

Classifying vortices in $S=3$ Bose-Einstein condensates

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Motivated by the recent realization of a ^{52}Cr Bose-Einstein condensate, we consider the phase diagram of a general spin-three condensate as a function of its scattering lengths. We classify each phase according to its reciprocal spinor, using a method developed in a previous work. We show that such a classification can be naturally extended to describe the vortices for a spinor condensate by using the topological theory of defects. To illustrate, we systematically describe the types of vortex excitations for each phase of the spin-three condensate.

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Over the past few years, there has been remarkable experimental progress in the study of spinor Bose-Einstein condensates (BECs) [1–5]. One of the most intriguing examples is the recent realization of a ^{52}Cr [4] condensate which has since received substantial theoretical attention [6–9]. Atomic chromium has six electrons in its outermost shell which combine into a state with maximal spin $S=3$ according to Hund’s rules. These electrons also give rise to a magnetic dipole moment which is much larger than that of the alkali-metal atoms where dipolar effects are typically unimportant. In fact, such dipolar effects have been observed in the expansion profiles of ^{52}Cr [10]. Dipolar effects are important for magnetic traps where the spin degrees are frozen out. However, when purely optical traps are used it has been argued that the spin exchange interaction will overwhelm the dipolar interaction [7]. Due to such spin interactions, a dilute gas of spin-three bosons will interact according to the pair potential

$$V_p(\mathbf{r}_1 - \mathbf{r}_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2)(g_0\mathcal{P}_0 + g_2\mathcal{P}_2 + g_4\mathcal{P}_2 + g_6\mathcal{P}_6), \quad (1)$$

where \mathcal{P}_S projects into the state with total spin S and $g_S = 4\pi\hbar^2 a_S/m$, and a_S is the scattering length corresponding to spin S . For the spin-three problem, this potential gives rise to a phase diagram (as a function of the possible values of the scattering lengths) of great richness as was revealed in [6,7]. In addition to having such rich phase diagrams, spinor condensates in general and the ^{52}Cr condensate in particular will have intriguing topological excitations. Topological excitations for spin-one, spin-three-halves, and spin-two condensates have received considerable attention in the literature [11–16] since the pioneering work of Ho [17] and Ohmi and Machida [18]. Also, recently topological spin textures have been observed in ^{87}Rb atoms in the spin-one hyperfine state [5].

In a previous publication [19], we have developed a way of classifying spinor BEC and Mott insulating states and illustrated the method with an application to the spin-two boson problem. More specifically, we showed that it is natural to identify a spin S state $|\psi\rangle = \sum_{\alpha=-S}^S A_\alpha |\alpha\rangle$ with $2S$ points on the unit sphere (θ, ϕ) . In fact, there is a one-to-one correspondence between a spinor and a “reciprocal spinor” up to phase and normalization

$$\{A_\alpha\} \leftrightarrow \{\zeta_i\}, \quad (2)$$

where $\zeta = \tan(\theta/2)e^{i\phi}$ is the stereographic image on the complex plane of the point (θ, ϕ) on the unit sphere. The set of such complex numbers $\{\zeta_i\}$ are explicitly constructed by finding the coherent states $|\zeta\rangle = \sum_{\alpha=0}^{2S} \sqrt{\binom{2S}{\alpha}} \zeta^\alpha |S-\alpha\rangle$, which are orthogonal to the spinor states $|\psi\rangle$. The characteristic equation $f_\psi(\zeta) \equiv \langle\psi|\zeta\rangle$ will then be a polynomial in ζ of order $2S$ and its $2S$ roots projected on the sphere will immediately give the symmetries of the spinor. Spin rotations which leave this set of points invariant will take a spinor A_α into itself modulo an overall phase which can be computed through geometrical considerations. Thus this method gives a complete description of the spinor state.

