Sensitivity of spin structures of small spin-1 condensates toward a magnetic field studied beyond the mean field theory

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Abstract
The spin structures of small spin-1 condensates \( N \leq 1000 \) under a magnetic field \( B \) have been studied beyond the mean field theory. Instead of the spinors, the many body spin eigenstates have been obtained. We have defined and calculated the spin correlative probabilities to extract information from these eigenstates. The correlation coefficients and the fidelity susceptibility have also been calculated. Thereby, the details of the spin structures responding to the variation of \( B \) can be better understood. In particular, from the correlation coefficients, which are the ratio of the two-body probability to the product of two one-body probabilities, strong correlation domains of \( B \) are found. The emphasis is placed on the sensitivity of the condensates toward \( B \). No phase transitions in spin structures are found. However, abrupt changes in the derivatives of observables (correlative probabilities) are found in some particular domains of \( B \). In these domains, the condensates are highly sensitive to \( B \). The effect of temperature is considered. The probabilities defined in the paper can work as a bridge to relate theories and experiments. Therefore, they can be used to discriminate various spin structures and refine the interactions.

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(Some figures may appear in colour only in the online journal)

1. Introduction

Bose–Einstein condensates are ideal artificial systems for quantum manipulation. The spinor condensates have very rich spin structures, and their swift response to the external field is notable [1]. Usually, a condensate would contain more than \( 10^4 \) atoms. Due to the progress in
techniques, much smaller condensates (say, particle number $N \leq 1000$) could be produced. Note that the strength of the effective interaction between the particles $C^2$ is proportional to the average particle density, which is proportional to $N^{-3/5}$ (evaluated based on the Thomas–Fermi approximation). Thus, the particles are subjected to a stronger interaction in smaller systems. In fact, in the study of spin dynamics, the rate of evolution depends on $\tau = C^2 t / \hbar$ rather than $t$ [2], where $t$ is the time. Therefore, the evolution is swifter in the smaller systems. Thus, they might be even more suitable for manipulation. In principle, these systems could be more precisely prepared (such as $N$ and $M$, the total magnetization, could be more rigorously given). Therefore, some properties not contained in large condensates might emerge (say, if $N < 50$, whether $N$ is even or odd might be serious), and some properties might depend on the external field very sensitively in some particular cases (as shown below).

There are already a number of references dedicated to large condensates of spin-1 atoms. The commonly used theoretical tool is the mean field theory (MFT) [3–10]. The ground states with the ferromagnetic and polar phases are found. Their modes of excitation and their dynamical behavior have been studied, and very rich physical phenomena have been found (say, the formation of spin domains and spin vortices). On the other hand, for small condensates, a theory that goes beyond the MFT might be more appropriate. In this paper, the spin structure of spin-1 small condensates under a magnetic field $B$ is studied by using a many-body theory in which the fractional parentage coefficients (FPC) of spin states are used as a basic tool. The FPC were firstly introduced by Racah for the calculation of matrix elements of fermion systems [11, 12]. Then, they were generalized and widely used in the theory of the interacting boson model (IBM) of nuclei [13]. In IBM, the boson is composed of two fermions and has an even spin. If the spin is odd, the relative spatial wavefunction of the two fermions would be anti-symmetric, and therefore harmful to stability. Hence, the spin-1 boson is scarcely considered in the IBM. On the other hand, in the study of spin-1 condensates, an analytical form of the FPC has been found [14, 15]. This will greatly facilitate the calculation.

The variation of $B$ is considered as adiabatic and the discussion is limited to static behavior. One- and two-body spin correlative probabilities are defined and calculated. They are used to extract information from the spin eigenstates [16]. Furthermore, the correlation coefficients are defined and calculated to measure quantitatively the spin correlation, and the fidelity susceptibilities are also calculated to measure quantitatively the sensitivity of the ground states toward the change of $B$. Thereby, a detailed and deeper description on spin–spin correlation has been obtained, which might lead to a better understanding of spin structures. In particular, the spin probabilities defined in this paper are observables, they might serve as a bridge to relate theories and experiments, thereby clarifying various spin structures and interactions. The emphasis is placed on the response of the condensates to $B$. The related knowledge might be useful for quantum manipulation. Both the cases with the temperature $T$ zero and nonzero are considered.

2. Hamiltonian and the eigenstates

In 1998, the MIT group first succeeded in trapping atoms in an optical trap by using laser beams [17]. This is an important technique in the research of cold atoms. In contrast to the magnetic trap, the spin degrees of freedom are free in the optical trap. Hence, the rich physics occurring in the spin space can be revealed. In theory, the effect of the trap can be embodied by a parabolic potential. Let $N$ spin-1 atoms be confined by an isotropic and parabolic potential with frequency $\omega$. Since the temperature in the experiments of cold atoms is very low, the kinetic energies of the atoms are very low. They interact with each other essentially via the
s-wave. Therefore, the feature of the condensate depends on the s-wave scattering lengths but not on the details of interaction. In theory, for convenience, the zero-range force is usually used, where the parameters are so chosen as to recover the correct s-wave scattering lengths. Thus, the spin-dependent inter-atomic interaction can be written as \( V_{ij} = \delta(r_i - r_j)(c_0 + c_2 f_i \cdot f_j) \), where \( r_i \) and \( f_i \) are, respectively, the position vector and the spin operator of the \( i \)th particle. The parameters \( c_0 \) and \( c_2 \) can be determined by experiments. An additional magnetic field \( B \) lying along the \( Z \)-axis is applied. We consider the case that the size of the condensate is small so that it is smaller than the spin healing length. In this case, the single-mode approximation (SMA) is applicable [18]. Under the SMA, all particles have the same spatial wavefunction \( \phi(r) \), and therefore the total spin wavefunction is totally symmetric. After the integration over the spatial degrees of freedom, we arrive at a model Hamiltonian

