General Structure of Bose-Einstein Condensates with Arbitrary Spin

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Motivated by the recent discoveries of spin-1 and pseudo-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.

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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 [1], the latter in magnetically trapped ^{87}Rb by rotating the hyperfine states $|f = 2, m = 1\rangle$ and $|f = 1, m = -1\rangle$ into each other through a slightly detuned rf field [2]. 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 has 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 [3,4]. The singlet state is a "fragmented" structure which bears no resemblance to the single condensate state [4]. 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 come into existence only within the last one and a half years. Very recently, the Colorado group has succeeded in Bose condensing ^{85}Rb in a magnetic trap, which will be a spin-2 Bose gas when loaded into an optical trap. The main reasons for our investigation, however, remain 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 $|F, F_z\rangle$ 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 $|F, F_z = F\rangle$ is made up of singlet and magnetic building units. A schematic representation of the structure of the spin state $|F, F\rangle$ for bosons with spins $f = 1, 2, 3$ and "pseudospin" $3/2$ are shown in Figs. 1(a)–1(d). They illustrate the intricate structure of these eigenstates and their increasing complexity with increasing f. For simplicity, we shall from now on refer to half integer pseudospins as "spins."

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. [4].) For a homogeneous dilute Bose gas, we first consider the condensate in the zero momentum mode (i.e., $\mathbf{k} = \mathbf{0}$), denoted by the annihilation operator $a_\mu \equiv a_\mu(\mathbf{k} = 0)$, where μ labels the $2f + 1$ spin components. The angular momentum operator then becomes $\hat{\mathbf{F}} = a^\dagger_\mu \mathbf{f}_{\mu\nu} a_\nu$, where $\mathbf{f}_{\mu\nu}$ is the spin matrix for a spin-f boson. The effect of the $\mathbf{k} \neq 0$ modes is to deplete the condensate. They can be ignored in the zeroth order approximation as they contribute only a small correction to the energy. (For trapped gases, the $\mathbf{k} = 0$ mode will be replaced by the lowest self-consistent mode that the system condenses into [3,4].) To construct the angular momentum eigenstates, it is sufficient to focus on the states $|F, F_z = F\rangle$ with maximum spin projections, since other states with $F_z < F$ can be obtained by applying to $|F, F\rangle$ the spin lowering operator $\hat{F}_- = \hat{F}_x - i\hat{F}_y$. 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 cases $f = 1/2$ and $3/2$. The case $f = 3$ is particularly subtle and will be considered last.

(I.1) Outline of the generating function method.—We first outline the logic of our method before presenting the detailed derivations. We begin by considering the total number of maximum spin states $|F, F\rangle$ for 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

$$G(x, y) = \sum_{N\geq 0} \sum_{F\geq 0} M_N(F) x^N y^F, \tag{1}$$

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

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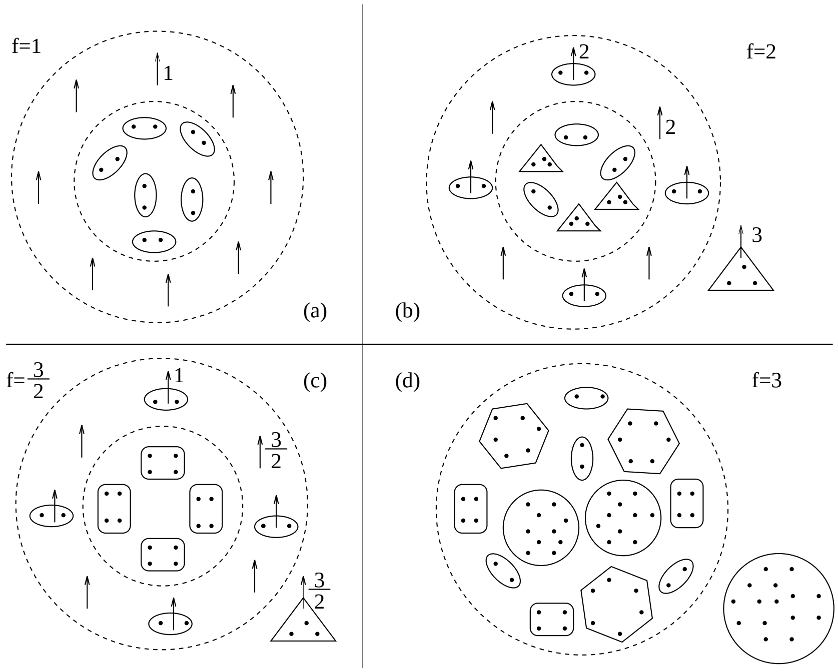