In this work, we show that such a method is also useful for classifying the spinor vortices. To illustrate, we focus on the spin-three problem, motivated by the recent experimental development [4]. We first reproduce the phase diagrams for spin-three condensates obtained previously in [6,7]. Then we find the symmetries of each phase (see Fig. 1) by applying the method developed in [19]. We then systematically describe the types of topological excitations for such a system

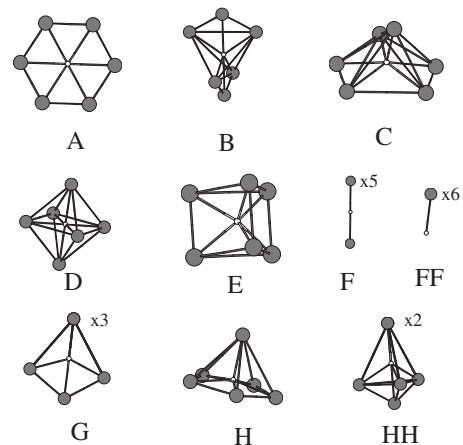


FIG. 1. Reciprocal spinors. Points on the unit sphere (gray spheres) having the transformation properties of the wave functions given in Table I. The small white spheres are put at the origin as a visual aid. Points which correspond to degenerate roots are marked.

TABLE I. Wave functions $|\psi\rangle = \frac{1}{\sqrt{N!}}(A_\alpha \alpha_\alpha^\dagger)^N|0\rangle$ for the possible spinor phases corresponding to global minima of Eq. (7) for particular scattering lengths up to SO(3) invariance. Also shown is the subgroup of SO(3) corresponding to the symmetries of the wave function. The last column gives the number of conjugacy classes of π_1 for each spin state, which gives the number of possible vortex excitations. The “ $\times \mathbb{Z}_v$ ” in this column reflects the fact that an arbitrary multiple of 2π can always be added to the winding in the superfluid phase.

	A_α	SO(3) subgroup	N_{vort}
A	$\left(\frac{1}{\sqrt{2}}, 0, 0, 0, 0, \frac{1}{\sqrt{2}}\right)$	D_6	$9 \times \mathbb{Z}_v$
B	$\left(0, \frac{\sin(\eta)}{\sqrt{2}}, 0, \cos(\eta), 0, -\frac{\sin(\eta)}{\sqrt{2}}, 0\right)$	D_2	$5 \times \mathbb{Z}_v$
C	$\left(0, \frac{\sin(\chi)\cos(\eta)}{\sqrt{2}}, \frac{i\sin(\chi)\sin(\eta)}{\sqrt{2}}, \cos(\chi), \frac{-i\sin(\chi)\sin(\eta)}{\sqrt{2}}, \frac{\sin(\chi)\cos(\eta)}{\sqrt{2}}, 0\right)$	C_2	$4 \times \mathbb{Z}_v$
D	$\left(0, \frac{1}{\sqrt{2}}, 0, 0, 0, \frac{1}{\sqrt{2}}, 0\right)$	O	$8 \times \mathbb{Z}_v$
E	$\left(\frac{\sin(\eta)}{\sqrt{2}}, 0, 0, \cos(\eta), 0, 0, \frac{\sin(\eta)}{\sqrt{2}}\right)$	D_3	$6 \times \mathbb{Z}_v$
F	$(0, 1, 0, 0, 0, 0, 0)$	U (1)	4
FF	$(1, 0, 0, 0, 0, 0, 0)$	U (1)	6
G	$(0, \sin(\eta), 0, \cos(\eta), 0, 0, 0)$	C_2	$4 \times \mathbb{Z}_v$
H	$(\sin(\eta), 0, 0, 0, 0, \cos(\eta), 0)$	C_5	$10 \times \mathbb{Z}_v$
HH	$(0, \sin(\eta), 0, 0, 0, \cos(\eta), 0, 0)$	C_3	$6 \times \mathbb{Z}_v$

using the topological theory of defects [20]. Such a scheme enumerates all possible types of vortex excitations, though it does not determine which are energetically stable against dividing into multiple vortices. Finally, we will briefly discuss the resulting microscopic wave functions for the vortex excitations. Such understanding of vortices will be relevant for rotating ^{52}Cr condensates in optical traps.

