SU(3) symmetry of spin-1 Bose-Einstein condensate

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Abstract. It is well-known that spin-1 atoms have SU(3) symmetry. In this work, we develop the theory for spin-1 Bose-Einstein condensate (BEC) based on SU(3) Lie group and predict that any spin-1 atom, for instance, ^{87}Rb can exist in either of two inequivalent fundamental representations of SU(3) namely $D(1,0)$ or $D(0,1)$. Furthermore, the SU(3) theoretical treatment results in either ferromagnetic or antiferromagnetic ground states of the spin-1 BEC depending on the sign of $a_{1,1}-a_{0,0}$, where $a_{1,1}$ and $a_{0,0}$ are the scattering lengths corresponding to $D(1,1)$ and $D(0,0)$ states. We also show that the coherent spin mixing process of spin-1 BEC is due to only the collisions between atoms in the $D(1,0)$ and $D(0,1)$ representations.

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1. Introduction

Lie groups and Lie algebras, and their representation theories are widely used in physics, and one of the best examples is the Bose-Einstein condensate (BEC) [1, 2, 3]. Indeed, symmetry properties are essential to the study of BEC being a boson with spin-1 [4, 5, 6, 7, 8].

So far, the commonly accepted theory of spin-1 BEC is based on SU(2) symmetry properties of a spin-1. According to this theory, the ground state properties of spin-1 BEC are determined by the s-wave scattering lengths a_0 and a_2 respectively for total spin 0 and 2. If $a_0 > a_2$ then the ground state of the BEC is ferromagnetic, otherwise, it is antiferromagnetic [9, 10, 11, 12, 13]. These results are the direct consequence of the SU(2) symmetric theory of the spin-1 BEC.

Interestingly, numerical values of a_0 and a_2 are found to be very close to each other for ^{87}Rb and ^{23}Na in Refs [10, 14, 15]. Thus, these similar values of s-wave scattering lengths imply that the total spin 0 and spin 2 may belong to one irreducible representation of SU(3). Motivated by this thought and the previous studies [16, 17, 18, 19], we develop the theory of spin-1 BEC using SU(3) — group of all three by three unitary matrices with determinant 1.

It is commonplace knowledge that the spin-1 has the SU(3) symmetry whereas spin-1/2 has SU(2) symmetry. For SU(2), its three generators (i.e. Pauli matrices) are related with three components of a spin magnetic-dipole moment. For SU(3), a similar situation can be easily observed, namely its eight generators correspond

to three components of a spin magnetic-dipole moment and five components of an electric-quadrupole moment. Therefore, it is obvious that the higher-order quadrupole moments can be considered with the use of SU(3) symmetry of a spin-1. Moreover, SU(3) symmetry allows us to consider electric-quadrupole moments in collisional processes of spin-1 BEC.

Another point of view is that by using SU(3) symmetry, we weaken symmetry restriction. Then, atom-atom collisional interaction Hamiltonian becomes SU(3) symmetric and as a result, no spin-dependent term exists in interaction Hamiltonian which implies the BEC is magnetically inactive. However, we identify two types of atoms associated to two fundamental representations of SU(3), and then, the Hamiltonian of collisional interactions between two types of atoms does depend on dipole-quadrupole moments. Due to this dipole-quadrupole moment-dependent Hamiltonian, spin-1 BEC exhibits either ferromagnetic or antiferromagnetic properties depending on interaction properties.

In this paper, we explore the SU(3) symmetry of spin-1 BEC and identify two types of spin-1 atoms associated with different fundamental representations. Moreover, a new SU(3) symmetric Hamiltonian of the interacting spin-1 BEC is written, and its ground state is analyzed. In addition, coherent spin mixing dynamics are discussed by using Gross-Pitaevskii equations.

2. SU(3) symmetry of spin-1 atoms

In the absence of the external magnetic and electric fields, spin-1 atoms are SU(3) symmetric. This means that three-dimensional spin space is isotropic i.e., there is no preferred direction in the spin space. It is well known that SU(3) algebra can have the Cartesian dipole-quadrupole basis composed of 8 generators consisting of three components of the spin magnetic-dipole moment and five components of the electric-quadrupole moment [20]. Nonetheless, the group theoretical treatment of the problem is more subtle since there are two fundamental irreducible representations $D(1,0)$ and $D(0,1)$ [21]. For the irreducible representation $D(1,0)$, eight generators are given by

$$\hat{s}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \hat{s}_y = \frac{i}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix},$$
$$\hat{s}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{1}$$

and

$$\hat{q}_{xy} = \{\hat{s}_x, \hat{s}_y\}, \quad \hat{q}_{xz} = \{\hat{s}_x, \hat{s}_z\}, \quad \hat{q}_{yz} = \{\hat{s}_y, \hat{s}_z\},$$
$$\hat{q}_{x^2-y^2} = \hat{s}_x^2 - \hat{s}_y^2, \quad \hat{q}_{3z^2-r^2} = \frac{1}{\sqrt{3}}(3\hat{s}_z^2 - \hat{s}^2), \tag{2}$$

where $\hat{s}^2 = \hat{s}_x^2 + \hat{s}_y^2 + \hat{s}_z^2$ and $\{\}$ denotes anti-commutator. However, the generators for $D(0,1)$ are expressed in terms of the generators for the representation $D(1,0)$ as follows

$$\hat{\bar{s}}_x = -\hat{s}_x, \quad \hat{\bar{s}}_y = \hat{s}_y, \quad \hat{\bar{s}}_z = -\hat{s}_z,$$
$$\hat{\bar{q}}_{xy} = \hat{q}_{xy}, \quad \hat{\bar{q}}_{xz} = -\hat{q}_{xz}, \quad \hat{\bar{q}}_{yz} = \hat{q}_{yz},$$
$$\hat{\bar{q}}_{x^2-y^2} = -\hat{q}_{x^2-y^2}, \quad \hat{\bar{q}}_{3z^2-r^2} = -\hat{q}_{3z^2-r^2}. \tag{3}$$

