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Term multiplicities in the *LS*-coupling scheme

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Abstract. Generating functions for the number of states with given total angular momentum and spin, for a system of identical fermions or bosons, are presented, along with generating functions for the number of states of a system of identical particles with any specified permutational symmetry and total spin. The spin of each particle could be any integral or half-integral number. A specific example for a system of particles with a pseudospin $s=\frac{3}{2}$ is presented. The extension of the generating functions for a system of particles which carry more than two angular momenta is made.

The determination of the number of states arising out of the coupling of N particles with a given elementary spin and statistics is a straightforward counting problem, which for few-particle systems can easily be carried out using elementary methods (de-Shalit and Talmi 1963). For a system consisting of a large number of particles this approach becomes prohibitively tedious. A more powerful method has recently been discussed (Katriel *et al* 1983, Sunko and Svrtan 1985, Sunko 1986). The central result, arrived at by somewhat different routes by Katriel *et al* (1983) and by Sunko and Svrtan (1985), is that a set of generating functions for the number of many-body states with a specific total spin and statistics can be constructed. These generating functions are very closely related to the Gaussian polynomials (Andrews 1976). A brief presentation of this method follows.

For N particles, each with spin l, we denote the number of states (NOS) with a given value M of the z component of the total spin by $f_M^{N,l}$ and $b_M^{N,l}$ for fermions and bosons, respectively. The generating functions

$$f^{N,l}(x)=\sum_M x^M f_M^{N,l} \tag{1a}$$

$$b^{N,l}(x)=\sum_M x^M b_M^{N,l} \tag{1b}$$

are defined. (The letters a and b in these and the following equation numbers refer to fermions and bosons, respectively.) These generating functions can be obtained for higher values of N and l using the recurrence relations they satisfy (Katriel *et al* 1983),

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or otherwise using the grand generating functions

$$f^{l}(x;z)=\prod_{m=-l}^{l}(1+zx^{m})=\sum_{N=0}^{2l+1}z^{N}f^{N,l}(x) \tag{2a}$$

$$b^{l}(x;z)=\prod_{m=-l}^{l}(1-zx^{m})^{-1}=\sum_{N=0}^{\infty}z^{N}b^{N,l}(x). \tag{2b}$$

These results provide the solution for the state enumeration problem for both fermions and bosons, in the *jj*-coupling scheme.

As a simple example consider a system of equivalent fermions with elementary angular momentum $j=\frac{3}{2}$. Using (2*a*) we obtain

$$\begin{aligned} f^{3/2}(x;z) &= (1+zx^{-3/2})(1+zx^{-1/2})(1+zx^{1/2})(1+zx^{3/2}) \\ &= 1+(z+z^{3})(x^{-3/2}+x^{-1/2}+x^{1/2}+x^{3/2})+z^{2}(x^{-2}+x^{-1}+2+x+x^{2})+z^{4} \end{aligned} \tag{3}$$

which means that for one and three particles the total angular momentum is $L=\frac{3}{2}$, for two particles $L=0$ or 2 and for four particles $L=0$. In none of the above cases is there any degeneracy.

The *LS*-coupling scheme, involving the simultaneous coupling of two types of angular momentum, has originally been introduced in atomic physics to describe the electronic states of light atoms in which spin-orbit coupling is small relative to the electrostatic interelectronic repulsion (Condon and Odabasi 1980). In a calculation involving many electrons the number of states with given total angular momentum and spin could be very large, possibly beyond current numerical computational limits. In such cases it is important to know this number *a priori*.

The *LS*-coupling scheme is important also for many other areas in physics, for example, in nuclear physics. When the shell model was introduced in nuclear physics it was realised that the strong spin-orbit coupling suggests *jj* coupling as the appropriate scheme for nuclear calculations. However, even in this context the introduction of isospin results in a situation analogous to the *LS*-coupling scheme (i.e. *JT* coupling). Furthermore, the *LS*-coupling scheme was used in the nuclear pseudo-SU(3) model (Arima *et al* 1969, Hecht and Adler 1969). Recently, the fermion dynamical symmetry model for nuclei was introduced (Wu *et al* 1986, 1987). In this model the total angular momentum of a nucleon is decomposed into a pseudo-orbital angular momentum $\boldsymbol{k}$ and a pseudospin $\boldsymbol{i}$.

