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Traces of products of angular momentum operators in the spherical basis

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Abstract. Analytic expressions are derived for the traces of products of angular momentum operators in the spherical basis. These expressions contain binomial coefficients and Stirling numbers of the second kind. In addition, some relations between Bernoulli polynomials and Stirling numbers are retrieved.

1. Introduction

Traces of products of angular momentum operators are common in the theory of atomic levels in fields, in the theory of nuclear orientation and of asymmetric top moments. Such traces were calculated and tabulated in two comprehensive articles by Ambler *et al* (1962a,b) using conventional angular momentum techniques. The analytical expressions for these traces are evaluated in a systematic way. This means that one starts in the spherical basis with the non-zero traces of J_z^2 and J_+J_- , goes on to $J_+J_zJ_-$ and then to traces which contain four angular momentum operators. All possible traces are evaluated for a given number of operators. The number of operators is then increased by one and the process repeated. It is quite clear that such calculations are difficult and cumbersome. Rose (1962) used recoupling and graphical methods to calculate traces of products of angular momentum operators. However, these methods are not simple to apply when the number of factors in the product is large. Witschel made use of the coupled boson representation, combined with operator algebra (Witschel 1971) and of a so called 'comparison method' (Witschel 1975). He illustrates both these techniques by deriving some traces already given by Ambler *et al* (1962a,b). Subramanian and Devanathan (1974) extended the results of Ambler *et al*. They proved that the trace is a polynomial in η where η is the eigenvalue of the J^2 operator, and that it can be expanded in terms of $\text{Tr}(J_z^{2p})$, where p is a positive integer.

The purpose of this paper is to derive analytic expressions for $\text{Tr}(J_a^p J_b^q J_c^r \dots)$ where a, b, c, \dots are equal to $+$, $-$ or z and p, q, r, \dots are non-negative integers. As far as we know, only an analytical expression for $\text{Tr}(J_-^k J_+^k)$ is available in the literature (Subramanian 1974). All traces are expressed as functions of well known mathematical objects, i.e. binomial coefficients, Bernoulli numbers and polynomials and Stirling

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numbers of the second kind. Although the evaluation of these traces has been the aim of this paper we give, in addition, some relations between Bernoulli polynomials and Stirling numbers of the first and second kind.

2. Analytic expression for $\text{Tr}(J_-^k J_+^k)$

An analytic expression for $\text{Tr}(J_-^k J_+^k)$ has been derived by Subramanian and Devanathan (1974) by using the definition and the special properties of the spherical tensor operator of rank k as introduced in nuclear spin orientation problems. We calculate that quantity directly by making use of the well known relations for the raising J_+ and lowering J_- operators (Edmonds 1957):

$$J_{\pm}|jm\rangle = [(j \mp m)(j \pm m + 1)]^{1/2}|j, m \pm 1\rangle. \tag{2.1}$$

A representation $|jm\rangle$ has been introduced in which J_z is diagonal. In this way $\text{Tr}(J_-^k J_+^k)$ can be evaluated as follows:

$$\text{Tr}(J_-^k J_+^k) = \sum_{m=-j}^j \langle jm|J_-^k J_+^k|jm\rangle = \sum_{m=-j}^{j-k} \frac{(j-m)!(j+m+k)!}{(j-m-k)!(j+m)!}, \tag{2.2}$$

which can be rewritten as:

$$\text{Tr}(J_-^k J_+^k) = \sum_{m=-j+k}^j \frac{(j+m)!(j-m+k)!}{(j+m-k)!(j-m)!}. \tag{2.3}$$

By substituting $t = j + m - k$ in (2.3), and introducing the notation

$$u = 2j - k \in \mathbb{Z}, \tag{2.4}$$

one gets

$$\text{Tr}(J_-^k J_+^k) = \sum_{t=0}^u \frac{(k+t)!(u+k-t)!}{t!(u-t)!} = k!^2 \sum_{t=0}^u \binom{k+t}{t} \binom{u+k-t}{u-t}. \tag{2.5}$$

In the last step, we have made use of the definition

$$\binom{a}{b} = \begin{cases} \frac{a(a-1)(a-2)\dots(a-b+1)}{b!} & \forall a \in \mathbb{R}, b \in \mathbb{N}, \\ 0 & \forall b \in \mathbb{Z}^0. \end{cases} \tag{2.6}$$

for the binomial coefficient.

2.1. Evaluation of (2.5) by simple algebraic methods

Putting for $0 < x < 1$ and $n \in \mathbb{N}^0$,

$$(1-x)^{-2n} = (1-x)^{-n}(1-x)^{-n},$$

expanding both sides by the binomial theorem, and equating coefficients of x^l on both sides of this identity, one gets the following relation:

$$\sum_{t=0}^l \binom{n+t-1}{n-1} \binom{n+l-t-1}{n-1} = \binom{2n+l-1}{2n-1}. \tag{2.7}$$

With the aid of (2.6) and (2.7) the expression (2.5) transforms to

$$\text{Tr}(J_-^k J_+^k) = k!^2 \binom{2k+1+u}{2k+1} = \frac{k!^2(2k+1+u)!}{(2k+1)!u!},$$

which by use of (2.4) reduces to

$$\text{Tr}(J_-^k J_+^k) = \frac{k!^2(2j+k+1)!}{(2k+1)!(2j-k)!} \tag{2.8}$$

This relation is identical to the result obtained by Subramanian and Devanathan (1974) and is valid for any $k \in \mathbb{N}$.

2.2. Evaluation of (2.5) by the aid of symbolic methods

Although the algebraical method presented in § 2.1 is simple and short, it cannot be used for the evaluation of $\text{Tr}(J_a^p J_b^q J_c^r \dots)$, where besides powers of J_- and J_+ factors of the form J_z^l appear. Therefore, we introduce here a symbolic method based upon the determination of differences of binomial coefficients with respect to the upper index (Jordan 1965).

