Magnetic and nematic phases in a Weyl type spin–orbit-coupled spin-1 Bose gas

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Abstract
We present a variational study of the spin-1 Bose gases in a harmonic trap with three-dimensional spin–orbit (SO) coupling of Weyl type. For weak SO coupling, we treat the single-particle ground states as the form of perturbational harmonic oscillator states in the lowest total angular momentum manifold with $j = 1, m_j = 1, 0, -1$. When the two-body interaction is considered, we set the trial order parameter as the superposition of three degenerate single-particle ground-states and the weight coefficients are determined by minimizing the energy functional. Two ground state phases, namely the magnetic and the nematic phases, are identified depending on the spin-independent and the spin-dependent interactions. Unlike the non-SO-coupled spin-1 Bose–Einstein condensate for which the phase boundary between the magnetic and the nematic phase lies exactly at zero spin-dependent interaction, the boundary is modified by the SO-coupling. We find the magnetic phase is featured with phase-separated density distributions, 3D skyrmion-like spin textures and competing magnetic and biaxial nematic orders, while the nematic phase is featured with miscible density distributions, zero magnetization and spatially modulated uniaxial nematic order. The emergence of higher spin order creates new opportunities for exploring spin-tensor-related physics in SO coupled superfluid.

1. Introduction
With the two-photon Raman coupling technique, a synthetic spin–orbit (SO) coupling has been realized in the pseudo-spin-1/2 Bose–Einstein condensates (BECs) [1, 2]. Since then, many theoretical [3–12] and experimental [13–17] works have been focused on this field including the unveiling of the well-known plane wave, stripe and zero-momentum phases [4]. In addition, the Raman-induced SO coupled spin-1 BEC has also been realized recently [18] which is unattainable in condensed matter materials, and spatially modulated nematic order is expected to appear in the stripe phase [19–22].

The Raman-induced SO coupling is a one-dimensional (1D) configuration as an equally weighted Rashba and Dresselhaus couplings. This year also witnessed the experimental progress in engineering the two-dimensional (2D) Rashba–Dresselhaus-type SO coupling in cold atom gases [23, 24]. Many interesting properties have been predicted for the Rashba SO coupled Bose gases [25–44], among which the weakly coupled BEC is found to condense into various half-quantum vortex phases [26, 27, 29, 30, 44] due to modification of the single particle spectrum by the trapping potential. All these efforts make the cold atom gases with the synthetic gauge field a rapidly developing field.

Researchers also go further to deal with the three-dimensional (3D) analogy of Rashba configuration, i.e. the Weyl SO coupling [45–54] and the experimental schemes for engineering the Weyl configuration in the ultracold gases have been proposed [55–57]. While the Weyl coupled spin-1/2 bosons in a homogeneous system reproduces the plane wave and the stripe phases [54], the 3D skyrmion mode with magnetic order [45, 47, 49, 53] spontaneously appears in the ground state of a trapped system.
For a trapped Weyl coupled spin-1 BEC, one expects the emergence of topological objects with even higher spin order, i.e. the nematic order. An immediate question is that, what will the phase diagram look like, and in what a way will the 3D skyrmion and (or) the nematic order manifest themselves in the individual phases. Here we consider a spin-1 bosonic system subject to a weak Weyl SO coupling of $\mathbf{s} \cdot \mathbf{p}$ type in a harmonic trap. We implement a standard variational approach [3, 4, 25, 26, 53] to give a phase diagram of the system in different interaction regimes. A magnetic phase and a nematic phase are predicted in the ground state, and the latter is entirely new and has no analogue in the 3D SO coupled pseudo-spin-1/2 bosonic gases [45, 47, 49, 53].

The paper is organized as follows. In section 2 the energy functional for the 3D SO coupled spin-1 condensate is introduced in harmonic oscillator units. In the weak coupling limit we construct our variational order parameter in section 3 and calculate the energy functional by means of the irreducible tensor method. The ground state phase diagram is determined by numerically minimizing the energy functional with respect to the variational parameters, and section 4 is devoted to an explicit illustration and detailed discussion of the densities and spin orders in the two ground state phases. We summarize our main results in section 5.