\[
H_{\text{mod}} = C_2 \hat{S}^2 - p \sum_i \hat{f}_i + q \sum_i (\hat{f}_i)^2,
\]

where \( \hat{S} \) is the total spin operator of the \( N \) particles, \( C_2 = c_2 \int d\sigma |\phi(r)|^4/2 \), \( \hat{f}_i \) is the \( z \)-component of \( f_i \), \( p = -\mu_B B/2 \), \( q = (\mu_B B)^2/4E_{\text{hf}} \), \( \mu_B \) is the Bohr magneton and \( E_{\text{hf}} \) is the hyperfine splitting energy. The last two terms of \( H_{\text{mod}} \) are the linear and quadratic Zeeman energies, respectively.

The eigenstates of \( H_{\text{mod}} \) have \( S \) and its \( z \)-component \( M \) (namely the magnetization, \( M > 0 \) is assumed) to be conserved when the quadratic term is neglected. Therefore, they can be denoted as \( \vartheta_{S,M}^{N} \), \( S = N, N - 2, \ldots, 0 \). It has been proved that \( \vartheta_{S,M}^{N} \) is unique without further degeneracy [19]. They together form a complete set for all the totally symmetric spin states of \( f = 1 \) systems. When the quadratic term is taken into account, \( M \) remains to be conserved, but not \( S \). In this case, \( \vartheta_{S,M}^{N} \) can be used as basis functions for the diagonalization of \( H_{\text{mod}} \). As a many-body wavefunction, the detailed expression of \( \vartheta_{S,M}^{N} \) is usually very complicated. However, due to the introduction of the FPC, the expression of \( \vartheta_{S,M}^{N} \) is not necessary. All the related physical quantities can be easily obtained by using the FPC.

Using the FPC, a particle (say, the particle 1) can be extracted from \( \vartheta_{S,M}^{N} \) as

\[
\vartheta_{S,M}^{N} = \sum_{\mu} \chi_{\mu}(1) \left[ a_{S,M\mu}^{(N)} \vartheta_{S+1,M-\mu}^{N-1} + b_{S,M\mu}^{(N)} \vartheta_{S-1,M+\mu}^{N-1} \right],
\]

where \( \chi_{\mu}(1) \) is the spin state of the particle 1 in component \( \mu = 0 \) or \( \pm 1 \). The FPC have analytical forms as

\[
a_{S,M\mu}^{(N)} = \sqrt{\frac{1 + (-1)^{N-S}(N+S)(S+1)}{2N(2S+1)}} C_{1\mu,S+1,M-\mu}^{SM},
\]

\[
b_{S,M\mu}^{(N)} = \sqrt{\frac{1 + (-1)^{N-S}S(N+S+1)}{2N(2S+1)}} C_{1\mu,S-1,M+\mu}^{SM},
\]

where the Clebsch–Gordan coefficients are introduced.

Once a particle has been extracted, the calculation of the matrix elements is straightforward, and we have

\[
\langle \vartheta_{S,M}^{N} | H_{\text{mod}} | \vartheta_{S,M}^{N} \rangle = \delta_{M,M'} [\delta_{S,S'} (C_2 S(S+1) - pM) + q Q_{SS'}^{NM}],
\]

where

\[
Q_{SS'}^{NM} = N \langle \vartheta_{S,M}^{N} | (\hat{f}_i)^2 | \vartheta_{S,M}^{N} \rangle = N \sum_{\mu} \mu^2 q_{SS'}^{NM\mu},
\]

\[
q_{SS'}^{NM\mu} = \delta_{S,S'} [a_{S,M\mu}^{(N)}]^2 + [b_{S,M\mu}^{(N)}]^2 + \delta_{S,S'} \delta_{M,M'} q_{SS'}^{NM\mu} + \delta_{S',S} 2a_{S-M\mu}^{(N)} b_{S+M\mu}^{(N)} + \delta_{S',S} 2b_{S-M\mu}^{(N)} b_{S+M\mu}^{(N)}].
\]
For an arbitrary \( N \), after a procedure of diagonalization, the set of eigenenergies \( E_i \) and the corresponding eigenstates \( \Theta_{\delta M} = \sum_i d^{iM}_S \phi_{\delta M}^i \) can be obtained, where \( E_i \) is in the order of increasing energy. Since the set \( \phi_{\delta M}^i \) is complete, the set \( \Theta_{\delta M} \) is exact for \( H_{\text{mod}} \).

