Phase characterization of spinor Bose-Einstein condensates: a Majorana stellar representation approach

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(Dated: February 21, 2023)

Many-body systems with spin degree of freedom may exhibit emergent phenomena described only by beyond mean-field (MF) theories. Here we present a rigorous method to determine the variational perturbations for the MF solution of an interacting spinor system with rotational symmetries. It is based on a generalization of the Majorana stellar representation for quantum mixed states, and it is amenable to any variational method with self-consistent symmetries and for any open ensemble of spinor-like particles. As an application of the formalism, we characterize the allowed phases in spin 1 and 2 Bose-Einstein condensates and calculate the finite-temperature phase diagram of spin-2 condensates.

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 (BEC) can be realized nowadays under highly controllable setups [1–5]. In BECs the spatial behavior of the ground state is basically defined by the type of the confinement trap, provided that neither spin-orbit coupling nor the dipolar interactions are of significance. Most notably, the spin domain behavior of spinor BECs can differ drastically over different atomic species [2]. For instance, it has been corroborated experimentally [6–9] that condensates of ^{23}Na and ^{78}Rb in an optical trap exhibits different ground spinor phases: the polar (P) and the ferromagnetic (FM) phases, respectively [1, 10]. Recent experimental advances allow us to 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 [7, 11–16]. Theoretically the study of the spin-phase diagram in spinor BECs via mean-field (MF) theories were introduced first for spin $f = 1$ [17, 18] and subsequently for higher spins [2, 19–22]. The MF theory consists to assume that all the atoms in the condensate share the same quantum state, which is defined by an average over the many-body quantum states of the condensate, and characterized by a spinor order-parameter $\mathbf{\Phi}$ obeying the spinor version of the well-known Gross-Pitaevskii (GP) equations [1, 2, 10].

Although the MF theory predicts qualitatively well the spin phases of a BEC, it fails to offer a satisfactory description of a wide range of physical effects as, its behavior at finite temperatures, quantum fluctuations, or nonlocal perturbations. The studies of the spinor BEC covering these aspects become essential to scrutinize other nontrivial physical phenomena such as deviations in the spin phase boundaries, metastable phases, tunneling effects, quench dynamics, or (dynamic/static) quantum phase transitions, among others phenomena [5, 8, 11, 23–38]. Some of the well-known beyond mean-field theories are the variational approaches which have proven in BECs to be well suitable near its MF phases [23, 39–44]. Physically, this entails that the condensate gas, represented by a mixed ensemble of particles, is described by a density matrix ρ. It is assumed to be comprised by two contributions such that $\rho = \rho^c + \rho^{nc}$, where $\rho^c = \mathbf{\Phi}^\dagger \mathbf{\Phi}$ is the atom fraction that remains in the same MF solution $\mathbf{\Phi}$, while ρ^{nc} is the ensemble of noncondensate atoms described by other quantum states to be determined [23, 27, 40].

Operationally, variational methods in condensates involve self-consistent solutions of the GP equations coupled to a set of equations that govern the noncondensate fraction. These methods are, however, computationally demanding and not free from numerical issues [23, 27, 39, 40].A way to circumvent this is to make use of variational methods with self-consistent symmetries [39], *i.e.*, approaches where the noncondensate fraction ρ^{nc} inherits the common symmetries between the Hamiltonian and the order parameter $\mathbf{\Phi}$ of the condensed fraction. In fact, and as a consequence of the Michel's theorem [45], the common symmetries of the Hamiltonian and $\mathbf{\Phi}$ are a nontrivial point group, *i.e.* a set of rotational and reflection symmetries. This result has been used to characterize MF solutions of spinor BEC [2, 20, 22, 46, 47]. The point group symmetries associated to spin phases are also of great interest due to its connection to the appearance of (Abelian or non-Abelian) vortices [48–50]. Notably, the inherited symmetries of ρ^{nc} has been exploited before to study the metastable phases of spinor BEC of spin-1 at finite temperatures [27].

In this Letter, we present a thoroughly systematic method based on the Majorana representation of spin mixed states [51, 52] and the use of self-consistent symmetries that allows to fully determine the non-condensed

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fraction ρ^{nc} of a spinor BEC with a certain point group symmetry. We exemplify the method by characterizing ρ^{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 [23, 39–41], that in turn predicts the appearance of a deviation with temperature of the cyclic-nematic phase boundary. Due to the nontrivial spin interactions a rich scenario emerges within the Hartree-Fock approximation for the noncondensate fraction in other symmetries and/or higher spins [2, 13, 14, 16]. This however, goes beyond the aim of this letter but it is covered in the companion paper [53].