2. Model

We start from the mean-field Gross–Pitaevskii (GP) energy functional of spin-1 bosons with a Weyl type 3D SO coupling in the presence of a harmonic trap

$$\mathcal{E} = \mathcal{E}_0 + \mathcal{E}_{\text{int}},$$

where the single particle part is

$$\mathcal{E}_0 = \int \! d^3r \psi^\dagger(r) \left( \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega^2 r^2 + \lambda \mathbf{s} \cdot \mathbf{p} \right) \psi(r),$$

with $m$ the atomic mass and $\omega$ the trap frequency. $\psi = (\psi_1, \psi_0, \psi_{-1})^T$ denotes the spinor order parameters for bosons with hyperfine components $1, 0, -1$ respectively, and $\mathbf{s} = (s_x, s_y, s_z)$ are spin-1 matrices. The Weyl SO coupling $\mathbf{s} \cdot \mathbf{p}$ with strength $\lambda$ is a 3D analogy of the Rashba configuration [56]. This SO coupling can be experimentally realized with pulsed inhomogeneous magnetic field on state-of-the-art atom chips [57]. Without the trapping potential, the momentum $\mathbf{p}$ and the helicity $\mathbf{s} \cdot \mathbf{p}/|\mathbf{p}|$ are constants of motion, and the single-particle ground states are highly degenerate, i.e. the lower-energy helical branch achieves a minimum along a sphere of radius $P_{SO} = m\lambda$, called SO sphere [45]. The presence of a trapping potential will partially lift this degeneracy, but at least a two-fold degeneracy related to the time-reversal (TR) symmetry will still remain [2]. The single particle Hamiltonian is also invariant under simultaneous rotation of spin and coordinate space SO(3) (except for a phase factor $\exp i \gamma$) that leaves the total (instead of spin) angular momentum a good quantum number [47]. This breaking of rotational symmetry in spin space leads to spin-textured ground states with magnetic and nematic orders, as previously studied in [20, 22, 25, 26, 53].

The interaction energy functional is formulated in the standard form [58–60]

$$\mathcal{E}_{\text{int}} = \frac{1}{2} \int \! d^3r (c_0 n^2 + c_2 S^2),$$

where $n(r) = n_1(r) + n_0(r) + n_{-1}(r)$ is the total particle density and $n_{1,0,-1}(r) = |\psi_{1,0,-1}(r)|^2$ are densities for the three components, respectively, and $S = \psi^\dagger \mathbf{s} \psi$ is spin density. $c_{0,2}$ are spin-independent and spin-dependent interaction strengths respectively, which are related to the two-body scattering lengths in the total spin-0 and spin-2 channels as $c_0 = 4\pi\hbar^2 (a_0 + 2a_2)/3m$ and $c_2 = 4\pi\hbar^2 (a_2 - a_0)/3m$. The interaction is TR symmetric under the operation $T = \exp(-i\pi S) K$ with $K$ the complex conjugate. Besides, this two-body interaction is also SU(2) spin-rotation symmetric, which is different from the spin-1/2 bosons [45, 47, 49, 53]. In the latter case the two body interaction is SU(2) symmetric only under the condition $g_{21} = g_{21} = g_{11}$, i.e. $c = c_{11}/g_{11} = 1$. We will see later that this highly symmetric interaction will lead to highly degenerate ground states. In harmonic oscillator units, the system has length scale $l_T = \sqrt{\hbar/m\omega}$, energy scale $\hbar\omega$, and SO coupling strength is in unit of $\sqrt{\hbar\omega/m}$. If we normalize the order parameter to unity, i.e., $\psi \rightarrow \sqrt{N}/l_T \psi$ with $N$ the total particle number in the condensate, the energy functional per particle is obtained as

$$\varepsilon = \int \! d^3r \psi^\dagger(r) \left\{ -\frac{\nabla^2}{2} + \frac{r^2}{2} + \lambda \mathbf{s} \cdot \mathbf{p} \right\} \psi(r) + \int \! d^3r \left( \frac{c_0}{2} n^2 + \frac{c_2}{2} S^2 \right).$$
and

\[ \phi_{n_{l_{jm_{i}}}}(r, \theta, \varphi) = R_{n_{l_{i}}}(r) Y_{j_{m_{i}}}^{l_{i}}(\Omega), \]  

where \( Y_{jm_{i}}^{l_{i}}(\Omega) = \sum_{m_{i}} \epsilon_{l_{i}m_{i}}^{j_{m_{i}}} Y_{m_{i}} Y_{m_{i}} \) is the vector spherical harmonics \[61\] with \( j = l + 1, l, |l - 1| \) (if \( l = 0, j = 1 \) only) and \( \epsilon_{l_{i}m_{i}}^{j_{m_{i}}} \) the Clebsch–Gordan coefficients. In the coupled representation, the ground state wave function has \( n_{l_{i}} = l = 0 \). This gives a total angular momentum \( j = 1 \) with \( m_{j_{l_{i}}} = 1, 0, -1 \) and the three ground states are

