Spinor Bose-Einstein condensates: self-consistent symmetries and characterization

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Quantum many-body systems with spin degree of freedom may exhibit novel phases and emergent phenomena that can only be described beyond mean-field theories. In this work, we present a generic and systematic method to fully determine the variational perturbations of a mean-field solution of interacting spinor systems with rotational symmetry. The method is based in a generalization of the Majorana stellar representation for quantum mixed states and group symmetry arguments. We apply the approach using the system of the spinor Bose-Einstein condensates (BECs) with spin 1 and 2. To further exemplify the advantages of the method, we calculate the phase diagram of a spin-2 BEC at finite temperatures.

Many-body quantum systems of interacting spins exhibit novel phases and fascinating physical phenomena. In the field of ultracold atoms, the phases occurring in spinor Bose-Einstein condensates can be realized nowadays under highly controllable setups. Whereas the spatial behavior of the ground state of BEC is basically defined by the type of the confinement trap, provided that neither spin-dependent coupling or dipolar interactions are considered, in spin BECs the ground-state behavior can differ drastically over different atomic species [1]. For instance, the condensates of $^{23}$Na and $^{87}$Rb in an optical trap exhibit different ground spinor phases: the ferromagnetic (FM) and the polar (P) phases, respectively [2, 3]. Both phases have been corroborated experimentally [4–7]. Recent experimental advances in the field of cold atoms allows us study the spin phases of BEC of several spin values, from 1 to 8, even in the presence of external fields and spin-orbit interactions [5, 8–13]. The study of the spin-phase diagram in spinor BECs via mean-field theories were introduced first for spin $f = 1$ [14, 15] and subsequently for higher spins [1, 16–19]. The mean-field theory consists to assume that all the atoms in the condensate are in the same quantum state, defined by an average over the interactions and characterized by the spinor order-parameter $\Phi$, which must obey the spinor version of the well-known Gross-Pitaevskii (GP) equations [1–3].

Although the mean-field theory predicts qualitatively well the spin phases of a BEC, it fails to offer a satisfactory description of aspects of crucial relevance as, finite temperature effects, quantum fluctuations, or non-local perturbations. The studies of the spinor BEC covering these aspects become essential to scrutinize other physical phenomena such as deviations in the spin phase boundaries, metastable phases, tunneling effects, quench dynamics, or (dynamic or static) quantum phase transitions, among others phenomena [6, 8, 20–36]. Some of the well-known beyond-mean-field theories are the variational approaches suitable for near the mean-field phases [20, 37–42]. Physically, this entails that the condensate gas, represented by a mixed ensemble of particles, is described by a density matrix $\rho$. It has two contributions such that $\rho = \rho^s + \rho^{nc}$, where $\rho^s = \Phi^\dagger \Phi$ is the atom fraction that remains in the same mean-field solution $\Phi$, while $\rho^{nc}$ is the ensemble of non-condensed atoms described by other quantum states [20, 24, 38].

Operationally, the variational methods lead to self-consistent calculations involving GP equations coupled to a set of equations that govern the noncondensate fraction. [20, 24, 37, 38]. A way to circumvent this rather extensive numerical calculations is to make use of the potential symmetries present in $\rho^{nc}$ and, consequently, reducing its degrees of freedom. Furthermore, it is exploited the fact that the noncondensate fraction $\rho^{nc}$ inherits the common symmetries between the Hamiltonian of the condensed and its order parameter. Within this scenario, it is established that the system has a self-consistent symmetry [37]. As suggested by the Michel theorem, several of the order parameters of the spin phases encounter in BECs [43] have rotational and reflection symmetries [1, 17, 19, 44, 45], i.e. a point group symmetry. More over, it is known that the complete Hamiltonian of the system in the absence of external fields have common symmetries of the point group of $\Phi$ [1, 2]. The spin phases with point group symmetries are also of great interest due to the appearance of (Abelian or non-Abelian) vortices [46–48]. The inherited symmetries of $\rho^{nc}$ has been used before to study the metastable phases of spinor BEC of spin-1 at finite temperatures [24].

In this Letter, we present a systematic method based on the Majorana representation of spin mixed states [49, 50] to determine the non-condensed fraction $\rho^{nc}$ with a certain point group of a spinor BEC. We exemplify the method by characterizing $\rho^{nc}$ of the spin phases of BEC of spin $f = 1$ and 2. As an application, we present the phase diagram of the spin-2 BEC at finite temperatures using the Hartree-Fock approximation [20, 37–39], where we observe a deviation in in the cyclic-nematic phase boundary. The joint work [51] of this letter includes the determination of the noncondensate fraction for other symmetries of higher spins in the Hartree-Fock approximation. Also, and with the help of the method

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described here, we can study with more detail the phases of the spin-2 BEC at finite temperatures.

