Motivated by the recent discoveries of spin-1 and spin-1/2 Bose gas, we have studied the general structure of the Bose gases with arbitrary spin. A general method is developed to uncover the elementary building blocks of the angular momentum eigenstates, as well as the relations (or interactions) between them. Applications of this method to Bose gas with integer spins \((f = 1, 2, 3)\) and half integer spins \((f = 1/2, 3/2)\) reveal many surprising structures.

Recent experiments on dilute quantum gases of alkali atoms have produced a spin-1 and (pseudo-) spin-1/2 Bose gas respectively. The former is produced in optically trapped \(^{23}\)Na [4], the latter in magnetically trapped \(^{87}\)Rb by rotating the hyperfine states \([f = 2, m = 1]\) and \([f = 1, m = -1]\) into each other through a slightly detuned rf-field [5]. Many macroscopic quantum phenomena have been observed in these systems. At present, these phenomena can be explained in terms of the single condensate picture. However, in the case of spin-1 Bose gas with antiferromagnetic interaction like \(^{23}\)Na, it is been pointed out very recently that as the magnetic field gradient is reduced, the single condensate will evolve toward an angular momentum eigenstate, which will become a spin singlet as the magnetic field is reduced to zero [6] [7]. The singlet state is a “fragmented” structure which bears no resemblance to the single condensate state [6]. That the ground state of a Bose system can be very different from a conventional single condensate when it acquires internal degrees of freedom is a surprise.

Motivated by the fragmented structure of the spin-1 Bose gas, we consider Bose gases with higher spins. Although Bose gases with spin \(f > 1\) have not yet been produced, it is conceivable that they can be realized in the future. After all, both spin-1 and spin-1/2 Bose gases have only come into existence within the last one and half year. Currently, there are also efforts to condense \(^{85}\)Rb, which will be a spin-2 Bose gas when loaded into an optical trap. The main reasons for our investigation, however, remains theoretical and conceptual. The nature of the ground states of Bose gases with internal degrees of freedom is of fundamental importance. It has a place in the lore of superfluid physics and significance that goes beyond to the study of Bose-Einstein condensation. Our goal is to present a general method to construct the (total) angular momentum eigenstates \([F, F_z = F]\) for Bose gases with arbitrary spin \(f\). The construction of these eigenstates is a crucial step in diagonalizing the Hamiltonian of the system. Our method reveals many surprising structures.

 Generally, the spin state \([F, F_z = F]\) is made up of singlet and magnetic building units. A schematic representation of the structure of the spin state \([F, F_z = F]\) for Bosons with spins \(f = 1, 2, 3\) and “pseudo-spin” \(3/2\) are shown in figure a to d. They illustrate the intricate structure of these eigenstates and their increasing complexity with increasing \(f\).

The essence of the problem can be illustrated by considering a homogeneous Bose gas with spin-\(f\). Its relation to a trapped gas can be understood either in terms of local density approximation and in the procedure outlined in ref. [3] [4]. For a homogeneous dilute Bose gas, we first consider the condensate in the zero momentum mode (i.e. \(k = 0\)), denoted by the annihilation operator \(a_{\mu} = a_{\mu}(k = 0)\), where \(\mu\) labels the \(2f + 1\) spin components. The angular momentum operator then becomes \(\hat{F} = a_{\mu}^\dagger f_{\mu\nu}a_{\nu}\), where \(f_{\mu\nu}\) is the spin matrix for a spin-\(f\) Boson. The effect of the \(k \neq 0\) modes is to deplete the condensate. However, they can be ignored in the zeroth order approximation as they only contribute a small correction to the energy. (For trapped gases, the \(k = 0\) mode will be replaced by the lowest self-consistent mode that the system condenses into [3] [5].)

To construct the angular momentum eigenstates, it is sufficient to focus on the states \([F, F_z = F]\) with maximum spin projections, since other states with \(F_z < F\) can be obtained by applying to \([F, F]\) the spin lowering operator \(\hat{F}_- = \hat{F}_z - i\hat{F}_y\). In the following, we shall first derive our method, and then illustrate its application for the integer cases \(f = 1\) to 3 and half integer case \(f = 1/2\) and 3/2. The case \(f = 3\) is particularly subtle and will be considered last.

