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COMMENT

Generating functions for angular momentum traces

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Abstract. Generating functions for $Tr(J_{\lambda}^{2p})$ are obtained, one of them being the character of a representation of the three-dimensional pure rotation group. Recurrence relations for the Bernoulli numbers and the Riemann zeta functions are deduced.

Interest in the study of traces of products of angular momentum matrices has so far been confined to (i) their evaluation (Ambler *et al* 1962a, b, Witschel 1971, 1975, Subramanian and Devanathan 1974, hereafter referred to as I, De Meyer and Vanden Berghe 1978a), (ii) obtaining recurrence relations (De Meyer and Vanden Berghe 1978b, Subramanian and Devanathan 1980, 1985, to be referred to hereafter as II and III, respectively) and (iii) expressing them in terms of familiar functions like the Bernoulli polynomials (Ambler *et al* 1962a, I), hypergeometric functions (Rashid 1979, Ullah 1980) and the Brillouin functions (Subramanian 1986, hereafter referred to as IV). It has been shown in I that the trace of a product of angular momentum matrices (given either in a cartesian or a spherical basis) can be expanded in terms of $Tr(J_{\lambda}^{2p})$, $\lambda = x$, y or z, J_{λ} being the operators for the three cartesian components of angular momentum.

The purpose of this comment is to obtain generating functions for $Tr(J_{\lambda}^{2p})$ and find the nature of its zeros. As a byproduct, sum rules for the Bernoulli numbers and hence for the Riemann zeta functions (Abramowitz and Stegun 1970, to be referred to hereafter as As) are derived.

It is shown in I that

$$\operatorname{Tr}(J_{\lambda}^{2p}) = \sum_{m=-j}^{j} m^{2p} = 2(2p+1)^{-1} B_{2p+1}(j+1)$$
(1)

with $p \ge 0$, j being the angular momentum quantum number in units of \hbar . The Bernoulli polynomials $B_n(x)$ are defined through the generating function (As)

$$f(x, t) = t \exp(xt)(\exp(t) - 1)^{-1}$$

= $\sum_{n=0}^{\infty} B_n(x)t^n/n!.$ (2)

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Now f(x, t) - f(x, -t), x = j + 1, yields, after some simple algebra,

$$g(j, t) = \sinh[(2j+1)t/2][\sinh(t/2)]^{-1}$$

= $\sum_{p=0}^{\infty} \operatorname{Tr}(J_{\lambda}^{2p})t^{2p}/(2p)!.$ (3)

As usual, for any matrix $\mathcal{J}, \mathcal{J}^0 = I$, the unit matrix. If η is the eigenvalue of the J^2 operator, then

$$\eta = j(j+1)$$
 $2j+1 = (4\eta + 1)^{1/2}$. (4)

It follows from equations (3) and (4) that

$$\mathscr{G}(\eta, t) = \sinh[(4\eta + 1)^{1/2} t/2] [\sinh(t/2)]^{-1}$$
$$= \sum_{p=0}^{\infty} \operatorname{Tr}(J_{\lambda}^{2p}) t^{2p} / (2p)!.$$
(5)

With t = x/j, j > 0, in equation (3), we have

$$G(j, x) = \sinh[(2j+1)x/2j][\sinh(x/2j)]^{-1}$$

= $\sum_{p=0}^{\infty} \operatorname{Tr}(J_{\lambda}^{2p})x^{2p}/((2p)!j^{2p}).$ (6)

Since $\partial G(j, x)/\partial x = G(j, x)B_j(x)$, where $B_j(x)$ is the Brillouin function (Van Vleck 1932), one can obtain expressions for $\text{Tr}(J_{\lambda}^{2p})$ in terms of (derivatives of) the Brillouin function (see also IV) as

$$\operatorname{Tr}(J_{\lambda}^{2p}) = j^{2p} \partial^{2p} G(j, x) / \partial x^{2p} \big|_{x=0}.$$
(7)

Substituting $t = i\theta$ in equation (3) and using $\sinh(i\theta) = i \sin \theta$, we have

$$\chi^{(j)}(\theta) = \sin[(2j+1)\theta/2][\sin(\theta/2)]^{-1}$$
$$= \sum_{p=0}^{\infty} (-1)^p \operatorname{Tr}(J_{\lambda}^{2p})\theta^{2p}/(2p)!.$$
(8)

Now $\chi^{(j)}(\theta)$ is the character of a representation—either single- or double-valued—of the three-dimensional pure rotation group, i.e. the trace of a rotation with rotation angle θ (Wigner 1959, Hamermesh 1962, Varshalovich *et al* 1975). Moreover (see Varshalovich *et al* 1975)

$$\chi^{(j)}(\theta) = U_{2j}(\cos(\theta/2)) = C_{2j}^{(1)}(\cos(\theta/2))$$

= $(2j+1) {}_{2}F_{1}(-2j, 2(j+1); \frac{3}{2}; \sin^{2}(\theta/4))$ (9)

