Two-body and three-body substructures served as building blocks in small spin-3 condensates

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It was found that stable few-body spin-structures, pairs and triplexes, may exist as basic constituents in small spin-3 condensates, and they will play the role as building blocks when the parameters of interaction are appropriate. Specific method is designed to find out these constituents.

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I. INTRODUCTION

When the structure of a few-body system is very stable, it may become a basic constituent of many-body systems. For an example, the structures of light nuclei can be explained based on the cluster model, where the α-particle is a building block. Another famous example is the Cooper pair in condensed matter. This pair is responsible for the superconductivity. For Bose-Einstein condensates of spin-1 and spin-2 atoms, basic few-body structures have already been proposed by theorists. For spin-1 condensates, the interaction can be written as

\[ V_{ij} = \delta(r_i - r_j) \sum_S g_S P_S, \]  

where \( S \) is the combined spin of \( i \) and \( j \) and has two choices 0 and 2. \( P_S \) is the projector of the \( S \)-channel, \( g_S \) is the strength proportional to the \( s \)-wave scattering length of the \( S \)-channel. When \( g_2 - g_0 \) is positive, the ground state will have total spin \( F = 0 \) (1) when the particle number \( N \) is even (odd). The ground state wave function \( \Psi_g \) is proportional to the pair-state \( \tilde{P}_N[(\varsigma\varsigma)0]^N/2 \) or \( \tilde{P}_N[(\varsigma\varsigma)0]^{(N-1)/2} \), where \( \varsigma \) denotes the spin-state of a spin-1 atom, a pair of them are coupled to zero, \( \tilde{P}_N \) is the symmetrizer (a summation over the \( N! \) permutation terms). For higher states, say, the one with \( F = 2 \) is proportional to \( \tilde{P}_N[(\varsigma\varsigma)2(\varsigma\varsigma)0]^{(N-2)/2} \). Thus, the singlet pair \((\varsigma\varsigma)0\) appears as a common building block. These pairs, together with a few other substructures, constitute the low-lying states.

For spin-2 condensates, the interaction can also be written as Eq. (1), but with \( S = 0, 2, \) and 4. A detailed classification of the spin-states based on the seniority and \( F \) was given in the Ref. [7]. When \( N \) is even and \( \frac{7}{10}(g_0 - g_4) < (g_2 - g_4) < -\frac{7}{10}(N-3)/(N-2)(g_0 - g_4) \), \( \Psi_g \) is also dominated by the singlet pairs, and is proportional to the pair-state \( \tilde{P}_N[(\eta\eta)0]^{N/2} \), where \( \eta \) denotes the spin-state of a spin-2 atom. When \( N \) is a multiple of 3, and \( (g_2 - g_4) \) is negative and smaller than \( \frac{7}{10}(g_0 - g_4) \), \( \Psi_g \) is nearly proportional to the triplex-state \( \tilde{P}_N[(\eta\eta)2\eta]0^{N/3} \). Obviously, the triplex \((\eta\eta)2\eta)0\) acts as a building block. Furthermore, when the parameters of interaction fall inside the indicated domain, the low-lying states are also dominated by these building blocks accompanied by a few other substructures.

![FIG. 1: Intuitive diagram of basic constituents of condensates: the pair (a) and triplex (b).](arXiv:1112.3722v1 [cond-mat.quant-gas] 16 Dec 2011)

It is evident that the existence of building blocks originates from the special feature of interaction. The pairs \((\varsigma\varsigma)S\) and \((\eta\eta)S\) may appear as building blocks whenever \( g_S \) is sufficiently negative. However, for spin-\( f \) atoms with \( f \) even, instead of the pairs, a more favorable substructure is a triplex. Let \( \vartheta \) denote the spin-state of a spin-\( f \) particle. For the triplex-state \( \tilde{P}_N[(\vartheta\vartheta)f\vartheta]0^\lambda_0 \), the symmetrizer \( \tilde{P}_N \) is not necessary when \( \lambda = 0 \) because \( ((\vartheta\vartheta)f\vartheta)0 \) itself is symmetric (i.e., \( ((\vartheta(i)\vartheta(j))f\vartheta(k))0 = ((\vartheta(j)\vartheta(k))f\vartheta(i))0 \) as can be verified by recoupling the spins). It implies that every two spins are coupled to \( f \). Thereby the binding would be maximized if \( g_f \) is sufficiently negative. Intuitively speaking, the three spins in the \( \lambda = 0 \) triplex will be coplanar and form a regular triangle. This is shown in Fig. (b), where the angle between every two spins is 120° so that they are coupled to \( f \). Therefore, for spin-\( f \) condensates, the \( \lambda = 0 \) triplex might serve as building blocks when \( g_f \) is sufficiently negative (note that the \( \lambda = 0 \) triplex is prohibited when \( f \) is...
odd).

The ground state structure of spin-3 condensates has already been studied based on the MFT.\[12–14\] In this theory the spin structure is described by the spinors. They will have the polar phase (corresponding to the pair-state) when $g_0$ is sufficiently negative, and have the cyclic phase (corresponding to the triplex-state) when $g_0$ becomes positive. If a magnetic field is applied, a number of phases will emerge. Instead of using the spinors, it is an attempt of this paper to describe the spin structures based on the basic constituents. From the experience of spin-1 and -2 condensates, it is expected that pairs and triplexes might also appear in spin-3 condensates when the parameters of interaction are appropriate. We are going to search for these basic constituents. Due to the difficulty in calculation, only small condensates ($N$ is small) are concerned. We believe that the knowledge from small systems will help us to understand better the larger systems. To the prohibition of the $\lambda = 0$ triplex, only the $\lambda \neq 0$ triplexes could emerge in spin-3 systems. Since each $\lambda$-triplex has $2\lambda + 1$ magnetic components, additional complexity will arise as shown below.

