Fragmented many-body states of a spin-2 Bose gas

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(Received 12 February 2015; revised manuscript received 9 April 2015; published 4 June 2015)

We investigate the fragmented many-body ground states of a spin-2 Bose gas in zero magnetic field. We point out that the exact ground state is not simply an average over rotationally-invariant mean-field states, in contrast to the spin-1 case with even number of particles N. While for some certain parameters the exact ground state is an averaged mean-field state like in the spin-1 case, for other parameters this is not so. We construct the exact ground states and compare them with the angular-averaged polar and cyclic states. The angular-averaged polar states in general fail to retrieve the exact eigenstate at $N \geqslant 6$ while angular-averaged cyclic states sustain only for N with a multiple of 3. We calculate the density matrices and two-particle density matrices to show how deviant the angular-averaged state is from the exact one.

DOI: 10.1103/PhysRevA.91.063603 PACS number(s): 03.75.Mn, 03.75.Hh, 67.10.Ba

I. INTRODUCTION

Since the advancement of optically trapped Bose-Einstein condensate (BEC) [1], spinor BEC [2] has provided a paradigm to study magnetism, spin textures, topological excitations, and quantum dynamics of associated many-body ground states [3,4]. The quantum phases of spin-f BEC can be ferromagnetic or polar for $f = 1,2$ [5,6], or cyclic ($f = 2$) [7–9] depending on two-body s-wave scattering lengths a_F of even total spin F' up to $2f$. Uniaxial and biaxial spin nematic phases can also be identified in spin-2 case when the degeneracy in polar phase is lifted by thermal or quantum fluctuations [10,11]. Higher spin Bose gas can involve even more complicated phases [12–15]. Rich spin mixing dynamics has been used to observe the ferromagnetic [16] and antiferromagnetic (polar) properties [17], respectively, for spin-1 ^{87}Rb and ^{23}Na Bose gases. In spin-2 cases, polar phase is the likely phase for ^{87}Rb [18,19]. Recent experimental developments in spinor BEC involve spin textures [20] and spin dynamics [21,22] under quadratic Zeeman shift. There are also studies of quantum phase transitions by Faraday rotation spectroscopy [23] or adiabatic microwave fields [24] and spin coherence measurements by Ramsey interferometry [25,26].

A condensate of bosons forms when one of its single-particle wave functions is macroscopically occupied [27]. The fragmentation of BEC becomes feasible when multiple macroscopic single-particle densities are degenerate in spinor Bose gases [28] though it is fragile in the presence of weak external magnetic fields or symmetry-breaking perturbations [29]. Lately many interests in fragmented BEC include dynamical formation of two-dimensional fragmented BEC [30], quadratic Zeeman effect on spin fragmentation [31,32], and fragmented many-body ground states with anisotropic long-range interactions [33] or trapping potentials [34]. It has been proposed that signatures of fragmentation can be probed by measuring density-density correlations [35], while fragmentation resulting from Goldstone magnon instability [36] and spin-orbit coupling [37] are also investigated.

The fragmented structure of the ground state in spin-1 Bose gases [29,38,39] originates from the rotational invariance in spin degrees of freedom. The symmetry-breaking mean-field (MF) treatment fails in describing the exact ground state for presumption of single spin coherent condensate. For scattering lengths obeying $a_2 > a_0$, the MF state is polar, but the exact ground state is fragmented and, for even number of particles N, can be viewed as a collection of two-particle spin singlets. This exact ground state has equal populations in the magnetic sublevels with large number fluctuations of order N [29], which is very different from MF states. It is claimed [39] that this exact ground state can be understood as the angular average of the MF polar states as an analog to the relation between Fock and coherent states in a double-well system [39]. This remains the view adopted by the most recent review articles [3,4]. Is this perspective of angular-averaged states universal and applicable in constructing the exact ground states for larger spins? In this paper, we investigate many-body ground states of a spin-2 Bose gas and demonstrate how angular-averaged states are unable to construct them except in certain cases. That the angular averaged MF states is the exact ground state is just a coincidence in the spin-1 system. We address the inapplicability of the angular-averaging process and show how the angular-averaged MF state deviates from the exact eigenstates by studying the two-particle density matrices.

II. SPIN-2 BOSE GAS

For a spin-f Bose gas at low temperature, the two-body particle interaction involves only scattering channels of even total hyperfine spin F' states up to $2f$ [5]. We shall consider the single-mode approximation (SMA) where the spatial part of the wave function is the same for all spin sublevels such that the field operator $\hat{\psi}_m(\mathbf{r}) = \sqrt{\rho(\mathbf{r})}\hat{a}_m$ with the density $\rho(\mathbf{r})$ and spinor operator $\hat{a}_m$. Since the spatial part is frozen, the effective Hamiltonian (in a zero magnetic field, to which we shall limit ourselves) involves only the interaction V, which reads [7]

$$V = \frac{1}{2}\int d\mathbf{r}\rho^2\Bigg(\sum_{m,m'=-2}^{2}\alpha\hat{a}_m^\dagger\hat{a}_{m'}^\dagger\hat{a}_{m'}\hat{a}_m + \sum_{\substack{m,n,m',\\ n'=-2}}^{2}\beta\hat{a}_m^\dagger\hat{a}_{m'}^\dagger\mathbf{f}_{mn}\cdot\mathbf{f}_{m'n'}\hat{a}_{n'}\hat{a}_n + \sum_{\substack{m,n,m',\\ n'=-2}}^{2}5\gamma\hat{a}_m^\dagger\hat{a}_{m'}^\dagger\langle 2m;2m'|00\rangle\langle 00|2n;2n'\rangle\hat{a}_n\hat{a}_{n'}\Bigg), \quad (1)$$

where the coefficients are $\alpha = (4g_2 + 3g_4)/7$, $\beta = (g_4 - g_2)/7$, and $\gamma = (g_0 - g_4)/5 - 2(g_2 - g_4)/7$. Here the interaction parameters $g_F \equiv 4\pi\hbar^2 a_F/M$ with the mass of the atom M and s-wave scattering length a_F, and $\langle 00|2n;2n'\rangle$ is the Clebsh-Gordan coefficient for the overlap between the states with two spin-2 bosons of $m_z = n,n'$ and the spin singlet $|00\rangle$.

In MF theory, bosons condense. Particles macroscopically occupy a single quantum state which can be described by a spin-2 wave function $(\varphi_{-2},\ldots,\varphi_2)$. In our case, there are three phases characterized by two order parameters of magnetization $\langle \hat{f}\rangle \equiv \sum_{m=-2}^{2} m\varphi_m^*\varphi_m$ and spin-singlet pair amplitude $\langle \hat{\Theta}_2\rangle$ [7,8], where

$$\hat{\Theta}_2 \equiv \sum_{m=-2}^{2} \sqrt{5}\langle 00|2m;2-m\rangle \hat{a}_m\hat{a}_{-m}$$

$$= 2\hat{a}_2\hat{a}_{-2} - 2\hat{a}_1\hat{a}_{-1} + \hat{a}_0^2 \quad (2)$$

is an operator which annihilates a singlet pair. That is, we have $\langle \hat{\Theta}_2\rangle = \sum_{m=-2}^{2}(-1)^m \varphi_m\varphi_{-m}$. There are three phases. The ferromagnetic (F) phase has a finite $\langle \hat{f}\rangle$ and zero $\langle \hat{\Theta}_2\rangle$, while the polar phase (P) has $\langle \hat{\Theta}_2\rangle = 1$ without $\langle \hat{f}\rangle$. When $\beta,\ \gamma > 0$, the cyclic (C) phase has the lowest mean-field energy for both zero $\langle \hat{\Theta}_2\rangle$ and $\langle \hat{f}\rangle$, breaking the time-reversal symmetry. The phase boundary between F and polar phases is delineated by the line $4\beta = \gamma$. The phase diagram is as shown in Fig. 1(a) [7,8]. Representative wave functions are (1,0,0,0,0) for F; $(1,0,0,\sqrt{2},1)$, which is equivalent by rotation to $(1,0,\sqrt{2},0,-1)$ for C [14]. Within the mean field, the polar phase P can have wave functions P0 = (0,0,1,0,0) or P2 = (1,0,0,0,1), or any real linear combinations thereof [40] (apart from rotations). This degeneracy, however, is lifted by fluctuations [10,11]. The resulting phase diagram, which we shall call the mean-field-plus (MF^+) phase diagram, is shown in Fig. 1(a). We note that P0(2) can be also represented by the polynomial forms via spherical harmonics as $(2z^2 - x^2 - y^2)$ and $(x^2 - y^2)$, respectively [14,40]. For ease of referral later, we shall call the regions in (β,γ) parameter space occupied by the F, C, P phases as F, C, P regions.

