Ground States of a Mixture of Two Species of Spinor Bose Gases with Interspecies Spin Exchange

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We consider a mixture of two species of spin-1 atoms with interspecies spin exchange, which may cooperate or compete with the intraspecies spin exchanges and thus dramatically affect the ground state. It represents a new class of bosonic gases differing from single-species spinor gases. We determine the exact ground states in several parameter regimes, and study the composite structures by using the generating function method generalized here to be applicable to a mixture of two species of spinor gases. The most interesting phase is the so-called entangled Bose-Einstein condensation (BEC), which is fragmented BEC with quantum entanglement between the two species, and with both interspecies and intraspecies singlet pairs. For comparison, we also apply the generating function method to a mixture of two species of pseudospin-$\frac{1}{2}$ atoms, for which the total spin quantum number of each species is fixed as half of the atom number, in contrast with the case of spin-1, for which it is a variable determined by energetics. Consequently, singlet pairs in entangled BEC of a pseudospin-$\frac{1}{2}$ mixture are all interspecies. Interspecies spin exchange leads to novel features beyond those of spinor BEC of a single species of atoms as well as mixtures without interspecies spin exchange.

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I. INTRODUCTION

Spin-exchange scattering between bosonic atoms leads to novel ground states and interesting phenomena unexplored previously [1]. This remarkable subject broadens the scope of magnetism, which is traditionally based on spin exchanges of fermions instead. Mixtures of two species without a spin degree of freedom or, equivalently, mixtures of atoms of the same species with two spin states whose occupation numbers are both conserved have also been studied [6]. What about a mixture of two different species with interspecies spin exchange, in addition to intraspecies spin exchanges? This question was first explored in a mixture of two species of pseudospin-$\frac{1}{2}$ atoms [7–10], where the most interesting phase was found to be BEC of interspecies singlet pairs, which was called entangled Bose-Einstein condensation (EBEC), or BEC with an entangled order parameter, emphasizing the aspect that it is in an entangled state of two distinguishable atoms that BEC occurs. More generally, here we define EBEC as multispecies BEC with interspecies entanglement. It is a special kind of fragmented BEC. In EBEC, quantum entanglement, which is the most essential quantum feature not existing in classical physics, is amplified to a macroscopic quantum phase, just as BEC in a superposed single-particle state amplifies single-particle superposition to a macroscopic phase, leading to the Josephson effect. EBEC also bears some similarities to the lowest energy state of a SU(2) symmetric model of a single species of pseudospin-$\frac{1}{2}$ atoms which are forced to occupy two orbital modes by conservation of the total spin in the cooling process [11], but there are also differences [10].

To pick out two hyperfine states of an alkali atom representing pseudospin-$\frac{1}{2}$ avoiding spin-exchange loss to other hyperfine states may require some careful tuning [10]. In addition, with the degree of freedom being pseudospin, there is no reason to expect rotation symmetry in the interaction. In contrast, in a mixture of two species of spin-1 atoms with full access to the spin-1 multiplet, the total single-particle energy of any two scattered particles is always conserved, whether in the absence or the presence of a magnetic field, hence spin-exchange scattering is energetically protected. Moreover, the total spin of each species is conserved by the intraspecies interaction, while the total spin of the whole mixture is conserved by the interspecies interaction. Therefore, if it is also a ground state of a mixture of two species of spin-1 atoms, EBEC may be more experimentally accessible and stable in such a mixture than in a pseudospin-$\frac{1}{2}$ mixture. However, our consideration of spin-1 mixture had been impeded by the apparent complexity of the spin-exchange interaction between two spin-1 atoms of different species, until it was shown recently that it is simply of Heisenberg form [12]. Some mean-field-like investigations of spin-1 mixtures have been carried out, but possible entanglement between the two species was ignored [12, 13].

In this article, we rigorously study the ground states of a mixture of two species of spin-1 atoms in various parameter regimes. Bosonic symmetry within each species and its absence between different species together lead to rich structures, with interesting features beyond those of a single species of spinor gas. For a spin-1 mixture, we find EBEC in certain parameter regimes, with the two
species significantly entangled. Two atoms of the two different species can form interspecies singlet pairs, with differences from a pseudospin-$\frac{1}{2}$ mixture, however; in EBEC of a spin-1 mixture, intraspecies and interspecies singlet pairs coexist.

The rest of the paper is organized as follows. The many-body Hamiltonian is given in Sec. II. Under a common assumption for spin-1 bose gases, the present Hamiltonian can be written solely in terms of spin operators of the two species and of the total system. Then in Sec. III, we find the ground states in terms of spin quantum numbers, in various parameter regimes. These ground states are given in terms of boson creation operators in Sec. IV. In Sec. V, composite structures of these ground states are studied by generalizing a generating function method from a single species to a mixture. In Sec. VI, we discuss a mixture of two species of pseudospin-$\frac{1}{2}$ bosons. The paper is summarized in Sec. VII.