II. HAMILTONIAN, EIGENSTATES AND PARTICLE CORRELATION

Let $N$ spin-3 atoms be confined by an isotropic and parabolic trap with frequency $\omega$. The interaction between particle $i$ and $j$ is $V_{ij} = \delta(r_i - r_j) \sum_S g_S P_S + V_{\text{dd}}$, where $V_{\text{dd}}$ is the dipole-dipole interaction. Let the wave function for the relative motion of $i$ and $j$ be $\psi_{ij|S}$, where $l$ is the relative orbital angular momentum, and $l$ the $S$ are coupled to $J$. Then, for $l = 0$, the matrix element $\langle \psi_{ij|S} | V_{\text{dd}} | \psi_{ij|S} \rangle$ is non-zero only if $l' = 2$. It implies that $V_{\text{dd}}$ would play its role only if a $d$-wave spatial excitation is accompanied. It is assumed that $\omega$ is so large that $\langle \psi_{ij|S} | V_{\text{dd}} | \psi_{ij|S} \rangle \ll 2\omega$. In this case the effect of $V_{\text{dd}}$ is suppressed so that it can be neglected. Note that, in general, $V_{\text{dd}}$ would be important in spin evolution where higher partial waves emerge. However, this is not the case of equilibrium state in strong isotropic trap at very low temperature.\[13\]\[15\] Furthermore, we consider a small condensate so that the size of the condensate is smaller than the spin healing length. In this case the single spatial mode approximation (SMA) is reasonable and is therefore adopted.\[16\]

Let the common spatial wave function be $\phi(r)$. Under the SMA, after an integration over the spatial degrees of freedom, we arrive at a model Hamiltonian

$$H_{\text{mod}} = \sum_{i<j} V'_{ij},$$

(2)

where $V'_{ij} = \sum_S g_S P_S$, $g_S = g_S \int |\phi(r)|^4 \,dr$.

For diagonalizing $H_{\text{mod}}$, the set of normalized and symmetrized Fock-states $|\alpha\rangle = |N^\alpha_3, N^\alpha_2, N^\alpha_1, N^\alpha_0, N^-\alpha_1, N^-\alpha_2, N^-\alpha_3\rangle$ are used as basis functions, where $N^\alpha_\mu$ is the number of particles in the $\mu$-spin-component, $\sum_\mu N^\alpha_\mu = N$ and $\sum_\mu \mu N^\alpha_\mu = M$, where $M$ is the magnetization. Since $|\alpha\rangle$ as a whole form a complete set, once the matrix elements $\langle \alpha' | H_{\text{mod}} | \alpha \rangle$ have been calculated, exact eigenenergies and eigenstates of $H_{\text{mod}}$ can be obtained via the diagonalization. Obviously, both the total spin $F$ and its $Z$-component $M$ are conserved when $V_{\text{dd}}$ is neglected.

Let the $i$-th eigenstate be denoted as $\psi_i$ with total spin $F(i)$ and magnetization $M(i)$. The state can be expanded as $\psi_i = \sum_\alpha c_\alpha |\alpha\rangle$. Since one can extract a particle from a Fock-state, one can also extract a particle from $\psi_i$ via the expansion as

$$\psi_i = \sum_\mu c_\mu \chi(1) \psi^i_\mu,$$

$$\psi^i_\mu = \sum_\alpha c_\alpha \sqrt{\frac{N^\alpha_\mu}{N}} |N^\alpha_\mu - 1, \cdots, 0, \cdots, 0\rangle,$$

(3)

where $\chi(1)$ is the spin-state of a $f = 3$ particle in component $\mu$ (from $-3$ to 3). With Eq. (3), we know that the probability of a particle in $\mu$ is just

$$P^i_\mu = \langle \psi^i_\mu | \psi^i_\mu \rangle.$$  

(4)

They fulfill $\sum_\mu P^i_\mu = 1$. $P^i_\mu$ is called the 1-body probability, and $NP^i_\mu$ is just the average population of the $\mu$ component.

If one more particle is further extracted, in a similar way, we have

$$\psi_i = \sum_\mu \chi(1) \chi(2) \psi^i_\mu.$$  

(5)

We define

$$P^i_{\mu \nu} = \langle \psi^i_\mu | \psi^i_\nu \rangle.$$  

(6)

They fulfill $P^i_{\mu \nu} = P^i_{\nu \mu} = \sum_\mu P^i_{\mu \nu} = 1$, and $P^i_{\mu \nu} = P^0_{\mu \nu}$. When two particles are observed simultaneously, obviously, the probability of one in $\mu$ and the other one in $\nu$ is $P^i_{\mu \nu} + P^0_{\mu \nu}$ (if $\mu \neq \nu$) or $P^i_{\mu \mu}$ (if $\mu = \nu$). $P^i_{\mu \nu}$ is called the correlation probability of spin-components.