III. MANY-BODY GROUND STATES

Let us now discuss the many-body ground states of a spin-2 Bose gas in zero magnetic field with SMA [8,41,42]. For a given N, the many-body ground states are characterized by two quantum numbers F and τ. F is the total spin, and the integer quantum number τ can be interpreted as the number of particles other than spin-singlet pairs; therefore τ is given by $3n_{30} + \lambda$ [8,42] where n_{30} is the number of spin-singlet trios and the integer λ indicates particles other than spin-singlet pairs and trios. These states are also eigenstates of the operator $\hat{\Lambda} \equiv \hat{\Theta}_2^\dagger\hat{\Theta}_2$ with eigenvalues $\Lambda = N(N+3) - \tau(\tau+3) = (N-\tau)(N+3+\tau)$, from which τ can be evaluated. The exact ground state energy is proportional to $\beta F(F+1) - \gamma\tau(\tau+3)$ aside from a term depending only on N. The phase diagram derived by minimizing the ground state energy is as sketched in Fig. 1 for $N = 2$ to 9. The line that separates the two phases in the $\beta < 0$, $\gamma < 0$ region is given by $(4N+2)\beta/(N+3) = \gamma$ for N even and $(4N+6)\beta/(N+4) = \gamma$ for N odd [42], which approaches the MF phase boundary in the thermodynamic limit.

The wave functions listed in Fig. 1 are constructed according to the eigenvalues F and τ which minimize the energy.

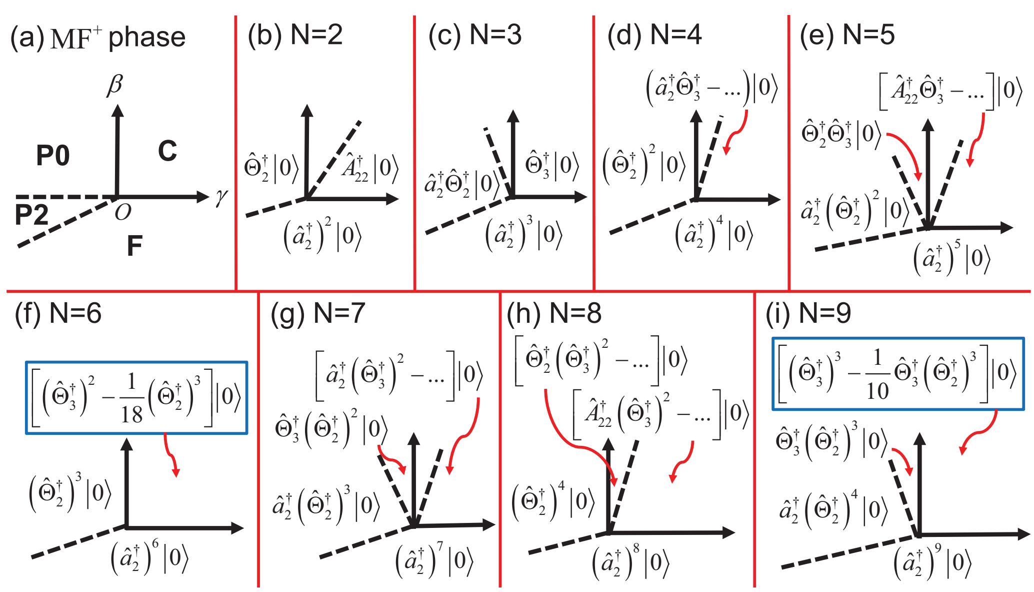

FIG. 1. (Color online) Mean-field-plus (MF^+) phase diagram and many-body ground states of spin-2 Bose gas in parameter space (γ,β). (a) Mean-field-plus phase diagram: ferromagnetic (F), polar (P0 and P2), and cyclic (C) phases. (b–i): phase diagram for exact many-body states with finite number of particles from $N = 2-9$. The form of the many-body ground states is shown. These states are constructed by spin-singlet pairs ($\hat{\Theta}_2^\dagger$) and trios ($\hat{\Theta}_3^\dagger$), and in certain regions, creation operator $a_2^\dagger$ ($A_{22}^\dagger$) for a single particle (pair of particles) with $f = 2, m = 2$ is also necessary (see text for definition of these operators). States that involve $\hat{a}_2^\dagger$ or $\hat{A}_{22}^\dagger$ explicitly are degenerate with their partners obtained by rotational symmetry (not shown). Dots in the formulas, when the complete expressions are not given, indicate that linear superposition with other terms is required. Wave functions shown here are not normalized. Dashed lines indicate the (schematic) phase boundaries.

The wave functions with appropriate quantum numbers F and τ can be written directly using their physical interpretation and, when necessary, supplemented with direct evaluation of τ (or equivalently Λ, which can be directly computed using the corresponding operator). In the ferromagnetic region F, they are $(\hat{a}_2^\dagger)^N|0\rangle$, hence identical with the mean-field states. (Here $|0\rangle$ denotes the vacuum.) For the polar P region, wave functions differ according to whether N is even or odd. For even N, the wave functions are $(\hat{\Theta}_2^\dagger)^{N/2}|0\rangle$ corresponding to $\tau = 0$, $F = 0$, and maximum possible Λ, which are $N(N+3)$ as can be seen in Eq. (A7),

$$\hat{\Theta}_2^\dagger \hat{\Theta}_2 (\hat{\Theta}_2^\dagger)^{N/2}|0\rangle = N(N+3)(\hat{\Theta}_2^\dagger)^{N/2}|0\rangle.$$

For odd N, the states that appear near the $-\gamma$ axis have wave functions $\hat{a}_2^\dagger(\hat{\Theta}_2^\dagger)^{(N-1)/2}|0\rangle$ (up to rotations) again correspond to states with maximum possible Λ, which are now $(N-1)(N+4)$ with $\tau = 1$ and $F = 2$. Near the $+\beta$ axis but still $\gamma < 0$, the states (for $N \geqslant 3$) have the form $\hat{\Theta}_3^\dagger(\hat{\Theta}_2^\dagger)^{(N-3)/2}|0\rangle$ where

$$\hat{\Theta}_3^\dagger = -\sqrt{6}\hat{a}_2^\dagger\hat{a}_0^\dagger\hat{a}_{-2}^\dagger + \frac{3}{2}(\hat{a}_1^\dagger)^2\hat{a}_{-2}^\dagger + \frac{3}{2}(\hat{a}_{-1}^\dagger)^2\hat{a}_2^\dagger - \sqrt{\frac{3}{2}}\hat{a}_1^\dagger\hat{a}_0^\dagger\hat{a}_{-1}^\dagger + \frac{1}{\sqrt{6}}(\hat{a}_0^\dagger)^3 \quad (3)$$

is an operator which creates a spin-0 trio (not normalized). These states have $\tau = 3$ [see Eq. (A6)] and $\Lambda = (N-3)(N+6)$ with $F = 0$.

In region C, if the particle numbers are multiple of 3, the ground state wave functions are singlets constructed by $\hat{\Theta}_3^\dagger$ and $\hat{\Theta}_2^\dagger$ with the eigenvalue $\Lambda = 0$. The wave functions are indicated in Fig. 1, and their derivation can be found in Eqs. (A8) and (A9). For other N, the C region is divided into two parts. The states near the $+\beta$ axis and $\gamma > 0$ are again spin singlets. If $N = 2(\text{mod}3)$, hence $N = 3R+2$, they are given by $\hat{\Theta}_2^\dagger|\Psi_{3R}\rangle$ (with $\tau = 3R$ and $F = 0$) where $|\Psi_{3R}\rangle$ is the corresponding ground state in region C for $3R$ particles. For $N = 1(\text{mod}3)$ and hence $N = 3R+4$ for integer R (when $N \geqslant 4$), then the wave functions are $(\hat{\Theta}_2^\dagger)^2|\Psi_{3R}\rangle$ and again $\tau = 3R$. For the N shown in Fig. 1, these states happen to be the same as the states near the $+\beta$ axis on the $\gamma < 0$ side so that they are the same phase, but this needs not hold for larger particle numbers $N \geqslant 11$. The states near the $+\gamma$ axis with $\beta > 0$ have instead finite magnetization of $F = 2$, which involve single- and two-particle creation operators of $\hat{a}_2^\dagger$ and $\hat{A}_{22}^\dagger$ (see its definition in Sec. V), respectively. We shall not discuss them in detail since they are not directly relevant here in the context of rotationally invariant states. We also note that Fig. 1 agrees with the results in Ref. [43].

IV. ANGULAR-AVERAGED MEAN-FIELD STATES

Now we turn to the angular-averaged MF states and compare with the corresponding exact eigenstates. First, we recall the corresponding results for spin-1. The MF ferromagnetic state corresponds to the exact solution. Their angular average actually vanishes. The polar mean-field state has a finite average only for N even and gives the correct exact many-body state [39]. We then demonstrate how for spin-2 the averaging process enables the fragmentation in both the polar and cyclic phases, but in general it fails to correctly construct the corresponding exact eigenstates at a given point (β,γ) in parameter space.