If E is an operator with the following property:

$$E \binom{a}{b} = \binom{a+1}{b}, \tag{2.9}$$

one can define the difference of the binomial coefficient with respect to the upper index as:

$$\Delta = E - 1, \tag{2.10}$$

such that

$$\Delta \binom{a}{b} = E \binom{a}{b} - \binom{a}{b} = \binom{a+1}{b} - \binom{a}{b} = \binom{a}{b-1}. \tag{2.11}$$

Therefore, one easily finds for $t \in \mathbb{N}$:

$$\Delta^t \binom{a}{b} = \binom{a}{b-t}. \tag{2.12}$$

It is important to note that for $t > b$ the right-hand side of (2.12) vanishes. The two binomial coefficients appearing in (2.5) can be rewritten as follows (Jordan 1965):

$$\binom{k+t}{t} = (-1)^t \binom{-k-1}{t}, \tag{2.13}$$

$$\binom{u+k-t}{u-t} = (-1)^{u-t} \binom{-k-1}{u-t}. \tag{2.14}$$

By formally applying (2.12), the coefficient in the right-hand side of (2.14) can be written as:

$$\binom{-k-1}{u-t} = \Delta^t \binom{-k-1}{u}.$$

In this way, the sum in (2.5) can be reduced to

$$\begin{aligned} & \sum_{t=0}^u \binom{k+t}{t} \binom{u+k-t}{u-t} \\ &= (-1)^u \left[\sum_{t=0}^u \binom{-k-1}{t} \Delta^t \right] \binom{-k-1}{u} \\ &= (-1)^u \left[\sum_{t=0}^{\infty} \binom{-k-1}{t} \Delta^t \right] \binom{-k-1}{u} = (-1)^u (1+\Delta)^{-k-1} \binom{-k-1}{u}. \end{aligned} \tag{2.15}$$

Putting $1 + \Delta = E$, in accordance with (2.10), and making use in a formal way of the definition (2.9) of E , one deduces:

$$\sum_{t=0}^u \binom{k+t}{t} \binom{u+k-t}{u-t} = (-1)^u E^{-k-1} \binom{-k-1}{u} = (-1)^u \binom{-2k-2}{u},$$

which, due to (2.13) and the general properties of binomial coefficients, can be written as follows:

$$\sum_{t=0}^u \binom{k+t}{t} \binom{u+k-t}{u-t} = \binom{2k+1+u}{u} = \binom{2k+1+u}{2k+1}. \tag{2.16}$$

Introducing (2.16) into (2.5) yields again the result (2.8) for $\text{Tr}(J_-^k J_z^k J_+^k)$.

3. Analytic expression for $\text{Tr}(J_-^k J_z^l J_+^k)$

In the same representation as in § 2, $\text{Tr}(J_-^k J_z^l J_+^k)$ is defined as:

$$\text{Tr}(J_-^k J_z^l J_+^k) = \sum_{m=-j}^j \langle j m | J_-^k J_z^l J_+^k | j m \rangle = \sum_{m=-j}^{j-k} (m+k)^l \frac{(j-m)!(j+m+k)!}{(j-m-k)!(j+m)!}, \tag{3.1}$$

from which it follows that

$$\text{Tr}(J_-^k J_z^l J_+^k) = \sum_{m=-j+k}^j (k-m)^l \frac{(j+m)!(j-m+k)!}{(j+m-k)!(j-m)!}. \tag{3.2}$$

Substituting $t = j + m - k$ in (3.2) one gets:

$$\text{Tr}(J_-^k J_z^l J_+^k) = \sum_{t=0}^{2j-k} (j-t)^l \frac{(k+t)!(2j-t)!}{t!(2j-k-t)!}. \tag{3.3}$$

Introducing again u defined by (2.4), and expanding $(j-t)^l$ in powers of j , (3.3) transforms to:

$$\text{Tr}(J_-^k J_z^l J_+^k) = k!^2 \sum_{i=0}^l \binom{l}{i} (-1)^i j^{l-i} \sum_{t=0}^u t^i \binom{k+t}{t} \binom{u+k-t}{u-t}. \tag{3.4}$$

3.1. Evaluation of the last sum in (3.4)

By using (2.12)–(2.15) the last sum in (3.4) can be brought to the form:

$$\sum_{t=0}^u t^i \binom{k+t}{t} \binom{u+k-t}{u-t} = (-1)^u \left[\sum_{t=0}^u t^i \binom{-k-1}{t} \Delta^t \right] \binom{-k-1}{u}. \tag{3.5}$$

The right-hand side of (3.5) can be written as:

$$\left(\frac{d}{d\alpha}\right)^i (-1)^u \left[\sum_{t=0}^u \binom{-k-1}{t} \Delta^t e^{\alpha t} \right] \binom{-k-1}{u} \Big|_{\alpha=0},$$

or as

$$\left(\frac{d}{d\alpha}\right)^i (-1)^u \left[\sum_{t=0}^{\infty} \binom{-k-1}{t} \Delta^t e^{\alpha t} \right] \binom{-k-1}{u} \Big|_{\alpha=0}, \tag{3.6}$$

since all terms with $t > u$ vanish. Replacing the expression in square brackets by the formal sum of the series, (3.6) becomes:

$$\left(\frac{d}{d\alpha}\right)^i (-1)^u (1 + \Delta e^{\alpha})^{-k-1} \binom{-k-1}{u} \Big|_{\alpha=0}. \tag{3.7}$$

Applying Faà di Bruno's formula (Abramowitz and Stegun 1970) to (3.7) one easily gets

$$\begin{aligned} & \sum_{t=0}^u t^i \binom{k+t}{t} \binom{u+k-t}{u-t} \\ &= (-1)^u \sum_{m=0}^i m! \binom{-k-1}{m} \mathbf{S}_i^{(m)} (1 + \Delta e^{\alpha})^{-k-1-m} (\Delta e^{\alpha})^m \Big|_{\alpha=0} \binom{-k-1}{u} \\ &= (-1)^u \sum_{m=0}^i m! \binom{-k-1}{m} \mathbf{S}_i^{(m)} E^{-k-1-m} \Delta^m \binom{-k-1}{u}. \end{aligned} \tag{3.8}$$

where $\mathbf{S}_i^{(m)}$ denotes a Stirling number of the second kind, which in closed form is defined by (Abramowitz and Stegun 1970)

$$\mathbf{S}_n^{(m)} = \frac{1}{m!} \sum_{k=0}^m (-1)^{m-k} \binom{m}{k} k^n. \tag{3.9}$$