In general, the topological vortex excitations (line defects) of an ordered medium are given by the first homotopy group $\pi_1(R)$ (the group of closed loops) of the order parameter space R . More specifically, the conjugacy classes of $\pi_1(R)$ correspond to the vortex types. Moreover, the way such vortices combine is determined by the multiplication table of the conjugacy classes. For a pedagogical review of the topological theory of defects, see [20] (whose notation we will adopt). A theorem from algebraic topology (see, e.g., Ref. [21]) which is used as a reliable tool for computing the first homotopy group is the following. Let G be a simply connected group and H be a subgroup of G . Then

$$\pi_1(G/H) = H/H_0, \quad (3)$$

where H_0 are the elements of H which are connected to the identity by continuous transformations. To apply this theorem to our system, we need to take G to be a group of operators that act transitively on the spin ground states and H to be the subgroup of G which leave the particular spinor state we are considering invariant. Then R has the same topology as G/H , so the theorem applies. The first guess would be to use elements such as $e^{i\alpha}e^{-i\mathbf{S}\cdot\hat{\mathbf{n}}\beta}$ (where \mathbf{S} are the spin-three matrices and $\hat{\mathbf{n}}$ is a unit vector) which act directly on the spinor states and superfluid phase. However, these

elements form a representation of $\text{SO}(3) \otimes \text{U}(1)$, which is not simply connected, so Eq. (3) will not apply. Thus we need instead to take the simply connected group $G = \text{SU}(2) \otimes T$, where T is the group of translations in one dimension with elements satisfying the property $T(x)T(y) = T(x+y)$ (which will be simply connected). This is the covering group of $\text{SO}(3) \otimes \text{U}(1)$. In this work we will use the representation of $\text{SU}(2)$ by Pauli matrices, thus we describe its elements in the form $e^{-i(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}/2)\Theta}$. We then use the homomorphism $\varphi: \text{SU}(2) \otimes T \rightarrow \text{SO}(3) \otimes \text{U}(1)$ given by $\varphi(T(x)e^{-i(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}/2)\Theta}) = e^{ix}e^{-i\mathbf{S}\cdot\hat{\mathbf{n}}\Theta}$ which “lifts” our group acting directly on the spinor states into the larger simply connected group, G . The subgroup $H \subseteq G$ will be the collection of elements $h \in G$ which leave the particular spinor under consideration invariant. Once H is constructed by such a method, Eq. (3) can then be directly applied to construct the first homotopy group.

As we will see, the majority of the phases in the spin-three phase diagram have only discrete symmetries. For such states, H_0 is the trivial group containing one element. For this situation, our computational theorem reduces to

$$\pi_1(G/H) = H. \quad (4)$$

Therefore, constructing π_1 for such states becomes straightforward: One first finds the rotations in $\text{SO}(3)$ which leave invariant the points on the unit sphere $\{\zeta_\alpha\}$ given by our classification scheme [19]. For this purpose, it is helpful to note the possible finite subgroups of $\text{SO}(3)$. They are the cyclic groups C_n , the dihedral groups D_n , the tetrahedral group T , the octahedral group O , and the icosahedral group Y (see Table I). One then lifts this subgroup of $\text{SO}(3)$ into the twice-as-large group $\text{SU}(2)$. On top of this “spinor scaffold-

ing” one can impose a superfluid winding x , but the allowed values of x are related to the spin rotation chosen. The winding is given in the form $x=-\lambda+2\pi k$, where the integer k is arbitrary. The offset λ is fixed and can be determined geometrically through the relation

$$\lambda = (r - S)\Theta, \quad (5)$$

where Θ is the angle of rotation, r is the multiplicity of the spin root on the axis of rotation, and S is the total spin (see Appendix for proof). This information on the superfluid phase determines the translation group elements $T(x)$. This provides a direct way of constructing H and therefore classifying the possible vortices which we illustrate below for the spin-three problem.