A. Polar states

The situation for the ferromagnetic state is exactly the same as the spin-1 case. We now consider the angular-averaged polar state of P0(2). Starting from the reference state (0,0,1,0,0), the state obtained by rotations via the Euler angels α,β,γ, which we denote collectively as $\hat{\Omega}$, is given by $\varphi_m^{P0}(\hat{\Omega}) = D_{m,0}^{(2)}(\hat{\Omega})$ where the matrix $D_{m,m'}^{(2)}(\hat{\Omega})$ is the spin-2 irreducible representation of the rotation operator [44] (see also Appendix B). The general (unnormalized) rotationally invariant state is constructed via

$$|\Psi\rangle_{av} = \frac{1}{\sqrt{N!}}\int_{\hat{\Omega}}[\hat{a}^\dagger(\hat{\Omega})]^N\ |0\rangle, \quad (4)$$

where we have defined $\int_{\hat{\Omega}} \equiv \int_0^{2\pi}\frac{d\alpha}{2\pi}\int_0^{\beta}\frac{d\beta\sin\beta}{\pi}\int_0^{2\pi}\frac{d\gamma}{2\pi}$. For our polar state P0, we thus use $\hat{a}^\dagger(\hat{\Omega}) \to \sum_m \hat{a}_m^\dagger\varphi_m^{P0}(\hat{\Omega})$. We call the resulting state $|\Psi_{P0}\rangle_{av}$. It is straightforward to evaluate the angular integrals. We find that $|\Psi_{P0}\rangle_{av}$ retrieves the exact ground states for even $N = 2,4$. For odd $N = 3,5,7$, we recover the spin singlet state located near the $+\beta$ axis as indicated in Fig. 1 (see more details in Appendix A). (Obviously the angular average cannot produce the states with finite magnetization near the $-\gamma$ axis.) However, for even $N \geqslant 6$ and odd $N \geqslant 9$, the angular-averaged states fail to construct the exact ground states. For example, for $N = 6$ it gives rather

$$|\Psi_{P0}\rangle_{av} = \frac{1}{7\times 11\times 13\sqrt{6!}}[5\times 3^2(\hat{\Theta}_2^\dagger)^3 + 3\times 2^4(\hat{\Theta}_3^\dagger)^2]|0\rangle,$$

which is in fact not even an eigenstate of the Hamiltonian in Eq. (1).

Similarly for P2, we can construct angular-averaged states as in Eq. (4) except now we use $\hat{a}^\dagger(\hat{\Omega}) \to \sum_m \hat{a}_m^\dagger\varphi_m^{P2}(\hat{\Omega})$ with $\varphi_m^{P2}(\hat{\Omega}) = \frac{1}{\sqrt{2}}(D_{m2}^{(2)} + D_{m,-2}^{(2)})(\hat{\Omega})$. In this case the angular average vanishes if N is odd. For N even again it produces the correct ground states for $N = 2,4$ but fails again at 6.

Actually why the angular averaged mean-field states can or cannot produce the many-body state is now clear. For N up to 5, the exact many-body singlet states are unique. Since angular averaged mean-field states must either be zero or they must be a rotationally invariant, they must either vanish or produce the singlet states. This is actually independent of whether the starting mean-field state is the corresponding ground state for the given parameters in the Hamiltonian. For $N = 6,8,9$, the many-body singlet states are no longer unique. The angular average, if it is not zero, just produces some linear combinations of these singlets. The resulting states have nothing to do with the ground state solutions of the Hamiltonian. That the angular average of the polar state for spin-1 produces correctly the exact many-body state for even N is purely because that, for spin-1, this singlet is unique.

Let us also consider the angular-averaged states for a linear combination of both P0(2) and use $\varphi_m^P(\hat{\Omega}) \equiv \cos\theta D^{(2)}_{m,0}(\hat{\Omega}) + \sin\theta[D^{(2)}_{m,2}(\hat{\Omega}) + D^{(2)}_{m,-2}(\hat{\Omega})]/\sqrt{2}$ in Eq. (4). For $N = 6$, and the angular-averaged polar state becomes (see Appendix C)

$$|\Psi_P(\theta)\rangle_{av} = \frac{1}{1001\sqrt{6!}}[(47 - 2\cos 6\theta)(\hat{\Theta}_2^\dagger)^3 + (12 + 36\cos 6\theta)(\hat{\Theta}_3^\dagger)^2]|0\rangle, \quad (5)$$

which in general again fails to become an eigenstate of Eq. (1). The θ dependence obtained above can be understood as follows. In the Cartesian representation, the general polar state is $\cos\theta(2z^2 - x^2 - y^2)/\sqrt{6} + \sin\theta(x^2 - y^2)/\sqrt{2}$. $\theta \to -\theta$ is equivalent to interchanging x and y, whereas $\theta \to \pi/3 - \theta$ has the effect of interchanging y and z as well as a sign change in the wave function. It follows that the angular averaged state must be invariant under $\theta \to -\theta$, while under $\theta \to \pi/3 - \theta$, it is multiplied by $(-1)^N$. On the other hand, for N particles, the θ dependence comes from terms of the form $\cos^n\theta \sin^{N-n}\theta$ where $n = 0,\ldots,N$ with real coefficients [see Eq. (C2)]. Hence it must be of the form $\sum_{k=-N}^{N} c_k e^{ik\theta}$ where $c_{-k} = c_k^*$. For even N, it follows that there is no θ dependence for $N \leqslant 4$, and the θ dependence for $6 \leqslant N \leqslant 10$ can only be a linear combination of a constant and another term $\propto \cos(6\theta)$ (only $c_{\pm 6}$ and c_0 are allowed). For odd N with $3 \leqslant N \leqslant 7$, the θ dependence is via $\cos(3\theta)$ (only $c_{\pm 3}$ allowed). The summation over k has the same parity as N when we combine all the symmetries we stated for θ, and therefore we have nonzero even/odd k ($6n$ and $6n + 3$ respectively with integer n) for even/odd N.

We note that the polar state P0 averages to $(\hat{\Theta}_3)^\dagger|0\rangle$ for $N = 3$, which happens to be the ground state also in the C region. While for $N = 6$, $|\Psi_P(\theta)\rangle_{av}$ never produces the many-body state $[(\hat{\Theta}_3^\dagger)^2 - \frac{1}{18}(\hat{\Theta}_2^\dagger)^3]|0\rangle$ in the C region for any choice of θ. It happens that when $\cos 6\theta = -1/3$, the angular-averaged polar state becomes the exact ground state $(\hat{\Theta}_2^\dagger)^3|0\rangle$ in the P region. The above special value of θ can be understood as follows. It can be shown that the weighted average $3/2\int_0^{\pi/3} d\theta \sin 3\theta$ over θ, together with the average over Euler angles above, is equivalent to an average over the 4-sphere in the quantum rotor picture of Ref. [45]. If we apply this average to $\varphi_m^P(\hat{\Omega})$, we obtain the exact many-body state $(\Theta_2^\dagger)^{N/2}|0\rangle$ for even N (the average vanishes for odd N). This is because the above mentioned averages guarantee that we obtain a state that is invariant under SO(5) rotations, and $(\Theta_2^\dagger)^{N/2}|0\rangle$ is the only such state (corresponding to $\tau = 0$ of Ref. [42]). The θ-averaged of $\cos(6\theta)$ is $-1/3$.

For even $N \geqslant 12$, the coefficients in the angular-averaged polar state would contain $\cos(12\theta)$ while for odd $N \geqslant 9$, they contain $\cos(9\theta)$ as expected. For $N = 12$ as an example, we expect three nonunique singlet states, which are $(\hat{\Theta}_2^\dagger)^6|0\rangle$, $(\hat{\Theta}_2^\dagger)^3(\hat{\Theta}_3^\dagger)^2|0\rangle$, and $(\hat{\Theta}_3^\dagger)^4|0\rangle$, with each coefficient a linear combination of constant, $\cos 6\theta$, and $\cos 12\theta$. We do not know whether the special θ^* with $\cos 6\theta = -1/3$ would retrieve the exact ground state for $N = 12$, but regard this as very unlikely.