\[ \phi_{001 \pm 1}(r) = R_{00}(r) Y_{1 \pm 1}^{0}(\Omega) \]  

and

\[ \phi_{0000}(r) = R_{00}(r) Y_{0}^{0}(\Omega) \]  

respectively. The lowest few levels of the 3D harmonic oscillator is shown in figure 1. The single particle spectrum may understood as a weak perturbation (slight level mixing) of the harmonic-oscillator energy levels in the case of weak SO coupling, which conserves the total angular momentum \( j \) and \( j_{l_{i}} \), but \( l \) is no longer a good quantum number. This means SO coupling term would couple \( s, p \) and even \( d \) waves into the ground state with the same \( j \) and \( j_{l_{i}} \) as illustrated in figure 1. In the case of strong SO coupling, the energy spectrum is weakly dispersive or nearly flat \[33, 45, 51\] which will not be considered in this work. The ground state wave functions are thus the superposition of the lowest \( s, p \) and \( d \) wave states with \( j = 1 \). The state with \( m_{j_{l_{i}}} = 1 \) is

\[ \Phi_{l_{i}1, m_{i}1} = A_{0} \phi_{001} + i A_{1} \phi_{011} - A_{2} \phi_{021}, \]  

Here \( A_{l_{i}} \) (\( l = 0, 1, 2 \)) are the weight coefficients with the normalization constraint \( \sum_{l_{i}m_{i}} |A_{l_{i}}|^2 = 1 \) and \( i \) in front of \( A_{1} \) comes from the pure imaginary matrix elements of SO coupling between \( \phi_{001} \) and \( \phi_{011} \) \[45, 51, 53\]. Explicitly this state is a spinor
Moreover, in the single particle level, the energies are irrelevant to the magnetic quantum number \(j_z\). Thus the other two states with \(m_j = 0\) and \(-1\) are

\[
\Phi_{j=1, m_j = 0} = \begin{pmatrix}
-A_0 R_{00} Y_{00} - i A_1 \sqrt{\frac{1}{2}} R_{01} Y_{10} - A_2 \sqrt{\frac{3}{10}} R_{02} Y_{20} \\
i A_1 \sqrt{\frac{1}{2}} R_{01} Y_{11} + A_2 \sqrt{\frac{3}{5}} R_{02} Y_{21} \\
-A_2 \sqrt{\frac{3}{5}} R_{02} Y_{22}
\end{pmatrix}
\]

(9)

and

\[
\Phi_{j=1, m_j = -1} = \begin{pmatrix}
-A_0 R_{00} Y_{00} + i A_1 \sqrt{\frac{1}{2}} R_{01} Y_{10} - A_2 \sqrt{\frac{3}{10}} R_{02} Y_{20} \\
-i A_1 \sqrt{\frac{1}{2}} R_{01} Y_{11} - A_2 \sqrt{\frac{3}{10}} R_{02} Y_{21} \\
A_2 \sqrt{\frac{3}{5}} R_{02} Y_{22}
\end{pmatrix}
\]

(10)

respectively. Note that the state \(\Phi_{j=1, m_j = -1}\) is the time reversal of \(\Phi_{j=1, m_j = 1}\), and \(T \Phi_{j=1, m_j = 0} = - \Phi_{j=1, m_j = 0}\). We have neglected contribution from the excited 1s wave state \(\phi_{1011}\) shown in figure 1 (gray dashed), which can be absorbed into the lowest 0s state \(\phi_{0011}\) owing to the same angular-spin wave function. For our interaction parameter regime, we found the weights of 1s state as well as the higher orbital channels \((l > 2)\) in the wavefunction are negligible, as indicated in figure 2. It has been verified that inclusion of these states in the calculation will not alter our main conclusion for interaction parameter \(c_0 < 20\).

