## RESEARCH ARTICLE

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# One-body and Two-body Fractional Parentage Coefficients for Spinor Bose–Einstein Condensation

**Abstract** A very effective tool, namely, the analytical expression of the fractional parentage coefficients (FPC), is introduced in this paper to deal with the total spin states of $N$-body spinor bosonic systems, where $N$ is supposed to be large and the spin of each boson is one. In particular, the analytical forms of the one-body and two-body FPC for the total spin states with $\{N\}$ and $\{N-1,1\}$ permutation symmetries have been derived. These coefficients facilitate greatly the calculation of related matrix elements, and they can be used even in the case of $N \to \infty$. They appear as a powerful tool for the establishment of an improved theory of spinor Bose–Einstein condensation, where the eigenstates have the total spin $S$ and its $Z$-component being both conserved.

**Keywords** total spin states of spinor bosonic systems, fractional parentage coefficients, permutation group, spinor Bose–Einstein condensates

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## 1 Introduction

Bose–Einstein condensate (BEc) is a new kind of aggregation of matter where numerous atoms are lying in the same single-particle state. In 1998, the Bose–Einstein condensation (BEC) of sodium atoms $^{23}$Na was experimentally realized in an optical trap by Stamper-Kurn et al. [1–3]. The use of the optical trap to replace the magnetic trap was an important step because the spin degrees of freedom of the $^{23}$Na atoms are thereby liberated. This success initiated the study of the spinor BEc as a hot topic. Afterwards, in addition to $^{23}$Na, the condensations of $^{39}$K and $^{87}$Rb atoms, which all have spin-one, have also been realized. These findings attracted strongly the attention of physicists. The BEc has a very special feature due to the

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Bose enhancement. For example, the magnetic moment of an individual atom is very small. However, in some BEcs, the moments of numerous atoms can be aligned, leading to a very large magnetic moment. Hence, some physical processes that hardly occur in individual atoms may occur in the BEc (e.g., the magnetic dipole transition, the correlation caused by magnetic dipole–dipole interaction, etc.). This implies that the BEc has a great potential in application, and therefore, the investigation of the spinor BEC has become a hot topic in recent years.

Theoretically, the addition of the spin degrees of freedom leads to complexity. In particular, in the eigenstates of such a spinor system, both the total spin $S$ and its $Z$-component $S_Z$ should be conserved. At the present stage, the theory is dominated by a three-component model, where the bosons are classified into three kinds according to $s_{iz}$, the $Z$-component of the spin of a boson, being equal to 1, 0, or $-1$. Each kind of boson would condense. Such a model is not appropriate to describe the eigenstates because, in this model, only $S_Z = \sum_i s_{iz}$ is conserved, $S$ is not. Obviously, a more precise theory should keep $S$ conserved. Accordingly, the eigenstates of $S$, which are called the total spin states, should be introduced, and related mathematical techniques should be developed. This paper is aimed at this purpose.

For a spinor $N$-boson system (where $N$ is the number of bosons), the eigenstates $\Psi_{LS}$ can be, in general, expanded as

$$\Psi_{LS} = \sum_{\lambda, w_\lambda} C_{LS\lambda, w_\lambda} \sum_i f^{w_\lambda}_{LS\lambda i} \chi^{w_\lambda}_{S,\lambda i} \tag{1}$$

where $L$ is the total orbital angular momentum, and $\lambda$ denotes a representation of the permutation group of order $N$ ($\lambda$ is labeled by a Young's diagram, e.g., when $N=4$ and $S=1$, $\lambda$ has two choices: $\{3,1\}$ and $\{2,1,1\}$). $f^{w_\lambda}_{LS\lambda i}$ and $\chi^{w_\lambda}_{S,\lambda i}$ are the spatial and spin parts of wave function, respectively, both belonging to the $i$th basis function of the $\lambda$ representation. Moreover, $\chi^{w_\lambda}_{S,\lambda i}$ is a normalized total spin state with good quantum numbers $\lambda$, $S$, and $S_Z$. The magnetic quantum numbers are irrelevant and have been neglected. The summation over $i$ is necessary to assure the correct

permutation symmetry of $\Psi_{LS}$. In some cases, the multiplicity (or the weight) of $\lambda$ is larger than 1; that is, when $S$ is given, there are more than one set of independent total spin states belonging to the $\lambda$ representation. Therefore, $w_\lambda$ is introduced to denote each of them. $C_{LS\lambda,w_\lambda}$ is a coefficient of combination. In what follows, we shall focus on the total spin state $\chi_{S,\lambda i}^{w_\lambda}$.

