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Fractional Parentage Coefficients for Spinor Bose-Einstein Condensation*

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Abstract: The total spin-states of a N-body system with spin-one bosons have been investigated. The fractional parentage coefficients for the total spin-states with $\{N\}$ and $\{N-1, 1\}$ symmetries have been derived. These coefficients facilitate greatly the calculation of related matrix elements, they appear as a powerful tool for the establishment of an improved theory for the spinor Bose-Einstein condensation, where the total spin S and its Z-component S_Z are both conserved.

Key words: Bose-Einstein condensation; spinor bosonic systems; fractional parentage coefficients
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Bose-Einstein condensation (BEC) is an important physical phenomenon predicted by Einstein. In 1998 the BEC of sodium atoms ^{23}Na was experimentally realized in an optical trap by Stamper-Kurn[1-3]. Since the ^{23}Na atom has spin one, the corresponding condensation is different from those of spin-zero bosons, and is called a spinor condensation. Afterwards, the condensations of ^{39}K and ^{87}Rb atoms, both have spin one, have also been observed. These findings implie the existence of a new kind of aggregation of matter, and therefore attract strongly the attention of physicists. The investigation of the spinor BEC becomes a hot topic in recent years.

In the theoretical aspect, the additional spin degrees of freedom lead to complicity. In particular, in 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 bosons would condense. Such a model is only an approximation, because in this model only $S_Z = \sum_i s_{iz}$ is conserved while S is not. Obviously, a more precise and advanced theory should keep S conserved. For this purpose, the eigenstates of S, which are called the total spin-states, should be introduced and related mathematical techniques should be developed. This paper aims at this purpose.

For a spinor N-boson system (where N is the number of bosons), the eigenstates Ψ_S can be in general expanded as

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

Where L is the total orbital angular momentum, λ denotes a representation of the permutation group of order N, it is labeled by a Young's diagram (e.g., when $N = 4$ and $S = 1$, λ have 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 λ representation. Moreover, $\chi^{w_\lambda}_{S\lambda i}$ is a normalized total spin state with good quantum numbers λ, S and S_Z. The summation over i is necessary to assure the correct permutation symmetry. In some cases the multiplicity (or the weight) of λ is larger than 1, i.e., when S is given, there are more than one set of total spin-states belonging to the λ-representation. Therefore w_λ 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 $\chi^{w_\lambda}_{S\lambda i}$.

When N is large, the explicit expression of $\chi^{w_\lambda}_{S\lambda i}$ is very difficult to obtain. However, it is clear from eq. (1) that the permutation symmetries of the spin part and spatial part are matched with each other. So, let us first study the spatial part. For the lowest state of a Bose-Einstein condensate (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 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 with the S unchanged, one of the boson would be in an excited state $\Psi_S(r_i)$, while $N-1$ bosons remain in $\phi_S(r_i)$, Ψ_S and ϕ_S are orthogonal with each other. In this case the spatial part is allowed to

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have both $\lambda = \{N\}$ and $\lambda = \{N-1, 1\}$ symmetries. Only the low-lying states of the BEC are concerned, therefore the study of the total spin-states can be limited to the two cases $\lambda = \{N\}$ and $\lambda = \{N-1, 1\}$.

In the case of $\lambda = \{N\}$, let the number of the totally symmetric spin-state $\chi^{w_\lambda}_{S;\lambda i}$ be denoted as $M(S)$, i.e., $M(S)$ is the multiplicity of the representation $\lambda = \{N\}$, and $w_{\{N\}}$ is ranged 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 with $s_z = 0$, 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

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

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

$$M(S) = K(S) - K(S+1) = \frac{1+(-1)^{N-S}}{2} \quad (3)$$

From eq. (3) we know that the number of $\chi^{w}_{S;\{N\} i}$ is one if $N - S$ is even, or is zero if $N - S$ is odd. Since the multiplicity is not larger than one, the superscript w_λ is redundant and can be neglected. For simplicity, from now on the totally symmetric spin-state is simply denoted as $\vartheta_S^{[N]} \equiv \chi^{w}_{S;\{N\} i}$. The total number of $\vartheta_S^{[N]}$ with $S = N, N-2, N-4, \cdots$ is nearly equal to $N/2$.