The presence of the trap has already lifted the degeneracy of the single-particle ground state to only three-fold degenerate for \(j = 1, m_j = 0, \pm 1\). In the language of Raman-induced SO coupling [1, 8, 15], the single particle ground state has three minima corresponding to three states \(\Phi_{j=1, m_j = 0, \pm 1}\). At the many-body level, the interaction will determine which minimum or minima the Bose gases will condense to by minimizing the GP energy functional [19]. We therefore set the variational wave function ansatz as

\[
\Psi = c_1 + c_1^\dagger \Phi_{j=1, m_j = 1} + \cdots + c_0^\dagger \Phi_{j=1, m_j = 0} + c_{-1} \Phi_{j=1, m_j = -1}
\]

(12)

with the normalization constraint \(c_{-1}^2 + c_0^2 + c_1^2 = 1\) that ensures the conservation of the particle numbers. The coefficients \(c_{-1}, c_0, c_1\), to be determined by the interaction, are generally complex. For the sake of simplicity, we restrict them to be real here. Later, we will discuss the consequences of such restriction. This variational wave function ansatz is extensively encountered in SO coupled cold atom gases [3, 4, 19, 20, 25, 26, 28, 31, 54]. In writing the variational wavefunction (12), we assume the Weyl coupled Bose
gases are condensed. All efforts concerning the condensation condition or fragmented condensation focus on the homogeneous system [62, 63]. It has been shown that the 3D SO coupled uniform gas can condense at least at zero temperature [37]. The trapped system is much easier to condense compared to the homogeneous one. So we present here only the result for zero-temperature phases.

3.2. Nematic order
Prior to the calculation of the energy functional, we first elucidate the meaning of our variational order parameter ansatz. Since our single-particle Hamiltonian respects the SO(3)$_{l=+1}$ symmetry, it is convenient to introduce the polarization operator [61] to describe the spin order. The polarization operators for spin- $s$ system $T_{m}^{(l)}(s)$ with $l = 0, 1, \ldots, 2s$ and $m_l = -l, -l + 1, \ldots, l$, are a set of $(2s + 1)^2$ operators which act on the spin wave functions and transform under the coordinate system rotation according to the irreducible representation of SO(3) group. In this sense, it is also an irreducible tensor of rank $l$.

For spin-1 objects, the nine polarization operators $T_{m}^{(1)}(s)$ with $l = 0, 1, 2$ constitute a complete set of square $3 \times 3$ matrices and are generators of the unitary group $U(3)$ in rotationally covariant Racah form [64]. The rank-0 operator is the unit $3 \times 3$ matrix $I$

$$T_0^{(0)}(s) = \frac{1}{\sqrt{2s + 1}} I.$$  
(13)

The rank-1 operators $T_{m}^{(1)}(s)$ are proportional to the irreducible rank-1 spin tensor with components

$$T_{m}^{(1)}(s) = \frac{\sqrt{3}}{s(s + 1)(2s + 1)} s_{m_l}^{(1)}(m_l = 0, \pm 1),$$  
(14)

where the spherical components of the irreducible rank-1 spin tensor $s_{m_l}^{(1)}$ are related to the cartesian ones as

$$s_{\pm 1}^{(1)} = \frac{1}{\sqrt{2}} (s_x \pm is_y), s_0^{(1)} = s_z.$$  
(15)

The rank-2 polarization operators $T_{m}^{(2)}(s)$ are

$$T_{m}^{(2)}(s) = \sum_{\mu, \nu = 0, \pm 1} C_{\mu\nu}^{2m_l} s_{\mu}^{(1)} s_{\nu}^{(1)} = \{s^{(1)} s^{(1)} m_l^{(2)} \}, \quad (\mu, \nu = 0, \pm 1),$$  
(16)

where $[A^{(n)} B^{(n)} ]^{(k)}$ defines the rank-$k$ tensor product of rank-$m$ irreducible tensor $A^{(m)}$ and rank-$n$ irreducible tensor $B^{(n)}$. $T_{m}^{(2)}(s)$ are equivalent to a symmetric traceless cartesian tensor of rank-2, i.e. the spin nematic tensor or quadrupole tensor $\mathbf{N}$ through the relation [61]

$$T_{2}^{(2)} = \frac{1}{2} (N_{xx} - N_{yy} \pm 2iN_{xy}),$$

$$T_{2}^{(2)} = \mp (N_{xx} \pm iN_{xz}),$$

$$T_{2}^{(2)} = \frac{3}{2} N_{zz}.$$  
(17)

The unit matrix $I$ is a spin-rotation invariant scalar which contains important information regarding the charge (density) order, three matrices $s_x, s_y, s_z$ form a vector which represents the local spin (magnetic) order, and five matrices $N_{ij}$ form a symmetric traceless tensor which represents the local spin fluctuations or nematic order [65–67]. The spin-1 systems therefore support spin nematic order in addition to the charge and magnetic ones. The magnetic and the nematic orders compete with each other as increasing one of them requires reducing the other [65].