II. THE MANY-BODY HAMILTONIAN

For two spin-$f$ atoms of different species, there is no permutation symmetry between them, hence the total spin can be $F = 0, \cdots 2f$. The effective interaction is thus

\[ V(r_a - r_b) = \delta(r_a - r_b) \sum_{F=0}^{2f} g_F^{ab} P_F \]

where $g_F^{ab}$ is the interaction strength proportional to the $F$-channel scattering length, and $P_F$ is the projection operator for the total spin $F$, and can be expanded in terms of $1, F_a \cdot F_b, \ldots, (F_a \cdot F_b)^{2f}$. For $f = 1$, $g_0^{ab} = -g_0^a/3 + g_0^b/3$, $g_1^{ab} = -g_0^a/2 + g_0^b/2$, and $g_2^{ab} = g_0^a/2 - g_0^b/2$. It has been shown that $c_{10}^{ab} = 3\sqrt{r}/4 + g_1^a/4 + g_1^b/4$, $c_{20}^{ab} = 0$, where $g_1$ and $g_2$ correspond to the triplet and singlet states of the two valence electrons of the scattering atoms [12].

Therefore the many-body Hamiltonian is

\[ \mathcal{H} = \mathcal{H}_a + \mathcal{H}_b + \mathcal{H}_{ab}, \]

where

\[ \mathcal{H}_a = \int dr \psi_{\alpha a}^+ h_\alpha(r) \psi_{\alpha a} + \frac{1}{2} \int dr \psi_{\alpha a}^+ \psi_{\alpha b} (c_0^{ab} \delta_{\mu \nu} \delta_{\rho \sigma} + c_2^{ab} F_{a \mu \nu} \cdot F_{a \rho \sigma}) \psi_{\alpha a} \]

is the well-known Hamiltonian of spin-1 atoms [1] of species $\alpha$ ($\alpha = a, b$), while

\[ \mathcal{H}_{ab} = \int dr \psi_{\alpha a}^+ \psi_{\beta b} (c_0^{ab} \delta_{\mu \nu} \delta_{\rho \sigma} + c_2^{ab} F_{a \mu \nu} \cdot F_{b \rho \sigma}) \psi_{\alpha a} \psi_{\beta b} \]

is the interspecies interaction. Here the field operator $\psi_{\alpha \mu}$ corresponds to spin $\mu$ component of species $\alpha$ ($\mu = -1, 0, 1$), and $F_{a \mu \nu}$ represents the $(\mu \nu)$ element of the spin-1 matrix of species $\alpha$.

\[ h_\alpha = -\hbar^2 2m_\alpha \nabla_\alpha^2 + U_\alpha(r) - \gamma_\alpha B \cdot F_\alpha \]

is the single particle Hamiltonian of species $\alpha$, $m_\alpha$ and $\gamma_\alpha$ are the mass and the gyromagnetic ratio of an atom of species $\alpha$, respectively, $B$ is a uniform magnetic field, and $U_\alpha$ is the trapping potential for an atom of species $\alpha$.

For the single-particle orbital wave function, certainly one can use the usual single-mode approximation to write $\psi_{\alpha \mu \nu}(r) = \phi_{\alpha \mu} \phi_{\alpha \nu}(r)$, where $\phi_{\alpha \mu}$ is the annihilation operator and $\phi_{\alpha \nu}$ is the lowest single-particle orbital wave function for species $\alpha$ and spin $\mu$. Then we obtain a Hamiltonian in terms of creation and annihilation operators, with integrals of various products of $\phi_{\alpha \mu}$’s and their complex conjugates entering as coefficients of the terms of the Hamiltonian.

Nevertheless, to simplify the matter, we can follow an additional common assumption for spin-1 bose gases, namely that the single particle orbital wave function is mainly determined by the spin-independent part of the Hamiltonian and is thus independent of spin; that is, $\phi_{\alpha \mu} = \phi_\alpha$ is independent of spin $\mu$. For a homogeneous system, $\phi_\alpha = 1/\sqrt{V}$, where $V$ is the volume. But our discussions also apply to the inhomogeneous case.

Therefore, the Hamiltonian can be simplified as

\[ \mathcal{H} = \frac{e_a}{2} S_a^2 + \frac{e_b}{2} S_b^2 + e_{ab} S_a \cdot S_b - \gamma_a B \cdot S_a - \gamma_b B \cdot S_b, \]

where

\[ S_a = \phi_{\alpha a}^+ F_{\alpha \mu \nu} \phi_{\alpha a} \]

is the total spin operator for species $\alpha$, $\gamma_a, \gamma_b > 0$,

\[ C = N_a \epsilon_a + N_b \epsilon_b + \frac{e_a}{2} (N_a^2 - N_a) + \frac{e_b}{2} (N_b^2 - N_b) - c_a N_a - c_b N_b + c_{ab} N_a N_b \]

is a constant, $c_{k} = \frac{e_k}{\hbar} \int d^3 r |\phi_{\alpha \mu}|^4$, $c_{ab} = \frac{e_{ab}}{\hbar} \int d^3 r |\phi_{\alpha \mu} \phi_{\beta \nu}|^2$, $(k = 0, 2)$, and we have simplified notations $c_2^a$ and $c_2^{ab}$ as $c_1^a$ and $c_1^{ab}$, respectively.

If $e_{ab} = 0$, then there is no entanglement between the two species of atoms, the ground state is simply a direct product of the ground states of the two species of spin-1 atoms.

We now set out to find the ground states of (7) in various parameter regimes.