We use a bar to indicate the irreducible representation $D(0,1)$ and use the lowercase letters to indicate single-atomic operators while the uppercase letters for total spin operators throughout this work. As long as there are two inequivalent fundamental representations of SU(3), we claim that there are two types of spin-1 bosons that differ by the corresponding irreducible representations. Two operators,

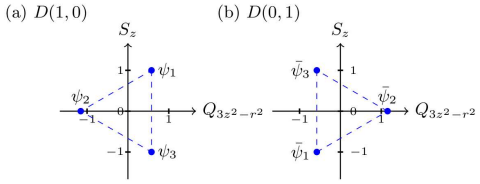

Figure 1. Two fundamental irreducible representations (a) $D(1,0)$ (b) $D(0,1)$ in the S_z and $Q_{3z^2-r^2}$ plane. Spin states are denoted by $\{\psi_1, \psi_2, \psi_3\}$ for $D(1,0)$ and $\{\bar{\psi}_1, \bar{\psi}_2, \bar{\psi}_3\}$ for $D(0,1)$.

namely $\hat{S}_z$ and $\hat{Q}_{3z^2-r^2}$ out of 8 generators, commute with each other so that the fundamental representations can be illustrated in the S_z and $Q_{3z^2-r^2}$ plane (see Fig. 1). Accordingly, $S_z = 1$ and $S_z = -1$ states have the same quadrupole moments, but the state $S_z = 0$ has the different $Q_{3z^2-r^2}$ from others. This is true for both fundamental representations.

In a nutshell, SU(3) symmetry of a spin-1 atom implies that the atom can be found in two inequivalent irreducible representations $D(1,0)$ and $D(0,1)$. This suggests that any atom of a single species, for example ^{87}Rb atom does exist in two types depending on the fundamental representations of SU(3). Note that this is the direct consequence of the SU(3) symmetry of spin-1 atoms. As shown in Fig. 1 different types of atoms are different by their electric quadrupolar moment $Q_{3z^2-r^2}$, and as a consequence, these atoms react to the electric field gradient of an external field differently. This basic clue could be used to experimentally distinguish the types of atoms.

On the other hand, SU(2) symmetry has only one fundamental, irreducible representation given by the generators $\hat{s}_x$, $\hat{s}_y$ and $\hat{s}_z$ (see eq. 1). Thus, all spin-1 atoms are of one type according to SU(2) symmetry. For instance, ψ_1 and $\bar{\psi}_3$ states that correspond to $s_z = 1$ state are treated as the same state according to the SU(2) symmetry.

3. SU(3) symmetric Hamiltonian of spin-1 BEC

In what follows, we consider mixture of the interacting spin-1 BEC with N_1 atoms in the states $D(1,0)$ and N_2 atoms in the states $D(0,1)$. It is worth pointing out that these two types of atoms are of a single species. Then, the free part of the Hamiltonian of the spin-1 BEC is written as

$$\hat{H}_0 = \int \left(\frac{\hbar^2}{2m} \nabla \hat{\psi}_a^\dagger \cdot \nabla \hat{\psi}_a + \hat{\psi}_a^\dagger U(\mathbf{r}) \hat{\psi}_a \right) d^3\mathbf{r} + \int \left(\frac{\hbar^2}{2m} \nabla \hat{\bar{\psi}}_a^\dagger \cdot \nabla \hat{\bar{\psi}}_a + \hat{\bar{\psi}}_a^\dagger U(\mathbf{r}) \hat{\bar{\psi}}_a \right) d^3\mathbf{r} \quad (4)$$

where $\hat{\psi}_a(\mathbf{r})$ and $\hat{\bar{\psi}}_a(\mathbf{r})$ $(a = 1, 2, 3)$ are field operators of two types of atoms. Mass of the atoms is denoted by m and $U(\mathbf{r})$ is trap potential energy.

3.1. Collisional interactions between atoms

There are three types of collisional interactions between condensed atoms namely (i) collision between $D(1,0)$ atoms (ii) collision between $D(0,1)$ atoms and (iii) collision between $D(1,0)$ and $D(0,1)$ atoms. First, we consider the collisional interaction between $D(1,0)$ atoms. When two atoms of type $D(1,0)$ collide, the state of the total system can be $D(2,0)$ and $D(0,1)$ since $D(1,0)\otimes D(1,0) = D(2,0)\oplus D(0,1)$. Using Clebsch-Gordan coefficients it is easy to verify that the subspace $D(2,0)$ is symmetric and $D(0,1)$ is anti-symmetric under the permutation of two atoms. Thus, the representation $D(0,1)$ is ruled out by symmetry consideration for bosons. Therefore, the collisional interaction potential energy $\hat{H}_{1,0}$ can be expressed as $\hat{H}_{1,0} = U_{2,0}\hat{P}_{2,0}$ where $\hat{P}_{2,0}$ is a projection operator that projects the state of two colliding atoms into the space $D(2,0)$ and $U_{2,0} = 4\pi\hbar^2 a_{2,0}/m$. Here $a_{2,0}$ stands for the scattering length corresponding to $D(2,0)$.

In order to write the interaction Hamiltonian in an appropriate form, we consider the quadratic Casimir operators which is denoted by $\hat{g}^2 = \sum_{i=1}^{8}\hat{g}_i^2$. Here we introduce the new notation for the $SU(3)$ generators as $\hat{g}_1 = \hat{s}_x$, $\hat{g}_2 = \hat{s}_y$, $\hat{g}_3 = \hat{s}_z$, $\hat{g}_4 = \hat{q}_{xy}$, $\hat{g}_5 = \hat{q}_{xz}$, $\hat{g}_6 = \hat{q}_{yz}$, $\hat{g}_7 = \hat{q}_{x^2-y^2}$, $\hat{g}_8 = \hat{q}_{3z^2-r^2}$. For two atoms, the Casimir operator of total system is given by $\hat{G}^2 = (\hat{\mathbf{g}}^{(1)} + \hat{\mathbf{g}}^{(2)})^2 = (\hat{g}^{(1)})^2 + (\hat{g}^{(2)})^2 + 2\hat{\mathbf{g}}^{(1)}\cdot\hat{\mathbf{g}}^{(2)}$ where the mixed product term can be expanded as $\hat{\mathbf{g}}^{(1)}\cdot\hat{\mathbf{g}}^{(2)} = 4\left(\hat{P}_{2,0} - 2\hat{I}/3\right)$ with being $\hat{I}$ the unit matrix. Hence, the interaction Hamiltonian is obtained as

$$\hat{H}_{1,0} = U_{2,0}\left(\frac{1}{4}\hat{\mathbf{g}}^{(1)}\cdot\hat{\mathbf{g}}^{(2)} + \frac{2}{3}\hat{I}\right). \tag{5}$$