3. Spin correlative probabilities

For the condensates with nonzero spins, it has been shown theoretically that there are various spin structures. In order to confirm these structures experimentally, one has to define some measurable physical quantities. For the spatial degrees of freedom, it is recalled that the one-body density \( \rho(r) \) can provide information on the spatial distribution of the particles, and the two-body density \( \rho(r_1, r_2) \) can describe the spatial correlation. Similar quantities can be defined in the spin space. Each spin eigenstate can be written as

\[
\Theta_{\delta M} = \sum_x d^{xM}_S \phi_{\delta M}^x S \equiv \sum_{\mu} \chi_{\mu}(1) \psi_{\mu}^{\text{ANSM}} M,
\]

where \( \psi_{\mu}^{\text{ANSM}} \) can be obtained by applying equation (2) to each total spin \( S \) component, and summing over \( S \). The normality \( 1 = (\Theta_{\delta M} | \Theta_{\delta M} ) = \sum_{\mu, \nu} \langle \phi_{\mu}^{\text{ANSM}} | \phi_{\nu}^{\text{ANSM}} \rangle \) implies that \( \langle \phi_{\mu}^{\text{ANSM}} | \phi_{\nu}^{\text{ANSM}} \rangle \) is the probability of particle 1 in \( \mu \)-component. Then, we define the one-body probability

\[
P_{\mu}^{\text{ANSM}} = \langle \phi_{\mu}^{\text{ANSM}} | \phi_{\mu}^{\text{ANSM}} \rangle = \sum_{SS'} d^{SS'}_S d^{\text{ANSM}}_{S' M} d^{\text{ANSM}}_{S' M},
\]

Note that \( NP_{\mu}^{\text{ANSM}} \) is just the average population of the \( \mu \)-component and is an observable which can be directly measured via the Stern–Gerlach technique.

In the case with \( B = 0 \), \( S \) is a good quantum number, and the \( \ell \)th state has \( S_\ell = N + 2 - 2i \) (if \( c_2 < 0 \) or \( S_\ell = 2(i - 1) \) (if \( c_2 > 0 \) [5]. In this case, \( d_{SS'}^{\text{ANSM}} = \delta_{S,S'}d_{S}^{\text{ANSM}} \), and we have

\[
P_{\mu}^{\text{ANSM}} = \left( d_{S,\mu}^{\text{ANSM}} \right)^2 + \left( b_{S,\mu}^{\text{ANSM}} \right)^2.
\]

When one more particle is extracted from the right side of equation (2), we have

\[
\theta_{\delta M}^N = \sum_{\mu, \nu} \chi_{\mu}(1) \chi_{\nu}(2) \sum_{SS'} A^{\text{ANSM}}_{\mu,\nu;S,M} \theta_{\delta M}^{N-2},
\]

where

\[
A^{\text{ANSM}}_{\mu,\nu;S,2} = d_{S,\mu}^{\text{ANSM}} d_{S,\nu}^{\text{ANSM}} d_{S+1,1-M,-\mu,-\nu}^{\text{ANSM}} S-1,1-M,-\nu,
\]

\[
A^{\text{ANSM}}_{\mu,\nu;S,S} = d_{S,\mu}^{\text{ANSM}} d_{S,\nu}^{\text{ANSM}} d_{S+1,1-M,-\mu,-\nu}^{\text{ANSM}} S-1,1-M,-\nu,
\]

or \( A^{\text{ANSM}}_{\mu,\nu;S,2} = 0 \) otherwise.

Then, the \( \ell \)th state can be rewritten as

\[
\Theta_{\delta M} = \sum_{\mu, \nu} \chi_{\mu}(1) \chi_{\nu}(2) \psi_{\mu,\nu}^{\text{ANSM}} M.
\]

From the normality as before, we have \( 1 = \sum_{\mu, \nu} \langle \psi_{\mu,\nu}^{\text{ANSM}} | \psi_{\mu,\nu}^{\text{ANSM}} \rangle \). Thus, it is straightforward to define the two-body spin correlative probability as

\[
P_{\mu,\nu}^{\text{ANSM}} = \langle \psi_{\mu,\nu}^{\text{ANSM}} | \psi_{\mu,\nu}^{\text{ANSM}} \rangle = \sum_{SS'} d^{SS'}_S d^{\text{ANSM}}_{S' M} A^{\text{ANSM}}_{\mu,\nu;S,M} A^{\text{ANSM}}_{\mu,\nu;S,2},
\]

\( P_{\mu,\nu}^{\text{ANSM}} \) is the probability that the spin of a particle is in \( \mu \), while another in \( \nu \) when the two are observed; obviously, \( P_{\mu,\mu}^{\text{ANSM}} = P_{\mu,\mu}^{\text{ANSM}} \). If more particles are extracted, then higher order spin correlative probabilities could also be similarly defined. These probabilities do not have a counterpart in the MFT, therefore additional information might be provided by them.
Incidentally, the technique for the measurement of the correlative probabilities is mature in particle physics and nuclear physics, but not in condensed matter physics. The development of the related technique is desired.

In general, one can define the correlation coefficient

$$\gamma_{\mu, \nu}^{1, M} = \frac{p_{\mu, \nu}^{1, M}}{p_{\mu}^{1, M} p_{\nu}^{1, M}}$$

(15)

to measure quantitatively how large the correlation is. If $\gamma_{\mu, \nu}^{1, M}$ deviates remarkably from 1, then the correlation is strong, whereas if $\gamma_{\mu, \nu}^{1, M} \approx 1$, then the correlation is weak, and the system can be well understood simply from the one-body probabilities.