III. GROUND STATES IN TERMS OF SPINS

We assume $\gamma_a = \gamma_b = \gamma \geq 0$, as satisfied by alkali atoms with the same nuclear spin, for example, $^7$Li, $^{23}$Na, $^{39}$K, $^{41}$K and $^{85}$Rb, all of which have nuclear spin 3/2.
Then $S_a$ and $S_b$ together with the total spin $S$ and its $z$-component $S_z$ are all conserved. Therefore, the ground state is

$$|G⟩ = |S_a, S_b, S, S_z⟩,$$

(9)

with the four spin quantum numbers being the integers that minimize the energy $E = \frac{c^a - c^{ab}}{2} S_a(S_a + 1) + \frac{c^b - c^{ab}}{2} S_b(S_b + 1) + \frac{c^{ab}}{2} S(S + 1) - \gamma B S_z$, where $B > 0$ is the magnitude of the magnetic field and the constant $C$ has been neglected. Note that the minimization of $E$ is under the constraints $|S_a - S_b| \leq S \leq S_a + S_b$ and $-S \leq S_z \leq S$.

Moreover, for a given $S$, $S_z = S$ minimizes the energy. Therefore the ground state must be

$$|G⟩ = |S^m_a, S^m_b, S^m, S^m⟩,$$

(10)

where $S^m_a$, $S^m_b$ and $S^m$ are, respectively, the values of $S_a$, $S_b$ and $S$ that minimize

$$E = \frac{c^a - c^{ab}}{2} S_a(S_a + 1) + \frac{c^b - c^{ab}}{2} S_b(S_b + 1) + \frac{c^{ab}}{2} S(S + 1) - \gamma BS.$$

(11)

In the following, we find the ground states in the form of (10), by minimizing (11), for various parameter regimes. For specification, we assume $N_a \geq N_b$ without loss of generality.

A. $c^{ab} < 0$

First, we consider the cases with $c^{ab} < 0$. Then for given $S_a$ and $S_b$, it is $S = S_z = S_a + S_b$ that minimizes the energy (11).

The ground state is thus

$$|G(c^{ab} < 0)⟩ = |S^m_a, S^m_b, S^m_a + S^m_b, S^m_a + S^m_b⟩,$$

(12)

where $S^m_a$ and $S^m_b$ are respectively the values of $S_a$ and $S_b$ that minimize $E(c^{ab} < 0) = \frac{c^a - c^{ab}}{2} S_a(S_a + 1) + \frac{c^b - c^{ab}}{2} S_b(S_b + 1) + \frac{c^{ab}}{2} (S_a + S_b)(S_a + S_b + 1) - \gamma B S_a S_b$, and must be calculated separately for different subcases.

In particular, here we consider $c^b < 0 < c^a < c^{ab}$ and $c^b < c^{ab}$. $E$ always decreases as $S_a$ or $S_b$ increases. For

$$|G⟩_I = |N_a, N_b, N_a + N_b, S_z⟩$$

(13)

where $S_z = -N_a - N_b, \ldots, N_a + N_b$, the prime in the subscript to $|G⟩_I$ represents the absence of a magnetic field, and $g_I(S_{bz})$ is the Clebsch-Gordan coefficient.

$$|G⟩_I = |N_a, N_b, N_a + N_b, S_z⟩$$

(15)

$$= \sum_{S_{bz} = -N_b}^N N_b g_I(S_{bz}) |N_a, S_z - S_{bz}⟩_a \otimes |N_b, S_{bz}⟩_b.$$

(16)

With $c^{ab} < 0$, one can see that the ground state remains as $|G⟩_I$ or $|G⟩_I'$ if $c^a = c^{ab}$ while $c^b < c^{ab}$, or $c^b = c^{ab}$ while $c^a < c^{ab}$, or $c^a = c^b = c^{ab}$. This is because to minimize $E$, first $S$ is maximized to the largest possible value $N_a + N_b$. Consequently $S_i$ and $S_b$ have to be maximized to $N_a$ and $N_b$, respectively, even though one or both disappear in $E$. Therefore regime I can be expanded as $c^{ab} < 0$, $c^a \leq c^{ab}$ and $c^b \leq c^{ab}$.
B. $c^{ab} > 0$

Now we turn to cases with $c^{ab} > 0$, for which it is useful to rewrite $E$ as $E(c^{ab} > 0) = \frac{a^2 - c^{ab}}{2} S_a (S_a + 1) - \frac{b^2 - c^{ab}}{2} S_b (S_b + 1) + c^{ab} (S + \frac{1}{2} - \gamma B)^2/2 - a^2 (\frac{1}{2} - \gamma B)^2/2$. When $c^{ab} \geq 2\gamma B$, $c^a - c^{ab} > 0$, and $c^b - c^{ab} > 0$, the ground state is

$$|G\rangle_{II} = |0, 0, 0, 0\rangle = |0, 0\rangle_a \otimes |0, 0\rangle_b,$$

which is a maximally entangled state, as one can easily see by considering the reduced density matrix of either species.

$$|G\rangle_{III} = |N, N, 0, 0\rangle = \frac{1}{2N+1} \sum_{m=-N}^{N} (-1)^m |N, m\rangle_a \otimes |N, -m\rangle_b,$$

which is a maximally entangled state.

If $c^{ab} \geq 2\gamma B > 0$ or $c^{ab} > 2\gamma B = 0$ under the constraint $N_a = N_b = N$, one can see that the ground state remains as $|G\rangle_{III}$ if $c^a < c^{ab}$ while $c^b = c^{ab}$, or $c^b < c^{ab}$ while $c^a = c^{ab}$. This is because to minimize $E$, $S$ is minimized to 0 while $S_a$ or $S_b$ is maximized to $N$ and, consequently, the other $S_b$ or $S_a$ is maximized to $N$ also, although it does not appear in $E$.

