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1990 J. Phys. A: Math. Gen. 23 2689

(http://iopscience.iop.org/0305-4470/23/12/041)

J. Phys. A: Math. Gen. 23 (1990) 2689-2694. Printed in the UK

COMMENT

The overlap integral of associated Legendre functions

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Received 23 March 1990

Abstract. Closed formulae have been derived for the definite integral $\int_0^\pi \mathscr{L}_n^k \mathscr{L}_m^{k+l} \sin\rho \,\mathrm{d}\rho$ where $0 \leqslant k \leqslant n$ and $0 \leqslant k+l \leqslant m$ involving two normalised associated Legendre functions. It has been shown that the selection rules are independent of the parity of k and depend only on the parities of l, n, and m. These results complete those obtained by Salem and Wio who have given closed expressions for the special $k=0$ case. As side results, closed formulae of the definite integral $\int_0^\pi (\sin\rho)^P (\cos\rho)^M \,\mathrm{d}\rho$ where P and M are integers and $0 \leqslant P, M$ as well as sum rules involving combinations of binomial coefficients have been obtained.

1. Introduction

Recently, Salem and Wio [1] have given closed expressions of the definite integral

$$\int_0^\pi \mathscr{L}_n^0 \mathscr{L}_m^l \sin\rho \,\mathrm{d}\rho$$

where $\mathscr{L}_n^0$ denotes the nth Legendre polynomial, $\mathscr{L}_m^l$ stands for an associated Legendre function and $0 \leqslant l \leqslant m$. This work aims at completing the results of [1] by evaluating the overlap integral of two normalised associated Legendre functions, i.e. the integral

$$\mathscr{I}(n, k, m, l) = \int_0^\pi \mathscr{L}_n^k \mathscr{L}_m^{k+l} \sin\rho \,\mathrm{d}\rho \tag{1}$$

where $0 \leqslant k \leqslant n$ and $0 \leqslant k+l \leqslant m$. Details of the calculations are given in section 2 and the results are presented in section 3. Section 4 summarises.

2. Evaluation of $\mathscr{I}(n, k, m, l)$

By definition the normalised associated Legendre function $\mathscr{L}_n^k$ is given by the equations

$$\mathscr{L}_n^k = N_n^k \mathscr{P}_n^k \tag{2}$$

$$N_n^k = \sqrt{\frac{(2n+1)(n-k)!}{2(n+k)!}} \tag{3}$$

$$\mathscr{P}_n^k = \frac{1}{2^n}\frac{1}{n!}(\sin\rho)^k \frac{\mathrm{d}^{n+k}(x^2-1)^n}{\mathrm{d}x^{n+k}} \tag{4}$$

where $x = \cos\rho$ and $0 \leqslant k \leqslant n$. Since

$$(a+b)^n = \sum_{s=0}^{n} \binom{n}{s} a^s b^{n-s} \tag{5}$$

we may write that

$$(x^2-1)^n = \sum_{s=0}^{n} \binom{n}{s} x^{2s}(-1)^{n-s} \tag{6}$$

and since

$$\frac{\mathrm{d}^{n+k}x^{2s}}{\mathrm{d}x^{n+k}} = \binom{2s}{n+k}(n+k)!\,x^{2s-n-k} \tag{7}$$

the associated Legendre function $\mathscr{P}_n^k$ may be written as

$$\mathscr{P}_n^k = \frac{1}{2^n}\frac{1}{n!}(n+k)! \sum_{s;2n\geqslant 2s\geqslant n+k}^{n} (-1)^{n-s}\binom{n}{s}\binom{2s}{n+k}(\sin\rho)^k(\cos\rho)^{2s-n-k}. \tag{8}$$

Therefore the integral we would like to calculate can be given by the expression

$$\begin{aligned}\mathscr{I}(n,k,m,l) = {} & N_n^k N_m^{k+l}\frac{1}{2^{n+m}}\frac{1}{n!}\frac{1}{m!}(n+k)!(m+k+l)! \\ & \times \sum_{s;2n\geqslant 2s\geqslant n+k}^{n}\ \sum_{p;2m\geqslant 2p\geqslant m+k+l}^{m} (-1)^{n+m-s-p}\binom{n}{s}\binom{2s}{n+k}\binom{m}{p}\binom{2p}{m+k+l} \\ & \times \int_0^{\pi} (\sin\rho)^{2k+l+1}(\cos\rho)^{2s+2p-n-m-2k-l}\,\mathrm{d}\rho\end{aligned} \tag{9}$$

and can be calculated immediately once a closed formula of the integral

$$\mathscr{I}(P,M) = \int_0^{\pi} (\sin\rho)^P(\cos\rho)^M\,\mathrm{d}\rho \tag{10}$$

where P and M are integers and $P, M \geqslant 0$ has been substituted into (9). The problem is that there has not been published any closed formula for $\mathscr{I}(P,M)$.