Now we move on to discuss the possible phases of the spin-three condensate in the absence of an external magnetic field. The interaction Hamiltonian determined by the pair potential equation (1) is given by

$$\mathcal{H}_{\text{int}} = \frac{1}{2L^3} \sum_{S,m} g_S a_\alpha^\dagger a_\beta^\dagger \langle \alpha\beta | Sm \rangle \langle Sm | \alpha' \beta' \rangle a_{\alpha'} a_{\beta'}, \quad (6)$$

where a_α^\dagger creates a zero-momentum boson in the spin α state, $\langle \alpha\beta | Sm \rangle$ are Clebsch-Gordan coefficients, and the sums over the Greek indices are implicit. Note that this interaction energy alone is sufficient to determine the spinor ground state since the rest of the Hamiltonian will not have a spinor preference. Using the variational state $|\psi\rangle = \frac{1}{\sqrt{N!}} (A_\alpha a_\alpha^\dagger)^N |0\rangle$, where the coefficients are normalized $A_\alpha^* A_\alpha = 1$, the interaction energy to leading order in N can be found by replacing a_α by the scalar $\sqrt{N} A_\alpha$, giving the interaction energy of

$$E_{\text{int}}/N^2 = \frac{1}{2L^3} \sum_S g_S P(S), \quad (7)$$

where

$$P(S) = \sum_m |A_\alpha^* A_\beta^* \langle \alpha\beta | Sm \rangle|^2. \quad (8)$$

We numerically minimize this energy as a function of the seven complex variational parameters A_α under the constraint of normalization $A_\alpha^* A_\alpha = 1$ for all possible values of the scattering lengths, and reproduce the phase diagram given in [6,7]. We give explicit forms of the wave functions up to $\text{SO}(3)$ rotation which are summarized in Table I where, for comparison, we use the same notation as was used in [7]. A subtle difference is that we find the additional state HH which is degenerate with the phase H reported in [7]. It is important to note that the unspecified angles η and χ will take unique values for particular regions in the phase diagram. That is, there is no mean-field degeneracy as was reported for the spin-two case [19].

We now apply the classification scheme developed in [19] to give the symmetries of the possible spinor condensates, and the results are given in Fig. 1. Shown are reciprocal spin-three spinors which are six points on the unit sphere which make the symmetries explicit. All of the phases except for F and FF have no continuous symmetries. As was explained in [6,7], all of the scattering lengths for ^{52}Cr are

known except a_0 . This gives a line in parameter space of possible ground states for such a condensate where the phases A , B , and C are the candidate ground states of the ^{52}Cr condensate.

We will now discuss the topological excitations of each phase. For each case we will take $G=T \otimes \text{SU}(2)$, which will act on the spinor states via the homomorphism φ . The goal is to find the isotropy group H which leaves the particular spinor state under consideration invariant. We start with the two states having continuous symmetries, namely F and FF . For state FF , taking the state to be oriented along the z axis, we find that the only operators leaving the spin state invariant are $e^{iS\Theta} e^{-iS_z\Theta}$ with $S=3$. Note that the phase factor $e^{iS\Theta}$ is necessary to cancel the phase from rotation. Immediately, we find that this gives the isotropy group

$$H = \{T(S\Theta + 2\pi n) e^{-i(\sigma_z/2)\Theta} : \Theta \in \mathbb{R}, n \in \mathbb{Z}\}, \quad (9)$$

$$H_0 = \{T(S\Theta) e^{-i(\sigma_z/2)\Theta} : \Theta \in \mathbb{R}\}. \quad (10)$$

The first homotopy group is then computed to be $\pi_1(FF) = H/H_0 = \mathbb{Z}_{2S}$ consistent with that in [14,15]. Carrying through the similar analysis for state F , we find $\pi_1(F) = \mathbb{Z}_{2(S-1)}$. Note that since these groups are Abelian, the conjugacy classes are the original group elements. The number of conjugacy classes for these cases are $2S=6$ (FF) and $2(S-1)=4$ (F). The number of possible types of vortex excitations is smaller by one here since the identity corresponds to the absence of a vortex. This is in contrast to the spinless case where there are infinitely many types of vortices corresponding to different windings in the superfluid phase as the vortex is circled (with $\pi_1 = \mathbb{Z}$). The underlying reason for this is that rotating such a spinor along its symmetry axis is identical to changing the superfluid phase.