The expressions of ϑ_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 2-boson system, we have

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

where χ is the spin-state of a single boson, 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].

$$\vartheta_3^{[3]}(123) = \{(\chi(1)\chi(2))_2\chi(3)\}_3 = \{\vartheta_2^{[2]}\chi(3)\}_3 \quad (5a)$$

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

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

Starting from eq. (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

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

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. This expansion holds because (i) based on the rule of the outer product of permutation groups, only the totally symmetric states of the $(N-1)$-subsystem are necessary to be considered, (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 zero and therefore can be dropped. From eq. (6), a similar formula can be written for $\vartheta_{S'}^{[N-1]}$ as

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

Inserting eq. (7) into (6), we have

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

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

$$\vartheta_S^{[N]} = P_{N,N-1}\vartheta_S^{[N]} \quad (9)$$

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

$$[W_S(S+1, S+1) - 1]\, a_S^{[N]}b_{S+1}^{[N-1]} + W_S(S-1, S+1)b_S^{[N]}a_{S-1}^{[N-1]} = 0 \quad (10a)$$

$$W_S(S+1, S-1)a_S^{[N]}b_{S+1}^{[N-1]} + [W_S(S-1, S-1) - 1]\, b_S^{[N]}a_{S-1}^{[N-1]} = 0 \quad (10b)$$

$$W_S(S+1, S)a_S^{[N]}b_{S+1}^{[N-1]} + W_S(S-1, S)b_S^{[N]}a_{S-1}^{[N-1]} = 0 \quad (10c)$$

where

$$W_S(T, T') = \sqrt{(2T+1)(2T'+1)}\; W(1SS1; TT') \quad (11)$$

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

$$a_S^{[N]} = \gamma_S^N \frac{\sqrt{2S-1}}{S\sqrt{2S+1}}/b_{S+1}^{[N-1]} \quad (12a)$$

$$b_S^{[N]} = \gamma_S^N \frac{\sqrt{2S+3}}{(S+1)\sqrt{2S+1}}/a_{S-1}^{[N-1]} \quad (12b)$$

if $N - S$ is even, or $a_S^{[N]} = b_S^{[N]} = 0$ if $N - S$ is odd, where the constant γ_S^N is to be determined. Eq. (12a) and (12b), together with the requirement of normalization

$$(a_S^{[N]})^2 + (b_S^{[N]})^2 = 1 \quad (12c)$$

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

$$a_S^{[N]} = \left[\frac{(1+(-1)^{N-S})(N-S)(S+1)}{(2N(2S+1))}\right]^{1/2} \quad (13a)$$

$$b_S^{[N]} = \left[\frac{(1+(-1)^{N-S})S(N+S+1)}{(2N(2S+1))}\right]^{1/2} \quad (13b)$$

$$\gamma_S^N = S(S+1)\left[\frac{(N-S)(N+S+1)}{(N(N-1)(2S+3)(2S-1))}\right]^{1/2} \tag{13c}$$

The coefficients $a_S^{[N]}$ and $b_S^{[N]}$ are called fractional parentage coefficients (FPC). With these coefficients, all the $\vartheta_S^{[N]}$ can be identified and can be written down by repeatedly using eq. (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. Only the FPC is sufficient to achieve an analytical form. Thus the FPC is a powerful tool for the spinor systems.