After operating with Δ^m and E^{-k-1-m} on the binomial coefficient, the expression (3.8) reduces to

$$\sum_{t=0}^u t^i \binom{k+t}{t} \binom{u+k-t}{u-t} = (-1)^u \sum_{m=0}^i m! \binom{-k-1}{m} \mathbf{S}_i^{(m)} \binom{-2k-2-m}{u-m}.$$

Making further use of (2.13) and (2.14) one deduces from this expression the formula

$$\sum_{t=0}^u t^i \binom{k+t}{t} \binom{u+k-t}{u-t} = \sum_{m=0}^i m! \mathbf{S}_i^{(m)} \binom{k+m}{m} \binom{2k+u+1}{2k+m+1}. \tag{3.10}$$

Substituting (3.10) into (3.4) one obtains:

$$\begin{aligned} \text{Tr}(J_-^k J_z^l J_+^k) &= k!^2 \sum_{i=0}^l \binom{l}{i} (-1)^i j^{l-i} \sum_{m=0}^i m! \mathbf{S}_i^{(m)} \binom{k+m}{m} \binom{2k+u+1}{2k+m+1} \\ &= k!^2 \sum_{m=0}^l m! \binom{k+m}{m} \binom{2k+u+1}{2k+m+1} \sum_{i=m}^l \binom{l}{i} (-1)^i j^{l-i} \mathbf{S}_i^{(m)}, \end{aligned} \tag{3.11}$$

which, due to (2.4) and (2.8), may be written as

$$\text{Tr}(J_-^k J_z^l J_+^k) = \text{Tr}(J_-^k J_+^k) A(j, k, l), \tag{3.12a}$$

$$A(j, k, l) = \sum_{m=0}^l \frac{(k+m)!(2k+1)(2j-k)!}{k!(2k+m+1)!(2j-k-m)!} \sum_{i=m}^l \binom{l}{i} (-1)^i j^{l-i} \mathbf{S}_i^{(m)}. \tag{3.12b}$$

$A(j, k, l)$ is polynomial with respect to j , of degree not exceeding the value l . Also, since $\mathbf{S}_0^{(0)} = 1$, it is clear from (3.12b) that $A(j, k, 0) = 1$.

In appendix 1 we present the explicit forms for $\text{Tr}(J_-^k J_z^l J_+^k)$ for $0 \leq l \leq 7$, and general k value. These expressions are expanded as powers of j and at the same time as powers of η with η the eigenvalue of the J^2 operator. We remark that all these traces are polynomials of η , a property generally proved by Subramanian and Devanathan (1974). These authors have shown that each trace of a product F of k operators J_- , k operators J_+ and l operators J_z can always be expanded as

$$\text{Tr } F = (2j+1)F(\eta), \tag{3.13}$$

where $F(\eta)$ is a polynomial in η , of degree $k + \frac{1}{2}l$ if l is even, and of degree $k + \frac{1}{2}(l-1)$ if l is odd. As a consequence one can write $\text{Tr}(J_-^k J_z^l J_+^k) = (2j+1)G(\eta)$, with $G(\eta)$ a polynomial in η of degree k . It then follows from (3.12) that $A(j, k, l)$ has to be a polynomial in η of degree $\frac{1}{2}l$ if l is even, and of degree $\frac{1}{2}(l-1)$ if l is odd. The reader can check that this is true for the special cases presented in appendix 1.

3.2. Coefficients of the powers j^l and j^{l-1} of $A(j, k, l)$

From (3.12b) it follows that $A(j, k, l)$ can be expanded as

$$A(j, k, l) = \sum_{i=0}^l j^i a_i(k, l), \tag{3.14}$$

and we proceed with the evaluation of the functions $a_i(k, l)$ and $a_{i-1}(k, l)$.

A careful analysis of the right-hand side of (3.12b) shows that the only contributions to $a_i(k, l)$ come from the terms with $i = m$, leaving us with the form

$$a_i(k, l) = \frac{(2k+1)!}{k!} \sum_{m=0}^l \frac{(k+m)!}{(2k+m+1)!} \binom{l}{m} (-2)^m. \tag{3.15}$$

In appendix 2 it is shown that (3.15) can be transformed to

$$a_i(k, l) = \frac{(2k+1)!}{k! 2^{2k+2}} \int_0^\pi d\theta \sin^{2k+1} \theta \cos^l \theta, \tag{3.16}$$

from which it is deduced that

$$a_i(k, l) = \begin{cases} 0 & \text{(odd } l), \\ \frac{l!}{((l/2)! 2^{l/2+1} (2k+3)(2k+5) \dots (2k+l+1))} & \text{(even } l \geq 2). \end{cases} \tag{3.17}$$

Analysing the expression (3.12b) further it is seen that there are terms with $i = m$ and $i = m + 1$ which contribute to $a_{i-1}(k, l)$, i.e.:

$$a_{i-1}(k, l) = \frac{(2k+1)!}{k!} \sum_{m=1}^l \frac{(k+m)!}{(2k+m+1)!} (-1)^{m-1} \left[2^m \binom{l}{m+1} \mathbf{S}_{m+1}^{(m)} + 2^{m-1} \binom{l}{m} \sum_{i=0}^{m-1} (k+i) \right]. \tag{3.18}$$

By using the relation

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

and with the aid of the formula (Abramowitz and Stegun 1970)

$$\mathbf{S}_{(m+1)}^{(m)} = \binom{m+1}{2},$$

(3.18) can be reduced to

$$a_{l-1}(k, l) = \frac{(2k+1)!}{k!} l(l+k-1) \sum_{m=1}^l \frac{(k+m)!}{(2k+m+1)!} \binom{l-1}{m-1} (-2)^{m-1} + \frac{(2k+1)!}{k!} l(l-1) \sum_{m=2}^l \frac{(k+m)!}{(2k+m+1)!} \binom{l-2}{m-2} (-2)^{m-2}. \quad (3.19)$$

In appendix 2 it is proved that

$$\frac{(2k+1)!}{k!} \sum_{m=1}^l \frac{(k+m)!}{(2k+m+1)!} \binom{l-1}{m-1} (-2)^{m-1} = \begin{cases} -\frac{1}{2}a_l(k, l) & (\text{even } l), \\ \frac{1}{2}a_{l-1}(k, l-1) & (\text{odd } l) \end{cases} \quad (3.20)$$

and

$$\frac{(2k+1)!}{k!} \sum_{m=2}^l \frac{(k+m)!}{(2k+m+1)!} \binom{l-2}{m-2} (-2)^{m-2} = \begin{cases} \frac{1}{4}(a_l(k, l) + a_{l-2}(k, l-2)) & (\text{even } l), \\ -\frac{1}{2}a_{l-1}(k, l-1) & (\text{odd } l). \end{cases} \quad (3.21)$$