### (I.1) Outline of the Generating Function Method:

To give an orientation of our discussions, we first outline the logic of our method before presenting the detailed derivations. We begin by considering the total number of maximum spin states \([F, F]\) for a systems of \(N\) particles, which we denote as \(M_N(F)\). To generate this number for all \(N\) and \(S\) simultaneously, we consider the generating function

\[
G(x, y) = \sum_{N \geq 0} \sum_{F \geq 0} M_N(F) x^N y^F.
\]  

where \(x\) and \(y\) are complex numbers within the unit circle \((|x|, |y| < 1)\) to ensure convergence. Once this function is constructed, we shall see that \(M_N(F)\) is given by the number of solutions of a set of equations obeyed by two sets of non-negative integers \(\{s_i \geq 0\}\) and \(\{m_j \geq 0\}\). The integer \(s_i\) is the number of singlet building unit \(\Theta_i\) which is made up of \(n_i^{(s)}\) Bosons and carries no spin, while \(m_j\) is the number of magnetic building unit \(\Gamma_j\) which is made up of \(n_j^{(m)}\) Bosons and carries spin \(\ell_j\). The integers \(\{s_i \geq 0\}\) and \(\{m_j \geq 0\}\) satisfy number and spin constraints

\[
\sum_i n_i^{(s)} s_i + \sum_j n_j^{(m)} m_j = N, \quad \sum_j \ell_j m_j = F,
\]  

for Bosons with spins \(f = 1, 2, 3\) and “pseudo-spin” \(3/2\) are.
as well as a set of conditions $\mathcal{L}_a$ that further limit the range of the integers $\{s_i\}$ and the $\{m_j\}$. These conditions $\mathcal{L}_a$ reflect the inter-dependence (or “interactions”) among the building units. The conditions $\mathcal{L}_a$ are very simple for spin $f < 3$ but become quite complicated as $f \geq 3$, illustrating the rapidly increasing complexity of the system as $f$ increases. The typical form of these conditions will become clear when we come to our examples.

The general structure of the maximum spin state is therefore $|F,F\rangle = \sum A(s_i, m_j) \prod_\alpha \Theta^{s_i}_\alpha \Gamma^{m_j}_\alpha |\text{vac}\rangle$, where the $A$'s are coefficients and the sum is over all non-negative integers $\{s_i \geq 0\}$ and $\{m_j \geq 0\}$ satisfying the constraints $\mathcal{L}_a$.

(I.2) Derivation of the Generating Function Method:
We begin with the observation that the integer $M_N(F)$ can be expressed as

$$M_N(F) = I_N(F) - I_N(F + 1),$$

(3)

where $I_N(F)$ is the total number of states with $F_z = F$, independent of the value of total spin $F$. Eq.(3) follows from the fact that all spin multiplets with total spin $F' > F$ will contain a state $|F', F_z = F\rangle$, which contribute 1 to both $I_N(F)$ and $I_N(F + 1)$, and hence 0 to $M_N(F)$. Only those spin states with total spin $F_{\text{total}} = F_z = F$ will be included in the integer $I_N(F)$ and not $I_N(F + 1)$. That eq.(3) is useful is because it is much easier to construct a generating function for $I_N(F)$ due to the removal of the spin constraint. Before proceeding, we note that while $M_N(F)$ is defined only for $F \geq 0$, $I_N(F)$ is defined for both positive and negative $F$ such that $I_N(F) = I_N(-F)$.

To find $I_N(F)$, we note that a many-body state with total spin projection $F_z = F$ is of the form

$$|F, F_z = F\rangle = \sum_{\{n_j\} \geq 0} B(\{n_j\}) \left( \prod_{j=-f}^{f} a_j^{n_j} \right) |\text{vac}\rangle$$

(4)

with $\sum_{j=-f}^{f} n_j = N$ and $\sum_{j=-f}^{f} j n_j = F$, where $\{n_j\}$ is a set of $2f+1$ non-negative integers, $a_j$ creates a Boson in spin state $j$, and $B$'s are coefficients. The number of states with $F_z = F$ is

$$I_N(F) = \sum_{\{n_j\} \geq 0} \Delta \left( \sum_{j=-f}^{f} n_j \right) \Delta \left( \sum_{j=-f}^{f} j n_j - F \right)$$

(5)

where $\Delta(x)$ is a delta-function ensuring the vanishing of $x$. The generating function eq.(3) can in principle be obtained by substituting eqs.(3) and (5) into eq.(1). However, the constraint $F \geq 0$ in eq.(3) prevents an efficient summation. We therefore consider the function

$$W(x, y) = \sum_{N \geq 0} \sum_{F} (I_N(F) - I_N(F + 1)) x^N y^F,$$

(6)

where the sum $F$ ranges over all integers. Clearly, $G(x, y)$ is $W(x, y)$ with all negative powers of $y$ eliminated. This elimination can be achieved by the following integration

$$G(x, y) = \int_0^{2\pi} \frac{d\theta}{2\pi} \sum_{\ell=0}^{\infty} \left[ (yz^{-1})^\ell W(x, z) \right]_{z=e^{i\theta}}.$$