where $U_n(x)$ are the Chebyshev polynomials of the second kind (As), $C_n^{(1)}(x)$ the Gegenbauer (ultraspherical) polynomials (As) and $_2F_1(a, b; c; x)$ the Gauss hypergeometric functions (As). It is now clear from equations (3)-(9) that g(j, t), $\mathcal{G}(\eta, t)$, G(j, x), $\chi^{(j)}(\theta)$, $U_{2j}(\cos(\theta/2))$, $C_{2j}^{(1)}(\cos(\theta/2))$, $(2j+1)_2F_1(-2j, 2(j+1); \frac{3}{2}; \sin^2(\theta/4))$ are all generating functions for $\operatorname{Tr}(J_{\lambda}^{2p})$. It is particularly pleasant to note that J_x , J_y and J_z are the generators of rotations (see, e.g., Merzbacher 1970) and the character of a rotation is a generating function for $\operatorname{Tr}(J_{\lambda}^{2p})$. As in the case of the familiar special functions due to, say, Hermite, Legendre and Laguerre, the power series expansion (PSE), pure recurrence relation, etc, can be obtained from the generating function (Rainville 1960, Bell 1968). Thus, for example, using the well known PSE for sinh x and cosech x (AS), we obtain, from equation (5), the PSE for $Tr(J_{\lambda}^{2p})$:

$$\operatorname{Tr}(J_{\lambda}^{2p}) = 2(2p+1)^{-1}4^{-p}(4\eta+1)^{1/2} \sum_{n=0}^{p} {\binom{2p+1}{2n}} (4\eta+1)^{p-n}(1-2^{2n-1})B_{2n}.$$
(10)

The binomial coefficients are denoted by $\binom{n}{r}$. It has been shown in I that for $p \ge 1$

$$\operatorname{Tr}(J_{\lambda}^{2p}) = \Omega G_{p-1}(\eta) = (4\eta + 1)^{1/2} \eta \sum_{i=0}^{p-1} a_i \eta^i$$
(11)

where $G_{p-1}(\eta)$ is a polynomial in η of degree p-1 and $\Omega = \text{Tr}(J^2) = (2j+1)\eta$. In other words, $\text{Tr}(J_{\lambda}^{2p})$ is $(4\eta+1)^{1/2}$ times a polynomial in η of degree p with no constant term. Since (see II)

$$a_0 = 2B_{2p} \qquad p \ge 1 \tag{12}$$

we obtain the following sum rules for B_{2n} from equations (10)-(12), remembering that $B_0 = 1$ (AS):

(i)
$$2\sum_{n=1}^{p} {\binom{2p+1}{2n}} (2^{2n-1}-1)B_{2n} = 1$$
 $p \ge 1$ (13)

(ii)
$$\sum_{n=1}^{p} {\binom{2p+1}{2n}} n(2^{2n-1}-1)B_{2n} = 4^{p-1}(2p+1)B_{2p} \qquad p \ge 2.$$
(14)

However, these sum rules seemed to have failed to attract the attention of Ramanujan (1927) who obtained a number of recurrence relations for B_{2n} using quite different mathematical techniques. As B_{2n} are intimately connected to the Riemann zeta functions $\zeta(2n)$ and $\zeta(1-2n)$ (see As), one can easily obtain from equations (13) and (14) corresponding recurrence relations for $\zeta(2n)$ and $\zeta(1-2n)$ (see also IV). Thus, for example,

$$4\sum_{n=1}^{p} {\binom{2p+1}{2n}} n(1-2^{2n-1})\zeta(1-2n) = 1 \qquad p \ge 1.$$
(15)

Relations (13)-(15) have been checked and found correct for $p \le 18$.

It is clear from equations (10) and (11) that $a_{p-1} = 1/(2p+1) \neq 0$, $p \ge 1$, and hence $G_q(\eta)$, $q \ge 0$, is precisely of degree q in η with real coefficients. Thus $\{G_q(\eta)\}$ form a simple set of real polynomials (Rainville 1960) and hence any real polynomial of degree $n \ge 0$ can be expressed as a unique linear combination of $G_q(\eta)$, $0 \le q \le n$. It has been shown in III that the adjacent coefficients of $G_q(\eta)$, $q \ge 1$, alternate in sign throughout. Hence $G_q(-\eta)$ has all the terms of the same sign (positive (negative) when q is even (odd), $q \ge 1$). Thus there is no variation in sign in the coefficients of $G_q(-\eta)$ has no positive zeros (i.e. $G_q(-\eta) = 0$ has no positive roots) and hence $G_q(\eta)$ has *no negative* zeros. It follows from the fundamental theorem of algebra (see, for example, Korn and Korn 1968) that the zeros of $G_q(\eta)$, $q \ge 1$, are either positive or complex. When $q \ge 1$ is odd, $G_q(\eta)$ has at least one positive zero, as the complex zeros occur in pairs of complex conjugates (cf Korn and Korn 1968). For $p \ge 2$, apart from the obvious zeros, namely 0 and $-\frac{1}{4}$, the zeros of $Tr(J_{\lambda}^{2p})$ (which is a function of

 η) are simply the zeros of $G_{p-1}(\eta)$ (see equations (10) and (11)). It is gratifying to note that the functional dependence of the angular momentum traces exhibits a symmetry between fermions (*j* half-integral) and bosons (*j* integral) as the trace has the same η dependence (see also I) whether *j* is a half-integer or integer.

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