The enumeration of the allowed states in the *LS*-coupling scheme using the elementary method (Breit 1926, Condon and Odabasi 1980) is tedious. Thus, a systematisation of this counting problem was proposed by Shudeman (1937). Another approach, based on the reduction of the representations of the symmetric group spanned by the many electron product states, was developed by Curl and Kilpatrick (1960). This approach results in a generating function for the number of states for N electrons with given values of the total orbital and spin angular momenta, and represents a significant improvement over the direct counting procedure. A further development of the group theoretical approach was introduced by Karayianis (1965), who derived recursion relations for the number of *LS* states. All these approaches were developed for spin-$\frac{1}{2}$ fermions.

In the present paper we formulate an approach which is a generalisation of the method described above for a system of particles with a single type of angular momentum. This method applies to both fermions and bosons, with arbitrary values of the single particle orbital and spin angular momenta. The generating functions obtained have a very compact and transparent form.

We denote by $F^{N,l,s}_{M,M_s}(B^{N,l,s}_{M,M_s})$ the number of antisymmetric (symmetric) states of a system of N particles, each with an angular momentum l and a spin s, whose total z components are M and M_s, respectively. The corresponding generating functions

$$F^{N,l,s}(x,y)=\sum_M\sum_{M_s} x^M y^{M_s} F^{N,l,s}_{M,M_s} \tag{4a}$$

$$B^{N,l,s}(x,y)=\sum_M\sum_{M_s} x^M y^{M_s} B^{N,l,s}_{M,M_s} \tag{4b}$$

are defined. The generating functions (4*a*) and (4*b*) for two angular momenta are the generalisation of the one angular momentum generating functions (1*a*) and (1*b*).

The grand generating functions

$$F^{l,s}(x,y;z)=\sum_{N=0}^{(2l+1)(2s+1)} z^N F^{N,l,s}(x,y) \tag{5a}$$

$$B^{l,s}(x,y;z)=\sum_{N=0}^{\infty} z^N B^{N,l,s}(x,y) \tag{5b}$$

are the generalisation of the grand generating functions (2*a*) and (2*b*) for two angular momenta. They can be written in the form

$$F^{l,s}(x,y;z)=\prod_{m=-l}^{l}\prod_{m_s=-s}^{s}(1+zx^m y^{m_s}) \tag{6a}$$

$$B^{l,s}(x,y;z)=\prod_{m=-l}^{l}\prod_{m_s=-s}^{s}(1-zx^m y^{m_s})^{-1}. \tag{6b}$$

These expressions can also be obtained by interpreting the present problem as a multipartite partition (Andrews 1976). Thus, the generalisation to a system of particles each one of which has three (or more) types of angular momenta (such as in *LST* coupling) is straightforward. The generalisation of the grand generating functions, (6*a*) and (6*b*), to the case of n types of angular momentum can be written in the form

$$F^{l_1,l_2,\ldots,l_n}(x_1,x_2,\ldots,x_n;z)=\prod_{i=1}^{n}\prod_{m_i=-l_i}^{l_i}\left(1+z\prod_{j=1}^{n}x_j^{m_j}\right) \tag{7a}$$

and

$$B^{l_1,l_2,\ldots,l_n}(x_1,x_2,\ldots,x_n;z)=\prod_{i=1}^{n}\prod_{m_i=-l_i}^{l_i}\left(1-z\prod_{j=1}^{n}x_j^{m_j}\right)^{-1}. \tag{7b}$$

Here, $l_1, l_2, \ldots, l_n$ are the values of the n different single particle angular momenta.

In (7*a*), the coefficient of $z^N \prod_{i=1}^n x_i^{M_i}$ is $F^{N,l_1,l_2,\ldots,l_n}_{M_1,M_2,\ldots,M_n}$, the number of fermion states of N particles with z components $M_1, M_2, \ldots, M_n$ of the n total angular momenta. For bosons, $B^{N,l_1,l_2,\ldots,l_n}_{M_1,M_2,\ldots,M_n}$ is similarly defined, and obtained from (7*b*).