FIG. 1. (a), (b), and (c) are schematic representations of the basis of the angular momentum state $|F, F\rangle$ for spin $f = 1$, 2, and 3/2, respectively. Enclosed units with and without arrows represent magnetic and singlet units, respectively. The number of dots indicates the number of particles in the unit. For example, in the spin-2 case (b), the state consists of two-particle and three-particle singlets (represented as arrow-free ellipses and triangles containing two and three dots, respectively), and a two-particle spin-2 pair (represented as an ellipse with two dots and an arrow). The three-particle spin-3 unit is represented as a triangle containing three 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. (d) is a schematic representation of the singlet structure of a spin-3 Bose gas, which consists of two-, four-, six- , and ten-particle singlets, and a "constraint" unit consisting of 15 particles, which is reducible to other existing singlet units when it appears more than once.

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 Θ_i which is made up of $n_i^{(s)}$ bosons and carries no spin, while m_j is the number of magnetic building unit Γ_j which is made up of $n_j^{(m)}$ bosons and carries spin ℓ_j. The integers $\{s_i \geq 0\}$ and $\{m_j \geq 0\}$ satisfy number and spin constraints

$$\sum_i n_i^{(s)} s_i + \sum_j n_j^{(m)} m_j = N, \qquad \sum_j \ell_j m_j = F\,, \quad (2)$$

as well as a set of conditions $\mathcal{L}_\alpha$ that further limit the range of the integers $\{s_i\}$ and the $\{m_j\}$. These conditions $\mathcal{L}_\alpha$ reflect the interdependence (or "interactions") among the building units. The conditions $\mathcal{L}_\alpha$ 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 $|F, F\rangle = \sum A(\{s_i\}, \{m_j\}) \prod_{i,j} \Theta_i^{\dagger s_i} \Gamma_j^{\dagger m_j} |\mathrm{vac}\rangle$, 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 $\mathcal{L}_\alpha$.

(I.2) Derivation of the generating function method.— We begin with the observation that the integer $M_N(F)$ can be expressed as

$$M_N(F) = I_N(F) - I_N(F + 1)\,, \quad (3)$$

where $I_N(F)$ is the total number of states with $F_z = F$, independent of the value of total spin F. Equation (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 $F^{\mathrm{total}} = F_z = F$ 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

$$|F, F_z = F\rangle = \sum_{\{n_j \geq 0\}} B(\{n_j\}) \left(\prod_{j=-f}^{f} a_j^{\dagger n_j} \right) |\mathrm{vac}\rangle \quad (4)$$

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, $a_j^\dagger$ creates a boson in spin state j, and B's are coefficients. The number of states with $F_z = F$ is

$$I_N(F) = \sum_{\{n_j \geq 0\}} \Delta\left(\sum_{j=-f}^{f} n_j \right) \Delta\left(\sum_{j=-f}^{f} j n_j - F \right), \quad (5)$$

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

$$W(x,y) = \sum_{N\geq 0} \sum_{F} [I_N(F) - I_N(F+1)] x^N y^F, \quad (6)$$

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:

$$G(x,y) = \int_0^{2\pi} \frac{d\theta}{2\pi} \sum_{\ell=0}^{\infty} [(yz^{-1})^{\ell} W(x,z)]_{z=e^{i\theta}}. \quad (7)$$

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

$$G(x,y) = \int_C \frac{dz}{2\pi i} \frac{W(x,z)}{z-y}. \quad (8)$$

The expression W can be obtained easily since F now runs through all integers. Substituting Eq. (5) into Eq. (6), and first sum over F and N, the functions W become

$$W(x,z) = (1 - z^{-1}) \left[\prod_{j=-f}^{f} \sum_{n_j=0}^{\infty} \right] \left(\prod_{j=-f}^{f} x^{n_j} z^{jn_j} \right) \quad (9)$$

$$= (1 - z^{-1}) \prod_{j=-f}^{f} \frac{1}{1 - xz^j}, \quad (10)$$

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

$$G(x,y) = \int_C \frac{dz}{2\pi i} \frac{1 - z^{-1}}{z - y} \prod_{j=-f}^{f} \frac{1}{1 - xz^j}. \quad (11)$$

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

$$G^{(f=1)}(x,y) = \frac{1}{(1-x^2)(1-xy)} \quad (12)$$

$$= \sum_{n_2\geq 0} \sum_{\ell_1 \geq 0} x^{2n_2+\ell_1} y^{\ell_1}. \quad (13)$$