Substituting the results (3.20) and (3.21) for odd l values in (3.18), one obtains

$$a_{l-1}(k, l) = \frac{1}{2}lka_{l-1}(k, l-1) \quad (\text{odd } l), \quad (3.22)$$

whereas for even l values one obtains

$$a_{l-1}(k, l) = \frac{1}{4}l[(l-1)a_{l-2}(k, l-2) - (l+2k-1)a_l(k, l)] = \frac{5}{2}la_l(k, l) \quad (\text{even } l). \quad (3.23)$$

In the last step use has been made of the relation

$$(l-1)a_{l-2}(k, l-2) = (2k+l+1)a_l(k, l),$$

which follows immediately from the explicit form (3.17). The reader can convince himself that the relations (3.17), (3.22) and (3.23) are indeed satisfied for the special cases mentioned in appendix 1.

4. Evaluation of other traces

Starting from the expression deduced for $\text{Tr}(J_-^k J_z^l J_+^k)$ one can derive several formulae of traces of arbitrary products of angular momentum operators. Therefore it is

necessary to use the commutation relations between the angular momentum operators in the spherical basis:

$$[J_z, J_{\pm}] = J_z J_{\pm} - J_{\pm} J_z = \pm J_{\pm}, \tag{4.1}$$

$$[J_+, J_-] = J_+ J_- - J_- J_+ = 2J_z. \tag{4.2}$$

The number of traces which have to be considered can be reduced due to symmetry arguments. The following rules simplify the calculations.

(a) Each trace in the spherical basis, where the number of raising operators is not equal to the number of lowering operators, is identical zero. This feature has been mentioned by Ambler *et al* (1962b) and has been proved by Subramanian and Devanathan (1974).

(b) Taking into account the explicit form (3.1) of $\text{Tr}(J_+^k J_z^l J_-^k)$ and the symmetry properties of this expression, one can easily verify that:

$$\begin{aligned} &\text{Tr}(J_-^k J_z^l J_+^k) \\ &= \sum (m+k)^l \frac{(j-m)!(j+m+k)!}{(j-m-k)!(j+m)!} \\ &= \sum (k-m)^l \frac{(j+m)!(j-m+k)!}{(j+m-k)!(j-m)!} = (-1)^l \text{Tr}(J_+^k J_z^l J_-^k). \end{aligned} \tag{4.3}$$

Thus, if J_- is substituted for J_+ and J_+ for J_- the trace $\text{Tr}(J_-^k J_z^l J_+^k)$ is unchanged when J_z occurs an even number of times, and changes only in sign when J_z occurs an odd number of times. Later on we shall show that all traces considered can be expressed in terms of traces of the form $\text{Tr}(J_-^k J_z^l J_+^k)$. In this way this substitution rule is a general rule, valid for all traces determined in the spherical basis.

4.1. Traces of the form $\text{Tr}(J_+^k J_z^{l-n} J_- J_z^n J_-^{k-1})$, $\text{Tr}(J_-^k J_z^{l-n} J_+ J_z^n J_+^{k-1})$ and $\text{Tr}(J_+^{k-1} J_z^m J_+ J_z^{l-n-m} J_- J_z^n J_-^{k-1})$

We start from $\text{Tr}(J_+^k J_z^l J_-^k)$, well defined by (4.3) and (3.12) and apply the commutation relation (4.1) to obtain:

$$\begin{aligned} &\text{Tr}(J_+^k J_z^l J_-^k) \\ &= \text{Tr}(J_+^k J_z^{l-1} (J_z J_-) J_-^{k-1}) \\ &= \text{Tr}(J_+^k J_z^{l-1} J_- J_z J_-^{k-1}) - \text{Tr}(J_+^k J_z^{l-1} J_-^k) \end{aligned}$$

from which it follows that

$$\text{Tr}(J_+^k J_z^{l-1} J_- J_z J_-^{k-1}) = \text{Tr}(J_+^k J_z^l J_-^k) + \text{Tr}(J_+^k J_z^{l-1} J_-^k). \tag{4.4}$$

Now applying (4.1) to (4.4), one gets:

$$\begin{aligned} &\text{Tr}(J_+^k J_z^{l-1} J_- J_z J_-^{k-1}) \\ &= \text{Tr}(J_+^k J_z^{l-2} (J_z J_-) J_z J_-^{k-1}) \\ &= \text{Tr}(J_+^k J_z^{l-2} J_- J_z^2 J_-^{k-1}) - \text{Tr}(J_+^k J_z^{l-2} J_- J_z J_-^{k-1}). \end{aligned}$$

Taking into account (4.4) and the preceding relation, one finds

$$\text{Tr}(J_+^k J_z^{l-2} J_- J_z^2 J_-^{k-1}) = \text{Tr}(J_+^k J_z^l J_-^k) + 2 \text{Tr}(J_+^k J_z^{l-1} J_-^k) + \text{Tr}(J_+^k J_z^{l-2} J_-^k). \tag{4.5}$$

The expressions (4.4) and (4.5) can be denoted, respectively for $s = 1$ and $s = 2$, as follows:

$$\text{Tr}(J_+^k J_z^{l-s} J_- J_z^s J_-^{k-1}) = \sum_{t=0}^s \binom{s}{t} \text{Tr}(J_+^k J_z^{l-t} J_-^t). \tag{4.6}$$