Similarly, the interaction Hamiltonian for $D(0,1)$ atoms is

$$\hat{H}_{0,1} = U_{0,2}\left(\frac{1}{4}\hat{\tilde{\mathbf{g}}}^{(1)}\cdot\hat{\tilde{\mathbf{g}}}^{(2)} + \frac{2}{3}\hat{I}\right), \tag{6}$$

where $\hat{\tilde{\mathbf{g}}}$ is general notation for the generators for $D(0,1)$ and $U_{0,2} = 4\pi\hbar^2 a_{0,2}/m$.

Next we consider the interaction between the condensed atoms in the states $D(1,0)$ and $D(0,1)$. Since $D(1,0)\otimes D(0,1) = D(1,1)\oplus D(0,0)$ these atoms scatter into $D(1,1)$ and $D(0,0)$ subspaces and consequently interaction Hamiltonian $\hat{H}_{\rm mix}$ can be written as

$$\hat{H}_{\rm mix} = U_{0,0}\hat{P}_{0,0} + U_{1,1}\hat{P}_{1,1}, \tag{7}$$

where $U_{0,0} = 4\pi\hbar^2 a_{0,0}/m$ and $U_{1,1} = 4\pi\hbar^2 a_{1,1}/m$.

Similar to $\hat{H}_{1,0}$ and $\hat{H}_{0,1}$, the Hamiltonian $\hat{H}_{\rm mix}$ can be expressed in terms of $\hat{\mathbf{g}}^{(1)}\cdot\hat{\tilde{\mathbf{g}}}^{(2)}$. Especially, the use of the expressions $\hat{P}_{0,0} + \hat{P}_{1,1} = \hat{I}$ and $\hat{\mathbf{g}}^{(1)}\cdot\hat{\tilde{\mathbf{g}}}^{(2)} = 6\hat{P}_{1,1} - 16\hat{I}/3$ yields $\hat{H}_{\rm mix}$ in the form of

$$\hat{H}_{\rm mix} = \frac{U_{0,0}+8U_{1,1}}{9}\hat{I} + \frac{1}{6}(U_{1,1}-U_{0,0})(\hat{\mathbf{g}}^{(1)}\cdot\hat{\tilde{\mathbf{g}}}^{(2)}). \tag{8}$$

Finally, total interaction Hamiltonian $\hat{H}_{\rm int}$ may be written in the second quantized form as

$$\begin{aligned}\hat{H}_{\rm int} &= \hat{H}_{1,0} + \hat{H}_{0,1} + \hat{H}_{\rm mix}\\ &= \int\left[\left(\frac{U_{0,0}+8U_{1,1}}{9}\right)\hat{\psi}_a^\dagger\hat{\tilde{\psi}}_{a'}^\dagger\hat{\tilde{\psi}}_{a'}\hat{\psi}_a\right.\end{aligned}$$

$$+\frac{U_{2,0}}{4}\hat{\psi}_a^\dagger\hat{\psi}_{a'}^\dagger\hat{\mathbf{g}}_{ab}^{(1)}\cdot\hat{\mathbf{g}}_{a'b'}^{(2)}\hat{\psi}_{b'}\hat{\psi}_b+\frac{2U_{2,0}}{3}\hat{\psi}_a^\dagger\hat{\psi}_{a'}^\dagger\hat{\psi}_{a'}\hat{\psi}_a$$
$$+\frac{U_{0,2}}{4}\hat{\bar{\psi}}_a^\dagger\hat{\bar{\psi}}_{a'}^\dagger\hat{\bar{\mathbf{g}}}_{ab}^{(1)}\cdot\hat{\bar{\mathbf{g}}}_{a'b'}^{(2)}\hat{\bar{\psi}}_{b'}\hat{\bar{\psi}}_b+\frac{2U_{0,2}}{3}\hat{\bar{\psi}}_a^\dagger\hat{\bar{\psi}}_{a'}^\dagger\hat{\bar{\psi}}_{a'}\hat{\bar{\psi}}_a$$
$$+\frac{1}{6}(U_{1,1}-U_{0,0})\hat{\psi}_a^\dagger\hat{\bar{\psi}}_{a'}^\dagger\hat{\mathbf{g}}_{ab}^{(1)}\cdot\hat{\bar{\mathbf{g}}}_{a'b'}^{(2)}\hat{\bar{\psi}}_{b'}\hat{\psi}_b\Bigg]d^3\mathbf{r}. \tag{9}$$

This Hamiltonian with the SU(3) symmetry of spin-1 atoms is the main result of the current paper.