We start by considering a BEC with spin $f$ in an optical trap. The system is assumed to be weakly interacting and sufficiently diluted such that only two-body collisions are predominant and the $s$-wave approximation is still valid. Since we are interested only in the spinorial sector of the atomic gas, we assume the the spatial part of the system can be factorized and then solved, independently. The previous restriction also considers the absence of topological spin disorders (vortices) over the atoms in the condensate gas, and then all the atoms of the BEC relies in the same mean-field spin state, even when the ground-state has degeneracies. The spinor sector of the full Hamiltonian, constituted by the single-particle and interaction terms, can be written in the spinor sector of the full Hamiltonian, constituted by the square of the number operator. The rest of the Hamiltonian of the spinor sector can be written as

$$\hat{H} = \sum_{F=0}^{f} \frac{c_F}{2} \mathcal{M}^{(F)}_{ijkl} \hat{\psi}^+_i \hat{\psi}^+_j \hat{\psi}^+_k \hat{\psi}^+_l,$$  

(1)

where $\mathcal{M}^{(F)}$ are numerical tensors associated to the two-body collisions [1]. For example, the interactions for a spin-2 BEC has only three interactions $F = 0, 1, 2$ with

$$\mathcal{M}^{(0)}_{ijkl} = \delta_{ij} \delta_{jk}, \quad \mathcal{M}^{(1)}_{ijkl} = (F_0)_{ij}(F_0)_{jk}, \quad \mathcal{M}^{(2)}_{ijkl} = \frac{(-1)^{i+k}}{5} \delta_{i,-j} \delta_{k,-l},$$

(2)

where $\delta_{ij}$ is a Kronecker delta and $F_0$ are the angular momentum matrices with $\alpha = x, y$ or $z$ and scaled by $\hbar$, then the $F_0$ matrices are dimensionless. For spin-1 condensates, only the first two interactions $c_0$ and $c_1$ appear in the Hamiltonian. The term associated to $c_0$ is called spin-independent interaction since is equivalent to the square of the number operator. The rest of the interactions are spin-dependent. The spinor-quantum field associated to the spinor condensate is denoted by $\Psi = (\hat{\psi}_f, \hat{\psi}_{f-1}, \ldots, \hat{\psi}_{-f})^T$, where $\hat{\psi}_m$ are the field operators with magnetic quantum number $m$, and $T$ denotes the transpose. The Hamiltonian (1) has a point group $SO(3) \times \mathbb{Z}_2$ constituted by the group of rotations $SO(3)$ and the inversion through the origin.

Mean-field approximation assumes that $\langle \Psi \rangle = \Phi$, where $\Phi = (\phi_f, \phi_{f-1}, \ldots, \phi_{-f})^T$ is the spinor order-parameter and $\Phi^\dagger \Phi = N$, with $N$ the total number of atoms in the condensate gas. The spin phase of the BEC is be the order parameter $\Phi$ that minimizes the functional mean-field energy $E[\Phi] = \langle \hat{H} \rangle$. The rotational symmetries of $\Phi$ can be found alternatively through the Majorana representation for pure states [49], which associates to each spin-$f$ state $\Phi$ with $2f$ points on the sphere, usually called (the Majorana) constellation of $\Phi$ and denoted by $C_\Phi$. The representation is defined via a polynomial that involves the coefficients of $\Phi$,

$$p_{\Phi}(z) = \sum_{m=-f}^{f} (-1)^{f-m} \sqrt{\frac{2f}{f-m}} f_m z^{f+m}.$$  

(3)

The polynomial $p_{\Phi}(z)$ has degree at most $2f$, and by a rule its set of roots $\{\zeta_k\}$ is always increased to $2f$ by adding the sufficient number of roots at the infinity $[49, 52]$. $C_\Phi$ is thus a set of $2f$ points on $S^2$, called stars, obtained with the stereographic projection from the south pole of the roots $\{\zeta_k\}_{k=1}^{2f}$. Hence, a root $\zeta_k = \tan(\theta_k/2)e^{i\varphi_k}$ is associated to the point on the sphere with spherical angles $(\theta, \varphi)$. When $\Phi$ is transformed by the unitary representation $D(R)$ of a rotation $R \in SO(3)$ in its Hilbert space, the constellation $C_\Phi$ rotates by $R$ on the physical space $\mathbb{R}^3$, where $D^{(\sigma)}(R) \equiv (\sigma, \mu')e^{-i\alpha S_\sigma e^{-i\beta S_\mu} e^{-i\gamma S_3}}|\sigma, \mu\rangle$ is the Wigner D-matrix of a rotation $R$ with Euler angles $(\alpha, \beta, \gamma)$ [53]. Therefore, the point group of the quantum state $\Phi$ is equal to the point group of the geometrical object associated to $C_\Phi$. This representation has been used successfully to classify the spin ground phases of BEC in the ideal case of the zero temperature [17, 19, 44].