The comparison between the angular-averaged polar state and the exact eigenstates can also be viewed in a different manner. Let us consider the operator $\hat{\Theta}_2^\dagger\hat{\Theta}_2$. We note that, for the normalized state $|\tilde{\Psi}_p(\theta)\rangle_{av}$ of $|\Psi_p(\theta)\rangle_{av}$, we have the expectation value

$$_{av}\langle\tilde{\Psi}_p(\theta)|\hat{\Theta}_2^\dagger\hat{\Theta}_2|\tilde{\Psi}_p(\theta)\rangle_{av} = N(N-1)X_{N-2}(\theta)/X_N(\theta), \quad (6)$$

where $X_N(\theta) \equiv_{av} \langle\Psi_p(\theta)|\Psi_p(\theta)\rangle_{av}$ and we have defined $X_0 = 1$. The derivation of Eq. (6) can be seen as follows. Consider operating $\hat{\Theta}_2$ on the unnormalized state $|\Psi_p(\theta)\rangle_{av}$, for example, of $\hat{a}_0^2$ in $\hat{\Theta}_2$, we would have a term of the form

$$\int_{\hat{\Omega}} \frac{\sqrt{N(N-1)}}{\sqrt{(N-2)!}}(\varphi_0^P)^2 \times \left(\varphi_2^P\hat{a}_2^\dagger + \varphi_1^P\hat{a}_1^\dagger + \varphi_0^P\hat{a}_0^\dagger + \varphi_{-1}^P\hat{a}_{-1}^\dagger + \varphi_{-2}^P\hat{a}_{-2}^\dagger\right)^{N-2}|0\rangle.$$

Similar derivations are for other operators in $\hat{\Theta}_2$. After summing over these contributions and using the identity $\sum_m(-1)^m\varphi_m^P(\hat{\Omega})\varphi_{-m}^P(\Omega) = 1$, we get

$$\int_{\hat{\Omega}} \frac{\sqrt{N(N-1)}}{\sqrt{(N-2)!}} \times \left(\varphi_2^P\hat{a}_2^\dagger+\varphi_1^P\hat{a}_1^\dagger+\varphi_0^P\hat{a}_0^\dagger+\varphi_{-1}^P\hat{a}_{-1}^\dagger+\varphi_{-2}^P\hat{a}_{-2}^\dagger\right)^{N-2}|0\rangle = \sqrt{N(N-1)}|\Psi_p(\theta)\rangle_{N-2}, \quad (7)$$

where $|\Psi_p(\theta)\rangle_{N-2}$ is the corresponding wave function for $N-2$ particles. Eq. (6) follows then just from the definition of $X_N(\theta)$, since its left-hand side is just the overlap of $\hat{\Theta}_2|\Psi_p(\theta)\rangle_{av}$ with its own complex conjugate.

While Eq. (6) is general, let us focus on P0. The evaluation of X_N at $\theta = 0$ are particularly straightforward. We have

$$X_N(0) \equiv_{av} \langle\Psi_p(0)|\Psi_p(0)\rangle_{av} = \int_{\hat{\Omega}} d\hat{\Omega}\left[D^{(2)}_{0,0}(\hat{\Omega})\right]^N, \quad (8)$$

where $\hat{\Omega} \equiv \hat{\Omega}_1^{-1}\hat{\Omega}_2$ represents the rotation $\hat{\Omega}_2$ followed by the inverse of $\hat{\Omega}_1$. Here we have used the relation $D^{(2)}_{0,0}(\hat{\Omega}) \equiv \sum_m D^{(2)*}_{m,0}(\hat{\Omega}_1)D^{(2)}_{m,0}(\hat{\Omega}_2)$ [44]. We obtain $X_1 = 0$, $X_2 = 1/5$, $X_3 = 2/35$, $X_4 = 3/35$, $X_5 = 4/77$, $X_6 = 53/(7\times 11\times 13)$, $X_7 = 6/(11\times 13)$, $X_8 = 5\times 19/(11\times 13\times 17)$, $X_9 = 2^3 \times 197/(11\times 13\times 17\times 19)$. On the other hand, as already mentioned, the exact eigenstates are also eigenvectors of the operator $\hat{\Lambda} \equiv \hat{\Theta}_2^\dagger\hat{\Theta}_2$. For even N, the states $(\hat{\Theta}_2^\dagger)^{N/2}|0\rangle$ have eigenvalues $\Lambda = N(N+3)$. For odd N, the exact eigenstates $(\hat{\Theta}_2^\dagger)^{(N-3)/2}\hat{\Theta}_3^\dagger|0\rangle$ have eigenvalues $(N-3)(N+6)$. We can check directly from Eq. (6) that the expectation values for $\hat{\Theta}_2^\dagger\hat{\Theta}_2$ equal these exact values for $N = 2, 3, 4, 5, 7$ but not 6, 8 or 9.

B. Cyclic states

We now study the angular-averaged cyclic states. It is simplest to use the reference state $\frac{1}{\sqrt{3}}(1,0,0,\sqrt{2},0)$ and hence $\varphi_m^C(\hat{\Omega}) = \frac{1}{\sqrt{3}}(D^{(2)}_{m,2} + \sqrt{2}D^{(2)}_{m,-1})(\hat{\Omega})$ in Eq. (4). The angular-averaged C states are nonvanishing only when N is a multiple of 3, which can be easily seen by considering the integral over the angle γ. It turns out that, in these cases, the angular-averaged C states do produce the correct many-body states. This is due to the fact that $\varphi_m^C(\hat{\Omega})$ obeys $\sum_m(-1)^m\varphi_m(\hat{\Omega})\varphi_{-m}(\hat{\Omega}) = 0$, and hence the angular averaged state is annihilated by $\hat{\Theta}_2$, so that the resulting state must satisfy $\Lambda = 0$ and hence correctly produce the corresponding many-body state. We have also verified this conclusion by direct angular averages in Appendix D.

V. REDUCED DENSITY MATRIX

As a further investigation, compare, for $N = 6$, the two-particle density matrices for the angular-averaged polar states with those for the exact many-body states $|\Psi_6\rangle \equiv \frac{1}{\sqrt{g(3)}}(\Theta_2^\dagger)^3|0\rangle$ where $g(3)$ is a normalization constant. (The one-particle density matrices are obviously identical since both states are rotational invariant.) It is simplest to present the results using the operators

$$\hat{A}_{JM} \equiv \sum_{m_1,m_2} \langle JM|22m_1m_2\rangle \hat{a}_{m_1}\hat{a}_{m_2}. \tag{9}$$

$\langle\Psi_6|\hat{A}^\dagger_{JM}\hat{A}_{J'M'}|\Psi_6\rangle$ is finite only when $J = J'$ and $M = M'$ and is further M independent, as expected by rotational invariance. These values are discussed in Appendix E. We have $\langle\Psi_6|\hat{A}^\dagger_{00}\hat{A}_{00}|\Psi_6\rangle = 54/5 = 10.8$, and $\langle\Psi_6|\hat{A}^\dagger_{2M}\hat{A}_{2M}|\Psi_6\rangle = \langle\Psi_6|\hat{A}^\dagger_{4M}\hat{A}_{4M}|\Psi_6\rangle = 48/35 \approx 1.37$.

The numerical results for the angular-averaged MF state is shown in Fig. 2. The values oscillate with θ with period $\pi/3$ due to the $\cos 6\theta$ factor in Eq. (5). For general θ, the difference between the angular-averaged MF and the spin-singlet pair states is less than 10%. For example, $\langle\hat{A}^\dagger_{00}\hat{A}_{00}\rangle = 10.8$ for the exact many-body state while $\langle\hat{A}^\dagger_{00}\hat{A}_{00}\rangle = 9.7$ in Fig. 2(a) at $\theta = 0$. The values are identical at $\cos(6\theta) = -1/3$.

While the density matrices at finite N in general differ, it can be shown in Appendix E that they have the same leading terms in the large N limit, so that the energy per particle remains the same up to corrections of order $1/N$, as in the case for spin-1 [29]. In the large N limit, the fragmented state has macroscopic number fluctuations while they decay rapidly as miniscule magnetization sets in, therefore it is fragile against symmetry-breaking perturbations. However, we expect that the fragmentation of many-body ground state can be observable in the few-particle system where its signature of two-particle correlations is more noticeable in contrast to the mean-field results.

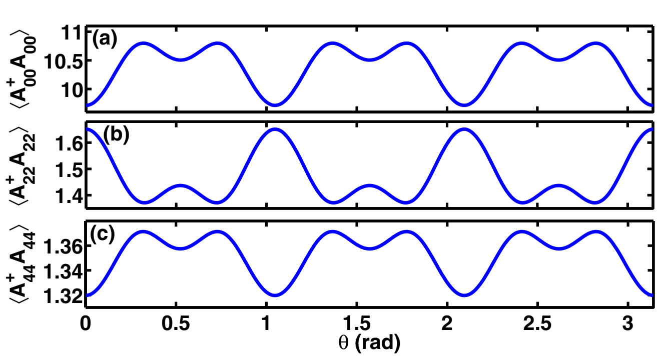

FIG. 2. (Color online) Two-particle density matrices for the angular-averaged polar state for $N = 6$. Three density matrices for $J = 0$, 2, 4 are shown in (a), (b), and (c), respectively.

VI. CONCLUSION

In conclusion, the many-body ground states of spin-2 Bose gas in zero magnetic field are in general fragmented, which is, however, not describable via angular-averaged MF states. For polar states the angular-averaged calculation fails to describe the exact eigenstates when even or odd $N \geqslant 6$ or 9 except in certain cases. For cyclic states, the angular-averaged treatment only sustains the exact ground states for particle number of a multiple of 3, which preserves the constraint of $\langle\hat{\Theta}_2^\dagger\hat{\Theta}_2\rangle = 0$. That the angular-averaged MF states for even Nin spin-1 Bose gas are equivalent to the exact ground states is simply a coincidence. For even higher spinor BEC ($f \geqslant 3$), we expect angular-averaged states fail to retrieve the exact eigenstates at an even smaller number of particles.