Furthermore, in the single mode approximation we take only $\mathbf{k}=0$ mode in the plane wave expansion $\hat{\psi}_a=\frac{1}{\sqrt{V}}\sum_{\mathbf{k}}\hat{\zeta}_{\mathbf{k},a}e^{i\mathbf{k}\cdot\mathbf{r}}$ of the field operators where $\hat{\zeta}_a$ is a spin field operator. Taking the expression $\hat{\psi}_a=\frac{1}{\sqrt{V}}\hat{\zeta}_a$ into account and integrating over whole space V, the Hamiltonian (9) may be written as

$$\hat{H}_{\rm int}=\frac{1}{V}\left(\frac{U_{0,0}+8U_{1,1}}{9}\right)\hat{\zeta}_a^\dagger\hat{\bar{\zeta}}_{a'}^\dagger\hat{\bar{\zeta}}_{a'}\hat{\zeta}_a$$
$$+\frac{U_{2,0}}{4V}\hat{\zeta}_a^\dagger\hat{\zeta}_{a'}^\dagger\hat{\mathbf{g}}_{ab}^{(1)}\cdot\hat{\mathbf{g}}_{a'b'}^{(2)}\hat{\zeta}_{b'}\hat{\zeta}_b+\frac{2U_{2,0}}{3V}\hat{\zeta}_a^\dagger\hat{\zeta}_{a'}^\dagger\hat{\zeta}_{a'}\hat{\zeta}_a$$
$$+\frac{U_{0,2}}{4V}\hat{\bar{\zeta}}_a^\dagger\hat{\bar{\zeta}}_{a'}^\dagger\hat{\bar{\mathbf{g}}}_{ab}^{(1)}\cdot\hat{\bar{\mathbf{g}}}_{a'b'}^{(2)}\hat{\bar{\zeta}}_{b'}\hat{\bar{\zeta}}_b+\frac{2U_{0,2}}{3V}\hat{\bar{\zeta}}_a^\dagger\hat{\bar{\zeta}}_{a'}^\dagger\hat{\bar{\zeta}}_{a'}\hat{\bar{\zeta}}_a$$
$$+\frac{1}{6V}(U_{1,1}-U_{0,0})\hat{\zeta}_a^\dagger\hat{\bar{\zeta}}_{a'}^\dagger\hat{\mathbf{g}}_{ab}^{(1)}\cdot\hat{\bar{\mathbf{g}}}_{a'b'}^{(2)}\hat{\bar{\zeta}}_{b'}\hat{\zeta}_b. \tag{10}$$

Now, we follow Ref.[9] to identify the algebraic structure of the Hamiltonian and obtain

$$\hat{H}_{\rm int}=\frac{U_{2,0}}{V}\left(\frac{1}{4}\hat{\mathbf{G}}\cdot\hat{\mathbf{G}}+\frac{2}{3}\hat{N}_1^2-2\hat{N}_1\right)$$
$$+\frac{U_{0,2}}{V}\left(\frac{1}{4}\hat{\bar{\mathbf{G}}}\cdot\hat{\bar{\mathbf{G}}}+\frac{2}{3}\hat{N}_2^2-2\hat{N}_2\right)$$
$$+\frac{1}{V}\left(U_{0,0}\hat{N}_1\hat{N}_2+\frac{1}{12}(U_{1,1}-U_{0,0})\hat{\mathcal{G}}\cdot\hat{\mathcal{G}}\right) \tag{11}$$

where we define the following new notations as $\hat{\mathbf{G}}=\sum_{i=1}^N\mathbf{g}_i$, $\hat{\bar{\mathbf{G}}}=\sum_{i=1}^N\bar{\mathbf{g}}_i$ and $\hat{\mathcal{G}}=\hat{\mathbf{G}}+\hat{\bar{\mathbf{G}}}$. See Appendix A for further details on the derivations of eq. (11)

3.2. Relationships between SU(2) *and* SU(3) *symmetric Hamiltonians*

Interestingly, a clear relationship between SU(3) symmetric Hamiltonian $\hat{H}_{1,0}=U_{2,0}\hat{P}_{2,0}$ and SU(2) symmetric Hamiltonian $\hat{H}_{\rm SU(2)}=U_0\hat{P}_0+U_2\hat{P}_2$ [10, 22] exists. For SU(2), the total spin F that can have two values 0 and 2 is exploited to index the irreducible representations. Thus, in the Hamiltonian $\hat{H}_{\rm SU(2)}$, $\hat{P}_i$ stands for projection operator for $i=F$ spin subspaces, $U_i=4\pi\hbar^2a_i/m$, $i=\{0,2\}$ and a_i is scattering lengths for $i=F$ irreducible representations. In particular, it is straightforward to prove that the subspace $\hat{P}_{2,0}$ for SU(3) is identical to the sum of subspaces $\hat{P}_0$ and $\hat{P}_2$ for SU(2). This can be done using Clebsch-Gordan coefficients of SU(2) and SU(3) groups. Moreover, it implies that two subspaces $\hat{P}_0$ and $\hat{P}_2$ of $SU(2)$ go to one big subspace of $SU(3)$. That could be the reason why we have almost the same numerical values for the low-energy scattering lengths a_0 and a_2 for the atoms ^{87}Rb and ^{23}Na [10, 14, 15] except ^{7}Li [23, 24].

In the case of SU(2), the eigenvalues of the Casimir operator $\hat{s}^2$ are determined to be 0 and 6 as long as $\hat{s}^2\hat{P}_0 = 0\hat{P}_0$ and $\hat{s}^2\hat{P}_2 = 6\hat{P}_2$. Therefore, small difference between the scattering lengths a_0 and a_2 leads to big change in the ground state of BEC (ferromagnetic or antiferromagnetic ground states). On the other hand, for $D(2,0)$, the eigenvalue of the Casimir operator $\sum_{i=1}^{8}\hat{g}_i^2$ of SU(3) is given by $\sum_{i=1}^{8}\hat{g}_i^2\hat{P}_{2,0} = (40/3)\hat{P}_{2,0}$ and there is no other subspace with different eigenvalue. Consequently, SU(3) symmetric Hamiltonian does not provide the different ground state phases when we only consider the collisional interaction between the same type of atoms.

But this is not the end of this story, the interaction Hamiltonian eq. (8) can feature the various types of magnetic phases of the ground state. Details will be given in the next section.