If $c^{ab} \geq 2\gamma B > 0$ or $c^{ab} > 2\gamma B = 0$, while $c^a = c^b$, then the ground state is degenerate, and is $|S_a, S_b, 0, 0\rangle$, with $0 \leq S_b \leq N_b$.

Finally, if $0 < c^{ab} \leq 2\gamma B$, $c^a - c^{ab} < 0$, and $c^b - c^{ab} < 0$, while $|N_a - N_b| \leq n \leq N_a + N_b$, where $n \equiv \text{Int}(\frac{2\gamma B}{\gamma B} - \frac{1}{2})$, then $E$ is minimized when $S_a = N_a$, $S_b = N_b$, and $S = n$. Here $\text{Int}(x)$ represents the integer closest to $x$ and in the legitimate range given above is the integer no larger than and closest to $x$. Hence the ground state is

$$|G\rangle_{IV} = |N_a, N_b, n, n\rangle = \sum_{S_{bc} = -N_b}^{N_b} g_{IV}(S_{bc}) |N_a, n - S_{bc}\rangle_a \otimes |N_b, S_{bc}\rangle_b,$$

where $g_{IV}(S_{bc})$ is the Clebsch-Gordon coefficient.

If $0 < c^{ab} \leq 2\gamma B$, and $c^a - c^{ab} < 0$ while $c^b = c^{ab}$, then the ground state is $|N_a, S_b, n, n\rangle$, under the constraint $|N_a - S_b| \leq n \leq N_a + S_b$. If $0 < c^{ab} \leq 2\gamma B$, and $c^b - c^{ab} < 0$ while $c^a = c^{ab}$, then the ground state is $|S_a, N_b, n, n\rangle$, under the constraint $|S_a - N_b| \leq n \leq S_a + N_b$. If $0 < c^{ab} \leq 2\gamma B$ while $c^a = c^b = c^{ab}$, then the ground state is $|S_a, S_b, n, n\rangle$, under the constraint $|S_a - S_b| \leq n \leq S_a + S_b$. If $0 < c^{ab} \leq 2\gamma B$ while $c^a - c^{ab} < 0$ and $c^b - c^{ab} < 0$, then the ground state is $|N_a, n - S_b\rangle_a \otimes |N_b, S_{bc}\rangle_b$, with $0 \leq S_b \leq N_b$.
Note that the preceding ground states are all unique, because in each case, not only \( S_a \) and \( S_b \), but also \( S_a \) and \( S_b \) are specified. It has been known that for a single species of spin-1 atoms, \(|S_a, S_a\rangle_α\) is unique \[14\]. Hence any spin basis state

\[
|S_a, S_{az}\rangle_α = [r(S_a) \cdots r(S_{az}+1)]^{-1}(S_{az})^{S_a-S_{az}}|S_a, S_a\rangle_α,
\]

is also unique, where

\[
S_{az} = \sqrt{2}(a^+_1 a_0 + a^+_0 a_{-1})
\]

is the spin lowering operator,

\[
r(m) \equiv \sqrt{(S + m)(S - m + 1)}.
\]

Therefore any state \(|S_a, S_b, S, S_z\rangle\) of a mixture of two species of spin-1 atoms, as can be obtained from the spin basis states of the two species, is unique.

IV. GROUND STATES IN TERMS OF BOSON OPERATORS

We now proceed to determine the expressions of these ground states in terms of boson operators. First, it is straightforward to obtain

\[
|G\rangle_I = |N_a, N_b, N_a + N_b, N_a + N_b\rangle
\]

and

\[
|G\rangle_I = \frac{1}{\sqrt{N_a!N_b!}}(a^+_1)^N_a (b^+_1)^N_b |0\rangle,
\]

where \(Z_I = [(N_a/2)!(N_b/2)!2^{(N_a+N_b)/2}(N_a+1)!!(N_b+1)!!]^{1/2}\) is the normalization constant \[3\]. From this expression, it can be seen that \(|G\rangle_I\) exists only if \(N_a\) and \(N_b\) are both even.

One can rewrite in terms of boson operators \(|G\rangle_I\), \(|G\rangle_{III}\) and \(|G\rangle_{IV}\), in which cases \(S_a\) takes the largest possible value \(N_α\), by calculating the spin basis states of each species using \(24\), with

\[
|N_α, N_α\rangle_α = \frac{1}{\sqrt{N_α!}} a^+_1^{N_α} |0\rangle,
\]

and then substituting them into \(16\), \(20\) and \(23\), respectively. For convenience in reading, we write them down explicitly in the following equations.