The generating functions just introduced ((6*a*, *b*) and (7*a*, *b*)) provide the multi-M-scheme multiplicity, forming the natural generalisation of the M-scheme generating functions, (2*a*) and (2*b*). The transition from the M scheme to the L scheme for a system of N fermions with a single kind of angular momentum is carried out by noting that the number of states (or the degeneracy of a state) with a given value L of the resultant angular momentum quantum number is given by (de-Shalit and Talmi 1963)

$$\Phi^{N,l}_L=F^{N,l}_L-F^{N,l}_{L+1}. \tag{8}$$

For a system of fermions possessing two kinds of angular momenta the number of states (or the degeneracy of a state) with given L and S is

$$\Phi^{N,l,s}_{L,S} = F^{N,l,s}_{L,S} - F^{N,l,s}_{L+1,S} - F^{N,l,s}_{L,S+1} + F^{N,l,s}_{L+1,S+1}. \tag{9}$$

The last expression, equation (9), resulted as a simple generalisation to LS coupling of (8). In this case we have to subtract from the NOS for $M = L$, $M_s = S$ the NOS for $M = L+1$, $M_s = S$ and $M = L$, $M_s' = S+1$. However, because the NOS for $M = L+1$, $M_s = S+1$ is subtracted twice in this way, it has to be added once. Applying the same argument for a system of fermions possessing three kinds of angular momentum l_1, l_2 and l_3, yields that the number of states with total angular momenta L_1, L_2 and L_3 is

$$\begin{aligned}\Phi^{N,l_1,l_2,l_3}_{L_1,L_2,L_3} &= F^{N,l_1,l_2,l_3}_{L_1,L_2,L_3} - (F^{N,l_1,l_2,l_3}_{L_1+1,L_2,L_3} + F^{N,l_1,l_2,l_3}_{L_1,L_2+1,L_3} + F^{N,l_1,l_2,l_3}_{L_1,L_2,L_3+1}) \\ &\quad + (F^{N,l_1,l_2,l_3}_{L_1+1,L_2+1,L_3} + F^{N,l_1,l_2,l_3}_{L_1+1,L_2,L_3+1} + F^{N,l_1,l_2,l_3}_{L_1,L_2+1,L_3+1}) - F^{N,l_1,l_2,l_3}_{L_1+1,L_2+1,L_3+1}.\end{aligned} \tag{10}$$

The generalisation of (10) to the case of n types of angular momentum can be written in the form

$$\Phi^{N,l_1,l_2,\ldots,l_n}_{L_1,L_2,\ldots,L_n} = \sum_{k=0}^{n} (-1)^k \sum_{i_1<i_2<\ldots<i_k}^{n} F^{N,l_1,l_2,\ldots,l_n}_{\ldots,L_{i_1}+1,\ldots,L_{i_2}+1,\ldots,L_{i_k}+1,\ldots} \tag{11}$$

where $l_1, l_2, \ldots, l_n$ are the n types of single particle angular momentum and $L_1, L_2, \ldots, L_n$ are the corresponding N-particle angular momenta. The integer k denotes the number of angular momenta in which the M value is increased by unity relative to the value of interest (i.e. $L_1, L_2, \ldots, L_n$). For any given value k, all the possibilities of taking k different types of angular momentum from n ones have to be taken into account, and this is done by the second summation in (11). Equation (11) can be rewritten in a form in which the parameter k does not appear explicitly

$$\Phi^{N,l_1,l_2,\ldots,l_n}_{L_1,L_2,\ldots,L_n} = \sum_{L_1'=L_1}^{L_1+1} \sum_{L_2'=L_2}^{L_2+1} \cdots \sum_{L_n'=L_n}^{L_n+1} (-1)^{\sum_{i=1}^{n}(L_i'-L_i)} F^{N,l_1,l_2,\ldots,l_n}_{L_1',L_2',\ldots,L_n'}. \tag{12}$$

The relations (8)-(12) also hold for boson systems, where the NOS factors F have to be replaced by the corresponding factors B.