We now prove by the method of induction that relation (4.6) is valid for $s = n + 1$, if it is true for $s = n$. Again applying the commutation relation (4.1) to (4.6) for $s = n$, one deduces

$$\begin{aligned} &\text{Tr}(J_+^k J_z^{l-n} J_- J_z^n J_-^{k-1}) \\ &= \text{Tr}(J_+^k J_z^{l-(n+1)} J_z J_- J_z^n J_-^{k-1}) \\ &= \text{Tr}(J_+^k J_z^{l-(n+1)} J_- J_z^{n+1} J_-^{k-1}) - \text{Tr}(J_+^k J_z^{l-(n+1)} J_- J_z^n J_-^{k-1}) \end{aligned}$$

from which it follows that:

$$\text{Tr}(J_+^k J_z^{l-(n+1)} J_- J_z^{n+1} J_-^{k-1}) = \text{Tr}(J_+^k J_z^{l-n} J_- J_z^n J_-^{k-1}) + \text{Tr}(J_+^k J_z^{(l-1)-n} J_- J_z^n J_-^{k-1}),$$

which, due to (4.6), transforms to:

$$\text{Tr}(J_+^k J_z^{l-(n+1)} J_- J_z^{n+1} J_-^{k-1}) = \sum_{t=0}^n \binom{n}{t} [\text{Tr}(J_+^k J_z^{l-t} J_-^t) + \text{Tr}(J_+^k J_z^{l-1-t} J_-^t)]$$

or

$$\begin{aligned} &\text{Tr}(J_+^k J_z^{l-(n+1)} J_- J_z^{n+1} J_-^{k-1}) \\ &= \sum_{t=0}^n \binom{n}{t} \text{Tr}(J_+^k J_z^{l-t} J_-^t) + \sum_{t=1}^{n+1} \binom{n}{t-1} \text{Tr}(J_+^k J_z^{l-t} J_-^t) \\ &= \text{Tr}(J_+^k J_z^l J_-^0) + \text{Tr}(J_+^k J_z^{l-n-1} J_-^0) + \sum_{t=1}^n \left[\binom{n}{t} + \binom{n}{t-1} \right] \text{Tr}(J_+^k J_z^{l-t} J_-^t). \end{aligned}$$

Since (Abramowitz and Stegun 1970)

$$\binom{n}{t} + \binom{n}{t-1} = \binom{n+1}{t},$$

the last equation can be written as

$$\text{Tr}(J_+^k J_z^{l-(n+1)} J_- J_z^{n+1} J_-^{k-1}) = \sum_{t=0}^{n+1} \binom{n+1}{t} \text{Tr}(J_+^k J_z^{l-t} J_-^t),$$

showing that (4.6) is generally valid for each $s \in \mathbb{N}$ such that $l - s \geq 0$. In an analogous way one can prove that

$$\text{Tr}(J_-^k J_z^{l-s} J_+ J_z^s J_+^{k-1}) = \sum_{t=0}^s (-1)^t \binom{s}{t} \text{Tr}(J_-^k J_z^{l-t} J_+^t),$$

which due to (4.3) reduces to:

$$\begin{aligned} &\text{Tr}(J_-^k J_z^{l-s} J_+ J_z^s J_+^{k-1}) \\ &= (-1)^l \sum_{t=0}^s \binom{s}{t} \text{Tr}(J_+^k J_z^{l-t} J_-^t) = (-1)^l \text{Tr}(J_+^k J_z^{l-s} J_- J_z^s J_-^{k-1}), \end{aligned} \tag{4.7}$$

which demonstrates that for this special trace the substitution rule (b) is indeed appropriate.

Proceeding in the same way and making use of (4.6) one easily gets:

$$\begin{aligned} \text{Tr}(J_+^{k-1} J_z^m J_+ J_z^{l-n-m} J_- J_z^n J_-^{k-1}) \\ = \sum_{t=0}^m \binom{m}{t} \text{Tr}(J_+^k J_z^{l-n-t} J_- J_z^n J_-^{k-1}) \\ = \sum_{s=0}^n \sum_{t=0}^m \binom{n}{s} \binom{m}{t} \text{Tr}(J_+^k J_z^{l-s-t} J_-^k). \end{aligned} \tag{4.8}$$

4.2. Analytic expression for some other traces

Again starting from $\text{Tr}(J_+^k J_z^l J_-^k)$ or from (4.6), (4.7) or (4.8) and using one of the commutation relations (4.1) and (4.2), one can show that many traces can be expressed in terms of traces of the form $\text{Tr}(J_+^k J_z^l J_-^k)$. Since the derivation of these expressions follows in a similar way to those discussed in the previous section, we shall state here only the results. With the aid of the formulae mentioned it is possible to derive, besides all the results tabulated by Ambler *et al* (1962a) for $\text{Tr}(J_a^p J_b^q J_c^r \dots)$ with a, b, c, \dots equal to $+, -$ or z and $p + q + r + \dots \leq 7$, also the expressions for an unlimited number of other traces. The following relations have been considered:

(a)

$$\text{Tr}(J_+^{k-1} J_- J_+ J_-^{k-1}) = \text{Tr}(J_+^k J_-^k) - 2 \text{Tr}(J_+^{k-1} J_z J_-^{k-1}), \tag{4.9}$$

(b)

$$\begin{aligned} \text{Tr}(J_+^{k-2} J_- J_+ J_- J_+ J_-^{k-2}) \\ = \text{Tr}(J_+^k J_-^k) - 6 \text{Tr}(J_+^{k-1} J_z J_-^{k-1}) + 4 \text{Tr}(J_+^{k-2} J_z^2 J_-^{k-2}) - 4 \text{Tr}(J_+^{k-1} J_-^{k-1}), \end{aligned} \tag{4.10}$$

(c)

$$\text{Tr}(J_+^{k-1} J_z^m J_- J_+ J_z^n J_-^{k-1}) = \text{Tr}(J_+^{k-1} J_z^m J_+ J_- J_z^n J_-^{k-1}) - 2 \text{Tr}(J_+^{k-1} J_z^{m+n+1} J_-^{k-1})$$

which, due to (4.8), reduces to

$$\begin{aligned} \text{Tr}(J_+^{k-1} J_z^m J_- J_+ J_z^n J_-^{k-1}) \\ = \sum_{s=0}^n \sum_{t=0}^m \binom{n}{s} \binom{m}{t} \text{Tr}(J_+^k J_z^{m+n-s-t} J_-^k) - 2 \text{Tr}(J_+^{k-1} J_z^{m+n+1} J_-^{k-1}), \end{aligned} \tag{4.11}$$

