Characters of Two-Row Representations of the Symmetric Group

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Abstract: Characters of irreducible representations (irreps) of the symmetric group corresponding to the two-row Young diagrams, i.e. describing transformation properties of N-electron eigenfunctions of the total spin operators, have been expressed as explicit functions of the number of electrons N and of the total spin quantum number S. The formulae are useful in various areas of theory of many-electron systems, particularly in designing algorithms for evaluation of spectral density moments.

Key words: Symmetric group, irreducible representations (irreps), Young diagrams, characters of irreps, statistical theory of spectra, N-electron spin eigenfunctions.

1. Introduction

The eigenfunctions of the square of the N-electron spin operator corresponding to an eigenvalue $S(S+1)$ form a basis for the irreducible representation (irreps) of the symmetric group $\mathcal{S}_N$ described by a two-row Young diagram with

$$p = \frac{N}{2} + S \tag{1}$$

boxes in the first row and

$$q = \frac{N}{2} - S \tag{2}$$

boxes in the second row. This property of the total spin eigen-spaces results in many applications, such as the development of the *symmetric group approach* to the theory of N-electron systems [1], the formulation of the so called *spin-free quantum chemistry* [2], numerous applications in the theory of atomic spectra [3], in the theory of magnetism [4], in the statistical theory of spectra [5], and so on. One of advantages of these approaches is a possibility of expressing the coupling constants which appear in formulae for quantum-mechanical expectation values, in terms of matrix elements of the appropriate representations of the symmetric group. In consequence, quantities, which are expressible in terms of traces of the operators (like e.g. averages and moments) depend upon the the characters of the pertinent representations. In these applications one is interested in formulae for the characters rather then character tables since having the formulae one can easily explore the dependence on the number of particles and on the spin quantum numbers.

The problem of evaluation of the characters of irreps of $\mathcal{S}_N$ has been solved many years ago [6]. General algorithms have been formulated by Gamba [7] and by Butler and King [8]. In all these works, procedures for the evaluation of the characters of a given representation of $\mathcal{S}_N$ have been formulated. In the case of two-row representations, these methods allow for the evaluation of the character for arbitrary, but specified, values of S and N. On the other hand, the characters in the form of explicit functions of N and S are needed in atomic and molecular structure theory. The character expressions for the identity permutation

$$\chi^{[p,q]}_{[1^N]} \equiv f(S,N) = \frac{2S+1}{N+1}\binom{N+1}{N/2-S}, \tag{3}$$

(equal to the dimension of the representation) and for the class of transpositions

$$\chi^{[p,q]}_{[1^{N-2}\,2]} = \frac{4S(S+1)+N(N-4)}{2N(N-1)} f(S,N) \tag{4}$$

have already been derived by Heisenberg [9]. Similar expressions for $[1^{N-t}\,t]$, $t=3,4,5$ and for $[1^{N-4}\,2^2]$ have been reported by Corson [10]. Recently, simple expressions for the classes $[1^{N-t}\,t]$ and $[1^{N-s-t}\,s\,t]$ with arbitrary s and t have been obtained from the Murnaghan-Nakayama rule [11]. In this note, a general expression for an arbitrary two-row representation character is given. The derivation is based on the algorithm of Butler and King [8].

2. The general algorithm

The two-row representation character $\chi^{[p,q]}_{(\alpha)}$ corresponding to the class of $\mathcal{S}_N$ defined by the partition

$$(\alpha) = (1^{\alpha_1}\, 2^{\alpha_2}\, \ldots t^{\alpha_t}), \tag{5}$$

with

$$\sum_{k=1}^{t} k\alpha_k = p + q = N, \tag{6}$$

is an integer function of $t+2$ parameters: of p, q (i.e. of N, S) and of α_k, $k = 1, 2, \ldots, t$. Due to the constraint (6) only t of them are independent. Most frequently one is interested in the dependence of the characters upon N and S for a fixed (α). For the two-row representations, Eq. (4.9) of Butler and King [8] may be rewritten as

$$\chi^{[p,q]}_{(\alpha)} = \sum_{x=0}^{q} \mathcal{C}(x)\, f^{<q-x>}_{\alpha_1}, \tag{7}$$

where

$$f^{<x>}_{\alpha_1} = \frac{(\alpha_1 + 1 - 2x)\alpha_1!}{x!\,(\alpha_1 + 1 - x)!}, \tag{8}$$

and

$$\mathcal{C}(x) = \sum_{(\beta)} \prod_{k=2}^{p+q} \binom{\alpha_k}{\beta_k}, \tag{9}$$

with

$$(\beta) = (2^{\beta_2}\, 3^{\beta_3}\, \ldots t^{\beta_t}) \tag{10}$$

standing for a partition of x with no part smaller than 2. Obviously,

$$\sum_{k=2}^{t} k\beta_k = x. \tag{11}$$

The values of $f_{\alpha_1}^{<x>}$ are related to the dimensions of the irreps of $\mathcal{S}_{\alpha_1}$:

$$f_{\alpha_1}^{<x>} = \begin{cases} \chi_{1^{\alpha_1}}^{[\alpha_1 - x, x]} & \text{if } 0 \leq x \leq \frac{\alpha_1}{2}, \\ -\chi_{1^{\alpha_1}}^{[x-1, \alpha_1 - x + 1]} & \text{if } \frac{\alpha_1}{2} < x \leq \alpha_1 + 1. \end{cases} \tag{12}$$