4. Ground state structure

For the fixed number of atoms, those terms in eq. (11) which depend only on $\hat{N}_1$ and $\hat{N}_2$ are constant operators. Therefore, it is sufficient to minimize the following Hamiltonian

$$\hat{H}_{\rm int} = \frac{U_{2,0}}{4V}\hat{\mathbf{G}}\cdot\hat{\mathbf{G}} + \frac{U_{0,2}}{4V}\hat{\bar{\mathbf{G}}}\cdot\hat{\bar{\mathbf{G}}} + \frac{1}{12V}(U_{1,1}-U_{0,0})\hat{\mathcal{G}}\cdot\hat{\mathcal{G}}. \tag{12}$$

First of all, we consider the first term of eq. (12). For N_1 atoms in the state $D(1,0)$, the possible states can be obtained by expanding the product of $D(1,0)$ representations as a sum of irreducible representations:

$$D(1,0)\otimes D(1,0)\otimes\cdots\otimes D(1,0) = \bigoplus_i \alpha_i D_i, \tag{13}$$

where α_i are some integers and D_i stands for the irreducible representations. In principle, atoms can be either one of the states D_i however only totally-symmetric states under permutations are allowed for bosons. In our case, totally-symmetric allowed states belong to $D(N_1,0)$ with degeneracy $(N_1+1)(N_1+2)/2$. This claim is also true for the atoms in $D(0,1)$ states. Particularly, the irreducible representation $D(0,N_2)$ with degeneracy $(N_2+1)(N_2+2)/2$ is the only possible case for $D(0,1)$ atoms.

For any state of $D(N_1,0)$, the expectation values of the Casimir operator $\hat{\mathbf{G}}\cdot\hat{\mathbf{G}}$ are given by

$$\langle\hat{\mathbf{G}}\cdot\hat{\mathbf{G}}\rangle = \frac{N_1^2}{3} + N_1 \tag{14}$$

(see eq. (B.3)). Similarly,

$$\langle\hat{\bar{\mathbf{G}}}\cdot\hat{\bar{\mathbf{G}}}\rangle = \frac{N_2^2}{3} + N_2 \tag{15}$$

for any state of $D(0,N_2)$. Since the above expectation values are constant for the corresponding representations, no minimization is required for the first two terms in eq. (12). Note that this is the manifestation of the SU(3) symmetry.

Next, when we consider all interactions in the system by taking all terms in eq. (11), the last term $\hat{\mathcal{G}}\cdot\hat{\mathcal{G}}$ does not require additional requirements due to symmetry

since there are two distinguishable atoms belonging to $D(1,0)$ and $D(0,1)$. Thus, the ground state can be classified depending on the sign of $U_{1,1}-U_{0,0}$ i.e., $a_{1,1}-a_{0,0}$.

In particular, when $a_{1,1}-a_{0,0}>0$ ground state is $D(N_1-N_2,0)$ if $N_1>N_2$ and $D(0,N_2-N_1)$ if $N_1<N_2$ (see Appendix B for details). The ground state energy is obtained as

$$E_0=\frac{U_{2,0}}{4V}N_1\left(N_1-1\right)+\frac{U_{0,2}}{4V}N_2\left(N_2-1\right)+\frac{U_{0,0}N_1N_2}{V}+\frac{U_{1,1}-U_{0,0}}{3V}\left(\frac{(N_1-N_2)^2}{3}+|N_1-N_2|\right). \tag{16}$$

When $N_1=N_2$, the ground state reduces to the singlet state $D(0,0)$ and it is totally antiferromagnetic because $\langle\hat{\mathcal{G}}\cdot\hat{\mathcal{G}}\rangle=0$ for this state. However, when $N_1\neq N_2$ the ground state is partially antiferromagnetic.

In the other case, when $a_{1,1}-a_{0,0}<0$, ground state is $D(N_1,N_2)$ (see Appendix B for details) and its energy is found to be

$$E_0=\frac{U_{2,0}}{4V}N_1\left(N_1-1\right)+\frac{U_{0,2}}{4V}N_2\left(N_2-1\right)+\frac{U_{0,0}N_1N_2}{V}+\frac{U_{1,1}-U_{0,0}}{3V}\left(\frac{N_1^2+N_1N_2+N_2^2}{3}+N_1+N_2\right). \tag{17}$$

Note that the order of degeneracy is $(N_1+1)(N_2+1)(N_1+N_2+2)/2$. This ground state has maximum expectation value of a Casimir operator calculated as $\langle\hat{\mathcal{G}}\cdot\hat{\mathcal{G}}\rangle=N_1+N_2+(N_1^2+N_1N_2+N_2^2)/3$ which implies ferromagnetic ground state.

5. Spin mixing dynamics

In the spin-1 BEC, the spin degree of freedom is completely released, and atoms can freely move between internal spin states. Particularly, the scattering of two atoms in the states with spin components $+1$ and -1 may result in the state with 0 net spin (an atom in the state ζ_1 scatters from another atom in the state ζ_3 and after scattering both atoms are in the states ζ_2) and the other way around. This spin mixing process was extensively studied [9, 25, 12, 15, 13, 26, 27] with the use of SU(2) symmetry.

Here, we aim to study the spin mixing dynamics by using the SU(3) symmetric Hamiltonian (12). The first two terms are obviously Casimir operators of the SU(3) and consequently, these terms do not provide spin mixing. A much better interpretation of this claim could use conservation of the quadrupole moment. For the simplicity, let us analyze only $\hat{\mathbf{G}}\cdot\hat{\mathbf{G}}$ term in eq. (11) for $D(1,0)$ representation. Then, for the scattering $\{\zeta_1,\zeta_3\}\rightarrow\{\zeta_2,\zeta_2\}$, total quadrupole moment $Q_{3z^2-r^2}$ is equal to $2/\sqrt{3}$ before the scattering and $-4/\sqrt{3}$ after the scattering. This means the total quadrupole moment is not conserved. For the $D(0,1)$, $Q_{3z^2-r^2}$ is also not conserved. Therefore, these kinds of scattering do not happen. However, the scattering of the different types of atoms $\{\zeta_1,\bar{\zeta}_1\}\rightarrow\{\zeta_2,\bar{\zeta}_2\}$ does conserve the quantity $Q_{3z^2-r^2}$. Thus, only the third term $(U_{1,1}-U_{0,0})\hat{\mathcal{G}}\cdot\hat{\mathcal{G}}/12V$ in eq. (11) leads to spin mixing.

