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Recursion relations for traces of products of angular momentum operators in the spherical basis

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Abstract. A set of recursion relations is derived by the aid of which analytical expressions for $\mathrm{Tr}(J_-^k J_z^l J_+^k)$ can be built up in a chain procedure.

1. Introduction

The problem of evaluating traces of products of angular momentum operators in the Cartesian and the spherical basis has been considered by several authors. Using conventional angular momentum techniques, Ambler *et al* (1962a, b) were the first to tabulate the results for an extensive list of such traces. As the calculations involved were rather cumbersome, alternative techniques have been developed by Rose (1962) and Witschel (1971, 1975). A common disadvantage of all these methods is the lack of formulae allowing the calculation of more than one trace at a time. To partially cover this shortcoming, Subramanian and Devanathan (1974) gave an analytical expression for the trace of k raising operators J_+ and k lowering operators J_- in the special form $\mathrm{Tr}(J_-^k J_+^k)$ for arbitrary positive integers k. Recently, the possibility to extend this result to a wider variety of traces, has been investigated by the present authors (De Meyer and Vanden Berghe 1978). It was shown that all considered traces of a product of a definite number of operators J_+, J_- and J_z, defined in the spherical basis, could be written as a sum of traces of the kind $\mathrm{Tr}(J_-^k J_z^l J_+^k)$. The latter are then expanded in terms of binomial coefficients and of Stirling numbers of the second kind, a fact which allowed us to tabulate expressions for $\mathrm{Tr}(J_-^k J_z^l J_+^k)$ for arbitrary k, and l fixed between 0 and 7. In this compact way almost all results of Ambler *et al* (1962b) could be reproduced. For larger l values the algebraic operations became too involved.

In the present paper an alternative technique to find analytical expressions for $\mathrm{Tr}(J_-^k J_z^l J_+^k)$ is presented. The essential point is the construction of relations which express recursivity with respect to the number of J_z operators. It turns out that a distinction has to be made between even and odd l values, leading to a different type of recursion relation for either case. As a by-product some properties of traces found earlier are retrieved.

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2. Recursion relations for odd *l*

Introducing the shorthand notation

$$\mathrm{Tr}(J_-^k J_z^l J_+^k) = \mathrm{Tr}(k, l), \tag{2.1}$$

a method is outlined to define the quantity (2.1) recursively with respect to the parameter l. Starting with the explicit form of (2.1) for $l = 0$ (Subramanian and Devanathan 1974, De Meyer and Vanden Berghe 1978), i.e.

$$\mathrm{Tr}(k, 0) = \frac{k!^2(2j+2k+1)!}{(2k+1)!\,(2j-k)!}, \tag{2.2}$$

it is possible to evaluate (2.1) for arbitrary l.

Working in a representation $|j\,m\rangle$ in which J_z is diagonal, use can be made of the well known relations (Edmonds 1957)

$$J_\pm|j\,m\rangle = [(j\mp m)(j\pm m+1)]^{1/2}|jm\pm 1\rangle, \tag{2.3}$$

to express (2.1) as follows:

$$\mathrm{Tr}(k, l) = \sum_{m=-j}^{j} \langle jm|J_-^k J_z^l J_+^k|jm\rangle = \sum_{m=-j}^{j-k} (m+k)^l \frac{(j-m)!\,(j+m+k)!}{(j-m-k)!\,(j+m)!}. \tag{2.4}$$

By formally changing m to $-m$, (2.4) is brought into a first equivalent form

$$\mathrm{Tr}(k, l) = \sum_{m=-j+k}^{j} (k-m)^l \frac{(j+m)!\,(j-m+k)!}{(j+m-k)!\,(j-m)!}. \tag{2.5}$$

If on the other hand m in (2.4) is changed to $m-k$, a second equivalent form of (2.4) is obtained:

$$\mathrm{Tr}(k, l) = \sum_{m=-j+k}^{j} m^l \frac{(j+m)!(j-m+k)!}{(j+m-k)!\,(j-m)!}. \tag{2.6}$$

Equating the right-hand sides of (2.5) and (2.6), and expanding $(k-m)^l$ by the binomial theorem, one finds:

$$\sum_{m=-j+k}^{j} m^l \frac{(j+m)!\,(j-m+k)!}{(j+m-k)!\,(j-m)!} = \sum_{m=-j+k}^{j} \sum_{i=0}^{l} \binom{l}{i} k^{l-i}(-m)^i \frac{(j+m)!\,(j-m+k)!}{(j+m-k)!\,(j-m)!},$$

or

$$\sum_{m=-j+k}^{j} m^l \frac{(j+m)!\,(j-m+k)!}{(j+m-k)!\,(j-m)!}$$
$$= \sum_{m=-j+k}^{j} \left[(-m)^l + \sum_{i=0}^{l-1} \binom{l}{i} k^{l-i}(-m)^i\right] \frac{(j+m)!\,(j-m+k)!}{(j+m-k)!\,(j-m)!}. \tag{2.7}$$