Numerical examples are given below. $\hbar \omega$ and $\sqrt{\mu/(\hbar \omega)}$ are used as units for energy and length, respectively, where $\hbar$ is the mass of atom. The spatial wavefunction $\phi(r)$ is obtained under the Thomas–Fermi approximation, and thereby we have the strength $C_2 = 0.154c_2/(NC_0)^{3/5}$. Since a slight inaccuracy that may exist in $\phi(r)$ would cause only a slight deviation in the magnitude of $C_2$, the approximation is acceptable in a qualitative sense. $\omega = 300 \times 2\pi \text{ (in sec}^{-1})$ and $N = 1000$ are, in general, assumed (unless particularly specified). $^{87}\text{Rb}$ and $^{23}\text{Na}$ condensates are used as examples for the $C_2 < 0$ and $C_2 > 0$ species, respectively. In the units adopted, we have $c_0 = 2.49 \times 10^{-3} \sqrt{\omega}$ and $c_2 = -1.16 \times 10^{-5} \sqrt{\omega}$ for $^{87}\text{Rb}$, and $c_0 = 6.77 \times 10^{-4} \sqrt{\omega}$ and $c_2 = 2.12 \times 10^{-5} \sqrt{\omega}$ for $^{23}\text{Na}$. The diagonalization of $H_{mod}$ is straightforward when all the parameters are given. Then, the coefficients $d_0^M$ can be known. From equations (9), (10) and (14), the one- and two-body probabilities can be obtained.

4. Low-temperature limit

The condensate will fall into its ground state $\Theta_{1, M}$ with a specified $M$ when $T = 0$. $M$ is determined by how the species is prepared. The case with $T \neq 0$ will be considered later.

4.1. Condensates with $c_2 < 0$

To evaluate how strong the correlation in $\Theta_{1, M}$ would be, the correlation coefficients $\gamma_{0, 0}^{1, M}$ of $^{87}\text{Rb}$ toward $B$ are shown in figure 1(a). The magnitudes of all the curves are extremely close to one in figure 1(a). This is also true for $\gamma_{\mu, \nu}^{1, M}$ with $(\mu, \nu) \neq (0, 0)$. It implies that the correlation in $\Theta_{1, M}$ is very weak.

When $B = 0$, $\Theta_{1, M}$ has $S = N$ [5, 20]. Its expression does not depend on the details of the interaction, but only on the sign of $c_2$, and can be uniquely written as

$$\Theta_{1, M} = \theta_{N, M}^N \equiv (\cdots ((\chi(1)\chi(2))_2 \chi(3))_3 \cdots \chi(N))_{N, M},$$

(16)

where $(\chi(A)\chi(B))_j$ implies that the spins of $\chi(A)$ and $\chi(B)$ are coupled to spin $\lambda$, and so on. The special way of spin coupling in equation (16) (i.e. the combined spin of an arbitrary group of $j$ particles is $j$) assures that the state is normalized and symmetrized. All the spins are roughly aligned along a common direction, but the azimuthal angle of this direction is arbitrary.

From equation (10), the analytical forms of $P_{\pm 1}^{1, M}$ can be derived as

$$P_{\pm 1}^{1, M} = \frac{(N \pm M)(N \pm M - 1)}{2N(2N - 1)},$$

(17)

$$P_0^{1, M} = \frac{(N - M)(N + M)}{N(2N - 1)}.$$  

(18)

\[ \text{J. Phys. A: Math. Theor. 45 (2012) 235002} \] C G Bao
Equation (18) can be approximately rewritten as $P_{0,M}^{1,M} \approx \frac{1}{2} \left( 1 - \frac{M^2}{N^2} \right)$. Thus, if $M = 0$, half of the particles would have $\mu = 0$. If $M \neq 0$, the increase of $M$ would lead to a decrease of $P_{0,M}^{1,M}$.

In particular, $P_{0,M}^{1,M} \to 0$ when $M \to N$ as expected. Incidentally, the above analytical forms of $P_{\mu,M}^{1,M}$ are identical to those from the MFT when $N \to \infty$ [7].

When $B$ varies, the one-body probabilities $P_{\mu,M}^{1,M}$ of $\Theta_{1M}$ toward $B$ are calculated and shown in figure 2. The left ends of the curves coincide exactly with those from the above analytical expressions. Note that the $\mu \neq 0$ particles will gain additional energy from the quadratic Zeeman term. In order to reduce the energy, the number of $\mu = 0$ particles increases with $B$. This is clearly shown in figure 2. For $M = 0$ as shown in figure 2(a), the derivative of $P_{0,0}^{1,0}$ varies very swiftly from a positive value to zero at the vicinity of a turning point $B = 0.28$ G where $P_{0,0}^{1,0} \approx 1$, i.e. the number of $\mu = 0$ particles, $N_0$ is very close to its limit $N$. The swift variation at the turning point becomes a sudden transition when $N$ is large, and the point becomes a critical point $B_{\text{crit}}$. Passing through this point, the derivative varies abruptly, but the spin state $\Theta_{10}$ itself varies continuously. When $B > B_{\text{crit}}$, the ground state remains unchanged as $\Theta_{10} = |0, N, 0\rangle \equiv (\chi_0)^N$, where $|N_1, N_0, N_{-1}\rangle$ is a Fock state with $N_1, N_0$ and $N_{-1}$ particles in $\mu = 1, 0$ and $-1$, respectively.
When \( M \neq 0 \), not all the particles can be changed to \( \mu = 0 \) because of the conservation of \( M \). Accordingly, the increase of \( P_{1,M}^{0} \) is hindered and the curves in figure 2(b) are smoother. When \( M \) is large, the curves are very flat implying that \( \Theta_{1,M} \) is affected by \( B \) very weakly. When \( B \to \infty \), we found that \( \Theta_{1,M} \to |M, N - M, 0\rangle \). Accordingly, \( P_{0,1}^{M} \to (N - M)/N \), \( P_{1}^{M} \to M/N \) and \( P_{-1}^{M} \to 0 \). In this way, \( N_0 = N - M \) is maximized so that the quadratic Zeeman energy is minimized.