Let Eq. (5) be rewritten as

$$\psi_i = \sum_{S,m_S} \left( \chi(1) \chi(2) \right)_{S,m_S} \sum_\mu C^{S,m_{S\mu},m_{S\mu} - \mu} \psi^i_{\mu,m_{S\mu} - \mu}.$$  

(7)

Then, the probability of a pair of particles coupled to $S$ and $m_S$ is

$$P^i_{S,m_S} = \sum_{\mu', \mu} C^{S,m_{S\mu},m_{S\mu} - \mu} C^{S,m_{S\nu},m_{S\nu} - \nu} \langle \psi^i_{\mu',m_{S\mu} - \mu} | \psi^i_{\mu,m_{S\mu} - \mu} \rangle.$$  

(8)

One can prove from symmetry that $P^i_{S,m_S} = P^i_{S,-m_S}$ when $M(i) = 0$, and the $2S + 1$ members $P^i_{S,m_S}$ are equal to each other when $F(i) = 0$. Furthermore, we define

$$\Psi_S^i = \sum_{m_S} P^i_{S,m_S},$$  

(9)
which is the probability that the spins of an arbitrary pair are coupled to $S$. In general, $\Psi_S^\text{free}$ can provide information on the possible existence of two-body substructures as shown below.

As an example, let the normalized pair-state be denoted as

$$
\Psi^\text{polar} = \gamma \tilde{P}_N [(\chi\chi)_{0}]^{N/2},
$$

(10)

where $\gamma = [N!(\frac{1}{2})^{N/2}((N/2)!)]^{1/2}$ is the constant for normalization (refer to Appendix I). Since

$$
\tilde{P}_N [(\chi\chi)_{0}]^{N/2} = \sum_{S,m_S} (\chi(1)\chi(2))_{S,m_S} B_{S,m_S}
$$

\[\tilde{P}_N - 2(\chi(1)\chi(2))_{S,m_S} [(\chi\chi)_{0}]^{(N-4)/2}, \]

(11)

where

$$
B_{S,m_S} = N(\delta_{S,0}\delta_{m_S,0} + (-1)^{m_S} 2(N/2 - 1)/7). \quad (12)
$$

By making use of the formulae in Appendix I, one can prove that all the $P^\nu_{m_S}$ of the pair-state are equal to $\frac{2(N-2)}{63(N-1)}$ with the only exception $P^\nu_{0,0} = \frac{9(N+5)}{63(N-1)}$. From these data, $\Psi_S^\text{polar}$ of the pair-state, denoted as $\Psi_S^\text{polar}$, are listed in Tab. I.

| $S$ | 0 | 2 | 4 | 6 |
|-----|---|---|---|---|
| $\Psi^\text{polar}$ | $5(N+5)$ | $10(N-1)$ | $15(N-1)$ | $20(N-1)$ |
| $\Psi_S^\text{free}$ | $6(N-1)$ | $6(N-1)$ | $6(N-1)$ | $6(N-1)$ |

Note that, if the two particles are completely free, simply from the geometry, we would have $\Psi_S^\text{free} = (2S + 1)/\sum_{S'}(2S' + 1)$, where $S'$ covers 0, 2, 4, and 6. Therefore, $\Psi_S^\text{free} = 0.036$, 0.179, 0.321, and 0.464 for $S = 0$, 2, 4, and 6, respectively. Whereas for the pair-state, $\Psi_S^\text{polar} = 0.143$, 0.158, 0.286, and 0.413 when $N \to \infty$. Thus the ratios $\Psi_S^\text{polar} / \Psi_S^\text{free}$ are 4.0, 0.89, 0.89, and 0.89, where the ratio with $S = 0$ is remarkably large. Thus the big ratio is a signal of the dominance of the singlet pairs.

The spin-spin correlation is not able to be studied perfectly by the MFT. The 1-body and correlational probabilities together will help us to understand better the spin-structures. In the fields of atomic and nuclear physics, it was found that the structures depend on $N$ sensitively (say, the property of an even-even nucleus is quite different from its neighboring even-odd nuclei). Since $N$ is assumed to be small in this paper, the $N$-dependence of condensates is also studied in the follows.

### III. POPULATIONS OF THE SPIN-COMPONENTS OF THE GROUND STATES

We shall first study the $^{52}\text{Cr}$ atoms as a representative of spin-3 species. These atoms have $g_0 = 59.40meV \cdot A^3$, $g_4 = 0.5178g_6$, and $g_2 = -0.0625g_6$, while $g_0$ is unknown. In what follows $G_\nu = g_0 \int |\phi(r)|^4 dr$ is considered as a unit of energy, and $g_0$ is variable. The 1-body probabilities $P^\nu_{\nu}$ are firstly studied.

When $N$ is even and $g_0 \to -\infty$, it has been proved that the ground state $\psi_1$ is exactly the pair-state $\Psi^\text{polar}$ written in Eq. (10). Obviously, the pair-state has $F = 0$. It is a common feature that $P^\nu_{\nu}$ of all the $F = 0$ states do not depend on $\nu$ due to the isotropism. Therefore, all of them are equal to $1/(2f + 1) = 1/7$. When $N$ is odd and $g_0 \to -\infty$, $\psi_1$ is just the odd pair-state written as

$$
\Psi_{\text{odd}−\text{polar},\nu} = \gamma' \tilde{P}_N [(\chi\chi)_{0}]^{(N-1)/2},
$$