We now briefly review some of the most well-known phases with a point group that appears in a spinor BEC of spin $f = 1, 2$. In particular, we write their order parameters, and their respective Majorana constellations (see Figs. 1 and 2), in a particular orientation:

(1) Ferromagnetic (FM) phase: The spinor order-parameter has only one non-zero coefficient, $\phi_f = \sqrt{N}$. It is symmetric under rotations about the $z$ axis, imposing that the symmetry group is isomorphic to $SO(2)$. Its Majorana constellation $C_\Phi$ consists of $2f$ coincident points on the North pole.

(2) Polar (P) phase: Here $\phi_m = \sqrt{N}\delta_{m0}$. Its symmetry group, which is isomorphic to $SO(2) \times \mathbb{Z}_2$, consists of rotations about the $z$ axis and the inversion through the origin. For spin $f = 2$ condensates, it belongs to the family of states called the nematic phase [17]. The constellation of the polar phase has $f$ points on each pole of the sphere.

(3) Antiferromagnetic (AF) phase: It consists of a family of spin-1 states $\Phi = \sqrt{N}(\cos \chi, 0, \sin \chi)^T$ with $\chi \in (0, \pi/4)$. A family of states that represents this phase are also called non-inert states [44]. The whole set is symmetric over two geometric operations, a rotation by $\pi$ about the $z$ axis, and a reflection across the $yz$-plane, implying that the symmetry group is isomorphic to $\mathbb{Z}_2 \times \mathbb{Z}_2$. Its Majorana constellation consists of two points on the $yz$ plane, and their angle is dependent on $\chi$ and is bisected by the $z$ axes.

(4) Square (S) phase: A spin-2 phase with non-zero order-parameter terms $\phi_2 = \phi_{-2} = \sqrt{N/2}$. Its Majorana constellation consists of a square. Hence, $\Phi$ has the diphedral point group denoted by $D_2$ in the Schönflies notation [54]. This phase belongs also to the family of the non-inert nematic spin-2 states [17].
(5) Cyclic (C) phase: This spin-2 phase is described with \( \Phi = (\sqrt{N/3}) (1, 0, 0, \sqrt{2}, 0)^T \). The order parameter has constellation equal to a tetrahedron and, hence, point group equal to \( T \) [54].

The point group of each spin state can be confirmed by looking at its respective Majorana constellation. The states mentioned above appear as ground phases in the mean-field solution \( \psi_i = \phi_i + \delta \phi_i \). The atoms in the condensate are now split in two fractions: the condensate (c) and noncondensate (nc) atoms represented by a density matrices \( \rho_{ij}^{c} = \phi_{i} \phi_{j}^{*} \) and \( \rho_{ij}^{nc} = (\delta_{i}^{j} \delta_{i}) \), respectively. \( N^{a} = \text{Tr}(\rho^{a}) \) for \( a = n, nc \) are the fractions in each part and they satisfy that \( N^{c} + N^{nc} = N \). In the case of a self-consistent symmetry, such as the case of a spinor BEC with Hamiltonian (1) and \( \rho^{c} \) equal to one of the phases mentioned above, \( \rho^{nc} \) possess a particular point group. We then need to determine the most general \( \rho^{nc} \) with a particular point group. For that purpose, we now review the basic elements of a generalization of the Majorana representation for mixed states [50].