When $N$ is large, the explicit expression of $\chi_{S,\lambda i}^{w_\lambda}$ is very difficult to obtain. However, it is clear from Eq. (1) that the permutation symmetries of the spin part and the spatial part are matched with each other. Thus, let us first study the spatial part. For the lowest state of a BEc with a given $S$, all the bosons are spatially condensed into a single-particle state denoted as $\phi_S(r_i)$, where the subscript $S$ has been introduced to be able to respond to the possibility that the single-particle state may depend on $S$. Evidently, in this case, the spatial part must be totally symmetric with respect to permutation; therefore, only $\lambda = \{N\}$ is involved. For the first order of excitation, one of the boson would be in an excited state $\psi_S$, while $N-1$ bosons remain in $\phi_S$; $\psi_S$ and $\phi_S$ are orthogonal with each other. In this case, the spatial part is allowed to have both $\lambda = \{N\}$ and $\lambda = \{N-1, 1\}$ symmetries. In this paper, only low-lying states of the BEc are discussed; therefore, the study of the total spin states can be limited to the two cases: $\lambda = \{N\}$ and $\lambda = \{N-1, 1\}$.

## 2 The totally symmetric total spin states and the fractional parentage coefficients

In the case of $\lambda = \{N\}$, let the number of the totally symmetric spin state $\chi_{S,\lambda i}^{w_\lambda}$ be denoted as $M(S)$; that is, $M(S)$ is the multiplicity of the representation $\{N\}$, and $w_{\{N\}}$ ranges from 1 to $M(S)$. On the other hand, let the number of totally symmetric spin states having only $S_Z$ to be conserved be denoted as $K(S_Z)$. Evidently, if a spin state has $S_Z + i$ bosons with $s_z=1$, $i$ bosons with $s_z=-1$, while the rest $N - S_Z - 2i$ bosons having $s_z=0$, then the state is one in $K(S_Z)$. From the requirement that $N - S_Z - 2i \geqslant 0$, we have $0 \leqslant i \leqslant (N - S_Z)/2$. Thus, we have

$$K(S_Z) = \left[ N - S_Z - \frac{1 - (-1)^{N - S_Z}}{2} \right] / 2 + 1 \qquad (2)$$

From this formula, the number of totally symmetric spin states, namely, $M(S)$ can be derived as

$$M(S) = K(S) - K(S+1) = [1 + (-1)^{N-S}]/2 \qquad (3)$$

From Eq. (3), we know that the multiplicity of $\chi_{S,\{N\}i}^{w_{\{N\}}}$ is 1 if $N-S$ is even and 0 if $N-S$ is odd. Since the multiplicity is not larger than 1, the superscript $w_\lambda$ is, in this case, redundant and can be neglected. For simplicity, from now on, the totally symmetric spin state is simply denoted as $\vartheta_S^{[N]} \equiv \chi_{S,\{N\}i}^{w_{\{N\}}}$.

The total number of $\vartheta_S^{[N]}$ with $S=N$, $N-2$, $N-4$,... is nearly equal to $N/2$.