(13)

where $\gamma' = [N![\frac{1}{2}(N-1)!(\frac{N-1}{2})!!]^{1/2}$ is the constant of normalization (refer to Appendix I). Obviously, this state has $F = 3$. The associated 1-body probability $P^\nu_{\text{odd}−\text{polar},\mu}$ has an analytical form as given in Tab. II (the derivation is referred to Appendix II). For the case with a large $N$, it is shown in this table that $P^\nu_{\text{odd}−\text{polar},\mu}$ depend on $N$ very weakly. Thus, the population of the unpaired particle has $\mu = 0$, we know from Tab. II that the average population with $\nu = 0$ is the largest and is nearly third times as large as those with $\nu \neq 0$. When $\mu \neq 0$, the populations with $\nu = \mu$ and $-\mu$ are the largest two and they are nearly two times as large as those with $\nu \neq |\mu|$. On the other hand, it is recalled that $P^\nu_{\text{polar}} = 1/7$ which is greatly different from $P^\nu_{\text{odd}−\text{polar},\mu}$. Thus, the populations of spin-components of a pair-state will undergo a great change when a particle with a given $\mu$ is added into the state. This will happen even when $N$ is very large. Such special even-odd dependence could be revealed by measuring the 1-body probabilities if the polar-state can be prepared.

| $\mu$ | $\nu = 0$ | $\nu = \mu$ | $\nu = -\mu$ | $\nu \neq |\mu|$ |
|-------|------------|-------------|-------------|----------------|
| $\nu = \nu$ | $\frac{2(N+3)}{2N+1}$ | $\frac{2(N-1)}{2N-1}$ | $\frac{N+1}{2N}$ | $\frac{3(N+2)}{2N}$ |

When $g_0$ increases from $-\infty$ but still negative, $\psi_1$ with an even $N$ would be still more or less close to $\Psi^\text{polar}$. If the magnitudes of $g_2$, $g_4$, and $g_6$ are small, then $\psi_1$ would be closer. However, for realistic $^{52}\text{Cr}$, $g_2$ and $g_6$ are not small. To see how large $\psi_1$ would deviate from the pair-state, $\langle \Psi^\text{polar}|\psi_1\rangle$ has been calculated. If $g_0/g_6 = -1$, $-2$, and $-4$, respectively, $\langle \Psi^\text{polar}|\psi_1\rangle = 0.838, 0.936, and 0.981$ when $N = 12$. This set of values would become $0.706, 0.841$, and 0.937 when $N = 18$. Thus the deviation is not small unless $g_0$ is very negative.

For $^{52}\text{Cr}$, the 1-body probabilities $P^\nu_{\psi_1}$ with $M = 0$ against $g_0/g_6$ are plotted in Fig. 2. The curves at the left side of Fig. 2b with an even $N$ are horizontal lines.
They have the same value $1/7$ implying that $\psi_1$ keeps $F = 0$. The curves at the left side of Fig. 2a with an odd $N$ are close to each other implying a weak dependence on $N$. They are flat and have their values $\approx 0.038$, which deviates explicitly from $P_{a,b,c}^{odd-polar,0} \approx 0.103$ given in Tab. III. It implies that the deviation between $\psi_1$ and $\psi_{odd-polar,0}$ is not small when $g_0 = -0.1$.

By comparing the right side of Fig. 2b with that of 2a, the even-odd dependence is clearly shown. In addition, the curves with $N = 15$ and 18 are distinguished. It implies that $N = 3K$ ($K$ is an integer) is special. It is recalled that, for spin-2 condensates with a sufficiently negative $g_0$, the ground state is formed by the triplex ($\eta_3 | \eta_0 \rangle, \eta_1 | \eta_0 \rangle$). The finding of the 3K-dependence in spin-3 condensates is a hint that 3-body substructures might exist as well.

In Fig. 2 the domain of $g_0$ is roughly divided into three regions. At the left side (region I) the curves depend on $g_0$ mildly, and the singlet pairs play an important role. At the right side (region III) the curves depend on $g_0$ also mildly, where three-body substructures might exist. In between (region II, roughly from $g_0/g_6 = 0$ to 0.1) the curves vary with $g_0$ very swiftly, implying a swift change in spin-structure. In addition, critical point may appear in this region (say, $g_0/g_6 = 0.079$) is a critical point when $N = 18$ and $M = 0$, where $P_{1}^{N}$ varies abruptly. Once $g_0$ crosses a critical point $F$ will change suddenly implying a transition of spin structure.

Incidentally, according to the MFT, there are also three regions. The phases of the ground state in these regions are named maximum polar(A), collinear polar(B), and biaxial nematic(C) in the Ref. 12 when $g_0$ varies from negative to positive. The associated spinors are $(1, 0, 0, 0, 0, 0, 1), (a, 0, b e^{i\theta}, 0, b e^{i\phi}, 0, a)$, and $(a, 0, b, 0, c, 0, d)$. The critical point between A and B is $g_0/g_6 = 0.079$. In the Ref. 13, the three phases are named the polar phase, the mixed phase, and the cyclic phase. The associated spinors are $(\cos \theta, 0, 0, 0, 0, 0, 0, \sin \theta)$, $(0, a, b, 0, a, 0)$ and $(a, 0, b, 0, b, 0, a)$, respectively (the third spinor may mix up with the second spinor in the mixed phase). In this paper a different language is used so that the structures can be understood via a different path.