To conclude this section, for small condensates of Rb, the ground state \( \Theta_{1,M} \) is continuously changed from \( \Theta_{NM} \) to \( |M, N - M, 0\rangle \) without a transition when \( B \) increases. However, the derivative \( \Delta N_0/\Delta B \) undergoes a transition at \( B_{\text{crit}} \) when \( M = 0 \). It is recalled that MFT, which is correct when \( N \) is very large, has predicted the transitions between the ferromagnetic, broken-axisymmetry and the polar phases [3, 9, 10]. The broken-axisymmetry phase is caused by a rapidly quenched field; therefore, it is not expected to appear in our case with \( B \) varying adiabatically.
4.2. Condensates with $c_2 > 0$

In contrast to the previous case, the spin correlation is very strong in the ground states $\Theta_{1,M}$ of $c_2 > 0$ condensates as shown by $\gamma_{0,0}^{1,M}$ in figure 1(b), where the left ends of all the curves are remarkably larger than 1. It implies that when two particles are observed, the probability of a particle in $\mu = 0$ would be much larger if the other one has $\nu = 0$. Starting from $B = 0$, there is a domain of $B$ where $\gamma_{0,0}^{1,M}$ remains large and nearly unchanged (refer to the $M = 100$ curve in figure 1(b)). Outside that domain, the correlation vanishes rapidly. The domain is called a strong correlation domain (SCD), where the spin structure at $B = 0$ remains unchanged toward the increase of $B$. The SCD does not have a clear border. For each curve in figure 1(b), let $B_{\text{scd}}$ be the value where $\gamma_{0,0}^{1,M} = \left(\gamma_{0,0}^{1,M}\right)_{\text{max}} + 1/2$. Then, $B_{\text{scd}}$ is considered as the outward border of the SCD. A larger $M$ leads to a larger $B_{\text{scd}}$ (say, for figure 1(b), if $M = 10$, 100 and 500, respectively, $B_{\text{scd}} \approx 0.002$ G, 0.015 G and 0.073 G). Thus, the spin structure at $B = 0$ better when $M$ is large.

When $B = 0$, the ground state will have $S$ as small as possible [5, 20]. Thus, $\Theta_{1,M} = \theta_{M,M}^N$ if $N - M$ is even, or $\Theta_{M+1,1,M} = \theta_{M+1,1,M}^N$ if $N - M$ is odd. Due to the fact that $\theta_{M,M}^N$ is unique, we have

$$\theta_{M,M}^N \propto \mathcal{P}\{(\chi \chi)_0|^N-M/2\},$$

(19)

where $\mathcal{P}$ is the symmetrizer, i.e. a summation over the $N$! particle permutations. So this state is composed of a group of $\mu = 1$ particles together with a group of singlet pairs. And

$$\theta_{M+1,1,M}^N \propto \mathcal{P}\{\theta_{M+1,1,M}^N(\chi \chi)_0|^N-M-1/2\},$$

(20)

which is composed of a group of $(M + 1)$-polarized particles (but the direction of polarization deviates a little from the $Z$-axis) together with a group of singlet pairs. From equation (10) the one-body probabilities are

$$p_{0,0}^{1,M} = \frac{|M|(2 - 1/N) - |M|^2/N - 1}{(2|M| + 3)(2|M| - 1)},$$

(21)

$$p_{0,0}^{1,M} = \frac{|M|(2 - 1/N) + |M|^2(4 + 2/N) \pm M(4|M|(|M| + 1) - 3)/N - 2}{2(2|M| + 3)(2|M| - 1)}.$$  

(22)

For the case $M = 0$ and $N$ being even, $\Theta_{1,M} = \theta_{0,0}^N \propto \mathcal{P}\{(\chi \chi)_0|^N\}$. This state is named the polar state where all the particles are in the singlet pairs. From equations (21) and (22), the polar state has $p_{0,0}^{1,0} = 1/3$ for all $\mu$. In other words, the particles are equally populated among the three components. This is a common property of $S = 0$ states.

When $B$ increases, $p_{0,0}^{1,0}$ toward $B$ are shown in figure 3. Since the ground state has thereby more and more $\mu = 0$ particles, $p_{0,0}^{1,0}$ increases sharply from 1/3 to $\approx$ 1 as shown in figure 3(a). Correspondingly, the ground state $\Theta_{1,0}$ is sharply transformed from $\theta_{0,0}^N$ to $\{0, N, 0\} \equiv \{\chi_0\}^N$. Comparing the curve of $p_{0,0}^{1,0}$ in figure 3(a) with the one in figure 2(a) for Rb, the rise of the former is much faster than the latter. Thus, the Na condensate is highly sensitive to the appearance of $B$ if $M = 0$. A very weak field (a few mG) is sufficient to break nearly all the pairs and turn every spin lying on the $X$–$Y$ plane independently. The independence is supported by the curve of $\gamma_{0,0}^{1,0}$ in figure 1(b), where $\gamma_{0,0}^{1,0} \approx 1$ except when $B$ is close to zero. However, the high sensitivity would be lost if $M \neq 0$.