Comparing with Eq. (1), we have

$$M_N(S) = \sum_{n_2\geq 0} \sum_{\ell_1\geq 0} \Delta(2n_2 + \ell_1 - N) \Delta(\ell_1 - F). \quad (14)$$

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

$$2 \times n_2 + 1 \times \ell_1 = N, \qquad 1 \times \ell_1 = F. \quad (15)$$

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. Equation (15) shows that the system consists of ℓ_1 magnetic structural units which are spin-1 bosons (a_1), and n_2 singlet pairs of bosons Θ_2. A simple exercise shows that $\Theta_2 = (2a_1a_{-1} - a_0^2)$. The (un-normalized) many-body state $|F, F_z = F\rangle$ is then given by $|F,F\rangle = a_1^{\dagger F} \Theta^{\dagger (N-F)/2} |\text{vac}\rangle$, which is the result given in Ref. [4]. (See also Fig. 1a.)

Spin-2 bosons: For $f = 2$, Eq. (11) gives

$$G^{(f=2)}(x,y) = \frac{1 + x^3y^3}{(1-x^2)(1-x^3)(1-xy^2)(1-x^2y^2)} \quad (16)$$

$$= \sum \sum_{m_3=0,1} x^{2s_2+3s_3+m_1+2m_2+3m_3} y^{2m_1+2m_2+3m_3}, \quad (17)$$

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

$$2s_2 + 3s_3 + m_1 + 2m_2 + 3m_3 = N, \quad (18)$$

$$2m_1 + 2m_2 + 3m_3 = F. \quad (19)$$

A solution of Eqs. (18) and (19) describes a state consisting of s_2 two-particle singlets Θ_2, s_3 three-particle singlets Θ_3, m_1 spin-2 bosons ($a_2^\dagger$), and m_2 two-particle spin-2 state $|2,2\rangle$ (denoted as Γ_2). Since $m_3 = 0$ and 1, the system may or may not contain a three-particle spin-3 state $|3,3\rangle$ (dented as Γ_3) depending on whether F is odd or even. It is straightforward to work out the expressions of these states, which are $\Theta_2 = a_2a_{-2} - a_1a_{-1} + \frac{1}{2}a_0^2$, $\Theta_3 = a_0(2a_2a_{-2} + a_1a_{-1} - \frac{1}{3}a_0^2) - \sqrt{3/2}(a_1^2a_{-2} + a_2a_{-1}^2)$, $\Gamma_2 = a_2a_0 - (\sqrt{6}/4)a_1^2$, and $\Gamma_3 = 2a_2^2a_{-1} - \sqrt{6}\, a_2a_1a_0 + a_1^3$. The general structure of the state $|F,F\rangle$ is then $|F,F\rangle = \sum A(\{s_i\},\{m_i\}) (a_2^{\dagger m_1} \Gamma_2^{\dagger m_2} \Gamma_3^{\dagger m_3}) \times \Theta_2^{\dagger s_2} \Theta_3^{\dagger s_3} |\text{vac}\rangle$.

The condition $m_3 = 0, 1$ is the additional constraint $\mathcal{L}_\alpha$ mentioned in section (I.1). If Γ_3 was a "free" unit that could appear as many times as possible, the numerator of Eq. (16) would be (instead of $1 + x^3y^3$) an infinite series $\sum_{m_3=0}^{\infty} (x^3y^3)^{m_3}$, which will turn into a factor $(1 - x^3y^3)^{-1}$ like other free building units (Θ_2, Θ_3, a_2, and Γ_2) in the denominators in Eq. (16). The fact that the series of x^3y^3 terminates at the first order means that a pair of three-particle singlets can be expressed in terms of all other free excitations (Θ_2, Θ_3, a_2, and Γ_2) and therefore has already been accounted for in the generating function. Indeed, when examining Γ_3 (because of the prediction of the generating function), one finds $\Gamma_3^2 = -(16\sqrt{6}/9)\Gamma_2^3 + (8\sqrt{2}/3)a_2^2\Gamma_2\Theta_2 - 4\sqrt{2/3}\, a_2^3\Theta_3$ [5]. Note, however, that Γ_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. 1b.)