IV. CORRELATIVE PROBABILITIES OF THE GROUND STATES

The curves at the left side of Fig. 2b are horizontal until the critical point. However, the spin-structures are in fact changing in this broad region. This example demonstrates that the information provided by the 1-body probabilities is not sufficient. Therefore, the correlative probabilities are further studied. Firstly, for the pair-state, the probabilities $P_{\mu \nu}^{polar}$ are given in Tab. III (the derivation is referred to Appendix III).

| $(\mu, \nu)$ | $(0, 0)$ | $(\mu \neq 0, -\mu)$ | $(\mu \neq 0, \mu)$ | otherwise |
|-------------|--------|-----------------|-----------------|----------|
| $P_{\mu \nu}^{polar}$ | $\frac{3(N+1)}{6(N-1)}$ | $\frac{2N+5}{6(N-1)}$ | $\frac{2(N-2)}{6(N-1)}$ | $\frac{N-2}{6(N-1)}$ |

It is shown that $P_{\mu \nu}^{polar}$ are all nearly independent on $N$ unless $N$ is small. The largest component is $P_{0,0}^{polar}$. The probabilities of being spin-parallel and spin-anti-parallel, i.e., $P_{\mu,\mu}^{polar}$ and $P_{\mu,-\mu}^{polar}$, are equal when $N \to \infty$.

Examples of $P_{\mu \nu}^{polar}$ of $\psi_1$ with an even $N$ are given in Fig. 3. The curves with $N = 18$ are also distinguished and jump up suddenly at the critical point. The jump is accompanied by a change of the total spin $F$ from 0 to 2 implying a transition. Since the curves vary rapidly in the neighborhood of the critical point, strong adjustment in structure happens right before and after the transition. The strong adjustment in the neighborhood of the critical point is a notable phenomenon. The curves with $N = 16$ and 20 are similar to each other. In particular, they keep their $F = 0$ and accordingly they do not have the sudden jump. The critical point will appear whenever $N$ is a multiple of 3, and will shift a little to the left when $N$ becomes larger (say, they appear at $g_0/g_6 = 0.252, 0.079,$
and 0.075, respectively, when \( N = 12, 18, \) and 24). The shift would be very small if \( \Delta N/N \) is small.

The curves of \( P^1_{\mu} \) with an odd \( N \) are in general very different from those with an even \( N \). They also exhibit the 3\( K \)-dependence and contain the critical points in region II. For an example, there are two critical points appearing at \( g_0/g_6 = 0.058 \) and 0.067 when \( N = 15 \) and \( M = 0 \). Accordingly, \( F \) jumps from 3 to 1, then to 2 when \( g_0 \) increases.

V. MIXING OF \( S = 0 \) AND 2 PAIRS

Let us study \( \Psi^1_{S} \), the probabilities of the spins of two particles coupled to \( S \). \( \Psi^1_{S} \) of \( \psi_1 \) is close to \( \Psi^\text{polar} \) when \( N \) is even and \( g_0 \to -\infty \). When \( g_0 \) is not so negative, examples of \( \Psi^1_{S}/\Psi^\text{free} \) are listed in Tab. \( \text{IV} \).\(^3\)

| \( \Psi^1_{S}/\Psi^\text{free} \) | \( S = 0 \) | \( S = 2 \) | \( S = 4 \) | \( S = 6 \) |
|-----------------|--------|--------|--------|--------|
| \( g_0/g_6 = -0.2 \) | 4.58   | 1.78   | 0.14   | 1.02   |
| \( g_0/g_6 = 0.07 \) | 2.44   | 1.90   | 0.50   | 0.89   |
| \( g_0/g_6 = 0.09 \) | 0.75   | 1.92   | 0.83   | 0.78   |
| \( g_0/g_6 = 0.5 \)  | 0.04   | 1.88   | 1.02   | 0.72   |
| \( g_0/g_6 = 1.0 \)  | 0.01   | 1.87   | 1.04   | 0.72   |

We found that \( \Psi^1_{S}/\Psi^\text{free} \) is quite large when \( g_0/g_6 = -0.2 \). It implies the preference for the singlet pairs. However, the four ratios \( \Psi^1_{S}/\Psi^\text{free} \) as a whole deviate explicitly from \( \Psi^\text{polar}/\Psi^\text{free} \). Therefore \( \psi_1 \) is quite different from the pair-state. When \( g_0 \) increases further, the ratio with \( S = 0 \) keeps on decreasing. In particular, it decreases very rapidly when \( g_0 \) is passing through the critical point. On the other hand, the probability of \( S = 2 \) pair remains to be larger. In particular, it becomes the largest when \( g_0 \) is larger than the critical value. Therefore, the dominance of the singlet pairs is gradually replaced by the \( S = 2 \) pairs. Hence, for \( N \) being even, we define a set of basis functions formed by the two kinds of pairs as

\[
\Phi_j^\text{pairs} = \beta_j P_N \{ [ (\chi \chi)_0 ]^K_2 [ (\chi \chi)_2 ]^K_2 
\]

\[
\cdots [ (\chi \chi)_{2,-2} ]^K_{-2} \},
\]

where \( j \) denotes the set \( (K_p, K_2, \cdots, K_{-2}) \) of non-negative integers, and their sum = \( N/2 \). \( \beta_j \) is for the normalization. The space expanded by \( \Phi_j^\text{pairs} \) is much smaller than that expanded by the Fock-state. Say, if \( N = 18 \) and \( M = 0 \), the numbers of Fock-states and \( \Phi_j^\text{pairs} \) are 3486 and 148, respectively. The eigenstates can be approximately expanded as

\[
\psi_i \approx \sum_j b_j \Phi_j^\text{pairs} \equiv \tilde{\psi}_i,
\]

where \( b_j \) can be obtained via a diagonalization of \( H_\text{mod} \) in the much smaller space (Note that \( \Phi_j^\text{pairs} \) are not exactly orthogonal to each other).