(7)

Performing the sum in eq.(7), $G$ becomes a contour integral around the unit circle $C$, $z = e^{i\theta}$,

$$G(x, y) = \int_0^{2\pi} \frac{dz}{2\pi i} \frac{W(x, z)}{z - y}$$

(8)

The expression $W$ can be obtained easily since $F$ now runs through all integers. Substituting eq.(3) into eq.(9), and first sum over $F$ and $N$, the functions $W$ becomes

$$W(x, z) = (1 - z^{-1}) \left[ \prod_{j=-f}^{f} x^{n_j} y^{j n_j} \right]$$

(9)

$$= (1 - z^{-1}) \prod_{j=-f}^{f} \frac{1}{1 - x z^j}.$$  

(10)

We then arrive at the key expression for the generating function,

$$G(x, y) = \int_C \frac{dz}{2\pi i} \frac{1 - z^{-1}}{z - y} \prod_{j=-f}^{f} \frac{1}{1 - x z^j}.$$  

(11)

To illustrate how eq.(11) can be used to obtain the structure of the maximum spin state $|F, F\rangle$, we consider the following examples.

Spin-1 Bosons: For $f = 1$, eq.(11) gives

$$G^{(f=1)}(x, y) = \frac{1}{(1 - x^2)(1 - xy)} = \sum_{n_2 \geq 0, \ell_2 \geq 0} x^{2n_2 + \ell_2} y^{\ell_2}.$$  

(12)

(13)

Comparing with eq.(3), we have

$$M_N(S) = \sum_{n_2 \geq 0, \ell_2 \geq 0} \Delta (2n_2 + \ell_2 - N) \Delta (\ell_2 - F).$$  

(14)

Eq.(14) shows that $M_N(S)$ is the number of the solutions of the equations

$$2 : n_2 + 1 \cdot \ell_2 = N, \quad 1 \cdot \ell_2 = F.$$  

(15)

It is clear that eq.(15) has a unique solution $n_0 = (N - F)/2, \ell_1 = F$. Hence $M_N^{(f=1)}(F) = 1$, i.e. there is only one maximum spin state $|F, F_z = F\rangle$. Next, we recall that the exponent of $x$ and $y$ are associated with particle number and spin respectively. Eq.(12) shows that the system consists of $\ell_1$ magnetic structural units which are spin-1 Bosons $(a_1)$, and $n_2$ singlet pairs of Bosons $\Theta_2$. A simple exercise shows that $\Theta_2 = (2a_1 a_{1\bar{1}} - \bar{a}_1^2)$. The (unnormalized) many-body state $|F, F_z = F\rangle$ is then given by $|F, F_z = F\rangle = a_1^{P+1} \Theta^{((N-F)/2)} |\text{vac}\rangle$, which is the results given in ref.(14). (See also fig.a).
Spin-2 Bosons: For \( f = 2 \), eq. (11) gives
\[
G^{(f=2)}(x, y) = \frac{1 + x^3 y^3}{(1-x^2)(1-x^3)(1-xy^2)(1-x^2 y^2)^2}.
\]
(16)

where the first sum is over the non-negative integers set \( \{s_2, s_3, m_1, m_2\} \). We then see that \( M_N(F) \) is given by the number of solutions to the equations
\[
2s_2 + 3s_3 + m_1 + 2m_2 + 3m_3 = N, \\
2m_1 + 2m_2 + 3m_3 = F.
\]
(18)
(19)

A solution of eqs. (18) and (19) describes a state consisting of two two-particle singlets \( \Theta_2 \), \( s_3 \) three-particle singlets \( \Theta_3 \), \( m_1 \) spin-2 Bosons \( a_i^2 \), and \( m_2 \) two-particle spin-2 state \( \{2,2\} \) (denoted as \( \Gamma_2 \)). Since \( m_3 = 0 \) and 1, the system may or may not contain a three-particle spin-3 state \( \{3,3\} \) (denoted as \( \Gamma_3 \)) depending on whether \( F \) is odd or even. It is straightforward to work out the expressions of these states, which are \( \Theta_2 = a_2a_2 - a_1a_1 + \frac{1}{2}a_0^2 \), \( \Theta_3 = a_0(2a_2a_2 - a_1a_1 - \frac{1}{2}a_0^2) - \sqrt{\frac{2}{3}}(a_1^2a_2 + a_2a_2^2) \), \( \Gamma_2 = a_2a_2 - \frac{\sqrt{2}}{2}a_1^2 \), and \( \Gamma_3 = 2a_2a_1 - \sqrt{3}a_1a_0 + a_0^2 \).