If $x = (\alpha_1 + 1)/2$ or $x > \alpha_1 + 1$, then $f_{\alpha_1}^{<x>} = 0$. Therefore, if $q > \alpha_1 + 1$, the lower limit of the sum over x in Eq. (7) may be set equal to $q - \alpha_1 - 1$. Besides, since

$$f_{\alpha_1}^{<x>} = -f_{\alpha_1}^{<\alpha_1 - x + 1>}, \tag{13}$$

Eq. (7) simplifies to

$$\chi_{(\alpha)}^{[p,q]} = \sum_{x=0}^{\left[\frac{\alpha_1}{2}\right]} \left[\mathcal{C}(q-x) - \mathcal{C}(q - \alpha_1 - 1 + x)\right] f_{\alpha_1}^{<x>}, \tag{14}$$

where $\left[\frac{\alpha_1}{2}\right]$ stands for the integer part of $\frac{\alpha_1}{2}$. In particular, if $\alpha_1 < 2$ then

$$\chi_{(\alpha)}^{[p,q]} = \mathcal{C}(q) - \mathcal{C}(b). \tag{15}$$

According to Eq. (9), $\mathcal{C}(x)$ is evaluated as follows:

(1) List the partitions of (x) having no part smaller than 2;

(2) Replace each partition $(2^{\beta_2}\, 3^{\beta_3}\, \ldots t^{\beta_t})$ by the binomial coefficient product $\binom{\alpha_2}{\beta_2}\binom{\alpha_3}{\beta_3}\cdots\binom{\alpha_t}{\beta_t}$

(3) Get $\mathcal{C}(x)$ as the sum of the binomial coefficient products found in (1).

Thus, the first few coefficients of the character formula become

$$\mathcal{C}(0)=1,\quad \mathcal{C}(1)=0,\quad \mathcal{C}(2)=\alpha_2,\quad \mathcal{C}(3)=\alpha_3,$$

$$\mathcal{C}(4)=\tfrac{1}{2}\alpha_2(\alpha_2-1)+\alpha_4,\quad \mathcal{C}(5)=\alpha_2\alpha_3+\alpha_5,$$

$$\mathcal{C}(6)=\tfrac{1}{6}\alpha_2(\alpha_2-1)(\alpha_2-2)+\tfrac{1}{2}\alpha_3(\alpha_3-1)+\alpha_2\alpha_4+\alpha_6,$$

$$\mathcal{C}(7)=\tfrac{1}{2}\alpha_2(\alpha_2-1)\alpha_3+\alpha_3\alpha_4+\alpha_2\alpha_5+\alpha_7,$$

$$\mathcal{C}(8)=\tfrac{1}{24}\alpha_2(\alpha_2-1)(\alpha_2-2)(\alpha_2-3)+\tfrac{1}{2}\alpha_2\alpha_3(\alpha_3-1)+\tfrac{1}{2}\alpha_2(\alpha_2-1)\alpha_4$$
$$+\tfrac{1}{2}\alpha_4(\alpha_4-1)+\alpha_3\alpha_5+\alpha_2\alpha_6+\alpha_8.$$

3. Stabilization Property

It is easy to see that, in general, $\mathcal{C}(x)$ does not depend upon α_y when $y>x$. Hence, according to Eq. (7), $\chi^{[p,q]}_{(\alpha)}$ does not depend upon those parts α_y of the partition of N which are larger than q. In particular,

$$\begin{aligned}
\chi^{[p,0]}_{(\alpha)} &= 1,\\
\chi^{[p,1]}_{(\alpha)} &= \alpha_1-1,\\
\chi^{[p,2]}_{(\alpha)} &= \frac{1}{2}\alpha_1(\alpha_1-3)+\alpha_2,\\
\chi^{[p,3]}_{(\alpha)} &= \frac{1}{6}\alpha_1(\alpha_1-1)(\alpha_1-5)+(\alpha_1-1)\alpha_2+\alpha_3.
\end{aligned}$$

Similar expressions for larger q values may readily be obtained by combining Eqs. (7), (8) and (9). This observation is a special case of a general *stabilization rule* for the symmetric group characters [12].