\[
|G\rangle_{II} = |0, 0, 0, 0\rangle
\]

\[
= Z_{II}[2a^+_1 a^+_0 - (a^+_0)^2]^{N_a/2}[2b^+_0 b^+_1 - (b^+_1)^2]^{N_b/2} |0\rangle,
\]

where

\[
Z_{II} = [(N_a/2)!(N_b/2)!2^{(N_a+N_b)/2}(N_a+1)!!(N_b+1)!!]^{1/2}
\]

and

\[
g_{II}(S_{bz}) = \sqrt{(2N_a)!(2N_b)!(N_a + N_b + S_z)!(N_a + N_b - S_z)!}
\]

\[
\times (a^+_0 a^+_1 + a^+_1 a^-_0) a^+_1^{N_a-S_z} + S_{bz} a^+_1^{N_a-S_z} (-1)^m [b^+_0 b^+_1 + b^+_1 b^-_0]^{N_b-S_{bz}} b^+_1^{N_b} |0\rangle,
\]

where

\[
|G\rangle_{III} = |N, N, 0, 0\rangle
\]

\[
= \frac{2^N}{(2N+1)!} \sum_{m=-N}^N (-1)^m
\]

\[
\times (a^+_0 a^+_1 + a^+_1 a^-_0)^{N-m} a^+_1^{N} (b^+_0 b^+_1 + b^+_1 b^-_0)^{N+m} b^+_1^{N} |0\rangle,
\]
\[ |G \rangle_{IV} = |N_a, N_b, n, n \rangle \]
\[ = \sum_{S_b = -N_b}^{N_b} \frac{g_{IV}(S_{bz})2^{N_a+N_b-n}}{\sqrt{N_a!N_b!r(N_a)\cdots r(n-S_{bz}+1)r(N_b)\cdots r(S_{bz}+1)}} \times (a_0^\dagger a_1 + a_1^\dagger a_0)^{N_a-n+S_{bz}}a_1^{N_a}(b_0^\dagger b_1 + b_1^\dagger b_0)^{N_b-S_{bz}}b_1^{N_b}|0\rangle, \]

where
\[ g_{IV}(S_{bz}) = (-1)^{S_b}\sqrt{\frac{(N_a + N_b - n)!(2n+1)!(N_a + n - S_{bz})!(N_b + S_{bz})!}{(N_a + N_b + n + 1)!(n + N_a - N_b)!(n - N_a + N_b)!(N_a - n + S_{bz})!(N_b - S_{bz})!}}. \]

\[ |S_b, S_b, 0, 0, \rangle \text{, which is the ground state in some boundary regime of regime III, can be given by \textbf{38}, with } N \text{ replaced by } S_b. \]
\[ |S_a, S_b, n, n, \rangle \text{, which is the ground state in some boundary regime of regime IV, can be given by \textbf{38} and \textbf{39}, with } N_a \text{ and } N_b \text{ replaced by } S_a \text{ and } S_b, \text{ respectively.} \]

A clearer picture of the composite structures of these ground states in terms of basic units is revealed by generalizing the method of generating function \textbf{3} and \textbf{14}, in the next section.

\[ |S_a, S_b, S, S \rangle = \sum A(|Q_{m_j, n_j, l_j}\rangle) \prod (\Theta_{m_j, n_j, l_j})^{Q_{m_j, n_j, l_j}}|0\rangle, \]

where \( A \) is a coefficient and the summation is over all possible values of \( \{Q_{m_j, n_j, l_j}\} \).

The possible values of \( m_j, n_j, l_j \) and \( Q_{m_j, n_j, l_j} \) are subject to the constraints from \( N_a \), \( N_b \) and \( S \),
\[ \sum_j n_j Q_{m_j, n_j, l_j} = N_a, \]
\[ \sum_j m_j Q_{m_j, n_j, l_j} = N_b, \]
\[ \sum_j l_j Q_{m_j, n_j, l_j} = S, \]

as well as the constraints from \( S_a \) and \( S_b \),
\[ S_a^2 |S_a, S_b, S, S \rangle = S_a(S_a + 1)|S_a, S_b, S, S \rangle, \]
\[ S_b^2 |S_a, S_b, S, S \rangle = S_b(S_b + 1)|S_a, S_b, S, S \rangle. \]

where \( S_a^2 = (a_1^\dagger a_1 - a_1 a_1^\dagger - 1)^2 + 2(a_0^\dagger)^2 a_1 a_1^\dagger - 1 + 2a_1^\dagger a_1^\dagger a_0^\dagger a_0 - 1 + 2a_0^\dagger a_0 a_0 a_0^\dagger - 2a_0^\dagger a_0 a_0^\dagger a_1 - 1, \) as one can easily find.

For an integer \( f \), we define the generating function as
\[ G(x_a, x_b, y) \equiv \sum_{N_a, N_b, S} M(N_a, N_b, S)x_a^{N_a}x_b^{N_b}y^S, \]
where \( x_a, x_b \) and \( y \) are complex numbers inside the unit circle and \( M(N_a, N_b, S) \) is the number of solutions of the sets of the nonnegative integers \( \{Q_{m_j, n_j, l_j}\} \). Following the method of \textbf{14}, we obtain that
\[ G(x_a, x_b, y) = \int C 2\pi i dz \frac{1}{z - y} \prod_{j_a = -f}^{f} \frac{1}{1 - x_a z^{j_a}(1 - x_b z^{j_a})} \]

where the contour integral is along the unit circle \( C \).