In figure 3(b), the curve of $p_{0,0}^{1,100}$ remains horizontal when $B < B_{\text{scd}} = 0.015$ G (refer also to the curve with $M = 100$ in figure 1(b)). Thus, the spin structure inside the SCD might remain unchanged. To clarify, the two-body probabilities are calculated and shown in figure 4, where all the $p_{0,0}^{1,0}$ remain unchanged in the SCD. Thus, the invariance of the structure toward $B$ is strongly supported. The invariance can also be seen by observing the overlap $\langle \phi_{1,1,0}^B \rangle \langle \phi_{1,1,0}^B \rangle \equiv \left| \theta_{1,1,0}^B \right|^2 \left| \phi_{1,1,0}^B \right|^2 \equiv \left( \theta_{1,1,0}^B \right)^2 \left( \theta_{1,1,0}^B \right)^2 \equiv \left( \theta_{1,1,0}^B \right)^2 \equiv \left( \theta_{1,1,0}^B \right)^2$ toward $B$ (and $M$ and $N$ are assumed to be even, 8
a superscript $B$ is added to emphasize the dependence on $B$). With the parameters of figure 3 and with $M = 100$, this overlap is $\geq 0.99$ when $B \leq 0.01$ G. Thus, the invariance is directly confirmed. However, it decreases very fast when $B$ is close to $B_{\text{scd}}$, and is equal to 0.58 when $B = B_{\text{scd}}$. Afterward, it tends to zero rapidly when $B$ increases further. The existence of the SCD demonstrates that the mixture of a group of singlet pairs together with a group of $M$ unpaired particles (each has $\mu = 1$) keeps its structure unchanged while $B$ increases. However, the capability would be lost if $B$ is close to or $> B_{\text{scd}}$. Afterward the mixture begins to change, and is characterized by the increase of $\mu = 0$ particles, which come from the breaking of pairs. Therefore, the change would be less probable if the original number of pairs is small. Thus, a larger $M$ (implying a fewer original pairs) leads to a better stability and therefore a larger $B_{\text{scd}}$. A larger $c_2$ leads also to a better stability and therefore a larger $B_{\text{scd}}$ (say, if $c_2 = 2(c_2)_{\text{Na}}$, i.e. the experimental value of Na was doubled, then $B_{\text{scd}}$ would be enlarged from 0.015 to 0.021 G for the curve with $M = 100$ in figure 3(b).

Since $M$ affects the stability, $P_{\mu}^{1,M}$ is in general sensitive to $M$. If $B$ is weak, the sensitivity would be very high when $M$ is small. For example, it is shown in figure 3(b) that $P_{\mu}^{1,M}$ decreases dramatically at $B = 3$ mG when $M/N$ is simply changed from 0 to 0.01.

When $B \to \infty$, all the pairs are destroyed and $\Theta_{1,M}$ tends to $|M, N - M, 0\rangle$. Thus, disregarding $c_2 < 0$ or $> 0$, both species tend to the same structure.
4.3. Fidelity susceptibility

In order to understand the sensitivity of the ground states \( \Theta_{1,M}^\theta \) toward \( B \) quantitatively, the fidelity susceptibility [21–23],

\[
\Gamma_M(B) = \lim_{\epsilon \to 0} \frac{2}{\epsilon^2} \left( 1 - \left| \langle \Theta_{1,M}^\theta + \epsilon | \Theta_{1,M}^\theta \rangle \right| \right), \tag{23}
\]

is calculated and given in figure 5. This figure demonstrates that each species has its own region highly sensitive to \( B \). For Rb, the most sensitive region is surrounding the critical point \( B_{\text{crit}} \) where the increase in \( \bar{N}_0 \) stops suddenly (refer to figure 2(a)). When \( B \) is small, the sensitivity does not depend on \( M \) and is in general very weak, whereas for Na, the most sensitive region is surrounding the border of SCD, \( B_{\text{scd}} \), where \( \bar{N}_0 \) begin to increase suddenly (refer to figure 3(b)). The fact that \( B_{\text{scd}} \) becomes larger with \( M \) is clearly shown in figure 5(b). The sensitivity can be very high when \( B \) is small if \( M \) is also small.

4.4. Effect of the trap and the particle number

Since the linear Zeeman term does not affect the spin structures, the ratio \( q/C_2 \) involved in \( H_{\text{mod}} \) is crucial. This quantity is proportional to \( B^2/\omega^{9/5} \). Therefore, a larger \( \omega \) would reduce the effect of \( B \). Consequently, for \( \omega' > \omega \), all the curves plotted in figures 1–4 extend horizontally to the right by a common factor \( (\omega'/\omega)^{3/5} \). In particular, the SCD becomes larger.