The condition \( m_3 = 0,1 \) is the additional constraint \( \mathcal{L}_\alpha \) mentioned in section (I.1). If \( \Gamma_3 \) was a “free” unit that could appear as many as times as possible, the numerator of eq. (16) would be (instead of \( 1 + x^3 y^3 \)) an infinite sum \( \sum_{n=0}^\infty (x^3 y^3)^n \), which will turn into a factor \( (1-x^3 y^3)^{-1} \) like other “free” building units (\( \Theta_2, \Theta_3, a_2, \) and \( \Gamma_2 \)) in the denominators in eq. (16). The fact that the series of \( x^3 y^3 \) terminates at the first order \( 3 \) at the beginning expresses the idea that a pair of three-particle singlets can be expressed in terms of all other “free” excitations (\( \Theta_2, \Theta_3, a_2, \) and \( \Gamma_2 \)) and therefore has already been accounted for in the generating function. Indeed, when examining \( \Gamma_3 \) (because of the prediction of the generating function), one finds
\[
\Gamma_3 = -ia_0^2 \Theta_3 + 4a_3^2 \Theta_2 a_2 - 4\sqrt{3}a_3^2 \Theta_3 \
\]
Note, however, that \( \Gamma_3 \) appears at most once. It therefore has no thermodynamic significance. This means that one can obtain the relevant thermodynamic structure by taking any term in the numerator of eq. (16). (See also fig.b).

(II). Bose gas with half integer spins: When \( f \) is a half integer, it is useful to consider the generating function
\[
G(x, y) = \sum_{N \geq 0} \sum_{F \geq 0} M_N(F)x^N y^F.
\]
(20)

Proceeding as the integer case, the function \( W(x, z) \) in eq. (14) becomes \( W(x, z) = (1-z^{-2}) \prod_{j=-f}^f (1-xz^{2j})^{-1} \).

Since \( f \) is a half-integer, \( W \) consists of even and odd powers of \( z \). Using the previous method to project out all the negative powers in \( y \), we have
\[
G(x, y) = \int_C \frac{dz}{2\pi i} \frac{e^{(1-z^{-2})}}{z^{-y} (1-xz^{2})^{-1}}.
\]
(21)

Spin 1/2 Bosons: For \( f = 1/2 \), we have
\[
G^{(f=1/2)}(x, y) = \frac{1}{1-x y} = \sum_{n \geq 0} x^n (y^2)^{n/2}
\]
(22)

Since the equation \( n = N, n/2 = F \) has only one solution and forces \( F = N/2 \), this means that the total spin of a system of spin-1/2 Bosons is fixed by the particle number \( N \) to be \( F = N/2 \), and \( |F, F = N/2 = a_{1/2}|_{\text{vac}} \). The system can be referred to as “statistical” since the ferromagnetism is forced by statistics.

Spin 3/2 Bosons: For \( f = 3/2 \), we have
\[
G^{(f=3/2)}(x, y) = \frac{1 + x^3 y^3}{(1-x^4)(1-xy^3)(1-x^2 y^2)^2}
\]
(23)

where the first sum is over non-negative integers \( s_4, m_1, m_2 \). The number of spin state \( |F, F \rangle \) is given by the number of the solution of
\[
4s_4 + m_1 + 2m_2 + 3m_3 = N, \quad \frac{3}{2}m_1 + m_2 + \frac{3}{2}m_3 = F
\]
(25)

which describes a state consisting of \( s_4 \) four-particle singlets \( \Theta_4 \), \( m_1 \) spin-3/2 Bosons (i.e. \( a_{3/2} \)), and \( m_2 \) spin-1/2 pairs \( \{1,1\} \) made up of two spin-1/2 particles (denoted as \( \Gamma_2 \)). Since \( m_3 = 0 \) and 1, the system may also contain a spin-3/2 three-particle state \( \{3,3,3\} \), (denoted as \( \Gamma_3/2 \)) which appears at most once. Thus, we have \( |F, F \rangle = \sum A\{s_4, m_1, m_2 \} \theta_4^{m_4} |\text{vac} \rangle \). (See also fig.c).