For even l the terms m^l in both sides of (2.7) cancel. Setting $l = 2n$, (2.7) reduces to:

$$\sum_{i=0}^{2n-1} \binom{2n}{i} (-k)^{2n-i} \sum_{m=-j+k}^{j} m^i \frac{(j+m)!\,(j-m+k)!}{(j+m-k)!\,(j-m)!} = 0,$$

or with the help of (2.6)

$$\sum_{i=0}^{2n-1} \binom{2n}{i} (-k)^{2n-i}\, \mathrm{Tr}(k, i) = 0. \tag{2.8}$$

For odd l, the terms m^l in both sides of (2.7) add, and setting $l=2n-1$ one obtains:

$$-\sum_{i=0}^{2n-2}\binom{2n-1}{i}(-k)^{2n-1-i}\sum_{m=-j+k}^{j} m^i\frac{(j+m)!\,(j-m+k)!}{(j+m-k)!\,(j-m)!}$$
$$=2\sum_{m=-j+k}^{j} m^{2n-1}\frac{(j+m)!\,(j-m+k)!}{(j+m-k)!\,(j-m)!},$$

which by the aid of (2.6) can be written as

$$\sum_{i=0}^{2n-2}\binom{2n-1}{i}(-k)^{2n-1-i}\,\mathrm{Tr}(k,i)=-2\,\mathrm{Tr}(k,2n-1). \tag{2.9}$$

Both (2.8) and (2.9) are recursion relations which allow us to express $\mathrm{Tr}(k,l)$ for odd l as a sum of quantities $\mathrm{Tr}(k,i)$ with $i<l$. As an example we calculate $\mathrm{Tr}(k,1)$. From (2.9) it immediately follows for $n=1$ that

$$\binom{1}{0}(-k)^1\mathrm{Tr}(k,0)=-2\mathrm{Tr}(k,1),$$

or

$$\mathrm{Tr}(k,1)=\tfrac{1}{2}k\,\mathrm{Tr}(k,0), \tag{2.10}$$

which is in perfect agreement with the result found by direct calculation (De Meyer and Vanden Berghe 1978).

Setting $n=1$ in the implicit relation (2.8), the same result (2.10) is obtained. It is clear that it is not possible yet to build up a chain of expressions for $\mathrm{Tr}(k,l)$, $l=1,2,\ldots$ with the relations (2.8) or (2.9) alone. Finally one remarks by inspection of (2.9) that in the expressions for $\mathrm{Tr}(k,l)$ with odd l, the parameter k can always be factorised.

3. A consistency recursion relation

Separating in (2.8) the terms with $\mathrm{Tr}(k,2n-1)$, $\mathrm{Tr}(k,2n-2)$, it follows that

$$-2nk\,\mathrm{Tr}(k,2n-1)+n(2n-1)k^2\,\mathrm{Tr}(k,2n-2)=-\sum_{i=0}^{2n-3}\binom{2n}{i}(-k)^{2n-i}\,\mathrm{Tr}(k,i), \tag{3.1}$$

whereas the same procedure reduces (2.9) to

$$-2\mathrm{Tr}(k,2n-1)+(2n-1)k\,\mathrm{Tr}(k,2n-2)=\sum_{i=0}^{2n-3}\binom{2n-1}{i}(-k)^{2n-1-i}\,\mathrm{Tr}(k,i). \tag{3.2}$$

The left-hand sides of (3.1) and (3.2) are proportional. Expressing that the equations (3.1), (3.2) are not contradictory, leads to the consistency relation

$$\sum_{i=0}^{2n-3}\left[n\binom{2n-1}{i}-\binom{2n}{i}\right](-k)^{2n-1-i}\,\mathrm{Tr}(k,i)=0. \tag{3.3}$$

Using the well known property of binomial coefficients:

$$2n\binom{2n-1}{i}=(2n-i)\binom{2n}{i},$$

the relation (3.3) can be rewritten as

$$\sum_{i=0}^{2n-3} (2n-2-i)\binom{2n}{i}(-k)^{2n-1-i}\,\mathrm{Tr}(k,i)=0. \tag{3.4}$$