A mixed state is represented by a density matrix, i.e., a \( (2f + 1) \times (2f + 1) \) complex matrix with a nonnegative eigenspectrum. The set of density matrices has an orthonormal basis given by the tensor operators \( \{ T_{\sigma \mu}^{ij} \}_{\sigma \mu} \) with \( \sigma = 0, \ldots, 2f \) and \( \mu = -\sigma, \ldots, \sigma \) [53, 55, 56], which are defined in terms of the Clebsch-Gordan coefficients \( C_{j_{1}i_{1}j_{2}i_{2}}^{(m)} \)

\[
T_{\sigma \mu}^{(f)} = \sum_{m,m'} (-1)^{f-m'} C_{f,m,-m'}^{\sigma \mu} |f,m\rangle \langle f,m'|. \tag{4}
\]

From now on, we omit the super index \((f)\) when there is no possible confusion. The tensor operators \( T_{\sigma \mu} \) satisfy

\[
\text{Tr}(T_{\sigma \mu}^{\dagger} T_{\sigma' \mu'}) = \delta_{\sigma \sigma'} \delta_{\mu \mu'}. \tag{5}
\]

The most important property of the \( T_{\sigma \mu} \) operators is that they transform block-diagonally under a unitary transformation \( U(R) \) representing a rotation \( R \in SO(3) \) (or equivalent, of \( SU(2) \)) according to an irrep of \( SO(3) \) \( D^{(\sigma)}(R) \),

\[
U(R) T_{\sigma \mu} U^{-1}(R) = \sum_{\mu'=-\sigma}^{\sigma} D_{\mu' \mu}^{(\sigma)}(R) T_{\sigma \mu'}. \tag{6}
\]

where \( \sigma = 0, 1, 2, \ldots \) labels the irrep. The density matrix \( \rho^{nc} \) can be written in the \( \{ T_{\sigma \mu} \} \) basis as

\[
\rho^{nc} = N^{nc} \left( \frac{1}{2f+1} + \sum_{\sigma=1}^{2f} \rho_{\sigma} \cdot T_{\sigma} \right), \tag{7}
\]

where \( \rho_{\sigma} = (\rho_{\sigma \sigma}, \ldots, \rho_{\sigma -\sigma}) \in \mathbb{C}^{2\sigma+1} \) with \( \rho_{\sigma \mu} = \text{Tr}(\rho T_{\sigma \mu}^{\dagger}) \), \( T_{\sigma} = (T_{\sigma \sigma}, \ldots, T_{\sigma -\sigma}) \) is a vector of matrices, and the dot product is short for \( \sum_{\mu=-\sigma}^{\sigma} \rho_{\mu \mu} T_{\sigma \mu} \). Each vector \( \rho_{\sigma} \), which transforms as a spinor of spin \( \sigma \) by Eq. (6), can be associated to a constellation à la Majorana [49] consisting of \( 2\sigma \) points on \( S^{2} \) obtained through a similar polynomial as Eq. (3) but defined with \( \rho_{\sigma \mu} \). The hermiticity condition of \( \rho^{nc} \) and Eq. (5) implies that every constellation \( C^{(\sigma)} \) has antipodal symmetry [50]. While a pure state \( \Phi \) is normalized and its global phase factor is physically irrelevant, the same quantities of \( \rho_{\sigma} \) carry now the necessary information to fully characterize \( \rho^{nc} \). However, this information can also be added in the Majorana representation of \( \rho^{nc} \). The norm of \( \rho_{\sigma} \), \( r_{\sigma} \), is associated to the radius of the sphere where the constellation of \( \rho_{\sigma} \) lies. On the other hand, the hermiticity property of \( \rho^{nc} \) implies that the global phase factor of \( \rho_{\sigma} \) can only have two choices [50], both differing by a minus sign. There exists a method to associate this sign to a certain equivalence class of the points of each constellation [50]. For simplicity, we do not dwell more on this work, more details are presented in the companion article [51]. Here, we just incorporate this choice of sign to the norm \( r_{\sigma} \). Hence, \( r_{\sigma} \) can have negative values that evidently does not affect the radius of the sphere. In summary, a mixed state will be associated to a set, denoted
by \( \mathcal{C}_{\rho^{nc}} \), of \( 2f \) constellations with antipodal symmetry and a number of stars equal to \( 2\sigma \), with \( \sigma = 1, \ldots, 2f \), over spheres with radii \( r_\sigma \), respectively.

We now determine the density matrices \( \rho^{nc} \) with a particular point group \( G \). By the property (6) of the Majorana representation, \( \rho^{nc} \) has the point group \( G \) if each \( \rho_\sigma \) fulfill the following condition

\[
D^{(\sigma)}(g)\rho_\sigma = \rho_\sigma , \quad \text{for each } g \in G .
\]

Let us remark that this condition is more restrictive than in the case of pure states, where a state \( \Phi \) is invariant under the element action \( g \in G \) if \( D(g)\Phi \) is equal to \( \Phi \) up to a global phase factor. The determination of pure spin states with a particular point group has been studied before in [57]. We use Eq. (8) to impose on \( \rho^{nc} \) the symmetries of the spin phases mentioned above. We plot their Majorana representations in figures 1 and 2. By looking at the constellations, one can deduce that the point group of \( \rho^{nc} \) is equal to their corresponding order parameter \( \Phi \). We summarize the most important characteristics of \( \mathcal{C}_{\rho^{nc}} \) of each phase:

(1-2) FM and P phases: \( \rho_\sigma \) have only the 0th-components different than zero \( \rho_{\sigma 0} = r_\sigma \). Their constellations are given by \( \sigma \) stars on each pole of the sphere. The additional symmetry of the P phase implies that the \( \rho_\sigma \) vectors with \( \sigma \) odd are zero.