As an example we consider a system of $N = 3$ fermions with $l = 1$ and pseudospin $s = \frac{3}{2}$. The coefficient of z^3 in the grand generating function, (6a), is

$$\begin{aligned}F^{3,1,3/2}(x,y) &= (y^{9/2} + 3y^{7/2} + 6y^{5/2} + 11y^{3/2} \\ &\quad + 13y^{1/2} + \mathrm{NP}) + (y^{7/2} + 2y^{5/2} + \mathrm{NP})(x^2 + 2x + \mathrm{NP}) \\ &\quad + (y^{3/2} + \mathrm{NP})(x^3 + 4x^2 + 8x + \mathrm{NP}) + (y^{1/2} + \mathrm{NP})(x^3 + 5x^2 + 10x + \mathrm{NP})\end{aligned} \tag{13}$$

where NP stands for the terms with negative powers which, because of the M, $-M$ symmetry, are in one-to-one correspondence with the terms with positive powers, presented. Using the M, M_s scheme multiplicities as determined by the generating function, (13), we transform to the LS scheme by the rule given above (equation (9)), finding that the following fermionic states can be formed:

$L = 0$, $S = \frac{9}{2}, \frac{5}{2}, \frac{3}{2}$ $\qquad$ $L = 1$, $S = \frac{7}{2}, \frac{5}{2}, \frac{3}{2}$(twice), $\frac{1}{2}$

$L = 2$, $S = \frac{7}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2}$ $\qquad$ $L = 3$, $S = \frac{3}{2}$.

The antisymmetric states in the LS-coupling scheme were enumerated above by using the grand generating function, (6a). On the other hand, these states can be constructed in terms of direct products of conjugate irreducible representations (irreps) of the unitary groups $U(2l+1)$ and $U(2s+1)$. These irreps are labelled by Young shapes (Wybourne 1970). Therefore, the generating function $F^{N,l,s}(x, y)$ can be expanded as

$$F^{N,l,s}(x,y)=\sum_{[\lambda_1,\lambda_2,\ldots,\lambda_k]}\{[\lambda_1,\lambda_2,\ldots,\lambda_k]\}^{N,l}(x)\{[\lambda_1,\lambda_2,\ldots,\lambda_k]^{\dagger}\}^{N,s}(y) \tag{14}$$

where

$$\{[\lambda_1,\lambda_2,\ldots,\lambda_k]\}^{N,l}(x)=\sum_M\{[\lambda_1,\lambda_2,\ldots,\lambda_k]\}^{N,l}_M x^M \tag{15}$$

is the generating function for the number of states of N particles with angular momentum l and total z component M, belonging to the irrep $[\lambda_1, \lambda_2, \ldots, \lambda_k]$. Note that $\{[N]\}^{N,l}(x) = b^{N,l}(x)$ and $\{[1^N]\}^{N,l}(x) = f^{N,l}(x)$, where $b^{N,l}(x)$ and $f^{N,l}(x)$ are the boson and fermion generating functions defined in (1a) and (1b). The grand generating functions $f^l(x, z)$ and $b^l(x, z)$ are the generating functions for the elementary symmetric functions and the homogeneous product sums, respectively (Wybourne 1970). Therefore, the generating functions $f^{N,l}(x)$ and $b^{N,l}(x)$ are the Schur functions corresponding to the symmetric and alternative representations of the symmetric group, in terms of the set of symmetric power sums

$$S_r=\sum_{m=-l}^{l}x^{rm}. \tag{16}$$

For an arbitrary irrep the generating function is the appropriate Schur function (Wybourne 1970, p 20).

As an illustration we consider the example treated above, i.e. $N = 3$, $l = 1$ and $s = \frac{3}{2}$. In this case the following irrep generating functions are needed:

$$\begin{aligned}
&\{[3]\}^{3,1}(x)=(S_1^3+3S_1S_2+2S_3)/6\\
&\{[2,1]\}^{3,1}(x)=(S_1^3-S_3)/3\\
&\{[1^3]\}^{3,1}(x)=(S_1^3-3S_1S_2+2S_3)/6
\end{aligned} \tag{17}$$

where the expressions for S_r ($r = 1, 2, 3$) are given in (16). In particular, for $l = 1$ and $s = \frac{3}{2}$ the irrep generating functions are:

$$\begin{aligned}
&\{[3]\}^{3,1}(x)=x^3+x^2+2x+2+\text{NP}\\
&\{[3]\}^{3,3/2}(x)=x^{9/2}+x^{7/2}+2x^{5/2}+3x^{3/2}+3x^{1/2}+\text{NP}\\
&\{[2,1]\}^{3,1}(x)=x^2+2x+2+\text{NP}\\
&\{[2,1]\}^{3,3/2}(x)=x^{7/2}+2x^{5/2}+3x^{3/2}+4x^{1/2}+\text{NP}\\
&\{[1^3]\}^{3,1}(x)=1\\
&\{[1^3]\}^{3,3/2}(x)=x^{3/2}+x^{1/2}+\text{NP}.
\end{aligned} \tag{18}$$