(d)

$$\begin{aligned} \text{Tr}(J_+^k J_z^{l-n} J_- J_z^{n-1} J_-^p J_z J_-^{k-p-1}) \\ = \text{Tr}(J_+^k J_z^{l-n} J_- J_z^n J_-^{k-1}) + p \text{Tr}(J_+^k J_z^{l-n} J_- J_z^{n-1} J_-^{k-1}) \\ = \sum_{s=0}^n \binom{n}{s} \text{Tr}(J_+^k J_z^{l-s} J_-^k) + p \sum_{s=0}^{n-1} \binom{n-1}{s} \text{Tr}(J_+^k J_z^{l-1-s} J_-^k), \end{aligned} \tag{4.12}$$

(e)

$$\begin{aligned} \text{Tr}(J_+^{k-1} J_z^m J_- J_+ J_z^{n-1} J_-^p J_z J_-^{k-p-1}) \\ = \text{Tr}(J_+^{k-1} J_z^m J_- J_+ J_z^n J_-^{k-1}) + p \text{Tr}(J_+^{k-1} J_z^m J_- J_+ J_z^{n-1} J_-^{k-1}). \end{aligned} \tag{4.13}$$

The right-hand side of (4.13) can be expressed, from (4.11), in terms of traces of the form $\text{Tr}(J_+^k J_z^l J_-^k)$.

(f)

$$\begin{aligned} &\text{Tr}(J_+^{k-1} J_z^m J_+ J_z^{l-n-m} J_- J_z^{n-1} J_- J_z J_-^{k-p-1}) \\ &= \text{Tr}(J_+^{k-1} J_z^m J_+ J_z^{l-n-m} J_- J_z^n J_-^{k-1}) + p \text{Tr}(J_+^{k-1} J_z^m J_+ J_z^{l-n-m} J_- J_z^{n-1} J_-^{k-1}), \end{aligned} \tag{4.14}$$

whereby the right-hand side can be written as sums over $\text{Tr}(J_+^k J_z^l J_-^k)$, due to (4.8).

(g)

$$\begin{aligned} &\text{Tr}(J_+^{k-1} J_z^l J_- J_+ J_-^{k-p}) \\ &= \text{Tr}(J_+^{k-1} J_z^l J_+ J_-^k) - 2 \sum_{t=0}^{p-1} \text{Tr}(J_+^{k-1} J_z^l J_- J_+ J_-^{k-t-1}). \end{aligned} \tag{4.15}$$

The right-hand side of (4.15) can be expressed, from (4.8) and (4.12), in terms of traces of the form $\text{Tr}(J_+^k J_z^l J_-^k)$.

4.3. Evaluation of $\text{Tr}(J_z^{2p})$

There are several possibilities to determine $\text{Tr}(J_z^{2p})$. In the framework of the present paper we can derive a general expression for that trace by putting $k = 0$ in (3.12). Secondly, one can show that:

$$\text{Tr}(J_z^{2p}) = \text{Tr}(J_- J_z^{2p-1} J_+), \tag{4.16}$$

a result which is easily calculable for $2p \leq 8$, from appendix 1. To prove (4.16) one starts from (3.1), written down for the special value $k = 1$,

$$\text{Tr}(J_- J_z^{2p-1} J_+) = \sum_{m=-j}^{j-1} (m+1)^{2p-1} (j-m)(j+m+1),$$

in which we replace $m + 1$ by m and adjust the lower and upper limits in the sum to obtain:

$$\text{Tr}(J_- J_z^{2p-1} J_+) = \sum_{m=-j-1}^j m^{2p-1} (j-m+1)(j+m).$$

One can easily see that this relation can be transformed to:

$$\begin{aligned} &\text{Tr}(J_- J_z^{2p-1} J_+) \\ &= \sum_{m=-j}^j m^{2p-1} (\eta + m - m^2) \\ &= \eta \text{Tr}(J_z^{2p-1}) + \text{Tr}(J_z^{2p}) - \text{Tr}(J_z^{2p+1}). \end{aligned}$$

Since traces of odd powers of J_z are identical zero, (4.16) has been proved. Thirdly, traces of the form $\text{Tr}(J_z^{2p})$ for $p \geq 1$ can be expressed in terms of Bernoulli polynomials B_{2p+1} . This method has been used in some previous papers (Ambler *et al* 1962b, Subramanian 1974). One gets the following result:

$$\text{Tr}(J_z^{2p}) = \frac{2}{2p+1} B_{2p+1}(j+1) \quad (p \geq 1). \tag{4.17}$$

A last method, which we would like to mention here, is based on properties of Stirling numbers of the first and second kind. The trace of J_z^{2p} in the representation $|j m\rangle$ (see § 2) is defined by:

$$\text{Tr}(J_z^{2p}) = \sum_{m=-j}^j \langle j m | J_z^{2p} | j m \rangle = \sum_{m=-j}^j m^{2p} = 2 \sum_{m=0}^j m^{2p} - \delta_{p0}.$$

The last sum can be expressed for all values of p by means of Stirling numbers of the second kind $\mathbf{S}_n^{(m)}$ (Abramowitz and Stegun 1970):

$$\begin{aligned} \text{Tr}(J_z^{2p}) &= 2 \sum_{m=0}^{2p} m! \mathbf{S}_{2p}^{(m)} \binom{j+1}{m+1} - \delta_{p0} \\ &= 2 \sum_{m=0}^{2p} \frac{1}{m+1} \mathbf{S}_{2p}^{(m)} (j+1)(j)(j-1) \dots (j-m+1) - \delta_{p0}. \end{aligned}$$

By using one of the generating functions for the Stirling numbers of the first kind $S_n^{(m)}$ (Abramowitz and Stegun 1970) the previous relation reduces to:

$$\text{Tr}(J_z^{2p}) = 2 \sum_{m=0}^{2p} \frac{1}{m+1} \mathbf{S}_{2p}^{(m)} \sum_{s=0}^{m+1} S_{m+1}^{(s)} (j+1)^s - \delta_{p0}. \tag{4.18}$$

By equating (4.17) and (4.18) we obtain a relation, which is valid for all $p \geq 1$ between the Bernoulli polynomials of odd rank and Stirling numbers of the first and second kind:

$$B_{2p+1}(j+1) = (2p+1) \sum_{m=0}^{2p} \frac{1}{m+1} \mathbf{S}_{2p}^{(m)} \sum_{s=0}^{m+1} S_{m+1}^{(s)} (j+1)^s. \tag{4.19}$$