(II). Bose gas with half integer spins.—When f is a half integer, it is useful to consider the generating function

$$G(x,y) = \sum_{N\geq 0} \sum_{F\geq 0} M_N(F) x^N y^{2F}. \quad (20)$$

Proceeding as the integer case, the function $W(x,z)$ in Eq. (10) 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

$$G(x, y) = \int_C \frac{dz}{2\pi i} \frac{1 - z^{-2}}{z - y} \prod_{j=-f}^{f} \frac{1}{1 - xz^{2j}} . \quad (21)$$

Spin-1/2 bosons: For $f = 1/2$, we have

$$G^{(f=1/2)}(x, y) = \frac{1}{1 - xy} = \sum_{n\geq 0} x^n (y^2)^{n/2}. \quad (22)$$

Since the equation $n = N, n/2 = F$ has only one solution and forces $F = N/2$. This means that the total spin of systems of spin-1/2 bosons is fixed by the particle number N to be $F = N/2$, and $|F, F = N/2\rangle = a_{1/2}^{\dagger N}|\text{vac}\rangle$. The system can be referred to as a "statistical ferromagnet" since the ferromagnetism is forced by statistics.

Spin-3/2 bosons: For $f = 3/2$, we have

$$G^{(f=3/2)}(x, y) = \frac{1 + x^3 y^3}{(1 - x^4)(1 - xy^3)(1 - x^2y^2)} \quad (23)$$

$$= \sum \sum_{m_3=0,1} x^{4s_4 + m_1 + 2m_2 + 3m_3} \times (y^2)^{(3/2)m_1 + m_2 + (3/2)m_3}, \quad (24)$$

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

$$4s_4 + m_1 + 2m_1 + 3m_3 = N , \qquad \frac{3}{2} m_1 + m_2 + \frac{3}{2} m_3 = F , \quad (25)$$

which describes a state consisting of s_4 four-particle singlets Θ_4, m_1 spin-3/2 bosons (i.e., $a_{3/2}$), and m_2 spin-1 pairs $|1, 1\rangle$ made up of two spin-3/2 particles (denoted as Γ_2). Since $m_3 = 0$ and 1, the system may also contain a spin-3/2 three-particle state $|\frac{3}{2}, \frac{3}{2}\rangle$ (denoted as $\Gamma_{3/2}$), which appears at most once. Thus, we have $|F, F\rangle = \sum A(\{s_i\}, \{m_i\}) (a_{3/2}^{\dagger m_1} \Gamma_2^{\dagger m_2} \Gamma_3^{\dagger m_3}) \Theta_4^{\dagger s_4}|\text{vac}\rangle$. (See also Fig. 1c.)

(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. (8) gives

$$G^{(f=3)}(x, y) = \frac{[1 + x^{15} + C(x, y)]D(x, y)}{(1 - x^2)(1 - x^4)(1 - x^6)(1 - x^{10})} , \quad (26)$$

$$D(x, y) = \frac{1}{(1 - xy^3)(1 - x^2y^2)(1 - x^2y^4)} . \quad (27)$$

The term $C(x, y)$ is a polynomial with about 50 terms of the form $x^a y^b$ with $(a, b > 0)$. Since $b > 0$, these terms represent magnetic structures. From Eq. (1), we see that the structure of the total singlet state $|F = 0, F_z = 0\rangle$ is given by $G(x, y = 0)$. Extracting $G(x, y = 0)$ from Eq. (16) (i.e., setting $C = 0$ and $D = 1$), we see that the singlet state is a linear combination of singlets consisting of two, four, six, and ten particles, denoted as Θ_2, Θ_4, Θ_6, and Θ_{10}, respectively. From our discussions for the spin-2 case, we see that all singlets except those made up of 15 particles (Θ_{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., Θ_{15}^2) are reducible to free singlet units. (See also Fig. 1d.)

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 ($|2, 2\rangle$), and two-particle spin-4 pairs ($|4, 4\rangle$). The major difference between the $f = 3$ and previous examples, however, is the appearance of a 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 Γ_i and Γ_j can be expressed in terms of other magnetic and nonmagnetic units. These are the "interaction" constraints $\mathcal{L}_\alpha$ we mentioned in section (I.1). Note that in the case of $f = 2$, the interaction constraints come from the reducibility of a single type of structure; i.e., Γ_3^2 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 Γ_3 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 cannot be simply a termination of the multiplicity of a particular pattern. We shall not analyze 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, and 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 are already huge in the spin-1 case in the low-field limit [4]) will increase as the number of different singlets increases.

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[5] The reducibility of Γ_3^2 implies the choice of free structural unit is not unique. Writing Eq. (16) as $G(x, y) = \frac{1+x^2y^2+x^4y^4}{(1-x^2)(1-x^3)(1-xy^2)(1-x^3y^3)}$ shows that the role of Γ_2 and Γ_3 can be interchanged. For higher spins, there can be many equivalent representations. One natural choice is to choose a representation where the free units have a minimum number of particles.