Since $S=\frac{N}{2}-q$, a knowledge of $\mathcal{C}(k)$, $k=0,1,\ldots,q$, is sufficient to determine all of the characters for systems with $S\geq\frac{N}{2}-q$. Therefore, in high-spin systems only the "short-cycle" part of the permutation defines the character formula. More specifically, if $S = \frac{N}{2} - q$, then the corresponding characters do not depend upon $\alpha_{q+1}, \alpha_{q+2}, \ldots$. Alternatively, it may be formulated as follows: Let (σ) be a partition of $p+q$ with no part larger than q and let (μ) be a partition of k with all parts larger than q, then

$$\chi^{[p+k,q]}_{(\mu\sigma)} = \chi^{[p,q]}_{(\sigma)}. \tag{16}$$

The irreps of $\mathcal{S}_N$ are labelled by ordered partitions of N. In the case of the two-row representations, the standard ordering implies that $q \leq p$. Partitions that are not in standard order can be modified to produce equivalent standard $\mathcal{S}_N$ irreps using the modification rules of Littlewood [13], [14]. For two-part partitions this amounts to $[p,q] \Rightarrow -[q-1,p+1]$. If $p = q-1$ then the result is null. Thus,

$$\chi^{[p,q]}_{(\sigma)} = -\chi^{[q-1,p+1]}_{(\sigma)}. \tag{17}$$

Combining the stabilization property and the $\mathcal{S}_N$ modification rule one may derive interesting symmetry relations between the two-row representation characters. Indeed, according to Eqs. (16) and (17), for every $k > p+1$, we have

$$\chi^{[p+k,q]}_{(\mu\sigma)} = \chi^{[pq]}_{(\sigma)} = -\chi^{[q-1,p+1]}_{(\sigma)} = -\chi^{[k+q-1,p+1]}_{(\mu\sigma)}. \tag{18}$$

Another interesting, though probably less important, relation holds for the dimensions of the irreps. Namely, as one can easily check,

$$f(S,n) \quad = f(S+1,n), \;\; \text{if} \;\; n = (2S+2)^2 - 2, \tag{19}$$

$$f(S,n) \quad = f(S+2,n), \;\; \text{if} \;\; n = (2S+3)^2 - 3. \tag{20}$$

It seems, however, that no similar relations exist between $f(S,n)$ and $f(S+\Delta,n)$ if $\Delta > 2$.

4. Some Special Cases

Cases where (α) is composed of only several different cycles are both the simplest and the most important in applications. If $(\alpha) = 1^{N-t}t$, then the only binomial coefficient which contributes to Eq. (9) is $\binom{1}{\beta_t}$. Hence,

$$\chi^{[p,q]}_{[1^{N-t}\,t]} = f^{<q>}_{N-t} + f^{<q-t>}_{N-t}. \tag{21}$$

This formula is equivalent to Eq. (29) of ref. [11]. It reduces to Eq. (4) for $t = 2$ and to the results of Corson [10] for $t = 3,4,5$. In the case of $(\alpha) = 1^{N-t\alpha_t}t^{\alpha_t}$, there may be several non-zero $\mathcal{C}$ coefficients: $\mathcal{C}(t) = \binom{\alpha_t}{1}$, $\mathcal{C}(2t) = \binom{\alpha_t}{2}$, ..., $\mathcal{C}(mt) = \binom{\alpha_t}{m}$, where $m = \min(\alpha_t, \left[\frac{q}{t}\right])$ and $\mathrm{int}(a)$. Then,

$$\chi^{[p,q]}_{[1^{\alpha_1}\,t^{\alpha_t}]} = \sum_{n=0}^{m} \binom{\alpha_t}{n} f^{<q-nt>}_{\alpha_1}, \tag{22}$$

with $\alpha_1 = N - t\alpha_t$.

A similar procedure may also be applied in more complicated cases. For example, if $(\alpha) = 1^{\alpha_1}s^{\alpha_s}t^{\alpha_t}$ with $\alpha_1 = N - s\alpha_s - t\alpha_t$ then

$$\chi^{[p,q]}_{[1^{\alpha_1}\,s^{\alpha_s}\,t^{\alpha_t}]} = \sum_{n_s n_t} \binom{\alpha_s}{n_s}\binom{\alpha_t}{n_t} f^{<q-n_s s-n_t t>}_{\alpha_1}, \tag{23}$$

where the sum is extended over all terms for which $n_s s + n_t t \le q$, $n_s \le \alpha_s$ and $n_t \le \alpha_t$.

5. Concluding Remarks

The formulae for the symmetric group characters presented in this paper supply a general tool for expressing spectral density distribution moments of the Heisenberg Hamiltonian in terms of the number of particles $N = p + q$ and of the total spin $S = \frac{1}{2}(p - q)$. For other model Hamiltonians, these formulae are also useful since the irreducible characters appear in numerous expressions defining the appropriate moments [5].

The stabilization property of the characters (16) may allow the expression of more complicated propagation coefficients in terms of simpler ones. Also the symmetry relation (18) may be essential for simplifying some asymptotic expressions. However their significance for statistical spectroscopy has to be explored in more detail.

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