Using the property which exists between the derivative of a Bernoulli polynomial and the polynomial itself:

$$B'_n(x) = nB_{n-1}(x),$$

one can deduce from (4.19) the following expression for the Bernoulli polynomials of even rank:

$$B_{2p}(j+1) = \sum_{m=0}^{2p} \frac{1}{m+1} \mathbf{S}_{2p}^{(m)} \sum_{s=0}^{m+1} S_{m+1}^{(s)} s (j+1)^{s-1}. \tag{4.20}$$

Following Abramowitz and Stegun (1970) we denote the polynomials as a series expansion in the following way:

$$B_n(x) = \sum_{k=0}^n b_k^{(n)} x^k$$

where the coefficients $b_k^{(n)}$ are tabulated in Abramowitz and Stegun (1970) up to $n = 15$. From (4.19) and (4.20) one easily deduces analytic expressions for these coefficients ($p \geq 1$):

$$b_k^{(2p+1)} = (2p+1) \sum_{m=0}^{2p} \frac{1}{m+1} \mathbf{S}_{2p}^{(m)} S_{m+1}^{(k)}, \tag{4.21a}$$

$$b_k^{(2p)} = \sum_{m=0}^{2p} \frac{k+1}{m+1} \mathbf{S}_{2p}^{(m)} S_{m+1}^{(k+1)}. \tag{4.21b}$$

The Bernoulli numbers, denoted by B_n , are equal to $b_0^{(n)}$. From (4.21a) it follows that all B_{2p+1} (for $p \geq 1$) are equal to zero, since $S_{m+1}^{(0)} = 0$ for all values of m . From (4.21b) one obtains for $p \geq 1$

$$B_{2p} \equiv b_0^{(2p)} = \sum_{m=0}^{2p} \frac{1}{m+1} \mathbf{S}_{2p}^{(m)} \mathbf{S}_{m+1}^{(1)}.$$

Since (Abramowitz and Stegun 1970):

$$S_{m+1}^{(1)} = (-1)^m m!$$

the last relation transforms to:

$$B_{2p} = \sum_{m=0}^{2p} (-1)^m \frac{m!}{m+1} \mathbf{S}_{2p}^{(m)}. \tag{4.22}$$

Similar relations for the coefficients $b_k^{(n)}$ and the Bernoulli numbers B_n have been deduced using completely different methods by Jordan (1965).

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Appendix 1. Explicit form of $\text{Tr}(J_-^k J_z^l J_+^k)$ for $0 \leq l \leq 7$

(a) $l = 0$

$$\text{Tr}(J_-^k J_+^k) = \frac{k!^2 (2j+k+1)!}{(2k+1)! (2j-k)!} = \begin{cases} 2j+1 & (k=0) \\ \frac{k!}{(2k+1)!} (2j+1) \prod_{i=1}^k (4\eta+1-i^2) & (k \neq 0). \end{cases}$$

(b) $l = 1$

$$\text{Tr}(J_-^k J_z J_+^k) = \frac{1}{2} k \text{Tr}(J_-^k J_+^k).$$

(c) $l = 2$

$$\begin{aligned} \text{Tr}(J_-^k J_z^2 J_+^k) &= \frac{1}{2(2k+3)} \text{Tr}(J_-^k J_+^k) [2j^2 + 2j + k(k^2 + k - 1)] \\ &= \frac{1}{2(2k+3)} \text{Tr}(J_-^k J_+^k) [2\eta + k(k^2 + k - 1)]. \end{aligned}$$

(d) $l = 3$

$$\begin{aligned} \text{Tr}(J_-^k J_z^3 J_+^k) &= \frac{k}{4(2k+3)} \text{Tr}(J_-^k J_+^k) [6j^2 + 6j + k(k^2 - 3)] \\ &= \frac{k}{4(2k+3)} \text{Tr}(J_-^k J_+^k) [6\eta + k(k^2 - 3)]. \end{aligned}$$

(e) $l = 4$

$$\begin{aligned} \text{Tr}(J_-^k J_z^4 J_+^k) &= \frac{1}{4(2k+3)(2k+5)} \text{Tr}(J_-^k J_+^k) [12j^4 + 24j^3 + 4(3k^3 + 6k^2 - 4k + 2)j^2 \\ &\quad + 4(3k^3 + 6k^2 - 4k - 1)j + k(k^5 + k^4 - 9k^3 - 11k^2 + 6k + 2)] \\ &= \frac{1}{4(2k+3)(2k+5)} \text{Tr}(J_-^k J_+^k) [12\eta^2 + 4(3k^3 + 6k^2 - 4k - 1)\eta \\ &\quad + k(k^5 + k^4 - 9k^3 - 11k^2 + 6k + 2)]. \end{aligned}$$

(f) $l = 5$

$$\begin{aligned} \text{Tr}(J_-^k J_z^5 J_+^k) &= \frac{k}{8(2k+3)(2k+5)} \text{Tr}(J_-^k J_+^k) [60j^4 + 120j^3 + 20(k^3 + k^2 - 4k + 2)j^2 \\ &\quad + 20(k^3 + k^2 - 4k - 1)j + k(k^5 - k^4 - 15k^3 - 5k^2 + 30k + 10)] \\ &= \frac{k}{8(2k+3)(2k+5)} \text{Tr}(J_-^k J_+^k) [60\eta^2 + 20(k^3 + k^2 - 4k - 1)\eta \\ &\quad + k(k^5 - k^4 - 15k^3 - 5k^2 + 30k + 10)]. \end{aligned}$$

(g) $l = 6$

$$\begin{aligned} \text{Tr}(J_-^k J_z^6 J_+^k) &= \frac{1}{8(2k+3)(2k+5)(2k+7)} \text{Tr}(J_-^k J_+^k) \\ &\quad \times [120j^6 + 360j^5 + 60(3k^3 + 9k^2 - 5k + 4)j^4 \\ &\quad + 40(9k^3 + 27k^2 - 15k - 3)j^3 \\ &\quad + 2(15k^6 + 45k^5 - 135k^4 - 285k^3 + 316k^2 - 54k - 40)j^2 \\ &\quad + 2(15k^6 + 45k^5 - 135k^4 - 375k^3 + 46k^2 + 96k + 20)j \\ &\quad + k^9 - 31k^7 - 45k^6 + 150k^5 + 277k^4 - 4k^3 - 76k^2 - 20k] \\ &= \frac{1}{8(2k+3)(2k+5)(2k+7)} \text{Tr}(J_-^k J_+^k) [120\eta^3 + 60(3k^3 + 9k^2 - 5k - 2)\eta^2 \\ &\quad + 2(15k^6 + 45k^5 - 135k^4 - 375k^3 + 46k^2 + 96k + 20)\eta \\ &\quad + k^9 - 31k^7 - 45k^6 + 150k^5 + 277k^4 - 4k^3 - 76k^2 - 20k]. \end{aligned}$$