The expressions of $\vartheta_S^{\{N\}}$ with distinct $N$ and $S$ and with $N-S$ even can be deduced based on an iteration procedure. Let us start from a two-boson system, we have

$$\vartheta_S^{[2]}(12) = (\chi(1)\chi(2))_S \qquad (4)$$

where $\chi$ is the spin state of a single boson, and the two spins are coupled to $S=0$ or 2. For $N=3$, there are two $\vartheta_S^{[N]}$, with $S=3$ and 1 [4]:

$$\vartheta_3^{[3]}(123) = \{(\chi(1)\chi(2))_2\chi(3)\}_3 = \{\vartheta_2^{[2]}\chi(3)\}_3 \qquad (5.1)$$

$$\vartheta_1^{[3]}(123) = \frac{2}{3}\{\vartheta_2^{[2]}\chi(3)\}_1 + \frac{\sqrt{5}}{3}\{\vartheta_0^{[2]}\chi(3)\}_1 \qquad (5.2)$$

where the spins of the first and second bosons are first coupled to 2 or 0, then they couple with the spin of the third to achieve $S=3$ or 1.

Starting from Eqs. (4) and (5), let us assume that all the $\vartheta_{S'}^{[N-1]}$ have been known; then $\vartheta_S^{[N]}$ with $N-S$ even and $S \leqslant N$ can be uniquely expanded as

$$\vartheta_S^{[N]} = a_S^{[N]}\{\vartheta_{S+1}^{[N-1]}\chi(N)\}_S + b_S^{[N]}\{\vartheta_{S-1}^{[N-1]}\chi(N)\}_S \qquad (6)$$

where $a_S^{[N]}$ and $b_S^{[N]}$ are two coefficients to be determined, and $(a_S^{[N]})^2 + (b_S^{[N]})^2 = 1$ is assumed to assure the normalization. This expansion holds because (i) based on the rule of outer product of permutation groups, only the totally symmetric states of the $(N-1)$ subsystem are involved. (ii) Although from the point of angular momenta coupling, the total spins of the $(N-1)$ body subsystem can be $S+1$, $S$, and $S-1$, however, since $N-1-S$ is odd, the term $\vartheta_S^{[N-1]}$ is 0 and therefore does not appear.

From Eq. (6), a similar formula can be written for $\vartheta_{S'}^{[N-1]}$ as

$$\vartheta_{S'}^{[N-1]} = a_{S'}^{[N-1]}\{\vartheta_{S'+1}^{[N-2]}\chi(N-1)\}_{S'} \qquad (7)$$
$$+ b_{S'}^{[N-1]}\{\vartheta_{S'-1}^{[N-2]}\chi(N-1)\}_{S'}$$

Inserting Eq. (7) into Eq. (8), we have

$$\vartheta_S^{[N]} = a_S^{[N]}a_{S+1}^{[N-1]}\{[\vartheta_{S+2}^{[N-2]}\chi(N-1)]_{S+1}\chi(N)\}_S$$
$$+ a_S^{[N]}b_{S+1}^{[N-1]}\{[\vartheta_S^{[N-2]}\chi(N-1)]_{S+1}\chi(N)\}_S$$
$$+ b_S^{[N]}a_{S-1}^{[N-1]}\{[\vartheta_S^{[N-2]}\chi(N-1)]_{S-1}\chi(N)\}_S$$
$$+ b_S^{[N]}b_{S-1}^{[N-1]}\{[\vartheta_{S-2}^{[N-2]}\chi(N-1)]_{S-1}\chi(N)\}_S \qquad (8)$$

On the other hand, since $\vartheta_S^{[N]}$ in Eq. (8) is required to be totally symmetric, it must be invariant against any interchange. Thus, we have

$$\vartheta_S^{[N]} = P_{N,N-1}\vartheta_S^{[N]} \tag{9}$$

where $P_{N,N-1}$ denotes the interchange of the $(N-1)$th and $N$th bosons. Inserting Eq. (8) into both sides of Eq. (9), making use of the theory of the recoupling of spins, we arrive at a set of three homogeneous equations:

$$[\hat{W}_S(S+1, S+1) - 1]a_S^{[N]}b_{S+1}^{[N-1]} \tag{10.1}$$
$$+\hat{W}_S(S-1, S+1)b_S^{[N]}a_{S-1}^{[N-1]}=0$$