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. We also consider that the atomic gas is factorizable into its spinorial and spatial sectors, and is without topological spin disorder. The spinor sector of the full Hamiltonian can be written in the second-quantization formalism in terms of the interaction channel with its respective coupling factors c_γ, where $\gamma = 0, 1, \dots f$, associated to the s-wave scattering lengths of the total spin channel [1, 2]. In a general form, the Hamiltonian of the spinor sector of the BEC can be written as

$$\hat{H} = \sum_{\gamma=0}^{f} \frac{c_\gamma}{2} \mathcal{M}^{(\gamma)}_{ijkl} \hat{\psi}^\dagger_i \hat{\psi}^\dagger_j \hat{\psi}_k \hat{\psi}_l \,, \tag{1}$$

where $\mathcal{M}^{(\gamma)}$ are numerical tensors associated to the two-body collisions [2]. For example, the interactions for a spin-2 BEC has three tensor elements given by [53]

$$\begin{aligned} \mathcal{M}^{(0)}_{ijkl} =& \delta_{il}\delta_{jk} \,, \quad \mathcal{M}^{(1)}_{ijkl} = (F_\nu)_{il}(F_\nu)_{jk} \,, \\ & \mathcal{M}^{(2)}_{ijkl} = \frac{(-1)^{i+k}}{5} \delta_{i,-j}\delta_{k,-l} \,, \end{aligned} \tag{2}$$

where δ_{ij} is the Kronecker delta, and F_ν are the components of the angular momentum matrices along the $\nu = x, y$ or z direction, which here are scaled by $\hbar$ making them dimensionless. For spin-1 condensates, only the first two interactions c_0 and c_1 appear in the Hamiltonian. The c_0-interaction is spin-independent since it is equivalent to the square of the number operator. The rest of the interactions are all spin-dependent. The spinor-quantum field associated to the spinor condensate is denoted by $\hat{\mathbf{\Psi}} = (\hat{\psi}_f\,, \hat{\psi}_{f-1}\,, \dots\,, \hat{\psi}_{-f})^{\mathrm{T}}$, where $\hat{\psi}_m$ are the field operators with magnetic quantum number m, and T denotes the transpose. The Hamiltonian (1) has a symmetry point group $SO(3) \times \mathbb{Z}_2$ constituted by the group of rotations $SO(3)$ and the inversion through the origin.

Mean-field (MF) approximation assumes that $\langle \hat{\mathbf{\Psi}} \rangle = \mathbf{\Phi}$, where $\mathbf{\Phi} = (\phi_f, \phi_{f-1}, \dots, \phi_{-f})^{\mathrm{T}}$, is the spinor order-parameter obeying $\mathbf{\Phi}^\dagger \mathbf{\Phi} = N$, being N the total number of atoms in the condensate gas [1, 2]. The spin phase of the BEC is thus the order parameter $\mathbf{\Phi}$ that minimizes the functional energy $E[\mathbf{\Phi}] = \langle \hat{H} \rangle$. The rotational symmetries of $\mathbf{\Phi}$ can be found through the Majorana representation for pure states [51], which associates each spin-f state $\mathbf{\Phi}$ with $2f$ points on the sphere, usually called the (Majorana) constellation of $\mathbf{\Phi}$ and denoted by $\mathcal{C}_{\mathbf{\Phi}}$. The representation is defined via a polynomial that involves the coefficients of $\mathbf{\Phi}$,

$$p_{\mathbf{\Phi}}(z) = \sum_{m=-f}^{f} (-1)^{f-m} \sqrt{\binom{2f}{f-m}} \phi_m z^{f+m} \,. \tag{3}$$