By the aid of the formula

$$i\binom{2n}{i}=2n\binom{2n-1}{i-1},$$

(3.4) can be transformed to

$$\sum_{i=0}^{2n-3} (2n-2)\binom{2n}{i}(-k)^{2n-1-i}\,\mathrm{Tr}(k,i)-2n\sum_{i=1}^{2n-3}\binom{2n-1}{i-1}(-k)^{2n-1-i}\,\mathrm{Tr}(k,i)=0,$$

or

$$(2n-2)\sum_{i=0}^{2n-3}\binom{2n}{i}(-k)^{2n-1-i}\,\mathrm{Tr}(k,i)=2n\sum_{i=0}^{2n-4}\binom{2n-1}{i}(-k)^{2n-2-i}\,\mathrm{Tr}(k,i+1).$$

By the use of (3.1), the last relation is written consecutively as

$$(2n-2)[-2n\,\mathrm{Tr}(k,2n-1)+n(2n-1)k\,\mathrm{Tr}(k,2n-2)]$$
$$=2n\sum_{i=0}^{2n-4}\binom{2n-1}{i}(-k)^{2n-2-i}\,\mathrm{Tr}(k,i+1),$$

or

$$\sum_{i=0}^{2n-4}\binom{2n-1}{i}(-k)^{2n-2-i}\,\mathrm{Tr}(k,i+1)-\frac{(2n-2)(2n-1)}{2}k\,\mathrm{Tr}(k,2n-2)$$
$$=-(2n-2)\,\mathrm{Tr}(k,n-1),$$

or

$$\sum_{i=0}^{2n-3}\binom{2n-1}{i}(-k)^{2n-2-i}\,\mathrm{Tr}(k,i+1)=-2(n-1)\,\mathrm{Tr}(k,2n-1). \tag{3.5}$$

The recurrence relation (3.5) can again be used to calculate $\mathrm{Tr}(k,l)$ for odd l, in terms of quantities $\mathrm{Tr}(k,i)$ with $i<l$.

4. Recursion relations for even l

Replacing m by $m+1$ in the expression (2.6) for $\mathrm{Tr}(k,l)$, one obtains the equivalent forms

$$\mathrm{Tr}(k,l)=\sum_{m=-j+k-1}^{j-1}(m+1)^l\frac{(j+m+1)!(j-m+k-1)!}{(j+m-k+1)!(j-m-1)!}$$
$$=\sum_{m=-j+k-1}^{j}(m+1)^l\frac{(j+m+1)!(j-m+k-1)!}{(j-m-1)!(j+m-k+1)!}, \tag{4.1}$$

where in the last step the zero contribution for $m=j$ has been added to the sum. Introducing the notation $\eta=j(j+1)$ for the eigenvalue of the J^2 operator, one deduces from (4.1)

$$\mathrm{Tr}(k,l)=\sum_{m=-j+(k-1)}^{j}(m+1)^l(j+m+1)(j-m)\frac{(j+m)![j-m+(k-1)]!}{(j-m)![j+m-(k-1)]!}$$
$$=\sum_{m=-j+(k-1)}^{j}(m+1)^l(\eta-m^2-m)\frac{(j+m)![j-m+(k-1)!}{(j-m)![j+m-(k-1)]!},$$

which by use of the binomial theorem is transformed to

$$\mathrm{Tr}(k,l)=\sum_{i=0}^{l}\binom{l}{i}\sum_{m=-j+(k-1)}^{j}m^i(\eta-m^2-m)\frac{(j+m)![j-m+(k-1)]!}{(j-m)!(j+m-(k-1)]!}. \qquad (4.2)$$

By the aid of formula (2.6), the relation (4.2) is compactly written as

$$\mathrm{Tr}(k,l)=\sum_{i=0}^{l}\binom{l}{i}[\eta\,\mathrm{Tr}(k-1,i)-\mathrm{Tr}(k-1,i+2)-\mathrm{Tr}(k-1,i+1)] \qquad (k\geq 1),$$

which by formally changing k to $k+1$, and by separating the term $\mathrm{Tr}(k, l+2)$, reduces to the more useful form

$$\mathrm{Tr}(k,l+2)=-\mathrm{Tr}(k+1,l)+\eta\sum_{i=0}^{l}\binom{l}{i}\mathrm{Tr}(k,i)$$
$$-\sum_{i=0}^{l}\binom{l}{i}\mathrm{Tr}(k,i+1)-\sum_{i=0}^{l-1}\binom{l}{i}\mathrm{Tr}(k,i+2). \qquad (4.3)$$

The recursion relation (4.3), which is valid for all $l\geq 0$, can be used in practice to evaluate $\mathrm{Tr}(k, l)$ for even l, in terms of quantities $\mathrm{Tr}(k, i)$ with $i<l$. For odd l, the recursion relations (2.8), (2.9) or (3.5) have the advantages of containing only one sum and also not depending explicitly on η. This shows that by going from $\mathrm{Tr}(k, 2n)$ to $\mathrm{Tr}(k, 2n+1)$ the degree of η of the resulting polynomial remains unchanged, while by going from $\mathrm{Tr}(k, 2n+1)$ to $\mathrm{Tr}(k, 2n+2)$ the degree of η is increased by one.

