger)^2 - \frac{1}{3} \hat{A}^\dagger \hat{B}^\dagger) |0\rangle. \end{aligned} \quad (24)$$

From the relation between these three states (24), we see that the AA phase of our system includes at least two pairing mechanism (i.e.,  $\hat{\Theta}_{12}^\dagger$  and  $\hat{A}^\dagger \hat{B}^\dagger$ ). As total spin  $F$  vanishes, the number distributions of these three states are all  $\langle n_1^{(j)} \rangle = \langle n_0^{(j)} \rangle = \langle n_{-1}^{(j)} \rangle = N/3$ , but the number fluctuation on these states are quite different. For the state  $(\hat{A}^\dagger)^{N/2} (\hat{B}^\dagger)^{N/2} |0\rangle$  [8], the results are

$$\begin{aligned} \langle \Delta n_1^{(j)} \rangle &= \langle \Delta n_0^{(j)} \rangle / 2 = \langle \Delta n_{-1}^{(j)} \rangle \\ &= \frac{\sqrt{N^2 + 3N}}{3\sqrt{5}}. \end{aligned} \quad (25)$$

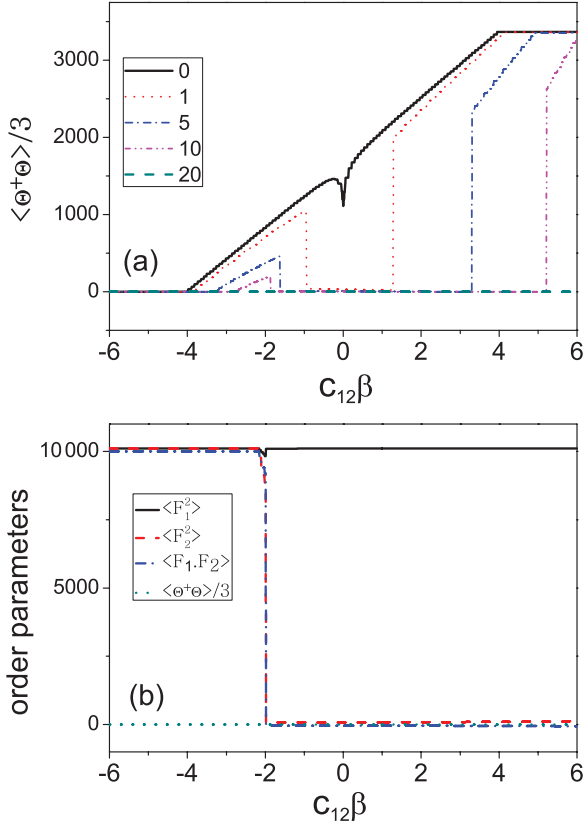


FIG. 4. (Color online) (a) The dependence of the fourth order parameter on the parameter  $c_{12}\beta$  for different interspecies pairing interaction parameters  $c_{12}\gamma = 0, 1, 5, 10, 20$ . (b) The dependence of ground-state order parameters on  $c_{12}\beta$  at fixed values of  $c_1\beta_1 = -1$ ,  $c_2\beta_2 = 2$ , and  $c_{12}\gamma = 20$ .

On the state  $|N, N, 0, 0\rangle$  [27], we have obtained in Eq. (22), in the case of large  $N$ , satisfying

$$\langle \Delta n_1^{(j)} \rangle = 2\langle \Delta n_0^{(j)} \rangle = \langle \Delta n_{-1}^{(j)} \rangle, \quad (26)$$

while for the state  $(\hat{\Theta}_{12}^\dagger)^N |0\rangle$ , we find that the number fluctuations are equally distributed [27], that is,

$$\langle \Delta n_1^{(j)} \rangle = \langle \Delta n_0^{(j)} \rangle = \langle \Delta n_{-1}^{(j)} \rangle$$

$$= \sqrt{\frac{N(N+1)}{6} - \frac{N^2}{9}}. \quad (27)$$

Finally we discuss briefly the situation when  $c_{12}\gamma > 0$ , in which case the ground state favors minimizing the  $\gamma$  term. We illustrate the competition between the interspecies coupling and singlet-pairing interactions numerically in Fig. 4(a). If  $c_{12}\gamma$  is far larger than any other parameters, the order parameter  $(\hat{\Theta}_{12}^\dagger \hat{\Theta}_{12})/3$  will vanish [see the dashed line in Fig. 4(a)]. All order parameters take the value 0 or  $\simeq N^2$  when  $c_1 2\gamma \gg 1$ , with the boundary determined by the corresponding amplitudes of spin-coupling strengths as shown in Fig. 4(b) for  $c_{12}\gamma = 20$ .

## V. CONCLUSION

In summary we studied the interspecies singlet pairing in the ground state of a binary mixture of spin-1 condensates in the absence of a magnetic field. In the case of  $c_{12}\gamma = 0$ , the exact quantum states can be constructed from angular momentum theory for the mixture of two ferromagnetic, two polar, and ferromagnetic-polar condensates. The ground state is classified into five types according to the interspecies coupling parameter  $c_{12}\beta$ . By means of the full quantum approach of exact diagonalization, a more general case of  $\gamma \neq 0$  is considered. We illustrate the competition between the two interspecies interactions  $c_{12}\beta$  and  $c_{12}\gamma$ , and find that if  $c_{12}\gamma \ll -1$  the ground state is a singlet of the total spin. There, however, exist different types of singlet formations determined by  $c_{12}\beta$ .

## ACKNOWLEDGMENTS

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