The degree of the polynomial $p_{\mathbf{\Phi}}(z)$ is at most $2f$, and by rule, its set of roots $\{\zeta_k\}$ is always increased to $2f$ by adding the sufficient number of roots at infinity [51, 54]. $\mathcal{C}_{\mathbf{\Phi}}$ is thus a set of $2f$ points on the sphere S^2, called *stars*, obtained with the stereographic projection from the south pole of the roots $\zeta_k = \tan(\theta_k/2)e^{i\varphi_k}$, with $(\theta_k\,, \varphi_k)$ the spherical angles. When $\mathbf{\Phi}$ is transformed by the unitary representation $D(\mathsf{R})$ of a rotation $\mathsf{R} \in SO(3)$ in its Hilbert space, the constellation $\mathcal{C}_{\mathbf{\Phi}}$ rotates by R on the physical space $\mathbb{R}^3$, where $D^{(\sigma)}_{\mu'\mu}(\mathsf{R}) \equiv \langle \sigma,\, \mu' | e^{-i\alpha F_z} e^{-i\beta F_y} e^{-i\gamma F_z} | \sigma,\, \mu \rangle$ is the Wigner D-matrix of a rotation R with Euler angles $(\alpha,\, \beta,\, \gamma)$ [55]. Therefore, the point group of the quantum state $\mathbf{\Phi}$ is equal to the point group of the geometrical object associated to $\mathcal{C}_{\mathbf{\Phi}}$. This representation has been used successfully to classify the spin ground phases of BEC in the ideal case of zero temperature [20, 22, 46].

We now briefly review some of the most well-known phases associated with a symmetry point group that appears as a MF solution of a BEC with spin $f = 1, 2$. In particular, we write its order parameters and respective Majorana constellations (Figs. 1 and 2) for a given 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 its symmetry group be isomorphic to $SO(2)$. Its constellation $\mathcal{C}_{\mathbf{\Phi}}$ 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 [20]. The constellation of the polar phase has f points on each pole of the sphere.

(3) Antiferromagnetic (AF) phase: It is a non-inert state [46] since it is represented by a family of spin-1 states $\mathbf{\Phi} = \sqrt{N}(\cos\chi, 0, \sin\chi)^{\mathrm{T}}$ with $\chi \in (0, \pi/4]$. The whole family is symmetric over two geometric operations, a rotation by π 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 χ and bisected by the z axis.

(4) Square (S) phase: A spin-2 phase with non-zero order-parameter terms $\phi_2 = \phi_{-2} = \sqrt{N/2}$. Its Majo-

rana constellation consists of a square. Hence, $\mathbf{\Phi}$ has the dihedral point group denoted by D_4 in the Schönflies notation [56]. This phase belongs also to the family of the nematic spin-2 states [20].

(5) Cyclic (C) phase: This spin-2 phase is described with $\mathbf{\Phi} = (\sqrt{N/3})(1, 0, 0, \sqrt{2}, 0)^{\mathrm{T}}$. The order parameter has constellation equal to a tetrahedron with point group T in the Schönflies notation [56].

The point group of each spin state can be established by seeking at its respective Majorana constellation. The spin phases mentioned above also appear as ground states for Hamiltonians with additional terms as Zeeman interactions, or others restrictions as fixed magnetization [2, 19].

We now consider a variational perturbation of the field operators $\hat{\delta}_j$ near the MF solution, such that $\hat{\psi}_j = \phi_j + \hat{\delta}_j$. The atoms in the condensate are now split in two fractions: those who describes the condensate (c) part, and those that specify the noncondensate (nc) fraction of atoms. They are represented by the density matrices $\rho^c_{ij} = \phi_i \phi^*_j$ and $\rho^{nc}_{ij} = \langle \hat{\delta}^\dagger_j \hat{\delta}_i \rangle$, respectively. Thus $N^a = \mathrm{Tr}(\rho^a)$ for $a = n, nc$ are the fractions in each part satisfying $N^c + N^{nc} = N$. In the case of a variational method with self-consistent symmetry, ρ^{nc} inherits a particular point group from the symmetries of the Hamiltonian (1) and ρ^c. We then need to determine the most general ρ^{nc} for a given point group symmetry. To that end, we make use of the Majorana representation for mixed states [52].

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 $T^{(f)}_{\sigma\mu}$ with $\sigma = 0, \ldots 2f$ and $\mu = -\sigma, \ldots, \sigma$ [55, 57, 58], which are defined in terms of the Clebsch-Gordan coefficients $C^{jm}_{j_1 m_1 j_2 m_2}$, and reads

$$T^{(f)}_{\sigma\mu} = \sum_{m,m'=-f}^{f} (-1)^{f-m'} C^{\sigma\mu}_{fm,f-m'} \left| f, m \right\rangle \left\langle f, m' \right| . \quad (4)$$

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

$$\mathrm{Tr}(T^\dagger_{\sigma_1\mu_1} T_{\sigma_2\mu_2}) = \delta_{\sigma_1\sigma_2}\delta_{\mu_1\mu_2} , \quad T^\dagger_{\sigma\mu} = (-1)^\mu T_{\sigma-\mu} . \quad (5)$$