We now move on to consider the remaining phases which have only discrete symmetries. For these situations, as mentioned before, H_0 is the trivial group, so we can apply Eq. (4) directly. We will start with the phases having the smallest isotropy groups, namely phases C and G . For phase G , with the spinor wave function written as in Table I, the only symmetry is a rotation by π about the z axis. Such an operation will not change the phase of the spinor, i.e., $e^{-iS_z\pi} |\psi\rangle = |\psi\rangle$. We then find for the isotropy group

$$\pi_1(G) = H = \{\pm \tau_0, \pm i\sigma_z\} \otimes \{T(2\pi n) : n \in \mathbb{Z}\}, \quad (11)$$

where τ_0 is the 2×2 identity matrix and we note that $e^{\pm i(\sigma_z/2)\pi} = \pm i\sigma_z$. This group is Abelian, so the conjugacy classes are just the group elements themselves. Note that the translational part of H merely tells us that an arbitrary winding in the superfluid phase can be imposed on any vortex state. *In the following, we will suppress the translational part of H , keeping this in mind.* The phase C will have a similar isotropy group, but we note here that rotation by π about the symmetry axis will give a phase of $e^{i\pi} = -1$.

Phases E , H , and HH have n -fold rotational symmetries about a particular axis. Phases E and HH have a threefold rotational symmetry about their symmetry axes, and the first homotopy group is found to be

$$\pi_1(E, HH) = \left\{ \pm \exp\left(-i \frac{\sigma_z 2\pi n}{2 \cdot 3}\right) : n = 1, 2, 3 \right\}. \quad (12)$$

On the other hand, phase H has a five-fold rotational symmetry, and its first homotopy group is similarly

$$\pi_1(H) = \left\{ \pm \exp\left(-i \frac{\sigma_z 2\pi n}{2 \cdot 5}\right) : n = 1, \dots, 5 \right\}. \quad (13)$$

As before, these groups are Abelian. Therefore, the types of possible vortices will correspond to rotating the polyhedra about the axes of symmetries n times as the vortex is circled. In addition, the phase winds by $-\lambda + 2\pi k$, where k is an arbitrary integer and $\lambda = 0, -\frac{4\pi n}{5}, -\frac{2\pi n}{3}$ for the phases E , H , and HH , respectively.

Phase B is the first phase we encounter that has a non-Abelian isotropy group. This phase has a rotational symmetry of π about the z axis. In addition, it also has the rotational symmetry about two axes in the xy plane, namely $(n_x, n_y) = \frac{1}{\sqrt{2}}(1, \pm 1)$. The isotropy group for this is

$$\pi_1(B) = \left\{ \pm \tau_0, \pm i\sigma_z, \pm \frac{i}{\sqrt{2}}(\sigma_x \pm \sigma_y) \right\}. \quad (14)$$

Since this group is non-Abelian, the conjugacy classes are not just the original group. This group is isomorphic to the quaternion group having eight elements. The conjugacy classes corresponding to each possible type of vortex excitation are

$$\begin{aligned} C_0 &= \{\tau_0\}, & \bar{C}_0 &= \{-\tau_0\}, & C_z &= \{\pm i\sigma_z\}, \\ C_{xy} &= \left\{ \pm \frac{i}{\sqrt{2}}(\sigma_x + \sigma_y) \right\}, \\ \bar{C}_{xy} &= \left\{ \pm \frac{i}{\sqrt{2}}(\sigma_x - \sigma_y) \right\}. \end{aligned} \quad (15)$$

Phases A and D have larger isotropy groups; we will not write out explicit representations here, but will merely state the results. For phase A which has the symmetry of the hexagon as seen in Fig. 1, there is a sixfold rotational symmetry about the z axis. In addition to this there are six axes in the xy plane for which there will be a twofold rotational symmetry. This will make $\pi_1(A)$ have 24 elements, which will have 9 conjugacy classes. Phase D has the symmetry of the octahedron. For this, $\pi_1(D)$ will have 48 elements and 8 conjugacy classes. All of these results are summarized in Table I.