As an example, let us calculate the matrix elements of the two-body interaction U_{ij} between the i-th and j-th bosons (the form of the interaction is not prescribed, however the total spin of the related two particles is assumed to be conserved). Inserting eq. (7) into (6), after a recoupling of the spins, we arrive at a new expression of the totally symmetric spin-state, namely

$$\vartheta_S^{[N]} = \sum_{\Lambda, T} h_{\Lambda, T}^{[N]S} \{[\chi(N-1)\chi(N)]_\Lambda \vartheta_T^{[N-2]}\}_S \tag{14}$$

where $(\Lambda, T) = (0, S)$, $(2, S+2)$, $(2, S)$, and $(2, S-2)$. When the Racah coefficients are written in analytical forms, we have

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

$$h_{2,S+2}^{[N]S} = a_S^{[N]} a_{S+1}^{[N-1]} \tag{15}$$

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

$$h_{2S-2}^{[N]S} = b_S^{[N]} b_{S-1}^{[N-1]}$$

Since $\vartheta_S^{[N]}$ is totally symmetric, the labels N and $N-1$ in the two-body spin-state $[\chi(N-1)\chi(N)]_\Lambda$ at the right of eq. (14) can be changed to i and j as well. Then the two-body matrix element reads

$$\langle \vartheta_S^{[N]} \mid U_{i,j} \mid \vartheta_S^{[N]} \rangle = \sum_{\Lambda, T} (h_{\Lambda, T}^{[N]S})^2 \langle [\chi(i)\chi(j)]_\Lambda \mid U_{i,j} \mid [\chi(i)\chi(j)]_\Lambda \rangle \tag{16}$$

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

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

$$\Theta_S^{[N], i} = b_S^{[N]} \{\vartheta_{S+1}^{[N-1]} \chi(i)\}_S - a_S^{[N]} \{\vartheta_{S-1}^{[N-1]} \chi(i)\}_S \quad (N-S \text{ is even}) \tag{17a}$$

$$\Theta_S^{[N], i} = \{\vartheta_S^{[N-1]} \chi(i)\}_S \quad (N-S \text{ is odd}) \tag{17b}$$

where $\vartheta_{S'}^{[N-1]}$ 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, $\Theta_S^{[N], i}$ will contain only the symmetries $\{N\}$ and $\{N-1, 1\}$. However, it has been stated above that the totally symmetric spin-state $\vartheta_S^{[N]}$ is unique. Hence, if $N-S$ is even and if (17a) is orthogonal to $\vartheta_S^{[N]}$, it must belong to the $\{N-1, 1\}$ symmetry. Comparing (17a) with (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, it has been stated above that totally symmetric spin-states do not exist, therefore $\Theta_S^{[N], i}$ has also 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 $\lambda = \{N-1, 1\}$. Furthermore, from the study in ref. [5], these states are unique (multiplicity is equal to one).

When S is given ($\neq N$ or 0), the index i of $\Theta_S^{[N], i}$ is ranged from 1 to N. This set of N states are not mutually orthogonal but linearly dependent. They satisfy

$$\sum_i \Theta_S^{[N], i} = 0 \tag{18}$$

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

Based on the total spin-states as given in (6) and (17), a variational procedure can be carried out where the total spin-states are introduced directly into the trial wave functions. This will lead to an improved theory for the BEC with both S and S_Z to be conserved. It is believed that the FPC introduced in this paper would be in general useful for various spinor systems.

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(下转第 76 页)

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Studies on the Ultrafast Relaxation of Coherent Control Photocurrent in AlGaAs/GaAs MQWs

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Abstract: The ultrafast dynamics of coherent control photocurrent in AsGaAs/GaAs MQWs at room temperature is studied theoretically and experimentally. A ballistic photocurrent relaxation time of ~600 fs is deduced with the theory of density matrix and electron-hole scattering relaxation model. This result is evidenced with the three color femtosecond pulse pump-probe measurements.

Key words: femtosecond pulses; semiconductor quantum wells; optical coherent control

（上接第 72 页）

母配分系数与旋量玻色—爱因斯坦凝聚

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摘 要：研究了由自旋为 1 的玻色子组成的 N-体系统的总自旋态。导出了具有 $\{N\}$ 和 $\{N-1, 1\}$ 对称性的总自旋态的母配分系数。这些系数使有关矩阵元的计算大为方便。因而它们将有助于建立一个关于旋量玻色爱因斯坦凝聚的改进了的理论，其中总自旋 S 及它的 Z-分量 S_Z 均得以守恒。

关键词：玻色—爱因斯坦凝聚；旋量玻色系；母配分系数

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