(3) AF phase: The vectors of \( \rho_\sigma \) are given by

\[
\rho_1 = r_1 (0,1,0) , \quad \rho_2 = r_2 \left( \frac{\cos x}{\sqrt{2}}, 0, \sin x, 0, \frac{\cos x}{\sqrt{2}} \right) ,
\]

\[
\rho_3 = r_3 (0,0,1,0,0) , \quad \rho_4 = r_4 \left( \frac{\cos y}{\sqrt{2}}, 0, 0, 0, \sin y, 0, 0, 0, \frac{\cos y}{\sqrt{2}} \right) .
\]

The constellation of \( \rho_1 \) has a star on each pole, and for \( \rho_2 \) it is a rectangle with sides parallels to the \( y \) and \( z \) axes with length dimensions dependent of the variable \( x \).

(4) S phase: \( \rho^{nc} \) has only two non-zero vectors \( \rho_\sigma \)

\[
\rho_2 = r_2 (0,0,1,0,0) , \quad \rho_4 = r_4 \left( \frac{\cos y}{\sqrt{2}}, 0, 0, 0, \sin y, 0, 0, 0, \frac{\cos y}{\sqrt{2}} \right) .
\]

The constellation of \( \rho_2 \) has two stars on each pole, and for \( \rho_4 \) it consists of a parallelepiped with faces parallel to the cartesian planes and length dimensions dependent of the variable \( y \).

(5) C phase: The \( \rho_\sigma \) non-zero vectors are

\[
\rho_1 = r_1 \left( -\sqrt{2}, 0, 0, \sqrt{5}, 0, 0, \sqrt{2} \right) / 3 ,
\]

\[
\rho_4 = r_4 \left( 0, -\sqrt{10}, 0, 0, -\sqrt{7}, 0, 0, \sqrt{10}, 0 \right) / \sqrt{27} .
\]

Their constellations are given by an octahedron and a constellation conformed by two antipodal tetrahedrons, respectively.

A generic \( \rho^{nc} \) has a total of \( (2f+1)^2 \) degrees of freedom constituted by the variables \( \rho_{\sigma \mu} \) and \( \mathcal{N}^{nc} \), with domain restricted by the properties of the density matrices \( \rho^{nc} \), unit trace, hermiticity and positive semidefinite condition [58], where the last one is complicated to implement in general but is satisfied for any physical system. However, the previous calculations show that the inherited symmetries of \( \rho^{nc} \) reduce the degrees of freedom considerably. For example, in spin-1 BEC, the number is reduced from
9 degrees to $3\left(N_{nc}, r_1, r_2\right)$ for the FM and P phases, and to $4\left(N_{nc}, r_1, r_2, x\right)$ in the AF phase. On the other hand, the degrees of freedom of the spin-2 phases, which are 25 in the general case, are reduced to 3 or 5, depending on the symmetry of its corresponding order parameter. As an application to these reductions, we calculate the spin phase diagram of a BEC of spin-2 at finite temperatures using the Hartree-Fock approximation [20, 37–39], and they are plotted in Fig. 3. We predict a deviation of the phase diagram of a BEC of spin-2 at finite temperatures by the Hartree-Fock approximation and as the other phase transitions that remain invariant. We also add the values of the coupling factors $(c_1, c_2)$ of several atomic species, with their respective uncertainties [16]. We can conclude that, while for $^{23}$Na and $^{87}$Rb gases the phases remain practically invariant with the temperature, the $^{87}$Rb condensates may exhibit a temperature-dependent spin-phase transition. Details of the Hartree-Fock approximation are presented in the companion article [51], including other results associated with other physical properties, such as magnetization and regions of metastability.

To conclude, we would like to emphasize that the characterization of the noncondensate fraction $\rho^{nc}$ is general for any variational approach with a self-consistent symmetry, and for any other spin or spin-like system. Moreover, the method presented here can be implemented in systems constituted by a tensor product of spin systems, where other generalizations of the Majorana representation may be necessary [59, 60].

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