With the polarization operators, our variational wavefunction (12) can be written as

$$\Psi = U(\mathbf{r}) \zeta,$$  
(18)

where $\zeta = (c_1, c_{10}, c_{1}^*)^T$ is a normalized spinor and the position-dependent transformation

$$U(\mathbf{r}) = \sqrt{\frac{2s + 1}{4\pi}} \sum_{l=0}^{2s} (-i)^l A_l R_{il} C^{(l)} \cdot T^{(l)}$$  
(19)

on the spinor $\zeta$ leads to the spin-textured ground states in the SO coupled cold atom gases. Here the dot defines the scalar product of the modified spherical harmonics $C^{(l)}$ and $T^{(l)}$. This local modulation operator is expanded in series of $C^{(0)}$, $T^{(1)}$ with the highest order $l = 2s$. The Hamiltonian is invariant under the simultaneous
rotation in spin and coordinate space SO(3)K, therefore trapped spinor condensate with SO coupling inevitably carries angular momentum by twisting its spinor order parameter [53, 65].

It is also intuitive to understand the modulation of spin-1/2 objects discussed in detail in [53], in which case the four polarization operators T_m^{(l)}(s) with l = 0, 1, or explicitly I, s^{(1)}, s^{(1)}, s^{(1)}, constitute a complete set of square 2 × 2 matrices. The transformation matrix U(r) can be rewritten as

$$U(r) = \sqrt{\Omega(r)} \exp[-i\omega(r)\hat{r} \cdot \hat{s}],$$

where the density and spin modulations are apparently separated owing to the absence of nematic order. The spin-1 system thus enables to explore spin-tensor-related physics in the SO coupling superfluid, which has fundamentally different rotation properties as in spin-1/2 system.

3.3. Energy functional

We now have six variational parameters $A_0$, $A_1$, $A_2$, $c_{1+}$, $c_{1-}$, $c_{-}$ in the trail variational order parameter. The energy functional of (4) can be calculated analytically using the proposed order parameter (12).

The single particle part of the energy functional consists of the kinetic energy, the trapping potential of the 3D harmonic oscillator, and the SO coupling term. As in the spin-1/2 case [53], the matrix elements for the kinetic energy and trapping potential are non-vanishing for states with the same parity, while the SO coupling term $s \cdot p$ will mix states with opposite parities. The result is

$$\int d^3r \Psi^\dagger(r) \left\{ -\frac{\nabla^2}{2} + \frac{r^2}{2} + \lambda s \cdot p \right\} \Psi(r) = \frac{3}{2} A_0^2 + \frac{5}{2} A_1^2 + 2\lambda A_0 A_1 + \Delta_0. \tag{21}$$

The contribution from the d-wave states is collected in $\Delta_0$

$$\Delta_0 = \frac{7}{2} A_2^2 - 2\lambda A_0 A_1 \sqrt{\frac{5}{6}}$$

and we have used

$$\langle \phi_{0011} | s \cdot p | \phi_{0111} \rangle = -i,$n

$$\langle \phi_{0011} | s \cdot p | \phi_{0211} \rangle = i \sqrt{\frac{5}{6}}. \tag{22}$$

We refer to [53] for details of the integral calculation in which the method of irreducible tensor algebra is employed [61].

The calculation of the interaction is tedious but straightforward which yields

$$\int d^3r \frac{\xi_0}{12} n^2 = \frac{\xi_0}{8\pi} \sqrt{\frac{2}{\pi}} \left[ A_0^4 + A_1^2 A_2^2 + \frac{1}{16} (7 + x) A_1^4 + \Delta_n \right]$$

and

$$\int d^3r \frac{\xi_2}{2} S^2 = \frac{\xi_2}{8\pi} \sqrt{\frac{2}{\pi}} \left[ A_0^4 + A_1^2 A_2^2 + \frac{5}{16} A_1^4 + \Delta \right] \left( 1 - x \right). \tag{24}$$

With $x = [1 - (c_{1+} + c_{1-})^2]^2$. Here $\Delta_n$ and $\Delta$, again denote the contributions from the d-wave states

$$\Delta_n = -\frac{1}{12000} \left[ (10A_0 A_1^2 A_2^2 - 7A_0 A_1^2) (1 + 3x) \right. \left. + \frac{3}{10} A_0^2 A_2^2 (2 + x) + \frac{7}{240} A_1^2 A_2^2 (19 - 3x) \right. \left. + \frac{63}{1600} A_2^4 (7 + x) \right] \tag{23}$$

$$\Delta = \sqrt{\frac{1}{480}} \left[ (10A_0 A_1^2 A_2^2 - 7A_0 A_1^2) + \frac{35}{48} A_0^2 A_2^2 + \frac{63}{320} A_2^4 \right]. \tag{25}$$

The energy functional per particle is simply the summation of equations (21), (23) and (24).