$$\hat{W}_S(S+1, S-1)a_S^{[N]}b_{S+1}^{[N-1]} \tag{10.2}$$
$$+[\hat{W}_S(S-1, S-1)-1]b_S^{[N]}a_{S-1}^{[N-1]} = 0$$

$$\hat{W}_S(S+1, S)a_S^{[N]}b_{S+1}^{[N-1]} \tag{10.3}$$
$$+\hat{W}_S(S-1, S)b_S^{[N]}a_{S-1}^{[N-1]}=0$$

where

$$\hat{W}_S(T, T') = \sqrt{(2T+1)(2T'+1)}W(1SS1; TT') \tag{11}$$

and $W(1SS1;TT')$ is the well-known Racah coefficients. It turns out that the set of equations (Eq. (10)) are linearly dependent. Taking into account the expressions of the Racah coefficients, from Eq. (10), we obtain

$$a_S^{[N]} = \gamma_S^N \frac{\sqrt{2S-1}}{S\sqrt{2S+1}}/b_{S+1}^{[N-1]} \tag{12.1}$$

$$b_S^{[N]} = \gamma_S^N \frac{\sqrt{2S+3}}{(S+1)\sqrt{2S+1}}/a_{S-1}^{[N-1]} \tag{12.2}$$

if $N-S$ is even, or $a_S^{[N]} = b_S^{[N]} = 0$ if $N-S$ is odd, where the constant $\gamma_S^N$ is to be determined. Equations (12.1) and (12.2), together with the requirement of normalization

$$(a_S^{[N]})^2 + (b_S^{[N]})^2 = 1 \tag{12.3}$$

constitute a set of three equations. The solution of this set is simply

$$a_S^{[N]}=[(1 + (-1)^{N-S})(N - S)(S + 1) \tag{13.1}$$
$$/(2N(2S+1))]^{1/2}$$

$$b_S^{[N]}=[(1 + (-1)^{N-S}) S (N + S + 1) \tag{13.2}$$
$$/(2N(2S+1))]^{1/2}$$

$$\gamma_S^N=S(S+1)[(N - S)(N + S + 1) \tag{13.3}$$
$$/(N(N - 1)(2S + 3)(2S - 1))]^{1/2}$$

The coefficients $a_S^{[N]}$ and $b_S^{[N]}$ are called one-body fractional parentage coefficients (one-body FPC). With these coefficients, all the $\vartheta_S^{[N]}$ can be identified and can be written down by using Eq. (4) and by repeatedly using Eqs. (6) and (13). When $N$ is large, the explicit form of $\vartheta_S^{[N]}$ is very lengthy. Fortunately, it turns out that, for calculating the matrix elements among the total spin states, the explicit form is, in general, not necessary. Knowing only the FPC is sufficient to achieve an analytical form as shown below. Thus, the FPC is a powerful tool for the spinor systems.

## 3 Total spin states with {N−1,1} permutation symmetry

Now, let us study the total spin states with $\lambda = \{N - 1, 1\}$. Making use of the FPC, we define the following spin state

$$\Theta_S^{[N],i}=b_S^{[N]}\{\vartheta_{S+1}^{[N-1]}(\overset{\times}{i})\,\chi(i)\}_S - a_S^{[N]}\{\vartheta_{S-1}^{[N-1]} \tag{14.1}$$
$$\times(\overset{\times}{i})\,\chi(i)\}_S \quad (N - S \text{ is even})$$

$$\Theta_S^{[N],i} = \{\vartheta_S^{[N-1]}(\overset{\times}{i})\,\chi(i)\}_S \quad (N - S \text{ is odd}) \tag{14.2}$$