ACKNOWLEDGMENTS

We thank Ryan Barnett and the referee for pointing out to us Ref. [45]. This work is supported by the Ministry of Science and Technology, Taiwan, under Grant No. MOST-101-2112-M-001-021-MY3.

APPENDIX A: WAVE FUNCTIONS FOR THE SINGLET MANY-BODY STATE WITH $\Lambda = 0$ IN THE C REGION

We show how to obtain the singlet wave functions in the C regions of Fig. 1. To simplify notations, we shall often simply write $\langle 00|n,n'\rangle$ for the Clebsch-Gordan coefficients $\langle 00|2n;2n'\rangle$ when no confusion arises. We observe that

$$\begin{aligned}\hat{\Theta}_3^\dagger &= c\sum_{m=-2}^{2}(-1)^m\hat{a}^\dagger_{-m}\hat{A}^\dagger_{2m},\\ &= \sqrt{5}c\sum_{m=-2}^{2}\langle 00|-m,m\rangle\hat{a}^\dagger_{-m}\hat{A}^\dagger_{2m},\end{aligned} \tag{A1}$$

where $c = -\frac{1}{2}(\frac{7}{3})^{1/2}$. Such a relation is expected since both sides create a singlet state of three particles. It is easy to see that

$$\begin{aligned}[\hat{a}_m,\hat{A}^\dagger_{2M}] &= 2\langle 2M|m,M-m\rangle\hat{a}^\dagger_{M-m}\\ &= 2(-1)^m\langle 2\ M-m|-m,M\rangle\hat{a}^\dagger_{M-m}.\end{aligned} \tag{A2}$$

It is useful to note that though $[\hat{a}_m,\hat{A}^\dagger_{2m}] \neq 0$, we have

$$\sum_{m=-2}^{2}[\hat{a}_m,\hat{A}^\dagger_{2m}] = 0. \tag{A3}$$

This relation is expected since the left-hand side is rotationally invariant but its right-hand side can involve only one creation operator. Indeed, $\sum_{m=-2}^{2}[\hat{a}_m,\hat{A}^\dagger_{2m}] = 2\sum_{\mu=-2}^{2}(-1)^\mu\langle 20|\mu,-\mu\rangle a_0^\dagger$ but the sum is proportional to $\sum_{\mu=-2}^{2}\langle 00|\mu,-\mu\rangle\langle 20|\mu,-\mu\rangle = 0$ due to the orthogonality between the states $|00\rangle$ and $|20\rangle$. From Eq. (A1) we can evaluate

$$[\hat{a}_{-m},\hat{\Theta}_3^\dagger] = -(-1)^m\frac{(3\times 7)^{1/2}}{2}\hat{A}^\dagger_{2,m}, \tag{A4}$$

and hence

$$[\hat{\Theta}_2,\hat{\Theta}_3^\dagger] = -\frac{(3\times 7)^{1/2}}{2}\sum_{m=-2}^{2}\{\hat{A}_{2m}^\dagger,\hat{a}_m\},$$
$$= -(3\times 7)^{1/2}\sum_{m=-2}^{2}\hat{A}_{2m}^\dagger\hat{a}_m, \tag{A5}$$

where in the last step we have used Eq. (A3).

From the above we find

$$\hat{\Theta}_2(\hat{\Theta}_2^\dagger)^Q\hat{\Theta}_3^{\dagger R}|0\rangle = 2Q(6R+2Q+3)(\hat{\Theta}_2^\dagger)^{Q-1}(\hat{\Theta}_3^\dagger)^R|0\rangle + \frac{3R(R-1)}{2}(\hat{\Theta}_2^\dagger)^{Q+2}(\hat{\Theta}_3^\dagger)^{R-2}|0\rangle. \tag{A6}$$

Note that this implies, for the special case $R=0$,

$$\hat{\Theta}_2^\dagger\hat{\Theta}_2(\hat{\Theta}_2^\dagger)^Q|0\rangle = 2Q(2Q+3)(\hat{\Theta}_2^\dagger)^Q|0\rangle, \tag{A7}$$

a result which we shall see again in Appendix E.

We can now derive the exact many-body wave function for the region C when N is a multiple of 3. The state $|\Psi_{3R}\rangle$ with $N=3R$ particles and $\tau=N$ with $N=3R$ being a multiple of 3 (i.e., $\hat{\Theta}_2^\dagger\hat{\Theta}_2|\Psi_{3R}\rangle = 0$ hence $\Lambda=0$) can then be constructed as

$$|\Psi_{3R}\rangle = b_0(\hat{\Theta}_3^\dagger)^R + b_1(\hat{\Theta}_2^\dagger)^3(\hat{\Theta}_3^\dagger)^{R-2} + \cdots + b_k(\hat{\Theta}_2^\dagger)^{3k}(\hat{\Theta}_3^\dagger)^{R-2k} + \cdots, \tag{A8}$$

where we have

$$\frac{b_{k+1}}{b_k} = -\frac{(R-2k)(R-2k-1)}{12(k+1)(2R-2k-1)}. \tag{A9}$$

We also note here that since $[\Theta_2, N(N+3) - \Theta_2^\dagger\Theta_2] = 0$, the states $(\Theta_2^\dagger)^Q|\Psi_{3R}\rangle$ have the same quantum number $\tau = 3R$ though different particle numbers $N = 2Q+3R$. From these we obtain the exact many-body ground states in region C of Fig. 1.

APPENDIX B: SPIN-2 IRREDUCIBLE REPRESENTATION OF $d^{(2)}_{m',m}(\beta)$

In this section, we reproduce the spin-2 irreducible representation of the rotation operator $\hat{D}^{(2)}_{m',m}(\alpha,\beta,\gamma) = e^{-i(m'\alpha+m\gamma)}d^{(2)}_{m',m}(\beta)$ [44] for Euler angles α, β, γ. In matrix form, $d^{(2)}_{m',m}(\beta)$ is

$$d^{(2)}_{m',m}(\beta) = \begin{pmatrix} \cos^4(\frac{\beta}{2}) & -\frac{\sin\beta}{2}(1+\cos\beta) & \sqrt{\frac{3}{8}}\sin^2\beta & \frac{\sin\beta}{2}(\cos\beta-1) & \sin^4\frac{\beta}{2} \\ \frac{\sin\beta}{2}(1+\cos\beta) & \frac{1}{2}(2\cos\beta-1)(\cos\beta+1) & -\sqrt{\frac{3}{2}}\sin\beta\cos\beta & \frac{1}{2}(2\cos\beta+1)(1-\cos\beta) & \frac{\sin\beta}{2}(\cos\beta-1) \\ \sqrt{\frac{3}{8}}\sin^2\beta & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \frac{1}{2}(3\cos^2\beta-1) & -\sqrt{\frac{3}{2}}\sin\beta\cos\beta & \sqrt{\frac{3}{8}}\sin^2\beta \\ \frac{\sin\beta}{2}(1-\cos\beta) & \frac{1}{2}(2\cos\beta+1)(1-\cos\beta) & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \frac{1}{2}(2\cos\beta-1)(\cos\beta+1) & -\frac{\sin\beta}{2}(1+\cos\beta) \\ \sin^4\frac{\beta}{2} & \frac{\sin\beta}{2}(1-\cos\beta) & \sqrt{\frac{3}{8}}\sin^2\beta & \frac{\sin\beta}{2}(\cos\beta+1) & \cos^4(\frac{\beta}{2}) \end{pmatrix}, \tag{B1}$$

which is expressed in terms of spin bases $(\varphi_2,\varphi_1,\varphi_0,\varphi_{-1},\varphi_{-2})$.

APPENDIX C: ANGULAR AVERAGE MEAN-FIELD POLAR STATES FOR FINITE NUMBER OF PARTICLES

From Eq. (4) with $\hat{a}^\dagger(\hat{\Omega}) = \sum a_m^\dagger\varphi_m^P(\hat{\Omega})$ where $\varphi_m^P(\hat{\Omega}) \equiv \cos\theta D^{(2)}_{m,0}(\hat{\Omega}) + \sin\theta(D^{(2)}_{m,2}(\hat{\Omega}) + D^{(2)}_{m,-2}(\hat{\Omega}))/\sqrt{2}$, we first average over α and γ, which gives

$$|\Psi'_P(\theta,\beta)\rangle_{av} = \sum_{n=0}^{N}\binom{N}{n}\left[\sum_{m'_1}\cos\theta\, d^{(2)}_{m'_1,0}(\beta)\hat{a}^\dagger_{m'_1}\right]^n\left(\frac{\sin\theta}{\sqrt{2}}\right)^{N-n}\left[\sum_{m'_2}d^{(2)}_{m'_2,2}(\beta)\hat{a}^\dagger_{m'_2} + \sum_{m'_3}d^{(2)}_{m'_3,-2}(\beta)\hat{a}^\dagger_{m'_3}\right]^{N-n}\delta_{f(m'),0}\delta_{f(m),0}, \tag{C1}$$

where $f(m) \equiv \sum_{m=m_{1,2,3}} m$. We may expand the above further and use one of the delta function constraint $\delta_{f(m),0}$, and the wave function becomes

$$|\Psi'_P(\theta,\beta)\rangle_{av} = \sum_{n=0}^{N}\binom{N}{n}\frac{\cos^n\theta\sin^{N-n}\theta}{2^{(N-n)/2}}\binom{N-n}{\frac{N-n}{2}}\left[\sum_{m'_1}d^{(2)}_{m'_1,0}(\beta)\hat{a}^\dagger_{m'_1}\right]^n\left[\sum_{m'_2}d^{(2)}_{m'_2,2}(\beta)\hat{a}^\dagger_{m'_2}\right]^{\frac{N-n}{2}}\left[\sum_{m'_3}d^{(2)}_{m'_3,-2}(\beta)\hat{a}^\dagger_{m'_3}\right]^{\frac{N-n}{2}}\delta_{f(m'),0}, \tag{C2}$$

where $(N-n)/2$ is integer. We then evaluate the β average either analytically or with the help of Mathematica. Below, we report the results for this angular-averaged polar states for finite number of particles $N=2$ to 10.