The overlap \( |\langle \tilde{\psi}_i | \psi_1 \rangle| \) of the approximate and exact ground states against \( g_0 \) is plotted in Fig. 4. The solid curve \( (N = 18) \) is extremely close to one when \( g_0 \) is smaller than the critical point. It confirms the physical picture that both the \( S = 0 \) and 2 pairs are building blocks. However, the solid curve has a sudden fall at the critical point. Thus the picture is spoiled when \( g_0 \) is larger, and we have to look for other structures. The dash curve \( (N = 16) \) represents the case without a transition, where a swift descending replaces the sudden fall.

VI. CANDIDATES OF THREE-BODY SUBSTRUCTURES AND THE TRIPLEX-STATES

In order to see whether 3-body substructures would exist in region III, let us first analyze a 3-body spin-3 system. Let

\[
\xi_{\sigma \lambda \lambda} = \beta \sigma \lambda P_N ( (\chi \chi) \sigma \lambda ) \lambda \lambda,
\]
be a spin-state of the 3-boson system, where two spins are firstly coupled to $\sigma$. Then, they are coupled to $\lambda$ and $m_\lambda$, the total spin and its Z-component. $\beta_{\sigma\lambda}$ is for the normalization. Totally there are $8$ independent $\xi_{\sigma\lambda}$ (the subscript $m_\lambda$ might be neglected) given in the top row of Tab.\textit{V}. Those not listed in the table are linear combination of them (Say, $\xi_{2,1} \equiv \xi_{1,1}$). Each of them represents a specific 3-body spin-structure. Incidentally, these eight $\xi_{\sigma\lambda}$ are exactly orthogonal to each other except $\xi_{2,3}$ and $\xi_{4,3}$.

By extracting two particles from $\xi_{\sigma\lambda}$, one can define and calculate the probabilities $p_{\sigma\lambda}^S$ that a pair of particles are coupled to $S$ in the 3-body states $\xi_{\sigma\lambda}$.

| $\sigma, \lambda$ | 2, 1 | 2, 2 | 3, 2 | 4, 2 | 5, 2 | 4, 3 | 5, 3 | 6, 3 | 6, 4 |
|------------------|------|------|------|------|------|------|------|------|------|
| $p_{0}^{2\lambda}$ | 0.524 | 0.094 | 0.108 | 0.011 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 |
| $p_{1}^{2\lambda}$ | 0.476 | 0.211 | 0.753 | 0.061 | 0.234 | 0.727 | 0.515 | 0.515 | 0.515 |
| $p_{2}^{\sigma\lambda}$ | 0.211 | 0.003 | 0.328 | 0.353 | 0.273 | 0.485 | 1.000 | 1.000 | 1.000 |

\textbf{TABLE V: The probabilities $p_{\sigma\lambda}^S$ that a pair of particles are coupled to $S$ in the 3-body states $\xi_{\sigma\lambda}$.}

\[ \Phi_{j}^{\text{triplex}} = \beta_{j}^{\prime} \hat{P}_{N} \{ [\xi_{4,3,3}]^{K_{1}} [\xi_{4,3,2}]^{K_{2}} \cdots [\xi_{4,3,-3}]^{K_{-3}} \}, \]

\textbf{TABLE VI: $\rho_{\sigma\lambda}^i$ of the ground state with $N = 18$. The parameters of interaction associated with the cases A and B are given in the text.}

| $\sigma, \lambda$ | 2, 1 | 2, 2 | 3, 2 | 4, 2 | 5, 2 | 4, 3 | 5, 3 | 6, 3 | 6, 4 |
|------------------|------|------|------|------|------|------|------|------|------|
| $\rho_{0}^{i\lambda}(A)$ | 0.999 | 0.119 | 0.425 | 0.032 | 0.069 | 1.813 | 0.967 | 0.204 | 0.967 |
| $\rho_{0}^{i\lambda}(B)$ | 3.485 | 1.180 | 1.011 | 2.399 | 1.231 | 0.728 | 0.752 | 0.390 | 0.390 |

It is shown that $\rho_{4,3}^i(A)$ is particularly large. Therefore $\xi_{4,3}$ is very preferred by the ground state as expected, and one might further expect that the triplex $\xi_{4,3}$ might play a role as a building block. To clarify, we introduce a set of basis functions for the case with $N = 3K$ as

\[ \Phi_{j}^{\text{triplex}} = \beta_{j}^{\prime} \hat{P}_{N} \{ [\xi_{4,3,3}]^{K_{1}} [\xi_{4,3,2}]^{K_{2}} \cdots [\xi_{4,3,-3}]^{K_{-3}} \}, \]

in which $\sum_{\mu} K_{\mu} = N/3$ and $\sum_{\mu} \mu K_{\mu} = M$. For $N = 18$ and $M = 0$, there are totally 58 basis functions, much smaller than 3486. After a diagonalization of $H_{\text{mod}}$ in the 58-dimensional space, we obtain the approximate eigenstates $\psi_{i}^{\text{triplex}} = \sum_{j} d_{j} \Phi_{j}^{\text{triplex}}$ to be compared with the exact eigenstates $\psi_{i}$. It turns out that $\langle \psi_{i}^{\text{triplex}} | \psi_{i} \rangle = 0.999$, 0.996, and 0.990 for $i = 1, 2,$ and 3, respectively (they are the three lowest states having $F(i) = 0, 4,$ and 6, respectively). Such a great overlap confirms that, similar to the spin-2 condensates, the triplex-structure exists also in spin-3 condensates. However, the triplex of spin-2 condensates has $\lambda = 0$, thus there is only one kind of building blocks. Whereas the triplex now has $\lambda = 3$ and therefore has $2\lambda + 1 = 7$ kinds of building blocks. This leads to complexity.