(III) Spin-3 Bosons: The case of \( f = 3 \) begins to illustrate the full complexity of the Bosons with higher spin. It is sufficiently intricate so we discuss it last. When \( f = 3 \), eq. (14) gives
\[
G^{(f=3)}(x, y) = \frac{[1 + x^{15} + C(x, y)] D(x, y)}{(1-x^2)(1-x^3)(1-x^6)(1-x^{10})}
\]
(26)

\[
D(x, y) = \frac{1}{(1-x^4)(1-x^2 y^2)(1-x^2 y^4)}
\]
(27)

The term \( C(x, y) \) is a polynomial with about fifty terms of the form \( x^a y^b \) with \( (a, b > 0) \). Since \( b > 0 \), these terms represent magnetic structures. From eq. (14), we see that
the structure of the total singlet state $|F = 0, F_z = 0\rangle$ is given by $G(x, y)$. Extracting $G(x, y)$ from eq. (16) (i.e. setting $C = 0$ and $D = 1$), we see that the singlet state is a linear combinations of singlets consisting of two, four, six, and ten particles, denoted as $\Theta_2, \Theta_4, \Theta_6, \Theta_{10}$ respectively. From our discussions for the spin-2 case, we see that all singlet except that made up of 15 particles ($\Theta_{15}$) can be expressed as products and sums of the “free” singlet set $\{\Theta_2, \Theta_4, \Theta_6, \Theta_{10}\}$. However, two 15-particle singlets (i.e. $\Theta_{15}^2$) is reducible to free singlet units. (See also fig.d).

As before, the elementary magnetic units $\{\Gamma_i\}$ are given by the denominator of $D$. They are single particle spin-3 Bosons ($a_3$), two-particle spin-2 pairs ($\langle 2, 2\rangle$), and two-particle spin-4 pairs ($\langle 4, 4\rangle$). The major difference between the $f = 3$ and previous examples, however, is the appearance of large number of terms in the numerator of the generating function (i.e. $C$), and the fact that about half of these terms have negative signs, which means disappearance rather than appearance of a configuration. The origin of the negative terms is due to the fact that a product of two or more different magnetic units $\Gamma_i$ and $\Gamma_j$ can be expressed in terms of other magnetic and non-magnetic units. These are the “interaction” constraints $L_\alpha$ we mentioned in section (1.1). Note that in the case of $f = 2$, the interaction constraints comes from the reducibility of a single type of structure, i.e. $\Gamma_2^3$ is reducible into other free units. As a result, all terms in the numerator of $G(f=2)$ are positive because one simply enumerates the multiplicity of $\Gamma_2$ until it becomes reducible. If, however, the interaction constraints involve the reducibility of the products of two or more different magnetic operators, as well as “scattering” such as $\Gamma_i \Gamma_j \rightarrow \Gamma_j \Gamma_k$ etc., then the counting process can be not be simply a termination of the multiplicity of a particular pattern. We shall not analyse the interaction constraint for the $f = 3$ case here because it is very involved. Despite this complexity, it is clear from the generating function what the elementary magnetic building units are.

In summary, we have illustrated the method to uncover the elementary building units of the angular momentum eigenstates of a spin-carrying Bose gas. The construction of these units is crucial for energy studies. Yet even without such studies, the present method has illustrated the complex structure of the ground state of these Bose gases as a function of magnetization. The fact that the number of independent singlet units proliferates as $f$ increases also means that the system becomes more fragmented, since spin fluctuations (which is already huge in the spin-1 case in the low field limit) will increase as the number of different singlets increases.

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Figure Captions: Figures a,b, and c are schematic representations of the basis of the angular momentum state $|F, F\rangle$ for spin $f = 1, 2,$ and $3/2$ respectively. Enclosed units with and without arrows represent magnetic and singlet units respectively. The number of dots indicates the number of particles in the unit. For example, in the spin-2 case (fig.b), the state consists of 2-particle and 3-particle singlets (represented as arrow-free ellipses and triangles containing two and three dots resp.), and a 2-particle spin-2 pair (represented as an ellipse with two dots and an arrow). The 3-particle spin-3 unit is represented as a triangle containing 3 dots and an arrow. The dashed circles in the interior are drawn to help to visualize the singlet and the magnetic units. They are not meant to imply the existence of a singlet core. Figure d is a schematic representation of the singlet structure of a spin-3 Bose gas, which consists of 2-, 4-, 6-, and 10-particle singlets, and a “constraint” unit consisting of 15 particles, which is reducible to other existing singlet units when appears more than once.