1. $N = 2$

From Eq. (C2), we have the angular-averaged polar state

$$|\Psi_P(\theta)\rangle_{av} = \frac{1}{2\sqrt{2!}}\int_0^\pi |\Psi'_p(\theta,\beta)\rangle \sin\beta d\beta,$$
$$= \frac{1}{5\sqrt{2}}[2\hat{a}_2^\dagger\hat{a}_{-2}^\dagger - 2\hat{a}_1^\dagger\hat{a}_{-1}^\dagger + (\hat{a}_0^\dagger)^2]|0\rangle,$$
$$= \frac{1}{5\sqrt{2}}\hat{\Theta}_2^\dagger|0\rangle. \quad \text{(C3)}$$

Note that it has no θ dependence. The angular-averaged MF state reproduces the exact many-body state.

2. $N = 3$

From Eq. (C2), we have the angular-averaged polar state

$$|\Psi_P(\theta)\rangle_{av} = \frac{1}{2\sqrt{3!}}\int_0^\pi |\Psi'_p(\theta,\beta)\rangle \sin\beta\, d\beta,$$
$$= \frac{2}{35}(\cos^3\theta - 3\cos\theta\sin^2\theta)\hat{\Theta}_3^\dagger|0\rangle$$
$$= \frac{2}{35}[\cos(3\theta)]\hat{\Theta}_3^\dagger|0\rangle, \quad \text{(C4)}$$

where $\hat{\Theta}_3$ is a three-particle singlet operator,

$$\hat{\Theta}_3^\dagger \equiv \frac{1}{\sqrt{6}}(\hat{a}_0^\dagger)^3 - \frac{3}{\sqrt{6}}\hat{a}_1^\dagger\hat{a}_0^\dagger\hat{a}_{-1}^\dagger + \frac{3}{2}(\hat{a}_1^\dagger)^2\hat{a}_{-2}^\dagger + \frac{3}{2}\hat{a}_2^\dagger(\hat{a}_{-1}^\dagger)^2 - \frac{6}{\sqrt{6}}\hat{a}_2^\dagger\hat{a}_0^\dagger\hat{a}_{-2}^\dagger. \quad \text{(C5)}$$

Note that this angular-averaged state has θ dependence with a period of $2\pi/3$ but always reproduces the exact many-body state for the region $\gamma < 0$ and near the $+\beta$ axis.

3. $N = 4$

For this even number of particles, we again have

$$|\Psi_P(\theta)\rangle_{av} = \frac{1}{2\sqrt{4!}}\int_0^\pi |\Psi'_p(\theta,\beta)\rangle \sin\beta\, d\beta,$$
$$= \frac{3}{35\sqrt{4!}}(\hat{\Theta}_2^\dagger)^2|0\rangle, \quad \text{(C6)}$$

where so far we still have a θ independent angular average. This state is a $N/2$ spin-singlet-pairs state, i.e., the exact eigenstate.

4. $N = 5$

From Eq. (C2), only $n = 1,3,5$ are possible for $(N-n)/2$ is an integer. The angular-averaged polar state is

$$|\Psi_P(\theta)\rangle_{av} = \frac{1}{2\sqrt{5!}}\int_0^\pi |\Psi'_p(\theta,\beta)\rangle \sin\beta\, d\beta,$$
$$= \frac{4\sqrt{6}}{77\sqrt{5!}}(\cos^5\theta - 3\cos\theta\sin^4\theta - 2\cos^3\theta\sin^2\theta)\hat{\Theta}_2^\dagger\hat{\Theta}_3^\dagger|0\rangle$$
$$= \frac{2}{77\sqrt{5}}[\cos(3\theta)]\hat{\Theta}_2^\dagger\hat{\Theta}_3^\dagger|0\rangle. \quad \text{(C7)}$$

Note that this angular-averaged state again has θ dependence with a period of $2\pi/3$ and reproduces the exact many-body state for the region $\gamma < 0$ and near the $+\beta$ axis.

5. $N = 6$

For this even number of particles, we expect a combination of two- and three-particle singlet states to appear. From Eq. (C2), we have

$$|\Psi_P(\theta)\rangle_{av} = \frac{1}{2\sqrt{6!}}\int_0^\pi |\Psi'_p(\theta,\beta)\rangle \sin\beta\, d\beta,$$
$$= \frac{1}{1001\sqrt{6!}}[(47 - 2\cos 6\theta)(\hat{\Theta}_2^\dagger)^3 + (12 + 36\cos 6\theta)(\hat{\Theta}_3^\dagger)^2]|0\rangle. \quad \text{(C8)}$$

We may express this wave function in terms of the normalized many-body state of two- and three-particle singlet states for N particles,

$$\left|\Psi_{N=6}^{(2)}\right\rangle = \frac{1}{\sqrt{2^4\cdot 3^3\cdot 5\cdot 7}}(\hat{\Theta}_2^\dagger)^3|0\rangle, \quad \text{(C9)}$$

$$|\Psi_{N=6}^{(3)}\rangle = \frac{1}{\sqrt{5\cdot 7^3}}(\hat{\Theta}_3^\dagger)^2|0\rangle. \quad \text{(C10)}$$

For $\theta = 0$, the normalized angular-averaged state is

$$|\tilde{\Psi}_P(0)\rangle_{av} = \frac{1}{\sqrt{11\times 13\times 53}}\left[5\times 3^{5/2}\left|\Psi_{N=6}^{(2)}\right\rangle + 2^2\times 7\left|\Psi_{N=6}^{(3)}\right\rangle\right], \quad \text{(C11)}$$

where we note the finite overlap $\langle\Psi_{N=6}^{(2)}|\Psi_{N=6}^{(3)}\rangle = 2/(\sqrt{3}\cdot 7)$. The angular average has θ dependence in general, and it can be expressed in terms of two-particle-singlets state only when $\cos 6\theta = -1/3$. In general the angular-averaged polar state fails to construct the exact ground states, which should be $N/2$ spin-singlet-pairs state.

6. $N = 8$

To investigate the θ dependence of even number of particles, we proceed to calculate the angular-averaged polar state of $N = 8$,

$$|\Psi_p(\theta)\rangle_{av} = \frac{1}{2\sqrt{8!}}\int_0^\pi |\Psi'_p(\theta,\beta)\rangle \sin\beta\, d\beta$$
$$= \frac{1}{2431\sqrt{8!}}[(71 - 8\cos 6\theta)(\hat{\Theta}_2^\dagger)^4 + 16(3 + 9\cos 6\theta)\hat{\Theta}_2^\dagger(\hat{\Theta}_3^\dagger)^2]|0\rangle. \quad \text{(C12)}$$

Using the normalized singlet states,

$$\left|\Psi_{N=8}^{(2)}\right\rangle = \frac{1}{\sqrt{2^7\times 3^3\times 5\times 7\times 11}}(\hat{\Theta}_2^\dagger)^4|0\rangle, \quad \text{(C13)}$$

$$\left|\Psi_{N=8}^{(2,3)}\right\rangle = \frac{1}{\sqrt{2\times 5\times 7\times 11\times 79}}\hat{\Theta}_2^\dagger(\hat{\Theta}_3^\dagger)^2|0\rangle, \quad \text{(C14)}$$

we may express the normalized angular-averaged state (consider $\theta = 0$) as

$$|\tilde{\Psi}_p(0)\rangle_{av} = \frac{1}{3\sqrt{2\times 5}}\left[\sqrt{3}\left|\Psi^{(2)}_{N=8}\right\rangle + \sqrt{79}\left|\Psi^{(2,3)}_{N=8}\right\rangle\right], \quad (C15)$$

where again we use $\langle\Psi^{(2)}_{N=8}|\Psi^{(2,3)}_{N=8}\rangle = 4/(\sqrt{3\times 79})$. Note that when $\cos 6\theta = -1/3$, the angular-averaged MF state becomes the exact many-body state.