By using the relation (4.3) in a trace calculation, one needs an expression of the form $\mathrm{Tr}(k+1, l)$, which can be deduced from $\mathrm{Tr}(k, l)$ by formally replacing k by $k+1$. However, as it turns out that this is not a simple algebraic operation, we look for a formula expressing $\mathrm{Tr}(k+1, l)$ in terms of quantities $\mathrm{Tr}(k, i)$. For this purpose, $\mathrm{Tr}(k+1, l)$ is brought into the form

$$\mathrm{Tr}(k+1,l)=\sum_{m=-j+k+1}^{j}m^l\frac{(j+m)!(j-m+k+1)!}{(j+m-k-1)!(j-m)!}$$
$$=\sum_{m=-j+k}^{j}m^l(j+m-k)(j-m+k+1)\frac{(j+m)!(j-m+k)!}{(j+m-k)!(j-m)!}$$
$$=\sum_{m=-j+k}^{j}m^l[\eta-m^2+(2k+1)m-k(k+1)]\frac{(j+m)!(j-m+k)!}{(j+m-k)!(j-m)!},$$

showing us that

$$\mathrm{Tr}(k+1,l)=\eta\,\mathrm{Tr}(k,l)-\mathrm{Tr}(k,l+2)+(2k+1)\,\mathrm{Tr}(k,l+1)-k(k+1)\mathrm{Tr}(k,l). \qquad (4.4)$$

Inserting (4.4) in (4.3) one obtains

$$0=\eta\sum_{i=0}^{l-1}\binom{l}{i}\mathrm{Tr}(k,i)-\sum_{i=0}^{l}\binom{l}{i}\mathrm{Tr}(k,i+1)-\sum_{i=0}^{l-1}\binom{l}{i}\mathrm{Tr}(k,i+2)$$
$$-(2k+1)\,\mathrm{Tr}(k,l+1)+k(k+1)\,\mathrm{Tr}(k,l),$$

or, after separating the terms with $\mathrm{Tr}(k, l+1)$:

$$(2k+l+2)\,\mathrm{Tr}(k,l+1)$$
$$=k(k+1)\,\mathrm{Tr}(k,l)+\eta\sum_{i=0}^{l-1}\binom{l}{i}\mathrm{Tr}(k,i)$$
$$-\sum_{i=0}^{l-1}\binom{l}{i}\mathrm{Tr}(k,i+1)-\sum_{i=0}^{l-2}\binom{l}{i}\mathrm{Tr}(k,i+2). \qquad (4.5)$$

As an example of the utility of formula (4.5) we calculate $\mathrm{Tr}(k, 2)$. Putting $l=1$ in (4.5) and with the aid of (2.10) one finds:

$$(2k+3)\,\mathrm{Tr}(k,2)$$
$$=k(k+1)\tfrac{1}{2}k\,\mathrm{Tr}(k,0)+\eta\,\mathrm{Tr}(k,0)-\tfrac{1}{2}k\,\mathrm{Tr}(k,0)$$
$$=(\tfrac{1}{2}k^3+\tfrac{1}{2}k^2-\tfrac{1}{2}k+\eta)\,\mathrm{Tr}(k,0)$$

or

$$\mathrm{Tr}(k,2)=\frac{1}{2(2k+3)}(2\eta+k^3+k^2-k)\,\mathrm{Tr}(k,0), \qquad (4.6)$$

a result which corresponds to the form found by direct calculation (De Meyer and Vanden Berghe 1978).

5. Conclusions

We have derived some recursion relations by which analytical expressions for $\mathrm{Tr}(J_-^k J_z^l J_+^k)$ can be determined. Evidently other and perhaps more powerful relations can be constructed from our results. As a check of the validity of the new technique, with the help of the relations (3.5) and (4.5) we have retrieved all the expressions for $\mathrm{Tr}(J_-^k J_z^l J_+^k)$ with $0 \leqslant l \leqslant 7$, already found by direct calculation (De Meyer and Vanden Berghe 1978). This was done in about one tenth of the time needed for direct calculation.

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