The most important property of the $T_{\sigma\mu}$ operators is that they transform block-diagonally under a unitary transformation $U(\mathsf{R})$, that represents a rotation $\mathsf{R} \in SO(3)$, according to an *irrep* of $SO(3)$ $D^{(\sigma)}(\mathsf{R})$, such that

$$U(\mathsf{R}) T_{\sigma\mu} U^{-1}(\mathsf{R}) = \sum_{\mu'=-\sigma}^{\sigma} D^{(\sigma)}_{\mu'\mu}(\mathsf{R}) T_{\sigma\mu'} , \quad (6)$$

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

$$\rho^{nc} = N^{nc} \left(\frac{\mathbb{1}_f}{2f+1} + \sum_{\sigma=1}^{2f} \boldsymbol{\rho}_\sigma \cdot \boldsymbol{T}_\sigma \right) , \quad (7)$$

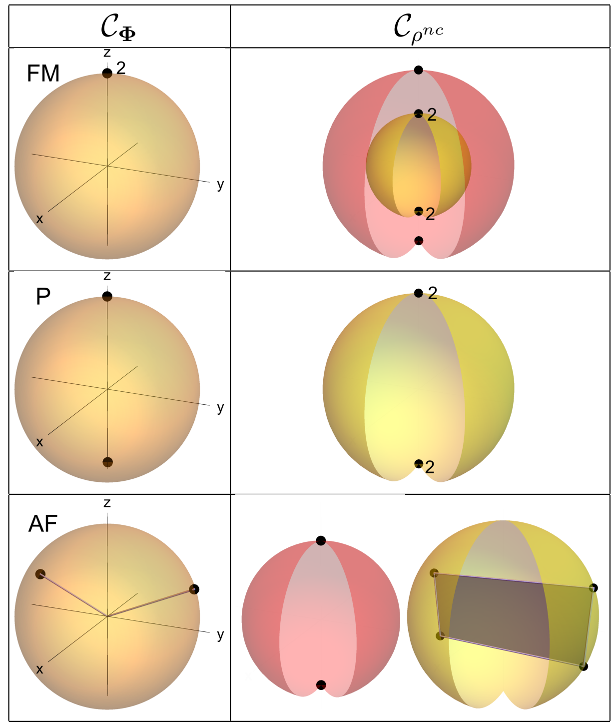

FIG. 1. Majorana representations of the order parameters $\mathbf{\Phi}$ (left) and noncondensed fraction ρ^{nc} (right) of spin phases of BEC of $f = 1$. The adjacent number in some points correspond to its degeneracy. Each nonzero vector $\boldsymbol{\rho}_\sigma$ of ρ^{nc} is associated to a constellation of 2σ points, which are also colored in red and yellow for $\sigma = 1$ and 2, respectively. For clarity, we omit the cartesian axis in the figures and split the constellations of the AF phase. The gray area in the second constellation of $\mathcal{C}_{\rho^{nc}}$ of the AF phase is the corresponding geometric object of the points.

where $\boldsymbol{\rho}_\sigma = (\rho_{\sigma\sigma}, \ldots, \rho_{\sigma-\sigma}) \in \mathbb{C}^{2\sigma+1}$ with $\rho_{\sigma\mu} = \mathrm{Tr}(\rho T^\dagger_{\sigma\mu})$, and $\boldsymbol{T}_\sigma = (T_{\sigma\sigma}, \ldots, T_{\sigma,-\sigma})$ is a vector of matrices. Here the dot product stands for $\sum_{\mu=-\sigma}^{\sigma} \rho_{\sigma\mu} T_{\sigma\mu}$. Each vector $\boldsymbol{\rho}_\sigma$, which transforms as a spinor of spin σ by Eq. (6), can be associated to a constellation *à la Majorana* [51] consisting of 2σ points on S^2 obtained through a similar polynomial as Eq. (3) but defined with $\rho_{\sigma\mu}$. The hermiticity condition of ρ^{nc} together with Eq. (5) implies that every constellation $\mathcal{C}^{(\sigma)}$ has antipodal symmetry [52]. While a pure state $\mathbf{\Phi}$ is normalized and its global phase factor is physically irrelevant, the same quantities of $\boldsymbol{\rho}_\sigma$ carry now the necessary information to fully characterize ρ^{nc}. However, this information can also be added in the Majorana representation of ρ^{nc}. The norm of $\boldsymbol{\rho}_\sigma$, r_σ, is associated to the radius of the sphere where the constellation of $\boldsymbol{\rho}_\sigma$ lies. On the other hand, the hermiticity property of ρ^{nc} implies that the global phase factor of $\boldsymbol{\rho}_\sigma$ can only have two choices [52], 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 [52] that is presented in the companion article [53]. Here, we just incorporate this choice of sign to the norm r_σ. Hence, r_σ 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 of $2f$ constellations, denoted by $\mathcal{C}_{\rho^{nc}}$, with antipodal symmetry and a number of stars equal to 2σ, with $\sigma = 1, \ldots, 2f$, over spheres with radii r_σ, respectively.