On the other hand, the change of \( N \) does not cause simply a change of scale, because the numbers of degrees of freedom are thereby changed. For an example, if \( N = 1000, 100 \) and \( 10, P_0^{1.0} \) of Rb would be equal to 0.99 when \( B = 0.277 \text{ G}, 0.178 \text{ G} \) and 0.134 G, respectively. Thus, the curve of \( P_0^{1.0} \) in figure 2(a) would rise up faster if \( N \) decreases from 1000. In contrast, if \( N = 1000, 100 \) and \( 10, P_0^{1.0} \) of Na would be equal to 0.90 when \( B = 0.0014 \text{ G}, 0.0084 \text{ G} \).
Figure 5. $\ln(\Gamma_M(B))$ toward $M/N$ and $B$ for the ground states of Rb (a) and Na (b) condensates. $B$ is in Gauss and $N = 1000$. The maximum of $\ln(\Gamma_M(B)) = 10.65$ (a) or 11.30 (b). The region surrounding the maximum is marked with ‘X’. The inmost contour of the X-region has the value 9.275 (a) or 9.541 (b). The difference of the values of a contour and its adjacent outer contour is 1.375 (a) or 1.760 (b).

and 0.0330 G, respectively. Thus, the curve of $P_{10}^{1,0}$ in figure 3(a) would rise up slower if $N$ decreases from 1000. Thus, the effect of $N$ on $c_2 < 0$ and $> 0$ species is different.

The effect of $N$ on $P_{10}^{1,M}$ with $M \neq 0$ is shown in figure 6. The curve with $N = 1000$ in figure 6(a) is identical to the curve with $M = 100$ in figure 2(b) for $c_2 < 0$. In figure 6(a) for Rb, the curves with a smaller $N$ rise up faster toward $B$ just as the previous case with $M = 0$. For $c_2 > 0$, the curve with $N = 1000$ in figure 6(b) is identical to the curve with $M = 100$ in figure 3(b). Similar to the case with $M = 0$, a smaller $N$ will cause also a smoother change. In particular, the abrupt change appearing in the vicinity of $B_{scd}$ as shown in figure 3(b) disappears when $N$ is small.

5. Finite temperature

Since the level density in a condensate is usually dense, thermal fluctuations are in general not negligible. What actually measured are the weighted probabilities $\bar{P}^M_\mu \equiv \sum_i W_i P^M_{\mu,i}$ and $\bar{P}_{\mu \nu}^M \equiv \sum_i W_i P^M_{\mu,i} P^M_{\nu,i}$, where $W_i = \exp(-E_i/k_BT) / \sum_j \exp(-E_j/k_BT)$ is the weight, $E_i$ is the energy, $T$ is the temperature and the summation in principle runs over all the states. However, when $T \ll \hbar \omega/k_B \equiv T_0$, the contribution arises essentially from the ground band, and all the higher states can be neglected [20]. The members of the ground band have nearly the same spatial wavefunctions, and their spin states together with $E_i$ can be obtained via the diagonalization of $H_{\text{mod}}$.

As an example, $\bar{P}_{00}^{1,0}$ of the condensates with $c_2 < 0$ at $T = T_0/10$ is plotted in figure 7(a). In order to see the effect of interaction, $c_2$ is given at three values. When $B$ is very small ($< 0.02$ G) or sufficiently large ($> 0.40$ G), the three curves associated with different
values of $c_2$ nearly overlap. However, in between, they are rather sensitive to $c$ as shown in figure 7(a). To see clearer, both $\bar{P}_{0}^{(b)}$ and $\bar{P}_{00}^{(b)}$ toward $c_2$ under $B = 0.2$ G are plotted in figure 7(b). The figure demonstrates that the weighted two-body probabilities are very sensitive to $c_2$. Furthermore, the patterns of the curves can be tuned by altering $B$. Therefore, the measurement of the weighted probabilities under various $B$ can provide rich information on the parameters of interaction.

One more example for the case $c_2 > 0$ is shown in figure 8. Similar to the previous case, high sensitivity to the interaction is found. In figure 8(a), the left ends of the curves are flat. This is caused by the existence of the SCD, where the spin structure remains nearly unchanged.

6. Final remarks

We have studied the spin structures of small spin-1 condensates ($N \lesssim 1000$) under a magnetic field $B$. The theory is beyond the MFT, and the single-mode approximation has been adopted. The fractional parentage coefficients have been used as a tool for the analytical derivation. The one-body, two-body and weighted probabilities are defined and calculated to extract information from the spin eigenstates. The correlation coefficients $\gamma_{\mu\nu}^{1,M}$ and the fidelity
Figure 7. The combined weighted probabilities for the condensates with \( c_2 < 0 \). \( T = T_0 / 10 \) is assumed. \( c_0 = (c_0)_{\text{Rb}} \) (i.e. the experimental value of \( ^{87}\text{Rb} \)) and \( c_2 = \alpha (c_2)_{\text{Rb}} \) are adopted, where \( \alpha \) is introduced to denote the ratio of the presumed \( c_2 \) to its realistic value. (a) \( \bar{P}_0^{(0)} \) toward \( B \) with \( \alpha \) given at three values marked beside the curves. (b) \( \bar{P}_0^{(0)} \) and \( \bar{P}_{\infty}^{(0)} \) toward \( \alpha \) with \( B = 0.2 \text{G} \).

Figure 8. Similar to figure 7 but for the condensates with \( c_2 > 0 \) and \( M = 100 \). \( c_0 = (c_0)_{\text{Na}} \) and \( c_2 = \alpha (c_2)_{\text{Na}} \) are adopted. Refer to figure 7.
susceptibility $\Gamma_M(B)$ have also been calculated. The following results are mentioned ($N - M$ is assumed to be even for simplicity).