The spin mixing dynamics are described by nine probability amplitudes denoted by $a_i(t)$ $(i=\{1,\ldots,9\})$ that characterize a general spin-1 state of BEC within tensor product space $D(1,0)\otimes D(0,1)$. Then, total state of the system reads as

$$\begin{aligned}|\Psi(t)\rangle=&\,a_1|\zeta_1\bar{\zeta}_1\rangle+a_2|\zeta_2\bar{\zeta}_1\rangle+a_3|\zeta_3\bar{\zeta}_1\rangle+a_4|\zeta_1\bar{\zeta}_2\rangle\\&+a_5|\zeta_2\bar{\zeta}_2\rangle+a_6|\zeta_3\bar{\zeta}_2\rangle+a_7|\zeta_1\bar{\zeta}_3\rangle+a_8|\zeta_2\bar{\zeta}_3\rangle\\&+a_9|\zeta_3\bar{\zeta}_3\rangle.\end{aligned} \tag{18}$$

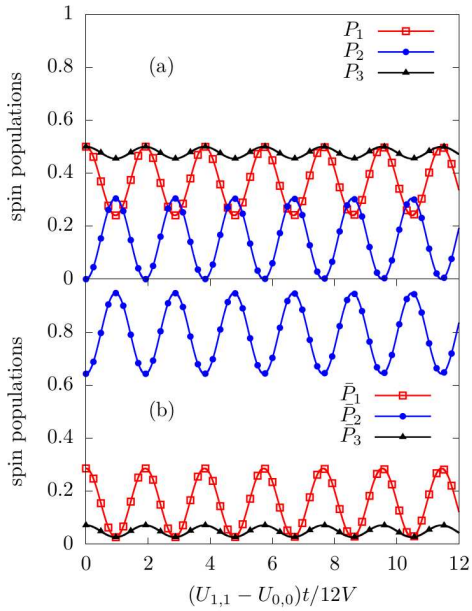

Figure 2. Coherent spin mixing dynamics of a spin-1 Bose-Einstein condensate. Spin populations as a function of time (a) for atoms in the $D(1,0)$ states and (b) for atoms in the $D(0,1)$ states. Initial values are given by $a_1 = a_3 = 2/\sqrt{28}$, $a_4 = a_6 = 3/\sqrt{28}$, $a_7 = a_9 = 1/\sqrt{28}$ and $a_2 = a_5 = a_8 = 0$.

The probability amplitudes $a_i(t)$ satisfy the following Gross-Pitaevskii equation

$$i\hbar\frac{\partial|\Psi(t)\rangle}{\partial t} = \frac{1}{12V}(U_{1,1} - U_{0,0})\langle\hat{\mathcal{G}}\rangle \cdot \hat{\mathcal{G}}|\Psi(t)\rangle. \tag{19}$$

Explicit form of this equation is too lengthy, and we do not present it here. However, we are able to perform numerical calculation of eq. (19) and obtain time dynamics of the following spin populations

$$\begin{aligned}
P_1(t) &= |a_1|^2 + |a_4|^2 + |a_7|^2,\\
P_2(t) &= |a_2|^2 + |a_5|^2 + |a_8|^2,\\
P_3(t) &= |a_3|^2 + |a_6|^2 + |a_9|^2,\\
\bar{P}_1(t) &= |a_1|^2 + |a_2|^2 + |a_3|^2,\\
\bar{P}_2(t) &= |a_4|^2 + |a_5|^2 + |a_6|^2,\\
\bar{P}_3(t) &= |a_7|^2 + |a_8|^2 + |a_9|^2.
\end{aligned} \tag{20}$$

Here, P_i are populations in the states $|\zeta_i\rangle$ and $\bar{P}_i$ are populations in the states $|\bar{\zeta}_i\rangle$. According to the results illustrated in Fig. (2), apparent spin mixing process exists due to collisional interactions between different types of atoms.

6. Scattering lengths

It is natural to arise the question how the $a_{1,1}$ and $a_{0,0}$ scattering lengths relate to well-known a_2 and a_0 scattering lengths? The answer to this question is intriguing and we present it below. As we discussed in Sec. (3), inelastic scattering of atoms of

different types is described by $D(1,1)$ and $D(0,0)$ subspaces spanned by the following states

$$D(1,1) = \left\{ \begin{array}{c} |\zeta_1\rangle \otimes |\bar{\zeta}_2\rangle, \\ |\zeta_2\rangle \otimes |\bar{\zeta}_1\rangle, \\ |\zeta_1\rangle \otimes |\bar{\zeta}_3\rangle, \\ |\zeta_3\rangle \otimes |\bar{\zeta}_1\rangle, \\ |\zeta_2\rangle \otimes |\bar{\zeta}_3\rangle, \\ |\zeta_3\rangle \otimes |\bar{\zeta}_2\rangle, \\ \dfrac{|\zeta_2\rangle \otimes |\bar{\zeta}_2\rangle + |\zeta_3\rangle \otimes |\bar{\zeta}_3\rangle}{\sqrt{2}}, \\ \dfrac{2|\zeta_1\rangle \otimes |\bar{\zeta}_1\rangle + |\zeta_2\rangle \otimes |\bar{\zeta}_2\rangle - |\zeta_3\rangle \otimes |\bar{\zeta}_3\rangle}{\sqrt{6}}, \end{array} \right.$$

$$D(0,0) = \left\{ \frac{|\zeta_1\rangle \otimes |\bar{\zeta}_1\rangle - |\zeta_2\rangle \otimes |\bar{\zeta}_2\rangle + |\zeta_3\rangle \otimes |\bar{\zeta}_3\rangle}{\sqrt{3}}. \right. \tag{21}$$

It is remarkable to see that the one-dimensional $D(0,0)$ subspace of SU(3) is exactly the same as $F = 0$ subspace of SU(2) when the following changes are made

$$|\bar{\zeta}_1\rangle \to |\zeta_3\rangle, \quad |\bar{\zeta}_2\rangle \to |\zeta_2\rangle, \quad |\bar{\zeta}_3\rangle \to |\zeta_1\rangle. \tag{22}$$

Indeed, $F = 0$ subspace is written as

$$\frac{1}{\sqrt{3}} \left(|\zeta_1\rangle \otimes |\zeta_3\rangle - |\zeta_2\rangle \otimes |\zeta_2\rangle + |\zeta_3\rangle \otimes |\zeta_1\rangle \right). \tag{23}$$

using Clebsch-Gordon coefficients of SU(2). Therefore, the identical subspaces $D(0,0)$ of SU(3) and $F = 0$ of SU(2) mean the same interaction potential energy of the colliding atoms in these two cases, and consequently, the numerical value of $a_{0,0}$ is equal to the experimentally determined value of the a_0.