We derive a closed formula of $\mathscr{I}(P,M)$. With

$$(\sin\rho)^P = (\mathrm{i})^P\frac{1}{2^P}\sum_{t=0}^{P}\binom{P}{t}(-1)^{P-t}\,\mathrm{e}^{\mathrm{i}(P-2t)\rho} \tag{11}$$

$$(\cos\rho)^M = \frac{1}{2^M}\sum_{q=0}^{M}\binom{M}{q}\mathrm{e}^{\mathrm{i}(M-2q)\rho} \tag{12}$$

we find that

$$\mathscr{I}(P,M) = (\mathrm{i})^P\frac{1}{2^{P+M}}\sum_{t=0}^{P}\sum_{q=0}^{M}(-1)^{P-t}\binom{P}{t}\binom{M}{q}\int_0^{\pi}\mathrm{e}^{\mathrm{i}(P+M-2t-2q)\rho}\,\mathrm{d}\rho \tag{13}$$

$$\begin{aligned} &= (\mathrm{i})^P\frac{1}{2^{P+M}}\sum_{t=0}^{P}\sum_{q;q\neq q^*(t)}^{M}\binom{P}{t}\binom{M}{q}(-1)^{P-t}\int_0^{\pi}\mathrm{e}^{\mathrm{i}(P+M-2t-2q)\rho}\,\mathrm{d}\rho \\ &\quad + (\mathrm{i})^P\frac{1}{2^{P+M}}\sum_{t=0}^{P}(-1)^{P-t}\binom{P}{t}\binom{M}{q^*(t)}\int_0^{\pi}\mathrm{d}\rho \\ &= (\mathrm{i})^{P-1}\frac{1}{2^{P+M}}\sum_{t=0}^{P}\sum_{q;q\neq q^*(t)}^{M}\frac{(-1)^{P-t}}{P+M-2t-2q}\binom{P}{t}\binom{M}{q}((-1)^{P+M-2t-2q}-1) \\ &\quad + (\mathrm{i})^P\frac{\pi}{2^{P+M}}\sum_{t=0}^{P}\binom{P}{t}\binom{M}{q^*(t)}(-1)^{P-t}\end{aligned} \tag{14}$$

where $2q^*(t) = P + M - 2t$ and the value of q^* must be restricted to $M \geq 2q^* \geq 0$, and q^* must be an integer.

Since $\mathscr{I}(P, M)$ must be a real number we can find the sum rules: for odd P

$$\sum_{t=0}^{P} \binom{P}{t} \binom{M}{q^*(t)} (-1)^{P-t} \equiv 0 \tag{15}$$

and for even P

$$\sum_{t=0}^{P} \sum_{q;q\neq q^*(t)}^{M} \frac{(-1)^{P-t}}{P+M-2t-2q} \binom{P}{t} \binom{M}{q} ((-1)^{P+M-2t-2q} - 1) \equiv 0 \tag{16}$$

where q^* is defined as above.

Now we shall discuss the selection rules. $\mathscr{I}(P, M)$ vanishes when P is odd and M is odd as well as when P is even and M is odd. In the latter case $\mathscr{I}$ vanishes since the first term in (14) must be zero otherwise we would end up at a complex $\mathscr{I}$ and the second term in (14) becomes zero for there is no appropriate q^* (consult the definition and restrictions on q^*). When P is odd and M is even $\mathscr{I}$ may be different from zero and

$$\mathscr{I}(P, M) = (\mathrm{i})^{P-1} \frac{1}{2^{P+M-1}} \sum_{t=0}^{P} \sum_{q=0}^{M} \frac{(-1)^{P-t+1}}{P+M-2t-2q} \binom{P}{t} \binom{M}{q} \tag{17}$$

where we have omitted restriction $q \neq q^*$ from the summation for no appropriate q^* exists i.e. q can take any values between 0 and M. When both P and M are even (i.e. $P = 2\bar{p}$, $M = 2\bar{m}$)

$$\mathscr{I}(P, M) = (-1)^{\bar{p}} \frac{\pi}{2^{P+M}} \sum_{t=t_{\min}}^{t_{\max}} \binom{P}{t} \binom{M}{\bar{p}+\bar{m}-t} (-1)^{P-t} \tag{18}$$

where $t_{\min} = 0$ and $t_{\max} = P$ when $P \leq M$ and $t_{\min} = \bar{p} - \bar{m}$ and $t_{\max} = \bar{p} + \bar{m}$ when $P > M$.

Thus we have essentially completed our task.

3. Expressions of $\mathscr{I}(n, k, m, l)$

In this section the closed formulae suitable for calculating the definite integral, (1), are presented in full detail along with a discussion of selection rules.

The definite integral, $\mathscr{I}(n, k, m, l)$, is equal to zero whenever $\mathscr{I}(P, M)$ vanishes. We shall consider the cases of $\mathscr{I}(P, M) \neq 0$. $\mathscr{I}(P, M)$ may be different from zero in the following cases.