(i) When $B = 0$, the ground state $\Theta_{1,M}$ is either the ferromagnetic state $\vartheta^N_{M}$, if $c_2 < 0$, or the polar state $\vartheta^0_{N,M}$, if $c_2 > 0$. For $\vartheta^N_{M}$, all the $N$ spins are coupled to total spin $S = N$, $\gamma_{1,M}$ is close to 1 and $\Gamma_M(0)$ is very small (figures 1 and 5). Hence, the ferromagnetic state does not have spin correlation, and is inert to $B$ when $B$ is small. The state $\vartheta^0_{N,M}$ has $M$ particles in $\chi_1$ together with $(N - M)/2$ singlet pairs, its $\gamma^1_{0,0}$ is very large. Thus, the polar state contains strong spin correlation. Furthermore, its $\Gamma_M(B = 0)$ is very large when $M$ is small. It implies a high sensitivity toward the appearance of $B$.

(ii) When $B$ increases, the number of $\mu = 0$ particles $\bar{N}_0$ in $\Theta_{1,M}$ increases in general so as to reduce the quadratic Zeeman energy. For $c_2 < 0$, $\Theta_{1,M}$ would be changed from $\vartheta^N_{N,M}$ to $\vartheta^N_{M, N - M}$ if $B$ increases from 0 to $\infty$. The change goes on continuously, no transition in the spin structure occur. In accord with the change of $\Theta_{1,M}$, $\bar{N}_0$ is changed from

$$\frac{(N - M)(N - 1)}{2N^2} \approx \frac{1 + M/N}{2} (N - M)$$

(refer to equation (18)) to $N - M$. Therefore, $(\bar{N}_0)_b - (\bar{N}_0)_{a=0} \approx (N - M)^2 / 2N \equiv N_{0, \text{diff}}$, which is the maximal number of particles allowed to be changed from being $\mu \neq 0$ to $\mu = 0$. When $M$ is close to $N$, $N_{0, \text{diff}}$ is very small implying that the room left for changing is very small; therefore $\Theta_{1,M}$ is inert to $B$ (refer to figure 2(b) where the curve with $M = 980$ is very flat). When $M$ is smaller, $\Theta_{1,M}$ has much room for changing and therefore would be more sensitive to $B$. In particular, when $M = 0$, there is a critical point $B_{\text{crit}}$. Once $B \geq B_{\text{crit}}$, $\bar{N}_0_b = N$ and the ground state no longer varies with $B$. There is an abrupt change in the derivative $\partial \bar{N}_0 / \partial B$ at $B_{\text{crit}}$. Thus, although the spin structures vary continuously with $B$, the related derivatives might not. $B_{\text{crit}}$ is equal to 0.28 G in figure 2. It is smaller when $N$ decreases, and larger when $\omega$ increases.

(iii) For $c_2 > 0$, the increase of $B$ from 0 to $\infty$ causes a change of $\Theta_{1,M}$ from $\vartheta^N_{N,M}$ (or $\vartheta^N_{N+1,M}$) to $\vartheta^N_{M, N - M}$, $\Theta_{1,M}$ of both cases $c_2 < 0$ and $c_2 > 0$ tend to the same state because it is the most advantageous state for reducing the quadratic Zeeman energy. The change of $\Theta_{1,M}$ goes on also continuously without transitions. In this process, $\bar{N}_0$ is in general increasing via a mechanism, i.e. a breaking of pairs as $(\chi_\chi)_0 \rightarrow \chi_0 \chi_0$ (whereas the process $(\chi \chi)_0 \rightarrow \chi_1 \chi_{-1}$ is suppressed under $B$ because it causes an increase of quadratic Zeeman energy). It is recalled that the particle correlation in $\Theta_{1,M}$ is very weak when $c_2 < 0$, but strong when $c_2 > 0$ due to the formation of pairs. When all the particles are paired (i.e. $M = 0$), the structure is extremely sensitive to $B$. A very weak $B$ (a few mG) is sufficient to break all the pairs. For a comparison, $P^{0,0}_{1,0}$ in figure 2(a) for Rb goes up to 0.9 when $B = 0.25$ G, but only $= 0.0014$ G in figure 3(a) for Na. However, when unpaired particles emerge (i.e. $M \neq 0$), the pairs have an additional ability to keep themselves. The mechanism underlying this phenomenon deserves to be studied further. This leads to the appearance of SCD ranging from $B = 0$ to $B_{\text{scd}}$. A larger $M$ leads to a larger $B_{\text{scd}}$, while $B_{\text{scd}} = 0$ when $M = 0$. The spin structure remains unchanged when $B < B_{\text{scd}}$, but $\bar{N}_0$ begins to increase when $B > B_{\text{scd}}$. The derivative of the probabilities varies very swiftly in the vicinity of $B_{\text{scd}}$. The swift variation becomes a sudden jump when $N$ is large (refer to figure 6(b)). Thus, $B_{\text{scd}}$ is also a critical point when $N$ is large. As a numerical example, when $N = 1000$ and $M = 100$, $B_{\text{scd}} = 0.015$ G in figure 3(b). Similar to $B_{\text{crit}}$, $B_{\text{scd}}$ becomes smaller when $N$ decreases (with $M/N$ remaining unchanged), and becomes larger when $\omega$ increases.

(iv) The sensitivity of the ground states toward $B$ is quantitatively shown in figure 5.

(v) When $B$ is appropriately chosen and $T$ is sufficiently low, the measurable weighted probabilities may provide rich information on the parameters of interaction.
(vi) Since there are strong correlation domains as shown in figure 1(b), the applicability of the MFT for Na in these domains is questionable.

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