Now that the classification scheme for vortices based on homotopy theory has been completed, we will briefly consider the resulting microscopic wave functions. We can express the order parameter explicitly in terms of the spinor as $\psi_\alpha(\mathbf{r}) = \psi(\mathbf{r}) A_\alpha(\mathbf{r})$ and write $\psi(\mathbf{r}) = |\psi_0| e^{i\theta(\mathbf{r})}$. Note that the amplitude of $\psi(\mathbf{r})$ is taken to have constant magnitude which is realistic provided we are sufficiently far from the vortex core. For $A_\alpha(\mathbf{r})$ it will prove useful to use the spinor-ket notation and write $|A_\alpha(\mathbf{r})\rangle = e^{-i\mathbf{S} \cdot \hat{\mathbf{n}} \beta(\mathbf{r})} |A_0\rangle$, where $|A_0\rangle$ is the reference state which can be taken as one of the spinors given in Table I. In this equation, $\hat{\mathbf{n}}$ is the axis about which the spinor is rotated as the vortex is circled and $\theta(\mathbf{r}), \beta(\mathbf{r})$ give the

spatial dependence of the superfluid phase and spinor rotation around the vortex. These functions must satisfy the requirement that the original wave function must be recovered after the vortex is completely circled. For instance, suppose the spinor state under consideration is invariant under a rotation by angle Θ . Then a vortex at the origin corresponding to this symmetry is given by $\theta(\mathbf{r}) = (-\frac{\lambda}{2\pi} + k)\varphi$ and $\beta(\mathbf{r}) = \frac{\Theta}{2\pi}\varphi$, where φ is the azimuthal angle, k is the winding number, and λ is given by Eq. (5).

Note added. After this work was completed, we became aware of a work by Yip [22] which considers a similar problem of vortices in spinor BECs, but uses a different approach.

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APPENDIX: PROOF OF EQ. (5)

The geometrical reciprocal spinors determine the rotational symmetries of the spinors. Associated with each such symmetry is a phase factor which we will calculate here. Suppose the rotation through an angle Θ about the axis $\hat{\mathbf{n}}$ is a symmetry of the reciprocal spinor of $|\psi\rangle$. Then

$$e^{-i\mathbf{S} \cdot \hat{\mathbf{n}} \Theta} |\psi\rangle = e^{i\lambda} |\psi\rangle, \quad (A1)$$

where λ is given by Eq. (5).

To prove this, it is convenient to choose (without loss of generality) the axis of rotation to be parallel to the z axis: $\hat{\mathbf{n}} = \hat{\mathbf{z}}$. Then by comparing the components of the spinors on the left- and right-hand sides of Eq. (A1) we see that

$$e^{-i\alpha\Theta} A_\alpha = e^{i\lambda} A_\alpha. \quad (A2)$$

This equation implies that the nonzero components of the spinor must satisfy

$$\lambda \equiv -\alpha\Theta \pmod{2\pi}. \quad (A3)$$

Let us compare this result to the multiplicity of the root at the north pole, which corresponds to $\zeta = 0$. The characteristic equation is

$$f_\psi(\zeta) = \sum_{\alpha=0}^{2S} \sqrt{\binom{2S}{\alpha}} A_{S-\alpha}^* \zeta^\alpha = 0. \quad (A4)$$

If the root at zero has multiplicity r , then the coefficients of the first r terms $\zeta^0, \dots, \zeta^{r-1}$ are all equal to zero, and the $r+1$ st coefficient is nonzero. This corresponds to the $r+1$ st component of the spinor being nonzero:

$$A_{S-r} \neq 0. \quad (A5)$$

Substituting $m = S - r$ into the condition for the nonzero components, Eq. (A3) gives the result equation (5) and the proof is complete. Note that our discussion has been for a rotational axis aligned with the z axis, but the result equation (5) has a conceptual formulation which does not depend on the coordinate system.

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