In the case of $D(1,1)$ subspace, it corresponds to the direct sum of two SU(2) subspaces namely, $F = 2$ and $F = 1$ when it transforms under eq. (22). However, the SU(2) treatment needs to apply the Pauli exclusion principle as long as the atoms are indistinguishable. For this reason, $F = 1$ subspace must be suppressed and only $F = 2$ subspace with dimension 5 is left. This discrepancy in the subspaces for SU(3) and SU(2) complicates obtaining relationships between a_2 and $a_{1,1}$.

7. Conclusions

To conclude, we propose two different types of spin-1 atoms which belong to two non-equivalent fundamental representations of the SU(3) Lie group, namely $D(1,0)$ and $D(0,1)$. For instance, an atom of ^{87}Rb can be in either of $D(1,0)$ and $D(0,1)$ states. When an atom is in the states $D(1,0)$, we call it type-1 and, in the other case, type-2. Essentially, different types of atoms interact with the electric field gradient in different ways due to their different quadrupole moment $Q_{3z^2-r^2}$. This is the most intriguing result of this paper.

Then, we consider the system composed of N_1 atoms in state $D(1,0)$ and N_2 atoms in state $D(0,1)$. In contrast to the single interaction term in the SU(2) theory of BEC, there are three different kinds of interactions: (i) scattering between $D(1,0)$ atoms (ii) scattering between $D(0,1)$ atoms and (iii) scattering between $D(1,0)$ and $D(0,1)$ atoms. Interactions between two different kinds of atoms depend on the dipole-quadrupole moment (last term in eq. (12)) and it leads to two different regimes of

ground state: either antiferromagnetic or ferromagnetic ground states depending on the magnitude of the coefficients $a_{0,0}$ and $a_{1,1}$. For the interactions between the same types of atoms, the interaction terms in the Hamiltonian do not depend on the dipole-quadrupole moments.

We also discover that the scattering length $a_{0,0}$ is equal to the experimentally measured value of a_0 but not to the theoretically calculated value. The reason for the latter is the current theoretical calculation of a_0 usually ignore the electric quadrupolar interaction, that is, a crucial element of SU(3).

Furthermore, spin mixing dynamics are studied by using SU(3) symmetric Hamiltonian. It shows the well-behaved pattern of spin mixing, that is, due to only the interaction between different types of atoms. This claim is also verified by the conservation law of the net quadrupole moments of atoms.

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Appendix A.

For the sake of clarity, we treat each term of eq. (10) one by one. The spin-independent terms can be re-expressed as

$$\begin{aligned}
\hat{\zeta}_a^\dagger \hat{\zeta}_{a'}^\dagger \hat{\zeta}_{a'} \hat{\zeta}_a &= \hat{N}_1(\hat{N}_1 - 1), \\
\hat{\bar{\zeta}}_a^\dagger \hat{\bar{\zeta}}_{a'}^\dagger \hat{\bar{\zeta}}_{a'} \hat{\bar{\zeta}}_a &= \hat{N}_2(\hat{N}_2 - 1), \\
\hat{\zeta}_a^\dagger \hat{\bar{\zeta}}_{a'}^\dagger \hat{\bar{\zeta}}_{a'} \hat{\zeta}_a &= \hat{N}_1 \hat{N}_2,
\end{aligned} \tag{A.1}$$

where $\hat{N}_1 = \hat{\zeta}_1^\dagger \hat{\zeta}_1 + \hat{\zeta}_0^\dagger \hat{\zeta}_0 + \hat{\zeta}_{-1}^\dagger \hat{\zeta}_{-1}$ and $\hat{N}_2 = \hat{\bar{\zeta}}_1^\dagger \hat{\bar{\zeta}}_1 + \hat{\bar{\zeta}}_0^\dagger \hat{\bar{\zeta}}_0 + \hat{\bar{\zeta}}_{-1}^\dagger \hat{\bar{\zeta}}_{-1}$ are the number operators and we use the bosonic commutation relations $[\hat{\zeta}_a, \hat{\zeta}_{a'}^\dagger] = \delta_{aa'}$, $[\hat{\bar{\zeta}}_a, \hat{\bar{\zeta}}_{a'}^\dagger] = \delta_{aa'}$ and $[\hat{\zeta}_a, \hat{\bar{\zeta}}_{a'}^\dagger] = 0$. For the spin-dependent terms, we have

$$\begin{aligned}
&\hat{\zeta}_a^\dagger \hat{\zeta}_{a'}^\dagger \hat{\mathbf{g}}_{ab}^{(1)} \cdot \hat{\mathbf{g}}_{a'b'}^{(2)} \hat{\zeta}_{b'} \hat{\zeta}_b \\
&\quad = \hat{\mathbf{g}}_{ab}^{(1)} \cdot \hat{\mathbf{g}}_{a'b'}^{(2)} \hat{\zeta}_a^\dagger \hat{\zeta}_b \hat{\zeta}_{a'}^\dagger \hat{\zeta}_{b'} - \hat{\mathbf{g}}_{ab}^{(1)} \cdot \hat{\mathbf{g}}_{a'b'}^{(2)} \hat{\zeta}_a^\dagger \delta_{a'b} \hat{\zeta}_{b'} \\
&\quad = \left(\hat{\zeta}_a^\dagger \hat{\mathbf{g}}_{ab}^{(1)} \hat{\zeta}_b \right) \cdot \left(\hat{\zeta}_{a'}^\dagger \hat{\mathbf{g}}_{a'b'}^{(2)} \hat{\zeta}_{b'} \right) - \hat{\mathbf{g}}_{ab}^{(1)} \cdot \hat{\mathbf{g}}_{bb'}^{(2)} \hat{\zeta}_a^\dagger \hat{\zeta}_{b'}.
\end{aligned} \tag{A.2}$$