4. Ground state phase diagram

We choose the SO coupling strength $\lambda = 0.4$ which can be implemented in the scheme proposed in [57] with pulsed magnetic field gradient in three spatial directions and the atom cloud trapped in a harmonic potential with $\omega = 2\pi \times 40$ Hz above the atomic chip. The typical dimensionless interaction strengths in current 3D
theoretical proposals are in the range 0.1–10^3, and can be tuned freely by properly choosing the number of trapped atoms and the laser fields that produce the harmonic confinement. Without loss of generality we choose c_0 = 10 for the alkali atom numbers ranging from a few hundred to several thousand, while typical spin-dependent interactions c_3 are determined by atomic species, i.e. c_3/c_0 ~ -0.005 for ^87Rb, c_3/c_0 ~ 0.04 for ^23Na, and c_3/c_0 ~ 0.5 for ^6Li [68]. The ground state c_0 2 c_2 phase diagram for these given coupling strength and interaction parameters can then obtained by minimizing the variational energy with respect to the parameters A_0 and x under two constraints \sum z_{\pm 0} |A_i|^2 = 1 and c_{z_1}^2 + c_{z_0}^2 + c_{z_1}^2 = 1. The latter further restricts x to the region [0,1]. Should the spin-independent interaction vanish c_0 = 0, we see from (24) that the optimized parameter x either takes value of 0 for c_2 < 0, or 1 for c_2 > 0 for negligibly small contribution \Delta, from the d-wave states. The analysis below will show that this assumption holds generally except for extremely strong interaction c_0. The variational ansatz characterizes two quantum phases: (I) the magnetic phase with a ferromagnetic manifold \zeta for c_2 < 0, as x = 0 means that (c_1 + c_2)^2 = 1 and the spin density S describes the magnetization. (II) the polar or nematic phase with a polar manifold \zeta for c_2 > 0, as x = 1 means (c_1 - c_2)^2 = 0 or 2 which leads to S \equiv 0. This is consistent with the conventional spin-1 BEC [58–60] where for c_2 < 0 (c_2 > 0) a ferromagnetic (polar) spinor is needed to minimize the mean-field energies. If c_0 > 0, the boundary between magnetic and nematic phases will drift a little to the positive c_2 side because the spin-independent interaction (23) which prefers x = 0, prevails in the c_2 > 0 regime over the spin–dependent one (24) which prefers x = 1. For the values of optimized parameters A_0 generally, the weights of p and d waves becomes more and more important with increasing interaction c_0, which effectively diminishes the partition of s wave. In the range of c_0 = 0 ~ 20 we considered here, |A_0|^2 decreases from 0.884 to 0.723, |A_i|^2 increases from 0.110 to 0.260, while |A_i|^2 from 0.003 to 0.014 which is always negligibly small. A typical phase diagram is shown in figure 2 where the phase boundary is calculated in three successive approximations: ‘sp’—only the lowest 0s and 0p states are considered in the approximation; ‘spd’—the 0d energy level is added; ‘spds’—the 1s energy level is added further. We can find that the boundary does not alter significantly when we include the excited s wave states \phi_{l01m} in the variational order parameter.

It has been pointed out that the SO coupling manifests itself in a way that the modulation of the ferromagnetic and polar spin textures in the pseudospin space could be transferred to patterned structures in orbit space even in the ground states [19]. The reason of this modulation lies in that, in the presence of SO coupling [69] or dipolar interaction [70], the spin-dependent interaction would inevitably influence the spatial motion, which leads to rich density pattern. We discuss this in the following for the magnetic and polar phases explicitly.