Substituting these expressions in (14) one obtains

$$\begin{aligned}
F^{3,1,3/2}(x,y)={}&(x^3+x^2+2x+2+\text{NP})(y^{3/2}+y^{1/2}+\text{NP})\\
&+(x^2+2x+2+\text{NP})(y^{7/2}+2y^{5/2}+3y^{3/2}+4y^{1/2}+\text{NP})\\
&+(y^{9/2}+y^{7/2}+2y^{5/2}+3y^{3/2}+3y^{1/2}+\text{NP}).
\end{aligned} \tag{19}$$

This expression is identical to the one obtained above (equation (13)), using the grand generating function $F^{1,3/2}(x, y, z)$.

A useful property which sometimes enables the reduction of an irrep generating function into the irrep generating function of a Young shape with a smaller number of boxes follows from the generating function appropriate for a closed shell. For particles with angular momentum l, a Young shape consisting of k columns, each one of which has $2l+1$ boxes, generates only the closed shell state with $L=0$. Therefore,

$$\{[k^{2l+1}]\}^{N=k(2l+1),l}(x)=1. \tag{20}$$

Consequently, a Young shape consisting of k columns of length $2l+1$ and additional columns of lengths $\lambda_{k+1}, \lambda_{k+2}, \ldots$ has the same generating function as the Young shape obtained by dropping the first k columns,

$$\{[(2l+1)^k, \lambda_{k+1}, \lambda_{k+2}, \ldots]^{\dagger}\}^{N,l}(x)=\{[\lambda_{k+1}, \lambda_{k+2}, \ldots]^{\dagger}\}^{N',l}(x) \tag{21}$$

where $N=(2l+1)k+N'$ and $N'=\lambda_{k+1}+\lambda_{k+2}+\ldots$.

From the closed shell property, (20), it also follows that the generating functions corresponding to two Young shapes which complement one another into a closed shell, are equal. Thus, a generating function for a Young shape with k columns is equal to the generating function for a Young shape with the same number of columns but with $2l+1-\lambda_{k-i+1}$ boxes in its ith column ($i=1,2,\ldots,k$), i.e.

$$\{[\lambda_1, \lambda_2, \ldots, \lambda_k]^{\dagger}\}^{N,l}(x)=\{[2l+1-\lambda_k, 2l+1-\lambda_{k-1}, \ldots, 2l+1-\lambda_1]^{\dagger}\}^{N',l}(x) \tag{22}$$

where $N'+N=(2l+1)k$. This equality corresponds to the well known particle-hole symmetry.

The following simple examples illustrate (21) and (22):

$$\{[3,2]\}^{5,1/2}(x)=\{[1]\}^{1,1/2}(x)=x^{1/2}+\text{NP} \tag{23}$$

$$\{[3,2]\}^{5,1}(x)=\{[3,1]\}^{4,1}(x)=x^3+2x^2+3x+3+\text{NP} \tag{24}$$

$$\{[3,1,1]\}^{5,1}(x)=\{[2]\}^{2,1}(x)=\{[2,2]\}^{4,1}=x^2+x+1+\text{NP}. \tag{25}$$

Equation (23) is an example of the property expressed by (21), equation (24) is an example of the particle-hole symmetry, (22), and in (25) we used both properties.

In conclusion, the form of the generating functions for the M, M_s scheme multiplicities in the LS-coupling scheme, and its generalisation to the case of n different types of angular momentum, for both fermions and bosons, has been reported. Furthermore, generating functions for the M-scheme multiplicities of states corresponding to any irrep of the symmetric group have been defined and their relation to the corresponding Schur functions has been pointed out.

The generating functions introduced in this work yield all the possible allowed LS states for fermions and bosons and all the allowed states for any Young shape (irrep of the symmetric group) without constructing explicitly the states, i.e. calculating their coefficients of fractional parentage (CFP) (Novoselsky *et al* 1988). Therefore, these generating functions are useful for any calculation in atomic, nuclear or quark physics which does not depend on the structure of the allowed states.

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