For \( f = 1 \), we obtain that
\[ G(x_a, x_b, y) = \sum x_a^{Q_{1,1,0}+2Q_{2,0,0}+Q_{0,1,0}+Q_{1,0,1}}x_b^{Q_{1,1,0}+2Q_{2,0,0}+Q_{0,1,0}+Q_{1,0,1}}y^{Q_{1,0,1}+Q_{0,1,1}}. \]

where the summations are over all possible values of \( Q_{1,1,0}, Q_{2,0,0}, Q_{0,1,0}, Q_{1,0,1} \) and \( Q_{0,1,1} \), all of which are nonnegative. Comparing \textbf{43} and \textbf{45}, we have
\[ M(N_a, N_b, S) = M_1(N_a, N_b, S) + M_2(N_a, N_b, S), \]

V. COMPOSITE STRUCTURES OF THE GROUND STATES

A. Generating function method for \( |S_a, S_b, S, S \rangle \)

Now we consider the construction of \( |S_a, S_b, S, S \rangle \) of a mixture of two species of spin-\( f \) atoms, with total spin and its \( z \)-component both being \( S \). With \( S_z \) being maximal, we may consider a configuration of the state \( |S_a, S_b, S, S \rangle \), in which there are \( Q_{m_j, n_j, l_j} \) copies of unit \( j \), which is made up of \( m_j \) \( a \)-atoms and \( n_j \) \( b \)-atoms and carrying spin \( l_j \). Denoting the creation operators for unit \( j \) as \( \Theta_{m_j, n_j, l_j} \), we have
where \( M_1(N_a, N_b, S) \) is the number of solutions to the set of equations
\[
Q_{1,1,0} + 2Q_{2,0,0} + Q_{1,0,1} = N_a, \\
Q_{1,1,0} + 2Q_{2,0,0} + Q_{0,1,1} = N_b, \\
Q_{1,0,1} + Q_{0,1,1} = S,
\]
while \( M_2(N_a, N_b, S) \) is the number of solutions to the set of equations
\[
Q_{1,1,0} + 2Q_{2,0,0} + Q_{1,0,1} + 1 = N_a, \\
Q_{1,1,0} + 2Q_{2,0,0} + Q_{0,1,1} + 1 = N_b, \\
Q_{1,0,1} + Q_{0,1,1} + 1 = S.
\]

In general, there may be multiple solutions to \( 47 \). In each solution, there are \( Q_{1,1,0} \) interspecies singlets consisting of one \( a \)-atom and one \( b \)-atom, \( Q_{2,0,0} \) singlets consisting of two \( a \)-atoms and \( Q_{0,2,0} \) singlets consisting of two \( b \)-atoms. In addition, there are \( Q_{1,0,1} \) \( a \)-atoms with \( z \)-component spin 1, as well as \( Q_{0,1,1} \) \( b \)-atoms with \( z \)-component spin 1.

There may also be multiple solutions to \( 48 \). In each solution, there are \( Q_{1,1,0} \) interspecies singlets consisting of one \( a \)-atom and one \( b \)-atom, \( Q_{2,0,0} \) singlets consisting of two \( a \)-atoms and \( Q_{0,2,0} \) singlets consisting of two \( b \)-atoms. Also, either there are \( Q_{1,0,1} \) \( a \)-atoms with \( z \)-component spin 1 together with one \( a \)-atom with \( z \)-component spin 0, as well as \( Q_{0,1,1} + 1 \) \( b \)-atoms with \( z \)-component spin 1; or there are \( Q_{0,1,1} \) \( b \)-atoms with \( z \)-component spin 1 together with one \( b \)-atom with \( z \)-component spin 1, as well as \( Q_{1,0,1} + 1 \) \( a \)-atoms with \( z \)-component spin 1.

\[ |S_a, S_b, 0, 0\rangle = \sum_{Q_{1,1,0}} A(Q_{1,1,0}) (\Theta_{1,1,0}^\dagger)^{Q_{1,1,0}} (\Theta_{2,0,0}^\dagger)^{Q_{0,1,1} - Q_{1,1,0}/2} (\Theta_{0,2,0}^\dagger)^{Q_{0,2,0}} |0\rangle, \]

where
\[
\Theta_{1,1,0}^\dagger = a_{1,1,0}^\dagger b_{1,1,0}^\dagger - a_{0,1,0}^\dagger b_{0,1,0}^\dagger + a_{0,1,0}^\dagger b_{1,1,0}^\dagger
\]
is the creation operator for an interspecies singlet pair, while \( \Theta_{2,0,0}^\dagger = 2a_{1,1,0}^\dagger a_{0,1,0}^\dagger - a_{0,1,0}^2 \) and \( \Theta_{0,2,0}^\dagger = 2b_{1,1,0}^\dagger b_{0,1,0}^\dagger - b_{0,1,0}^2 \) are creation operators of intraspecies singlet pairs of \( a \)-atoms and \( b \)-atoms, respectively.

As a simple example, we can verify that \( |G\rangle_I = |N_a, N_b, N_a + N_b\rangle = |N_a, N_a\rangle_a \otimes |N_b, N_b\rangle_b \) is indeed as given in \( 23 \). For \( S = N_a + N_b \), the only solution to \( 47 \) is \( Q_{1,0,1} = N_a, Q_{0,1,1} = N_b, \) and \( Q_{1,1,0} = Q_{2,0,0} = Q_{0,2,0} = 0 \), while there is no solution to \( 48 \). Hence in this case, \( |G\rangle_I \) must be given by \( 23 \), which is obviously an eigenstate of \( S_a^2 \) and \( S_b^2 \) as it should be.