We go back to the case of $^{52}\text{Cr}$ atoms. Let $g_{2}$, $g_{4}$, and $g_{6}$ be given at the experimental values and $g_{0}/g_{6}$ is given at some presumed values. Note that, in addition to $g_{0}$, $g_{4}$ is also quite positive. Since $\xi_{4,3}$ has a large $P_{4}^{\sigma\lambda}$, it is no more superior. Instead, $\xi_{2,4}$ might be important due to having a very small $P_{4}^{\sigma\lambda}$. When $g_{0}/g_{6} = 0.5$, the ratios denoted as $\rho_{0}^{i\lambda}(B)$ have been calculated and listed in the
The ratios theoretically the existence of stable 2-body and 3-body theory is used in this paper. We have shown another set of basis functions as

$$\Phi^{i,\text{tri}}_j = \beta''_j \hat{P}_N \{ \prod_{m_a} [\xi_{2,1,m_a}^{K_a,m_a}] \} \prod_{m_b} [\xi_{2,4,m_b}^{K_b,m_b}], \quad (18)$$

where $m_a$ is from $-1$ to $1$, $m_b$ is from $-4$ to $4$, $\sum_{m_a} K_a m_a + \sum_{m_b} K_b m_b = N/3$, and $\sum_{m_z} m_a K_a m_a + \sum_{m_z} m_b K_b m_b = M$. The number of $\Phi^{i,\text{tri}}_j$ is 758 when $N = 18$ and $M = 0$. However, only 615 of them are linearly independent. With $\Phi^{i,\text{tri}}_j$, we have calculated the approximate eigenstate $\psi^{i,\text{tri}}_j$ at five values of $g_0/g_6$, and the overlaps $|\langle \psi^{i,\text{tri}}_j | \psi_i \rangle|$ are listed in Tab. VII. It is reminded that $g_0/g_6 = 0.079$ is a critical point. Once $g_0/g_6$ is larger than the critical point, the overlaps are very close to one. Thus the picture of trplexes is theoretically confirmed. Whereas this picture is not well established when $g_0$ is smaller than the critical point, where the $S = 0$ and 2 pairs are dominant.

VII. FINAL REMARKS

Instead of using the MFT, a language from the few-body theory is used in this paper. We have shown theoretically the existence of stable 2-body and 3-body structures as building blocks in small spin-3 condensates. The ratios $P_{\text{tri}}/P_{\text{free}}$ and $Q_{\text{tri}}/Q_{\text{free}} \equiv \rho_{\text{tri}}^2$ defined in this paper are crucial in the search of these basic constituents. The reason leading to the appearance of these constituents is explained based on the feature of interaction. Whereas, in the MFT, the physics underlying the appearance of a specific spinor is not easy to clarify.

The calculation in this paper concerns only small spin-3 condensates ($N \leq 24$). For spin-2 condensates, it has been proved theoretically that the fact that pairs and trplexes appear as building blocks does not depend on $N$ (In fact, the picture of the trplexes would become even clearer when $N \to \infty$ [7]). It has also been proved that the existence of the pairs in spin-3 condensates does not depend on $N$. [7,17] Thus the existence of trplexes as building blocks in large spin-3 condensates is very probable, nonetheless it deserves a further study.

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Appendix A: Iteration relations

For the pair-state and odd-pair-state the following equations relating a $N$-body and a $(N-2)$-body systems are very useful:

$$N_0^{(N)} = \langle \hat{P}_N | (\chi \chi)_0 | \hat{P}_N | (\chi \chi)_0 \rangle^{N/2}, \quad (A1)$$

$$N_{\text{odd}}^{(N)} = \langle \hat{P}_N \chi_{\mu} | (\chi \chi)_0 | \hat{P}_N \chi_{\mu} \rangle^{(N-1)/2}, \quad (A2)$$

$$N_{\text{odd}}^{(N-2)} = \langle \hat{P}_N \chi \chi S_{m_\mu m_\nu} | (\chi \chi)_0 | \hat{P}_N \chi \chi S_{m_\mu m_\nu} \rangle^{(N-2)/2}, \quad (A3)$$

where $\hat{P}_N$ denotes a summation over the $N!$ permutation terms, Eq. (A3) holds only if $S \neq 0$ (if $S = 0$, then Eq. (A1) should be used). Making use of these equations related matrix elements can be derived via iteration. For examples, the constant of normalization $\gamma$ can be obtained from Eq. (A1), $\gamma'$ from Eq. (A2).