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

$$D^{(\sigma)}(g)\boldsymbol{\rho}_\sigma = \boldsymbol{\rho}_\sigma\,, \quad \text{for each } g \in G\,. \tag{8}$$

Let us remark that this condition is more restrictive that in the case of pure states, where a state $\boldsymbol{\Phi}$ is invariant under the element action $g \in G$ if $D(g)\boldsymbol{\Phi}$ is equal to $\boldsymbol{\Phi}$ up to a global phase factor. The determination of pure spin states with a particular point group has been studied before in [59]. We use Eq. (8) to impose on ρ^{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 ρ^{nc} is equal to their corresponding order parameter $\boldsymbol{\Phi}$. We summarize the most important characteristics of $\mathcal{C}_{\rho^{nc}}$ of each phase:

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

(3) AF phase: The vectors of $\boldsymbol{\rho}_\sigma$ are given by

$$\boldsymbol{\rho}_1 = r_1\,(0,1,0)\,,\ \boldsymbol{\rho}_2 = r_2\left(\frac{\cos x}{\sqrt{2}}, 0, \sin x, 0, \frac{\cos x}{\sqrt{2}}\right)\,. \tag{9}$$

The constellations of $\boldsymbol{\rho}_1$ has a star on each pole, and for $\boldsymbol{\rho}_2$ it is a rectangle with sides parallels to the y and z axes with length dimensions dependent of the variable x.

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

$$\begin{aligned}\boldsymbol{\rho}_2 =& r_2\,(0\,,0\,,1\,,0\,,0)\,,\\ \boldsymbol{\rho}_4 =& r_4\left(\frac{\cos y}{\sqrt{2}}\,,0\,,0\,,0\,,\sin y\,,0\,,0\,,0\,,\frac{\cos y}{\sqrt{2}}\right)\,.\end{aligned} \tag{10}$$

The constellation of $\boldsymbol{\rho}_2$ has two stars on each pole, and for $\boldsymbol{\rho}_4$ it consists of a parallelepiped with faces parallel to the cartesian planes and length dimensions dependent of the variable y.

(5) C phase: The $\boldsymbol{\rho}_\sigma$ non-zero vectors are

$$\begin{aligned}\boldsymbol{\rho}_3 =& r_3\left(-\sqrt{2}\,,0\,,0\,,\sqrt{5}\,,0\,,0\,,\sqrt{2}\right)/3\,, \qquad (11)\\ \boldsymbol{\rho}_4 =& r_4\left(0\,,-\sqrt{10}\,,0\,,0\,,-\sqrt{7}\,,0\,,0\,,\sqrt{10}\,,0\right)/\sqrt{27}\,.\end{aligned}$$

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

A generic ρ^{nc} has a total of $(2f+1)^2$ degrees of freedom constituted by the variables $\rho_{\sigma\mu}$ and N^{nc}, with domain restricted by the properties of the density matrices ρ^{nc},