Now we look at \( |G\rangle_{III} = |N, N, 0, 0\rangle \). Equation \( 20 \) already indicates that the two species are strongly entangled, therefore \( |G\rangle_{III} \) is in the form of \( 19 \).

For \( |G\rangle_{IV} \), one considers \( 17 \) and \( 18 \) with \( S = S_z = n \). It can be found that the solution to \( 17 \) is
\[
\begin{align*}
Q_{1,0,1} &= \frac{N_a - N_b + n}{2} + Q_{2,0,0} - Q_{0,2,0}, \\
Q_{0,1,1} &= \frac{N_b - N_a + n}{2} + Q_{0,2,0} - Q_{2,0,0}.
\end{align*}
\]

which is valid if \( N_a + N_b - n \) is even, while the solution to \( 18 \) is
\[
\begin{align*}
Q_{1,0,1} &= \frac{N_a - N_b + n - 1}{2} + Q_{2,0,0} - Q_{0,2,0}, \\
Q_{0,1,1} &= \frac{N_b - N_a + n - 1}{2} + Q_{0,2,0} - Q_{2,0,0}.
\end{align*}
\]

which is valid if \( N_a + N_b - n \) is odd.

Hence, if \( N_a + N_b - n \) is even,
where $Q_{1,0,1}$ and $Q_{0,1,1}$ are given by (51) while if $N_a + N_b - n$ is odd,

$$|G′⟩_{IV} = |N_a, N_b, n, n⟩ = \sum A(Q_{1,1,0}, Q_{2,0,0}, Q_{2,0,0})a†_0Q_{1,0,1}b†_0Q_{0,1,1} + \sum A′(Q_{1,1,0}, Q_{2,0,0}, Q_{2,0,0})a†_1Q_{1,1,0}b†_1Q_{0,1,1} + \sum A(Q_{2,0,0}, Q_{2,0,0}, Q_{2,0,0})a†_0Q_{2,0,0}b†_0Q_{0,2,0} + \sum A′(Q_{2,0,0}, Q_{2,0,0}, Q_{2,0,0})a†_1Q_{2,0,0}b†_1Q_{0,2,0} |0⟩,$$

where $Q_{1,0,1}$ and $Q_{0,1,1}$ are given by (52). In both (53) and (54), the summations are over $Q_{1,1,0}$, $Q_{2,0,0}$ and $Q_{0,2,0}$. The coefficients $A$ and $A'$ are determined by constraints (12) with $S_a = N_a$ and $S_b = N_b$.

VI. COMPOSITE STRUCTURES OF $|S, S⟩$ OF A PSEUDOSPIN-1/2 MIXTURE

As a comparison, we now apply the generating function method to determine $|S, S⟩$ of a mixture of two species of pseudospin-1/2 atoms. Unlike the case of spin-1, for each species $α$ of pseudospin-$\frac{1}{2}$, the total spin is always fixed to be $S_α = N_α/2$. With $N_a$ and $N_b$ fixed, the spin state of the pseudospin-$\frac{1}{2}$ mixture is only determined by $S$ and $S_z$ of the total spin; that is,

$$|S, S_z⟩ \equiv \frac{1}{2} N_a, \frac{1}{2} N_b, S, S_z⟩.$$

(55)

The basic method for constructing the maximally polarized $|S, S⟩$ remains the same as that for a spin-1 mixture, as described in Sec. V.A. In a configuration of the state $|S, S⟩$, there are $Q_{m_1,n_1,l_1}$ copies of unit $j$, which is made up of $m_1$ $a$-atoms and $n_1$ $b$-atoms and carries spin $l_1/2$. The generating function is now defined as

$$G(x_a, x_b, y) = \sum_{N,a,N_b,S} M(N_a, N_b, S)x_a^{N_a}x_b^{N_b}y^{2S}.$$

(56)

where the normalization constant is neglected, and

$$Φ_{1,1,0} = a†_1S+(N_a-N_b)/2 b†_1S+(N_b-N_a)/2 Φ_{1,1,0} |0⟩,$$

(61)

is the interspecies singlet creation operator for a pseudospin-$\frac{1}{2}$ mixture. A sufficient and necessary condition for $Q_{1,1,0}$, $Q_{1,0,1}$ and $Q_{0,1,1}$ all to be integers is that $2S + N_a + N_b$ is an even integer.

When $S = 0$, the only consistent solution of (61) is

$$Q_{1,0,1} = Q_{0,1,1} = 0$ while $Q_{1,1,0} = N$ if and only if $N_a = N_b = N$. The state is then the global singlet

$$|0, 0⟩ = Φ_{1,1,0}^N |0⟩.$$

(63)

When $N_a \geq N_b$, the smallest value of $S$ is $(N_a - N_b)/2$, for which $Q_{1,1,0} = N_b, Q_{1,0,1} = N_a - N_b, and Q_{0,1,1} = 0$, hence

$$Q_{1,0,1} = Q_{0,1,1} = 0$ while $Q_{1,1,0} = N$ if and only if $N_a = N_b = N$. The state is then the global singlet

$$|0, 0⟩ = Φ_{1,1,0}^N |0⟩.$$

(64)

VII. SUMMARY

To summarize, we have considered a mixture of two different species of spin-1 gases with interspecies spin-
exchange scattering, as an extension of our previous work on a mixture of two different species of pseudospin-\(\frac{1}{2}\) gases, going beyond the usual spinor bose gases and BEC mixtures without interspecies entanglement. Interspecies spin exchange favors spin ordering between different species, while intraspecies spin exchange favors spin ordering within each species. The ground state of such a mixture thus depends on the parameters in the many-body Hamiltonian, which we have shown to be reduced to a Hamiltonian of two giant spins.