Appendix B: The 1-body probabilities of odd-pair-states

One can extract a particle (say, particle 1) from an odd-pair-state as

$$\hat{P}_N \chi_{\mu} | (\chi \chi)_0 \rangle^K = \sum_{\nu} \chi_{\nu} (1) \langle \delta_{\mu,\nu} \hat{P}_{N-1} | (\chi \chi)_0 \rangle^K$$

$$- (N-1) (\chi \chi S_{\mu,\nu})$$

$$\hat{P}_{N-1} | (\chi \chi) S_{\mu,\nu} \rangle | (\chi \chi)_0 \rangle^{K-1}. \quad (B1)$$

where $K = (N-1)/2$, the Clebsch-Gordan coefficients have been introduced, and only even $S$ are included in the summation. Then, from the definition of the 1-body probability, we have

$$P_{\nu}^{\text{odd-polar}} = \delta_{\mu,\nu} \frac{4K + 7}{4} \frac{N_0^{(N-1)}}{N_{\text{odd}}^{(N)}}$$

$$+ \frac{4K^2}{4} \sum_{S} (C_{S,\mu,\nu}^3)^2 \frac{N_{S,\mu,\nu}^{(N-1)}}{N_{\text{odd}}^{(N)}}. \quad (B2)$$

It is mentioned that the expression of $\mathcal{A}_{S,\mu,\nu}^{(N-1)}$ depends on whether $S$ is zero or nonzero. With this in mind, after a simplification, Eq. (B2) leads to the expressions given in the text.
TABLE VII: The overlap $|\langle \psi_{i}^{\text{tri,tri}} | \psi_{j} \rangle|$, where $\psi_{i}^{\text{tri,tri}}$ is the triplex-state formed by using $\xi_{2,1,m_{i}}$ and $\xi_{2,4,m_{i}}$ as building blocks. $N = 18$ and $12$, and $M = 0$ are given. The parameters $g_{2}$, $g_{4}$, and $g_{6}$ are from the experimental data of $^{52}$Cr, while $g_{0} / g_{6}$ is denoted as $g'$ given at five values. $i'$ is so chosen that, if $\psi_{i}$ is the $k$-th eigenstate of the series with $F = F(i)$, then $\psi_{i'}^{\text{tri,tri}}$ is also the $k$-th state of the series of triplex-states with $F(i') = F(i)$. $F(i)$ are given in the parentheses following the overlaps.

| $|\langle \psi_{i}^{\text{tri,tri}} | \psi_{j} \rangle|_{N=18}$ | $|\langle \psi_{i}^{\text{tri,tri}} | \psi_{j} \rangle|_{N=12}$ |
|-----------------------------------------------|-----------------------------------------------|
| $g' = -1$ | $g' = 1$ |
| 0.908 (0) | 0.915 (4) |
| 0.870 (2) | 0.861 (0) |
| 0.955 (0) | 0.959 (4) |
| 1.000 (2) | 1.000 (0) |
| 0.998 (2) | 0.999 (0) |
| 0.983 (2) | 0.981 (2) |

Appendix C: The correlative probabilities of pair-states

One can extract two particles (say, 1 and 2) from a pair-state as

$$\hat{P}_{N}[(\chi \chi)_{0}]^{N/2} = N \sum_{\mu \nu} \chi_{\mu}(1) \chi_{\nu}(2) \delta_{\mu, -\nu} C_{3, \mu, 3}^{0, 0} \hat{P}_{N-2}[(\chi \chi)_{0}]^{(N-2)/2}$$

$$+ (N - 2) \sum_{S} (2S + 1) U \begin{pmatrix} 3 & 3 & 0 \\ 3 & 3 & 0 \\ S & S & 0 \end{pmatrix} C_{3, \mu, 3}^{0, 0} \hat{P}_{N-2}[(\chi \chi)_{S, -\nu}][(\chi \chi)_{0}]^{(N-4)/2} \quad (C1)$$

where the Clebsch-Gordan and $9j$-coefficients have been introduced, and only even $S$ are included in the summation. Then, from the definition of the correlative probability, we have

$$P_{\mu \nu}^{\text{polar}} = \left( \frac{N}{2} \right) C_{3, \mu, 3}^{0, 0} \hat{P}_{N}[(\chi \chi)_{0}]^{N/2}$$

$$+ (N - 2) \sum_{S} \left( C_{3, \mu, 3}^{S, \mu + \nu} \right)^{2} \hat{P}_{N-2}[(\chi \chi)_{S, -\nu}] \quad (C2)$$

After a simplification, Eq. (C2) leads to the expressions given in the text.

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[15] The suppression of $V_{dd}$ in strong isotropic trap can also be seen under the framework of MFT. In this theory, the effect of $V_{dd}$ is embodied by the factor $c_d \Gamma_0$, where $c_d$ is the strength and is usually small ($c_d \approx 0.0036g_6$ for $^{52}\text{Cr}$), and $\Gamma_0 = \int dR dr |\phi(r_1)|^2 |\phi(r_2)|^2 Y_{20}(\hat{r})/|r|^3$, where $\phi(r_i)$ is the spatial wave function of the $i$-th particle, $R = (r_1 + r_2)/2$, and $r = r_1 - r_2$. A part of the integrand can be in general expanded as $|\phi(r_1)|^2 |\phi(r_2)|^2 = \sum_{l_a, l_b, L} B_{l_a, l_b, L}(R, r)(Y_{l_a}(\hat{R})Y_{l_b}(\hat{r}))_L$, where $l_a$ and $l_b$ denote the partial waves and they are coupled to $L$. Since $\phi$ is close to be isotropic when the trap is strong, the $L \neq 0$ terms can be neglected. This leads to $\Gamma_0 = 0$. Thus the effect of $V_{dd}$ is suppressed.

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