(h) $l = 7$

$$\begin{aligned} \text{Tr}(J_-^k J_z^7 J_+^k) &= \frac{k}{8(2k+3)(2k+5)(2k+7)} \text{Tr}(J_-^k J_+^k) [840j^6 + 2520j^5 \\ &\quad + 420(k^3 + 2k^2 - 5k + 4)j^4 + 840(k^3 + 2k^2 - 5k - 1)j^3 \\ &\quad + 7(6k^6 + 6k^5 - 110k^4 - 90k^3 + 352k^2 - 108k - 80)j^2 \\ &\quad + 7(6k^6 + 6k^5 - 110k^4 - 150k^3 + 232k^2 + 192k + 40)j \\ &\quad + k^9 - 3k^8 - 40k^7 + 14k^6 + 385k^5 + 329k^4 - 518k^3 - 532k^2 - 140k] \\ &= \frac{k}{8(2k+3)(2k+5)(2k+7)} \text{Tr}(J_-^k J_+^k) [840\eta^3 + 420(k^3 + 2k^2 - 5k - 2)\eta^2 \end{aligned}$$

$$+ 7(6k^6 + 6k^5 - 110k^4 - 150k^3 + 232k^2 + 192k + 40)\eta + k^9 - 3k^8 - 40k^7 + 14k^6 + 385k^5 + 329k^4 - 518k^3 - 532k^2 - 140k].$$

Appendix 2. Formulae for the evaluation of $a_l(k, l)$ and $a_{l-1}(k, l)$

Using the integral representation (Dingle 1973)

$$\frac{(s + \alpha)!}{(s + \beta)!} = \frac{1}{\beta - \alpha - 1} \int_0^1 du u^{s+\alpha} (1-u)^{\beta-\alpha-1}, \tag{A.2.1}$$

(3.15) is transformed to:

$$\begin{aligned} a_l(k, l) &= \frac{(2k + 1)!}{k!^2} \int_0^1 du u^k (1-u)^k \sum_{m=0}^l \binom{l}{m} (-2u)^m \\ &= \frac{(2k + 1)!}{k!^2} \int_0^1 du u^k (1-u)^k (1-2u)^l \\ &= \frac{(2k + 1)!}{k!^2} \frac{1}{2^{2k+2}} \int_0^\pi d\theta \sin^{2k+1} \theta \cos^l \theta, \end{aligned} \tag{A.2.2}$$

where in the last step the substitution $u = \sin^2 \theta/2$ has been made. It is clear that for odd l the integral in (A.2.2) vanishes. For even l using one of the integral representations of the beta function (Gradshteyn and Ryzhik 1965), i.e.

$$\int_0^{\pi/2} d\theta \sin^{\mu-1} \theta \cos^{\nu-1} \theta = \frac{1}{2} B(\mu/2, \nu/2) \tag{A.2.3}$$

one obtains successively instead of (A.2.2):

$$\begin{aligned} a_l(k, l) &= \frac{(2k + 1)!}{k!^2} \frac{1}{2^{2k+2}} B\left(k + 1, \frac{l+1}{2}\right) = \frac{(2k + 1)!}{k!} \frac{1}{2^{2k+2}} \frac{\Gamma((l+1)/2)}{\Gamma((2k+l+3)/2)} \\ &= \frac{(2k + 1)!}{k!} \frac{1}{2^{2k+2}} 2^{(2k+2)/2} \frac{(l-1)(l-3)\dots 3 \cdot 1}{(2k+l+1)(2k+l-1)\dots 3 \cdot 1} \\ &= \frac{1}{2^{k+1}} \frac{(2k+1)(2k-1)\dots 3 \cdot 1 k! 2^k}{k!(2k+l+1)(2k+l-1)\dots 3 \cdot 1} \frac{l(l-1)(l-2)\dots 2 \cdot 1}{2^{l/2} l! (\frac{1}{2}l-1)\dots 2 \cdot 1} \\ &= \frac{l!}{(\frac{1}{2}l)! 2^{l/2-1}} \frac{1}{(2k+3)(2k+5)\dots (2k+l+1)}. \end{aligned} \tag{A.2.4}$$

We calculate the expression

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

for $i = 1, 2$. Proceeding in the same way as in deriving (A.2.2), one obtains:

$$\phi_i(k, l) = \frac{(2k + 1)!}{k!^2} \frac{1}{2^{2k+i+2}} \int_0^\pi \sin^{2k+1} \theta \cos^{l-i} \theta (1 - \cos \theta)^i d\theta. \tag{A.2.5}$$

In particular one has

$$\phi_1(k, l) = \frac{1}{2} \frac{(2k+1)!}{k!^2} \frac{1}{2^{2k+2}} \int_0^\pi \sin^{2k+1} \theta (\cos^{l-1} \theta - \cos^l \theta) d\theta,$$

or

$$\phi_1(k, l) = \begin{cases} -\frac{1}{2} a_l(k, l) & \text{if } l \text{ is even,} \\ \frac{1}{2} a_{l-1}(k, l-1) & \text{if } l \text{ is odd,} \end{cases} \quad (\text{A.2.6})$$

where (A.2.2) has been used in reversed order. In the same way one obtains:

$$\phi_2(k, l) = \frac{1}{4} \frac{(2k+1)!}{k!^2} \frac{1}{2^{2k+2}} \int_0^\pi \sin^{2k+1} \theta (\cos^{l-2} \theta - 2 \cos^{l-1} \theta + \cos^l \theta) d\theta,$$

or

$$\phi_2(k, l) = \begin{cases} \frac{1}{4} (a_{l-2}(k, l-2) + a_l(k, l)) & \text{if } l \text{ is even} \\ -\frac{1}{2} a_{l-1}(k, l-1) & \text{if } l \text{ is odd.} \end{cases} \quad (\text{A.2.7})$$

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