We have worked out the ground states in four typical parameter regimes, which are now reported in Table I. It is straightforward to verify that they are all fragmented BEC, by calculating one-particle reduced density matrices. When \(c^a\) and \(c^b\) are both less than \(c^{ab}\), which is negative or 0, all atoms of each species form a ferromagnetic state with the spin of each atom being \(\mu = 1\); that is, the ground state of the mixture is the direct product of two independent ferromagnetic states. When \(c^a\) and \(c^b\) are both larger than \(c^{ab}\), which is larger than or equal to \(2\gamma B\), the atoms of each species form a singlet state, with the total spin of each species being 0; that is, the ground state of the mixture is the direct product of two independent singlet states, subject to the condition that \(N_a\) and \(N_b\) are even (otherwise there is minute deviation). These two ground states are disentangled between the two species. For \(N_a = N_b = N\), when \(c^{ab} \geq 2\gamma B > 0\) or \(c^{ab} > 2\gamma B = 0\), while \(c^a\) and \(c^b\) are both less than \(c^{ab}\), the ground state is a global singlet state \(|G\rangle_{IV} = |N,N,n,n\rangle\), with total spin zero. When \(0 < c^{ab} \leq 2\gamma B\), and \(c^a\) and \(c^b\) are both less than \(c^{ab} < 0\), the ground state is \(|G\rangle_{IV} = |N_a, N_b, n, n\rangle\), where \(n \equiv \text{Int}(\frac{N_B}{2} - \frac{1}{2})\).

The latter two ground states exhibit EBEC, displaying strong interspecies entanglement. A consequence of this entanglement is that the particle number in each spin state of each species is subject to strong quantum fluctuation. There are rich composite structures due to interspecies entanglement. By using the generating function method, it has been revealed that \(|G\rangle_{III}\) and \(|G\rangle_{IV}\) are each superpositions of configurations with both intraspecies and interspecies singlet pairs. It is interesting to note that \(|G\rangle_{III} = |G\rangle_{IV}\) when \(c^{ab} = 2\gamma B, N_a = N_b\), implying that \(|G\rangle_{III}\) and \(|G\rangle_{IV}\) belong to the same quantum phase.

We have also used the generating function method to find the spin state \(|S, S\rangle\) of a mixture of two species of pseudospin-\(\frac{1}{2}\) atoms with interspecies spin exchange. As the total spin of each species of pseudospin-\(\frac{1}{2}\) atoms is always half of the atom number, the composite structure of a pseudospin-\(\frac{1}{2}\) atoms is simpler, with only one configuration. Consequently, there are only interspecies singlet pairs when the total spin of the mixture is zero, hence EBEC in such a case is simply BEC occurring in an interspecies singlet state. Such a simplicity is lost in a spin-1 mixture, in which intraspecies singlet pair states coexist with interspecies singlet pairs, and EBEC is generally defined as BEC with interspecies entanglement. Previous studies on pseudospin-\(\frac{1}{2}\) mixture demonstrated that BEC leads to various physical properties different from those of usual BEC, to be similarly studied in spin-1 mixtures.

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**Note added:** Recently we became aware of a paper [10] that simply gives \(|N_a, N_b, N_a - N_b, S_2\rangle\) as the ground state “for large antiferromagnetic spin-exchange interaction between the two species”, without actually showing it gives the lowest energy. We had determined that the ground state varies with the parameters, and is not always this state even for large antiferromagnetic interspecies spin-exchange interaction. They also applied the same generating function method as ours to the Hamiltonian with an additional \(P_0\) term, which, to our understanding, had been shown to vanish by Luo et al. [12].

We also disagree with their statement that there is no interspecies singlet pairing when this additional \(P_0\) term vanishes. We have worked out all possible ground states, which will be discussed elsewhere.

| No. | Parameter regimes | Ground states |
|-----|-------------------|---------------|
| I   | \(c^{ab} \leq 0\), \(c^a < c^{ab}\), \(c^b < c^{ab}\). | \(|G\rangle_I = |N_a, N_b, N_a + N_b, N_a + N_b\rangle = |N_a, N_b, 0\rangle_a \otimes |N_a, N_b, 0\rangle_b\) (disentangled) |
| II  | \(c^{ab} \geq 2\gamma B\), \(c^a > c^{ab}\), \(c^b > c^{ab}\). | \(|G\rangle_{II} = |0, 0, 0, 0\rangle_{a} \otimes |0, 0\rangle_{b}\) (disentangled) |
| III | \(c^{ab} \geq 2\gamma B > 0\) or \(c^{ab} > 2\gamma B = 0\), \(c^a < c^{ab}\), \(c^b < c^{ab}\). | \(|G\rangle_{III} = |N, N, 0, 0\rangle\) (entangled) |
| IV  | \(0 < c^{ab} \leq 2\gamma B\), \(c^a < c^{ab}\), \(c^b < c^{ab}\). | \(|G\rangle_{IV} = |N_a, N_b, n, n\rangle\), \(n \equiv \text{Int}(\frac{N_B}{2} - \frac{1}{2})\) (entangled) |
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