4.1. Magnetic phase
This phase lies in the lower part of the parameter space with the states featured as c_1 + c_2 = ±1. The corresponding spinor \zeta in (18) denotes a ferromagnetic state with magnetization along any axis in the xz plane. This asymmetry between x-, z- and y-directions is a consequence of our simplified treatment which restricts the coefficients c_1, c_0, c_2 to be real, such that the spinor \zeta is unable to describe the state with magnetization along y direction, defined as \zeta with vanishes for real c_1, c_0, c_2. If we relax this restriction to allow complex coefficients c_1, c_0, c_2, all states with spinors \zeta magnetized along any spatial direction belong to this magnetic phase, which is related to the spin–rotation symmetric interaction. Two typical spinors are \zeta = (1, 0, 0)^T and \zeta = (1/2, 1/\sqrt{2}, 1/2)^T which are longitudinally and transversely magnetized ferromagnetic states respectively. This phase spontaneously breaks the TR symmetry which leads to spontaneous magnetization along the xz plane. The situation is just like spin half case we have studied before [53].

We first consider the longitudinally magnetized state \zeta = (1, 0, 0)^T with the time reversal state being \zeta = (0, 0, 1)^T. We plot the ground state density distribution for the three components in figure 3(a), which show clearly cylindrical symmetry. While the spin component 1 is dominantly occupied in the center, which allows the condensate to develop a longitudinal magnetization, the components 0 and −1 form two toruses surrounding the central part. It can be seen that the outermost shell of spin-1 density is negligibly small which is entirely attributed to the involvement of the d wave fraction in the order parameter. To visualize the d wave nature we need to zoom out 100 times in the density plot. Generally only less populated spin component can develop d-wave characters in the ground states because these complex structure in the high density spin components would cost too much kinetic energy [71]. For its TR degenerate state \zeta the spin components 1 and −1 are inversely populated.

The spin texture of the longitudinally magnetized state is plotted in figure 3(b) where we find a synchronous modulation between the particle density and the spin density owing to the breaking of spin rotation symmetry. In the trap center, the spins are aligned along the z-axis due to the dominant occupation of spin-1 component. The successive population of the 0 and −1 components forms a local spin texture \textbf{S(r)/n(r)} where the spin density vectors deflect continuously to the xy plane away from the center. This is a 3D magnetic skyrmion-like...
The main features of the 3D skyrmion can be extracted from the cut-plane plots. It is seen that the spin texture is a 2D skyrmion in the $xy$ plane, where the spin distribution forms a pattern, the in-plane components of the local spin are along the tangential direction. In the parallel planes shifted along the positive (negative) direction of the broken symmetry axis, the 2D skyrmion-like pattern remains, with its in-plane components nevertheless twisted outward (inward) around the broken symmetry axis. The spin vector field lines develop into a bundle of fountain-like streamlines close to the $z$-axis around which a torus is formed near the $xy$ plane.

The density distribution for the transversely magnetized state $\zeta_z = (1/2, 1/\sqrt{2}, 1/2)^T$ with the time reversal state $\zeta_{-z} = (1/2, -1/\sqrt{2}, 1/2)^T$ looks quite differently as shown in figure 4(a). With half of the atoms filled in the spin-0 component, the components $\pm 1$ becomes equally populated and spatially separated, which leads to a significant transverse magnetization. The density distributions of three components are separated in an alternative way, i.e., the $-1 (+1)$ component lies mainly in the $-y (+y)$ half-space and its peak density center is along the direction joining the III and VIII octants (I and VI octants), while the 0 component is embedded between them with a density profile along the $x$-axis. This leads to a magnetic skyrmion-like texture with the spins in the trap center transversely aligned along the $x$-axis as shown in figure 4(b), and the increasing population of $\pm 1$ components away from the trap center makes the spin density vector forms a torus near the $yz$ plane.
plane. Owing to the non-commutative nature of position-dependent transformation (19) and the spin rotation, the spin texture of the longitudinally magnetized state is different from the \( \frac{\pi}{2} \) spin rotation around \( y \)-axis of the transversely magnetized state, though the spinor wave functions themselves \( \zeta_z \) and \( \zeta_x \) are related by such a rotation. All other states degenerate with these two magnetic states have similar properties, except that the magnetization axes may be in any direction determined by the values of parameters \( c_s' \).

4.2. Nematic phase
This phase lies in the upper part of the parameter space with the states featured as \( \zeta_1^+ + \zeta_1^- = 0 \) or \( \sqrt{2} \). The corresponding spinor \( \zeta \) in (18) denotes a polar state with zero magnetization \( S(r) = 0 \) everywhere. Two typical spinors are \( \zeta_{p1} = \frac{1}{\sqrt{2}} (1, 0, -1)^T \) and \( \zeta_{p2} = (0, 1, 0)^T \). The TR symmetry is preserved in this phase, so the ground state has no spontaneous magnetization as the non-magnetic phase in the Raman induced SO coupled two-component Bose gases [1, 4, 8, 15]. This is a new phase and no analogy in spin half case we considered before [53].