The first term in RHS of the above equation is recognized as a tensor product, and as a consequence, it gives $\hat{\mathbf{G}} \cdot \hat{\mathbf{G}}$. In the second term, $\hat{\mathbf{g}}_{ab}^{(1)} \cdot \hat{\mathbf{g}}_{bb'}^{(2)}$ is a Casimir operator and it is equal to $(16/3)\delta_{ab'}$ for the considered representation $D(1,0)$. Then, eq. (A.2) becomes

$$\hat{\zeta}_a^\dagger \hat{\zeta}_{a'}^\dagger \hat{\mathbf{g}}_{ab}^{(1)} \cdot \hat{\mathbf{g}}_{a'b'}^{(2)} \hat{\zeta}_{b'} \hat{\zeta}_b = \hat{\mathbf{G}} \cdot \hat{\mathbf{G}} - \frac{16}{3} \hat{N}_1. \tag{A.3}$$

Similarly, for the representation $D(0,1)$, it turns out to be

$$\hat{\bar{\zeta}}_a^\dagger \hat{\bar{\zeta}}_{a'}^\dagger \hat{\bar{\mathbf{g}}}_{ab}^{(1)} \cdot \hat{\bar{\mathbf{g}}}_{a'b'}^{(2)} \hat{\bar{\zeta}}_{b'} \hat{\bar{\zeta}}_b = \hat{\bar{\mathbf{G}}} \cdot \hat{\bar{\mathbf{G}}} - \frac{16}{3} \hat{N}_2. \tag{A.4}$$

In order to rewrite the last term in eq. (10), we consider the sum of two generators $\hat{\mathbf{g}}_{ac}$ and $\hat{\bar{\mathbf{g}}}_{a'd}$ as defined

$$\hat{\mathcal{G}}_{aa',cd} = \hat{\mathbf{g}}_{ac} \delta_{a'd} + \hat{\bar{\mathbf{g}}}_{a'd} \delta_{ac}. \tag{A.5}$$

With the use of the following useful relation

$$\hat{\mathcal{G}}_{aa',cd}\cdot\hat{\mathcal{G}}_{cd,bb'} = 2\hat{\mathbf{g}}_{ab}\hat{\bar{\mathbf{g}}}_{a'b'} + \hat{\mathbf{g}}_{ac}\hat{\mathbf{g}}_{cb}\delta_{a'b'} + \hat{\bar{\mathbf{g}}}_{a'd}\hat{\bar{\mathbf{g}}}_{db'}\delta_{ab} \tag{A.6}$$

we rewrite the last term as follows

$$\begin{aligned}
&\zeta_a^\dagger\bar{\zeta}_{a'}^\dagger\hat{\mathbf{g}}_{ab}\cdot\hat{\bar{\mathbf{g}}}_{a'b'}\bar{\zeta}_{b'}\zeta_b \\
&= \frac{1}{2}\left(\hat{\mathcal{G}}\cdot\hat{\mathcal{G}} - \hat{N}_2\zeta_a^\dagger\hat{\mathbf{g}}_{ac}\hat{\mathbf{g}}_{cb}\zeta_b - \hat{N}_1\bar{\zeta}_{a'}^\dagger\hat{\bar{\mathbf{g}}}_{a'd}\hat{\bar{\mathbf{g}}}_{db'}\bar{\zeta}_{b'}\right) \\
&= \frac{1}{2}\left(\hat{\mathcal{G}}\cdot\hat{\mathcal{G}} - \hat{N}_2\hat{N}_1\left[\frac{16}{3}\right] - \hat{N}_1\hat{N}_2\left[\frac{16}{3}\right]\right) \\
&= \frac{1}{2}\hat{\mathcal{G}}\cdot\hat{\mathcal{G}} - \frac{16}{3}\hat{N}_1\hat{N}_2.
\end{aligned} \tag{A.7}$$

By substituting eqs. (A.1), (A.3), (A.4) and (A.7) into eq. (10) we get the desired eq. (11).

Appendix B.

The spin space of N_1 atoms of type-1 and N_2 atoms of type-2 is described by the tensor product $D(N_1,0)\otimes D(0,N_2)$. This product space can be expanded as a sum of irreducible representations. The explicit form of this expansion is given by

$$\begin{aligned}
&D(N_1,0)\otimes D(0,N_2) = D(N_1,N_2)\oplus D(N_1-1,N_2-1) \\
&\oplus D(N_1-2,N_2-2)\oplus\cdots\oplus D(N_1-N_2,0)
\end{aligned} \tag{B.1}$$

if $N_1 \geq N_2$ and

$$\begin{aligned}
&D(N_1,0)\otimes D(0,N_2) = D(N_1,N_2)\oplus D(N_1-1,N_2-1) \\
&\oplus D(N_1-2,N_2-2)\oplus\cdots\oplus D(0,N_2-N_1)
\end{aligned} \tag{B.2}$$

if $N_1 \leq N_2$. With the use of quadratic Casimir operator formula for the representation $D(p,q)$ given by

$$\hat{\mathbf{G}}\cdot\hat{\mathbf{G}} = 4\left(\frac{p^2+pq+q^2}{3}+p+q\right)\hat{I} \tag{B.3}$$

we find that $D(N_1-N_2,0)$ or $D(0,N_2-N_1)$ states yield the minimum expectation values of $\langle\hat{\mathcal{G}}\cdot\hat{\mathcal{G}}\rangle$ depending on which type of atoms are greater. Equivalently, $D(N_1,N_2)$ representation gives the maximum expectation values of $\langle\hat{\mathcal{G}}\cdot\hat{\mathcal{G}}\rangle$ no matter which one of N_1 and N_2 is greater.

To obtain the ground state energy, we need to find the expectation value of eq. (11). Using eq. (B.3), (14) and (15), we find the energy of ground states as given by eq. (16) and (17).

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