7. $N = 10$

We may further investigate the angular-averaged MF state for even N. From Eq. (C2), we have

$$\begin{aligned}|\Psi_P(\theta)\rangle_{av} &= \frac{1}{2\sqrt{10!}}\int_0^\pi |\Psi'_p(\theta,\beta)\rangle \sin\beta\, d\beta,\\ &\propto [(101 - 20\cos 6\theta)(\hat{\Theta}_2^\dagger)^5\\ &\quad + 120(1+3\cos 6\theta)(\hat{\Theta}_2^\dagger\hat{\Theta}_3^\dagger)^2]|0\rangle. \quad (C16)\end{aligned}$$

Note that a special angle of $\cos 6\theta = -1/3$ appears similar to the cases of $N = 6,8$.

APPENDIX D: ANGULAR-AVERAGED MEAN-FIELD CYCLIC STATES FOR FINITE N

When we angular averaged the mean-field cyclic state, we obtain, for $N = 3$,

$$|\Psi_C\rangle_{av} = \frac{4\sqrt{3}}{35\times\sqrt{3!}}\hat{\Theta}_3^\dagger|0\rangle. \quad (D1)$$

For $N = 6$, we have

$$|\Psi_C\rangle_{av} = \frac{8}{7\times 11\times 13\sqrt{6!}}[-(\hat{\Theta}_2^\dagger)^3 + 18(\hat{\Theta}_3^\dagger)^2]|0\rangle. \quad (D2)$$

In both cases, we produce the exact many-body states in the C region.

APPENDIX E: REDUCED DENSITY MATRIX CALCULATION

We here consider the $N = 2Q$ singlet state

$$|\Psi_{2Q}\rangle = \frac{1}{\sqrt{g(Q)}}\hat{\Theta}_2^{\dagger Q}|0\rangle, \quad (E1)$$

where $g(Q)$ is a normalization constant. $g(Q)$ can be evaluated (see also below) by the repeated use of the commutation relation $[\hat{\Theta},\hat{\Theta}^\dagger] = 2(2\hat{N}+5)$ where $\hat{N}$ is the number operator. We then obtain

$$g(Q) = 2^Q Q!(2Q+3)!!/3. \quad (E2)$$

Some special values are $g(1) = 10$, $g(2) = 2^3\times 5\times 7$, and $g(3) = 2^4\times 3^3\times 5\times 7$. It turns out that $g(Q) = f(1,Q)$ of Ref. [29].

The expectation values for the two-particle density matrices $\langle\Psi_{2Q}|\hat{A}^\dagger_{JM}\hat{A}_{JM}|\Psi_{2Q}\rangle$ needed can be read off from the energy $E = \frac{1}{2}[\alpha N(N-1) + \beta(F(F+1) - 6N) + \gamma\Lambda]$ where $\Lambda = 2Q(2Q+3)$ since this must also be $E = \frac{1}{2}\sum_{JM} g_F\langle\Psi_{2Q}|\hat{A}^\dagger_{JM}\hat{A}_{JM}|\Psi_{2Q}\rangle$ where the sum over J is for 0,2,4 only. We have

$$\langle\Psi_{2Q}|\hat{A}^\dagger_{00}\hat{A}_{00}|\Psi_{2Q}\rangle = 2Q(2Q+3)/5, \quad (E3)$$

$$\langle\Psi_{2Q}|\hat{A}^\dagger_{2M}\hat{A}_{2M}|\Psi_{2Q}\rangle = 8Q(Q-1)/35, \quad (E4)$$

$$\langle\Psi_{2Q}|\hat{A}^\dagger_{4M}\hat{A}_{4M}|\Psi_{2Q}\rangle = 8Q(Q-1)/35. \quad (E5)$$

The equality between the values between $J = 2$ and $J = 4$ is due to the special properties of the state $|\Psi_{2Q}\rangle$. Below we also show an alternate derivation of Eqs. (E3)–(E5)

The state (E1) can be expressed in terms of the basis $|n_2,n_1,n_0,n_{-1},n_{-2}\rangle$, where n_m is the number of particles in the state m. We get

$$\begin{aligned}|\Psi_{2Q}\rangle =& \left[\frac{3\times 2^Q Q!}{(2Q+3)!!}\right]^{1/2}\sum_{k_0,k_1,k_2}^{Q}{}' (-1)^{k_1}\frac{[(2k_0)!]^{1/2}}{2^{k_0}k_0!}\\ &\times |k_2,k_1,2k_0,k_1,k_2\rangle, \quad (E6)\end{aligned}$$

where the sum is over all non-negative integers k_0, k_1, k_2 with the restriction (denoted by the prime) $k_0+k_1+k_2 = Q$. The density matrices are obtained by operating $\hat{a}_{m_1}\hat{a}_{m_2}$ on $|\Psi_{2Q}\rangle$ and then evaluating the appropriate inner products. The required sums are evaluated below.

We show here how to evaluate the sums involved. They are of the form

$$S_Q \equiv \sum_{k=0}^{Q} b_k, \quad (E7)$$

where b_k are the products of polynomials in k with $c_k \equiv \frac{(2k)!}{2^{2k}(k!)^2} = \frac{(2k-1)!!}{2^k k!}$. For this, we notice that if the function $f(y) \equiv \sum_{k=0}^\infty b_k y^k$ is known, then (by straightforward verification) S_Q is simply the coefficient of y^Q of the function $F(y) \equiv f(y)/(1-y)$. Now, we note that $f_1(y) \equiv \sum_{k=0}^\infty c_k y^k$ is given simply by $(1-y)^{-1/2}$. Hence the sum $S_{1,Q} \equiv \sum_{k=0}^Q c_k$ is given by the y^Q coefficient of $(1-y)^{-3/2}$, and hence

$$S_{1,Q} \equiv \sum_{k=0}^{Q} c_k = \frac{(2Q+1)!!}{2^Q Q!}. \quad (E8)$$

Similarly, for the sum $S_{2,Q} \equiv \sum_{k=0}^Q kc_k$, the function $f_2(y) \equiv \sum_{k=0}^\infty kc_k y^k$ can be obtained from $y\frac{d}{dy}f_1(y) = \frac{y}{2}(1-y)^{-3/2}$. Hence $S_{2,Q}$ is the y^Q coefficient of $F_2(y) = \frac{y}{2}(1-y)^{-5/2}$, and hence

$$S_{2,Q} \equiv \sum_{k=0}^{Q} kc_k = \frac{Q}{3}\frac{(2Q+1)!!}{2^Q Q!}. \quad (E9)$$

We can proceed similarly to get

$$S_{3,Q} \equiv \sum_{k=0}^{Q} k(k-1)c_k = \frac{Q(Q-1)}{5}\frac{(2Q+1)!!}{2^Q Q!}, \quad (E10)$$

$$\begin{aligned}S_{4,Q} &\equiv \sum_{k=0}^{Q} k(k-1)(k-2)c_k\\ &= \frac{Q(Q-1)(Q-2)}{7}\frac{(2Q+1)!!}{2^Q Q!}. \quad (E11)\end{aligned}$$

With the above sums, we can also obtain

$$\sum_{k=0}^{Q}(Q+1-k)c_k = \frac{1}{3}\frac{(2Q+3)!!}{2^Q Q!}, \tag{E12}$$

$$\sum_{k=0}^{Q}(Q-k)(Q-k+1)c_k = \frac{4Q}{15}\frac{(2Q+3)!!}{2^Q Q!} \tag{E13}$$

[using $(Q-k)(Q-k+1) = k(k-1) - 2Qk + Q(Q+1)$], and

$$\sum_{k=0}^{Q}(Q-k-1)(Q-k)(Q-k+1)c_k = \frac{8Q(Q-1)}{35}\frac{(2Q+3)!!}{2^Q Q!} \tag{E14}$$

[using $(Q-k-1)(Q-k)(Q-k+1) = -k(k-1)(k-2) + 3(Q-1)k(k-1) - 3Q(Q-1)k + (Q-1)Q(Q+1)$].

We demonstrate the use of the above relations by checking here the normalization of $|\Psi_{2Q}\rangle$. $\langle\Psi_{2Q}|\Psi_{2Q}\rangle$ is given by $[\frac{3\times 2^Q Q!}{(2Q+3)!!}]\sum_{k_0,k_1,k_2}^{Q}{}' c_{k_0}$. Due to the restriction $k_0+k_1+k_2 = Q$, the sum is therefore given by $\sum_{k_0=0}^{Q}[\sum_{k_1=0}^{Q-k_0} 1] = \sum_k^Q c_k(Q-k+1)$, which is $\frac{(2Q+3)!!}{3\times 2^Q Q!}$ from Eq. (E13). The density matrices are obtained by first operating $\hat{a}_m$ or $\hat{a}_{m_1}\hat{a}_{m_2}$ on $|\Psi_{2Q}\rangle$ and then evaluating the appropriate interproducts with the help of the above formulas.