The density distribution of the state \( \zeta_{p1} \) is plotted in figure 5(a). A signature of the d-wave is seen in the 100 times zoomed density of 0 component in the \( xz \) plane, which comes from the d-wave contribution in the variational order parameter. The phase separation among three components, which is possible only in the case of TR symmetry breaking [72], i.e. the magnetic phase, is not seen for this nematic phase which preserves the TR symmetry and the \( \pm 1 \) components are miscible.
We define the nematicity density tensor $\mathcal{N} = \Psi^\dagger N \Psi$ to characterize the nematic order due to the absence of the magnetization. In the nematic phase $\zeta_{p1}$ or $\zeta_{p2}$, the normalized nematicity density tensor $\mathcal{N}/n$ has eigenvalues $\{1/3, 1/3, -2/3\}$ everywhere, therefore describing a uniaxial nematic state. The eigenvector associated with eigenvalue $-2/3$ defines the nematic director which is plotted in figure 5(b) together with the tensor magnetization density $\mathcal{M}_{zz} = \Psi^\dagger N_{zz} \Psi$. The nematic directors form a lantern-like structure with the principle axis along the $x$-direction. The spatially modulation of the nematic directors, shown as headless vectors in the $xy$, $yz$ and $xz$ planes, reflects indirectly the modulation of nematicity density tensor themselves. In the trap center, where the spinor wavefunction $\zeta_{p1}$ describes a transverse polar state, the nematic director points along the $x$-axis. Away from the trap center, the 0 component is gradually populated and the nematic director are continuously modulated into concentric circles in the $yz$ plane. For the state $\zeta_{p2}$, the 0 component in the trap center will allow a longitudinal polar state and we find an alternative modulation of the nematic directors. The tensor magnetization $\mathcal{M}_{zz}$ [18, 21] has been adopted to resolve the order of the phase transition in the Raman-induced SO coupled spin-1 condensate, and the spatial modulation of $\mathcal{M}_{zz}$ along direction of the SO coupling has been noticed [20, 22].

The magnetic phase is also featured with a nematic order and the competing orders in both phases are shown in figure 6. These two spin orders are competing with each other [65] to meet the requirement.
This prevents us from writing the transformation (19) into a local spin rotation as (20). Diagonalizing the nematicity density tensor yields three distinct eigenvalues which are spatially modulated as well as the nematicity density tensor themselves [22]. Thus the magnetic phase has both magnetic and biaxial nematic orders, while the nematic phase exhibits only a uniaxial nematic order.

Finally, we remind that our variational order parameter based on the perturbation expansion may not be applicable in the limit of strong SO coupling [29, 44, 45, 49] where a skyrmion-lattice-like ground state may appear. Moreover, when two-body interaction is strong enough, the variational order parameter starts to involve higher angular momentum \( j \) states which will break the SO(3) rotational symmetry, and the Bose gases will condense into the plane wave or stripe phases instead [27, 45, 54].

5. Summary

We establish the ground state phase diagram of the weakly 3D SO coupled spin-1 bosons theoretically. The ground state may be in a magnetic or a nematic phase determined by the competing between the spin-independent and the spin-dependent two-body interaction. The nematic phase is a new phase that is absent in a 3D SO coupled pseudo-spin-1/2 bosonic system. We discuss the density distribution and spin orders of the two phases in detail. The magnetic phase permits both a magnetic order and a biaxial nematic order, while the nematic phase is featured by a uniaxial nematic order. These novel phases are in current experimental reach benefiting from the rapid progress of cold gases with artificial gauge field.

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Figure 6. Competing orders in the magnetic and the nematic phases along x-axis. They are \( \frac{1}{2} \left| \mathbf{S} \right|^2 \) (red) and \( \text{Tr} \left( \frac{\mathbf{S} \mathbf{S}}{n} \right)^2 \) (blue) respectively. Solid curves are for the magnetic phase and dashed lines for the nematic phase.

\[
\frac{1}{2} \left| \mathbf{S} \right|^2 + \text{Tr} \left( \frac{\mathbf{S} \mathbf{S}}{n} \right)^2 = \frac{2}{3}.
\]
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