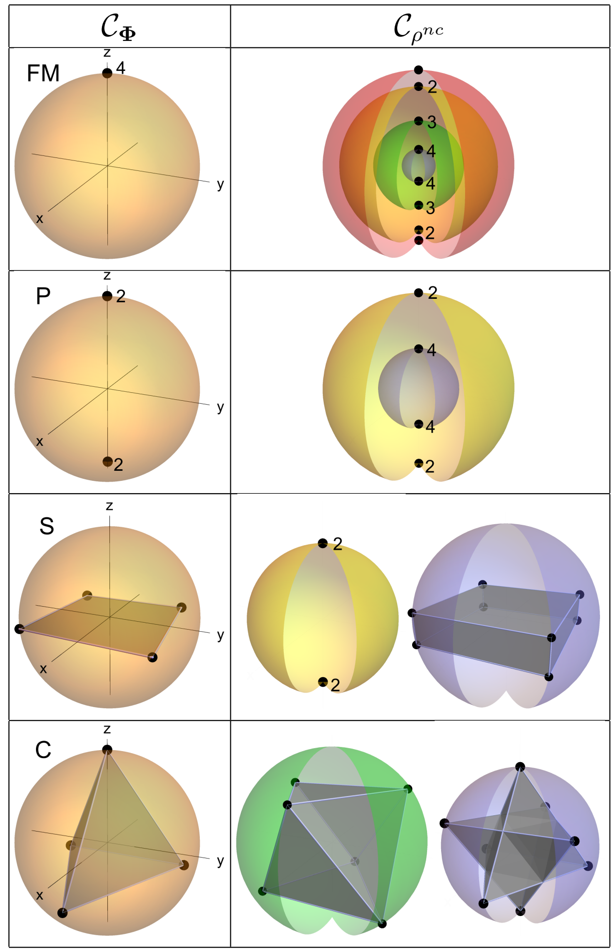

FIG. 2. Majorana representations of Φ (left) and ρ^{nc} (right) of spin phases of BEC of spin-2, where we follow the same conventions as in Fig. 1. The constellations of $\boldsymbol{\rho}_\sigma$ for $\sigma = 3, 4$, correspond to the constellations with six (green sphere) and eight (blue sphere) points, respectively.

unit trace, hermiticity and positive semidefinite condition [60]. The latter is intricate to implement but is still hold true in general for any physical system. Notwithstanding, the previous calculations show that the inherited symmetries of ρ^{nc} reduce the degrees of freedom considerably. For example, in spin-1 BEC, the number is reduced from 9 degrees to 3 (N^{nc}, r_1, r_2) for the FM and P phases, and to 4 (N^{nc}, r_1, r_2, x) in the AF phase. On the other hand, the degrees of freedom of the spin-2 phases, which add to 25 in the general case, are significantly reduced to 3 or 5, depending upon the symmetry of its corresponding order-parameter. As an application to the power of these reductions, we have calculated with this approach the spin phase diagram of a BEC of spin-2 at finite temperatures using the Hartree-Fock approximation [23, 39–41] (See Fig. 3). We predict a deviation of the C-P phase-transition dependent of the temperature, as opposite as the other phase transitions that remain invariant with the temperature. We can conclude that, whilst for ^{23}Na and ^{83}Rb cold gases the phases remain practically insen-

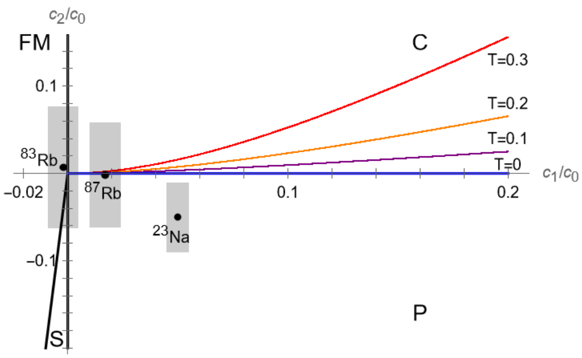

FIG. 3. Phase diagram of the spin-2 BEC in the space of the spin-dependent coupling factors (c_1, c_2). The C-P phase transition (color curves) depends on the temperature, while the rest of the phase transitions remain invariant (black lines). We also add the values of the coupling factors (c_1, c_2) of several atomic species along with its respective uncertainties [19].

sible to temperature, the ^{87}Rb condensates may exhibit a temperature-dependent spin-phase transition. Details of the calculations are presented in the companion article [53], including additional material related to the magnetization and the characterization of the allowed regions of the spin phases.

To summarize, we introduced a rigorous method capable of characterize the MF variational perturbations of an interacting spinor system with a self-consistent rotational symmetry. Our method is based in a generalization of the Majorana stellar representation for quantum mixed states in conjunction with point group symmetry arguments. A distinctive feature of the approach is that is general for any variational approach with a self-consistent symmetry, and for any other spin or spin-like physical 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 [61, 62].

E.S.-E. acknowledges support from the postdoctoral fellowships offered by DGAPA-UNAM and the IPD-STEMA program of the University of Liège. F.M. acknowledges the support of DGAPA-UNAM through the project PAPIIT No. IN113920.

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