where $\vartheta_{S'}^{[N-1]}(\overset{\times}{i})$ are the totally symmetric spin states of the 1 to $N$ bosons, except the $i$th. It is recalled that $a_S^{[N]}$ would be zero if $S=N$, $b_S^{[N]}$ would be zero if $S=0$ (refer to Eq. (13)), and $S\leqslant N$ is required in $\vartheta_S^{[N]}$. Thus, $\Theta_S^{[N],i}$ is well defined if $1\leqslant S\leqslant N-1$. From the rule of outer product, $\Theta_S^{[N],i}$ may contain the symmetries $\{N\}$ and $\{N-1,1\}$. However, it has been stated that the totally symmetric spin state $\vartheta_S^{[N]}$ is unique. Hence, if $N-S$ is even and if Eq. (14.1) is orthogonal to $\vartheta_S^{[N]}$, it must belong to the $\{N-1,1\}$ symmetry. Comparing Eq. (14.1) with Eq. (6) (where the $N$ in $\chi(N)$ can be changed to $i$), it is obvious that $\Theta_S^{[N],i}$ and $\vartheta_S^{[N]}$ are orthogonal; therefore, $\Theta_S^{[N],i}$ has the pure $\{N-1,1\}$ symmetry. When $N-S$ is odd, totally symmetric spin states do not exist, as has been discussed; therefore, $\Theta_S^{[N],i}$ also has the pure $\{N-1,1\}$ symmetry. Thus, the suggested $\Theta_S^{[N],i}$ ranging from $S=1$ to $N-1$ are just the total spin states with $\lambda = \{N - 1, 1\}$.

When $S$ is given ($\neq N$ and $\neq 0$), the index $i$ of $\Theta_S^{[N],i}$ ranges from 1 to $N$. Furthermore, from the study in [5], the weight of the $\{N-1,1\}$ representation (multiplicity) is equal to one. Thus, the set of $N$ states $\Theta_S^{[N],i}$ are sufficient. However, they are not mutually orthogonal but linearly dependent, and they satisfy

$$\sum_i \Theta_S^i = 0 \tag{15}$$

This arises because the summation over $i$ leads to symmetrization, and a state with $\lambda \neq \{N\}$ will not survive after the symmetrization. Nonetheless, $N-1$ are linearly independent, and they can be used as basis functions to span the $\{N-1,1\}$ representation.

## 4 Analytical derivation of two-body matrix elements

As an example, let us derive the matrix elements of the two-body interaction $U_{ij}$ between the totally symmetric total spin states. The form of the interaction is not prescribed; however, the total spin and its $Z$-component of the related two-body subsystem are assumed to be conserved under the interaction. Inserting Eq. (7) into Eq. (6), after a recoupling of the spins, we arrive at a new expression of the totally symmetric spin state, namely,

$$\vartheta_S^{[N]} = \sum_{\lambda,\,T} h_{\lambda,T}^{[N]S} \{[\chi(i)\chi(j)]_\lambda \vartheta_T^{[N-2]}\}_S \tag{16}$$

where $(\lambda, T) = $ (0,S), (2,S+2), (2,S), and (2,S−2). The coefficient $h_{\lambda,T}^{[N]S}$ can be defined as the two-body FPC; it contains the one-body FPC and the Racah coefficients arising from angular momenta recoupling. When the Racah coefficients are written in analytical forms, we have

$$h_{0,S}^{[N]S}=\left(\frac{(2S+3)}{3(2S+1)}\right)^{1/2} a_S^{[N]} b_{S+1}^{[N-1]} + \left(\frac{(2S-1)}{3(2S+1)}\right)^{1/2} b_S^{[N]} a_{S-1}^{[N-1]}$$

$$h_{2,S+2}^{[N]S} = a_S^{[N]} a_{S+1}^{[N-1]}$$

$$h_{2,S}^{[N]S}=\left(\frac{S(2S-1)}{3(2S+1)(2S+2)}\right)^{1/2} a_S^{[N]} b_{S+1}^{[N-1]}$$
$$+\left(\frac{(2S+2)(2S+3)}{12(2S+1)S}\right)^{1/2} b_S^{[N]} a_{S-1}^{[N-1]}$$

$$h_{2,S-2}^{[N]S} = b_S^{[N]} b_{S-1}^{[N-1]} \tag{17}$$

Then the two-body matrix element reads

$$\langle\vartheta_S^{[N]}|U_{i,j}|\vartheta_S^{[N]}\rangle$$
$$= \sum_{\lambda,T}(h_{\lambda,T}^{[N]S})^2 \langle[\chi(i)\chi(j)]_\lambda |U_{i,j}| [\chi(i)\chi(j)]_\lambda\rangle \tag{18}$$

Thus, once $a_S^{[N]}$ and $b_S^{[N]}$ are known, $h_{\lambda,T}^{[N]S}$ can be known, and the matrix element can be obtained analytically.