We list here also the two-particle density matrices $\langle\Psi_{2Q}|\hat{a}_{m_1}^\dagger\hat{a}_{m_2}^\dagger\hat{a}_{m_3}\hat{a}_{m_4}|\Psi_{2Q}\rangle$. We list them starting from the largest $M \equiv m_1+m_2 = m_3+m_4$. For $M=4$,

$$\langle\Psi_{2Q}|\hat{a}_2^\dagger\hat{a}_2^\dagger\hat{a}_2\hat{a}_2|\Psi_{2Q}\rangle = 8Q(Q-1)/35. \tag{E15}$$

For $M=3$

$$\langle\Psi_{2Q}|\hat{a}_2^\dagger\hat{a}_1^\dagger\hat{a}_1\hat{a}_2|\Psi_{2Q}\rangle = 4Q(Q-1)/35, \tag{E16}$$

corresponding to $\langle\Psi_{2Q}|\hat{A}_{4M}^\dagger\hat{A}_{4M}|\Psi_{2Q}\rangle = 8Q(Q-1)/35$. For $M=2$, we have two operators $\hat{a}_0\hat{a}_2$ and $\hat{a}_1\hat{a}_1$ and their conjugates. We obtain

$$\langle\Psi_{2Q}|\hat{a}_2^\dagger\hat{a}_0^\dagger\hat{a}_0\hat{a}_2|\Psi_{2Q}\rangle = 4Q(Q-1)/35, \tag{E17}$$

$$\langle\Psi_{2Q}|\hat{a}_1^\dagger\hat{a}_1^\dagger\hat{a}_1\hat{a}_1|\Psi_{2Q}\rangle = 8Q(Q-1)/35, \tag{E18}$$

whereas

$$\langle\Psi_{2Q}|\hat{a}_2^\dagger\hat{a}_0^\dagger\hat{a}_1\hat{a}_1|\Psi_{2Q}\rangle = 0. \tag{E19}$$

The last result can be most easily seen when Ψ_{2Q} is expanded in the number basis. This is reflected in the equality between Eqs. (E4) and (E5).

For $M=1$, there are two operators $\hat{a}_1\hat{a}_0$ and $\hat{a}_2\hat{a}_{-1}$. We have

$$\langle\Psi_{2Q}|\hat{a}_1^\dagger\hat{a}_0^\dagger\hat{a}_0\hat{a}_1|\Psi_{2Q}\rangle = \langle\Psi_{2Q}|\hat{a}_2^\dagger\hat{a}_{-1}^\dagger\hat{a}_{-1}\hat{a}_2|\Psi_{2Q}\rangle, \tag{E20}$$

$$= 4Q(Q-1)/35, \tag{E21}$$

and there are no cross elements. Similar remarks we made for the $M=2$ sector also applies here.

For $M=0$, there are three operators, $\hat{a}_2\hat{a}_{-2}$ and $\hat{a}_1\hat{a}_{-1}$ and $\hat{a}_0\hat{a}_0$. This part of the density matrix is, with rows and columns in order of these three operators, given by

$$\frac{2Q}{35}\begin{pmatrix} (4Q+3) & -(2Q+5) & (2Q+5) \\ -(2Q+5) & (4Q+3) & -(2Q+5) \\ (2Q+5) & -(2Q+5) & (6Q+1)\end{pmatrix}. \tag{E22}$$

The equality between the first two diagonal elements, as well as among the off-diagonal elements except signs, follows from the fact that $|\Psi_{2Q}\rangle$ is invariant under $\hat{a}_{\pm 2}\to\hat{a}_{\pm 1}$ up to a sign. From the above formulas, we can recover Eqs. (E3)–(E5).

It is straightforward to obtain the number fluctuations from above: $\langle\hat{N}_2\hat{N}_2\rangle = \langle\hat{N}_1\hat{N}_1\rangle = \langle\hat{N}_2\hat{N}_{-2}\rangle = \langle\hat{N}_1\hat{N}_{-1}\rangle = 2Q(4Q+3)/35$, $\langle\hat{N}_0\hat{N}_0\rangle = 4Q(3Q+4)/35$, $\langle\hat{N}_2\hat{N}_1\rangle = \langle\hat{N}_2\hat{N}_0\rangle = \langle\hat{N}_2\hat{N}_{-1}\rangle = \langle\hat{N}_1\hat{N}_0\rangle = 4Q(Q-1)/35$. The above expressions are valid also when replacing m by $-m$. $\langle\hat{N}_2\hat{N}_2\rangle = \langle\hat{N}_2\hat{N}_{-2}\rangle$ etc follows immediately also from (E6), since for each of the states on the right-hand side, $n_2 = n_{-2}$.

We now consider the density matrices for $|\Psi_P\rangle_{av}$ in large N limit. We have

$$\langle\hat{a}_{m_1}^\dagger\hat{a}_{m_1}^\dagger\hat{a}_{m_3}\hat{a}_{m_4}\rangle = N(N-1)\frac{\int_{\hat{\Omega}_1,\hat{\Omega}_2}\varphi_{m_1}^*(\hat{\Omega}_1)\varphi_{m_2}^*(\hat{\Omega}_1)\varphi_{m_3}(\hat{\Omega}_2)\varphi_{m_4}(\hat{\Omega}_2)\left[\sum_m\varphi_m^*(\hat{\Omega}_1)\varphi_m(\hat{\Omega}_2)\right]^{N-2}}{\int_{\hat{\Omega}_1,\hat{\Omega}_2}\left[\sum_m\varphi_m^*(\hat{\Omega}_1)\varphi_m(\hat{\Omega}_2)\right]^N}. \tag{E23}$$

(We leave out the explicit labels $|\Psi_P\rangle_{av}$ to simplify our notations.) For large N, the overlap $[\sum_m\varphi_m^*(\hat{\Omega}_1)\varphi_m(\hat{\Omega}_2)]^N$ is negligible unless $\hat{\Omega}_1$ is very close to $\hat{\Omega}_2$ (rigorously speaking, also $\hat{\Omega}_2 - \hat{\Omega}_1$, but we can check easily that this does not affect the following argument). Hence we can identify the $\hat{\Omega}$ in the arguments of $\varphi_{m_1}\ldots\varphi_{m_4}$ in the integrand of the numerator. Canceling the common factors (the normalization coefficient is $\propto N^{-1}$ for large N) we are left with

$$\langle\hat{a}_{m_1}^\dagger\hat{a}_{m_1}^\dagger\hat{a}_{m_3}\hat{a}_{m_4}\rangle = N(N-1)\int_{\hat{\Omega}}\varphi_{m_1}^*(\hat{\Omega})\varphi_{m_2}^*(\hat{\Omega})\varphi_{m_3}(\hat{\Omega})\varphi_{m_4}(\hat{\Omega}). \tag{E24}$$

Now we observe that, for our state, $\varphi_m^*(\hat{\Omega}) = (-1)^m\varphi_{-m}(\hat{\Omega})$, since $d_{-m,-n}^{(2)} = (-1)^{m+n}d_{m,n}^{(2)}$ where $\hat{D}_{m',m}^{(2)}(\alpha,\beta,\gamma) \equiv e^{-i(m'\alpha+m\gamma)}d_{m',m}^{(2)}(\beta)$. Therefore the integral above is the same as

$$(-1)^{m_1+m_2}\int_{\hat{\Omega}}\varphi_{-m_1}(\hat{\Omega})\varphi_{-m_2}(\hat{\Omega})\varphi_{m_3}(\hat{\Omega})\varphi_{m_4}(\hat{\Omega}).$$

We notice that this latter integral is the same as the one that occurs in our evaluation of the coefficient of $\hat{a}_{-m_1}^\dagger\hat{a}_{-m_2}^\dagger\hat{a}_{m_3}^\dagger\hat{a}_{m_4}^\dagger$ for the wave function $|\Psi_P\rangle_{av}$ for four particles, except combinatorial factors. For example, the value of $\langle\hat{a}_2^\dagger\hat{a}_1^\dagger\hat{a}_1\hat{a}_2\rangle$ is just $-N(N-1)$ times the coefficient of $\hat{a}^\dagger_{-2}\hat{a}^\dagger_{-1}\hat{a}^\dagger_1\hat{a}^\dagger_2$ in $|\Psi_P\rangle_{av}$ [see Eq. (C6)] divided by 4!. Using our previous calculations we therefore obtain, in the large N limit, $\langle\hat{a}^\dagger_2\hat{a}^\dagger_1\hat{a}_1\hat{a}_2\rangle = N^2/35$, $\langle\hat{a}^\dagger_2\hat{a}^\dagger_0\hat{a}_0\hat{a}_2\rangle = N^2/35$, etc. It is again most economical to express the final results using $\hat{A}_{JM}$. We get $\langle\hat{A}^\dagger_{00}\hat{A}_{00}\rangle = N^2/5$ and $\langle\hat{A}^\dagger_{2M}\hat{A}_{2M}\rangle = \langle\hat{A}^\dagger_{4M}\hat{A}_{4M}\rangle = 2N^2/35$. Hence the N^2 terms in two-particle density matrix in the state obtained by angular average is the same as that of Eq. (E1), and the differences arise only in lower powers in N. Therefore the interaction energies per particle for these states are equal except for terms that are of order 1.

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