Let us further derive the two-body FPC of the total spin states with the $\{N-1,1\}$ symmetry. Inserting Eq. (7) into Eq. (14), after a recoupling of the spins, we have

$$\Theta_S^{[N],i} = \sum_{\lambda,\,T} g_{\lambda,T}^{[N]S} \{[\chi(i)\chi(j)]_\lambda \vartheta_T^{[N-2]}\}_S \tag{19}$$

When $N-S$ is even,

$$g_{2,S+2}^{[N]S} = b_S^{[N]} a_{S+1}^{[N-1]}$$

$$g_{2,S}^{[N]S}=\left(\frac{S(2S-1)}{3(2S+1)(2S+2)}\right)^{1/2} b_S^{[N]} b_{S+1}^{[N-1]}$$
$$-\left(\frac{(2S+2)(2S+3)}{12(2S+1)S}\right)^{1/2} a_S^{[N]} a_{S-1}^{[N-1]}$$

$$g_{2,S-2}^{[N]S} = -a_S^{[N]} b_{S-1}^{[N-1]}$$

$$g_{1,S}^{[N]S}=\left(\frac{S(2S+3)}{(2S+1)(2S+2)}\right)^{1/2} b_S^{[N]} b_{S+1}^{[N-1]}$$
$$+\left(\frac{(2S+2)(2S-1)}{4(2S+1)S}\right)^{1/2} a_S^{[N]} a_{S-1}^{[N-1]}$$

$$g_{0,S}^{[N]S}=\left(\frac{2S+3}{3(2S+1)}\right)^{1/2} b_S^{[N]} b_{S+1}^{[N-1]} - \left(\frac{2S-1}{3(2S+1)}\right)^{1/2} a_S^{[N]} a_{S-1}^{[N-1]}$$

When $N-S$ is odd,

$$g_{2,S+1}^{[N]S} = -\left(\frac{S+2}{2(S+1)}\right)^{1/2} a_S^{[N-1]}$$

$$g_{2,S-1}^{[N]S} = -\left(\frac{S-1}{2S}\right)^{1/2} b_S^{[N-1]}$$

$$g_{1,S+1}^{[N]S} = \left(\frac{S}{2(S+1)}\right)^{1/2} a_S^{[N-1]}$$

$$g_{1,S-1}^{[N]S} = -\left(\frac{S+1}{2S}\right)^{1/2} b_S^{[N-1]}$$

In both cases, the two-body FPC $g_{\lambda,T}^{[N]S}$ not appearing in the above formulae are zero.

Using Eq. (19) or (16) for the $(N-1)$-body subsystem not containing the $i$th particle, any pair of particles can be extracted from $\Theta_S^{[N],i}$; thereby, two-body matrix elements can be calculated.

## 5 Final remarks

Based on the total spin states with both $S$ and $S_Z$ being conserved, and with a specified permutation symmetry as given in Eqs. (6) and (14), trial wave functions for the

ground band and for the first excited band of the BEc can be set up. Since the related matrix elements of the Hamiltonian can be obtained by using the one-body and two-body FPC, a traditional variational procedure can be carried out, and accordingly, generalized Gross–Pitaevskii equations for the ground band and the first excited band would be achieved. This will lead to an improved theory for the BEC, with both $S$ and $S_Z$ being conserved. This issue will be discussed elsewhere.

It is noted that the FPC has long been successfully used for few-body systems [6]. However, it has never been used in many-body systems. Due to having obtained the analytical forms in this paper, these coefficients can now be used for systems with a very large $N$; they can even be used for the limit $N \rightarrow \infty$ . Therefore, in addition to the BEC, they can be used for various systems, with each particle having spin-one or having one unit of orbital angular momentum.

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