(i) P is odd and M is even that is, when l is even and n and m is of the same parity (i.e. they are either odd or even). (To relate P and M to n, k, m and l compare (9) and (10).) Let subscripts o, e and p denote that the variable they are attached to is odd, even and either odd or even, respectively. Then

$$\begin{aligned}\mathscr{I}(n_p, m_p, k_{p'}, l_e) = {} & \left(\frac{(2n+1)(n-k)!(2m+1)(m-k-l)!}{4(n+k)!(m+k+l)!}\right)^{1/2} \\ & \times \frac{1}{2^{n+m}} \frac{1}{n!} \frac{1}{m!} (n+k)!(m+k+l)! \\ & \times \sum_s^n \sum_p^m \left[(-1)^{n+m-s-p} \binom{n}{s} \binom{2s}{n+k} \binom{m}{p} \binom{2p}{m+k+l} \right. \\ & \left. \times (-1)^{P-1/2} \frac{1}{2^{P+M-1}} \sum_{t=0}^{P} \sum_{q=0}^{M} \frac{(-1)^{P-t+1}}{P+M-2t-2q} \binom{P}{t} \binom{M}{q} \right]\end{aligned} \tag{19}$$

where

$$2n \geqslant 2s \geqslant n+k$$

$$2m \geqslant 2p \geqslant m+k+l$$

$$P = 2\bar{p}+1 = 2k+l+1$$

$$M = 2\bar{m} = 2(s+p)-(n+k)-(m+k+l).$$

(ii) $\mathscr{I}(n, k, m, l)$ may be different from zero when P is even and M is even that is, l is odd and n and m is of different parity. Then

$$\mathscr{I}(n_p, k_{p'}, m_{p''}, l_o) = \left(\frac{(2n+1)(n-k)!(2m+1)(m-k-l)!}{2(n+k)!2(m+k+l)!}\right)^{1/2}$$
$$\times \frac{1}{2^{n+m}} \frac{1}{n!} \frac{1}{m!} (n+k)!(m+k+l)!$$
$$\times \sum_s^n \sum_p^m \left[(-1)^{n+m-s-p} \binom{n}{s} \binom{2s}{n+k} \binom{m}{p} \binom{2p}{m+k+l} \right.$$
$$\left. \times (-1)^{P/2} \frac{\pi}{2^{P+M}} \sum_{t_{\min}}^{t_{\max}} \binom{P}{t} \binom{M}{\bar{p}+\bar{m}-t} (-1)^{P-t} \right] \tag{20}$$

where

$$2n \geqslant 2s \geqslant n+k$$

$$2m \geqslant 2p \geqslant m+k+l$$

$$P = 2\bar{p} = 2k+l+1$$

$$M = 2\bar{m} = 2(s+p)-(n+k)-(m+k+l)$$

$$t_{\min} = 0 \qquad \text{and} \qquad t_{\max} = P \text{ if } P \leqslant M$$

$$t_{\min} = \bar{p}-\bar{m} \qquad \text{and} \qquad t_{\max} = \bar{p}+\bar{m} \text{ if } P > M$$

and for the subscripts we have the restriction $p \neq p''$. It is interesting to note the selection rules are independent of the parity of k. Therefore the same selection rules apply to the $k \neq 0$ cases than to the $k = 0$ ones and as can be shown are in agreement with those obtained in [1]. However, the selection rule

$$\mathscr{I}(n_p, 0, m_p, l_e) = 0 \qquad \text{if } n_p > m_p \tag{21}$$

corresponding to that of equation (1.6) in [1] did not drop out from our derivation of $\mathscr{I}(n, k, m, l)$. Nevertheless the numerical results obtained by using the formulae in (19) and (20) confirm this selection rule as well as agree exactly with those of [1] obtained for the overlap integral between a normalised Legendre polynomial and a normalised associated Legendre function, thus confirming the correctness of our

Table 1. Overlap integral of associated Legendre functions.

k	n	$k+l$	m	$\mathscr{I}(n, k, m, l)$
1	1	2	2	0.987 864 57
1	1	2	4	0.142 585 97
1	1	2	6	0.052 058 68
1	1	2	8	0.025 777 84
1	2	2	3	0.974 047 60
1	2	2	5	0.201 909 40
1	2	2	7	0.083 879 99
1	3	2	2	−0.154 010 45
1	3	2	4	0.950 310 85
1	3	2	6	0.235 366 10
1	3	2	8	0.106 498 92
1	4	2	3	−0.223 679 96
1	4	2	5	0.927 328 14
1	4	2	7	0.255 402 13
2	2	3	3	0.994 133 17
2	2	3	5	0.103 036 46
2	2	3	7	0.029 656 05
2	2	3	9	0.012 154 82
2	3	3	4	0.986 335 93
2	3	3	6	0.153 991 65
2	3	3	8	0.051 622 77
2	4	3	3	−0.107 618 07
2	4	3	5	0.972 630 89
2	4	3	7	0.189 054 65
5	5	6	6	0.998 403 79
5	5	6	8	0.055 567 85
5	5	6	10	0.009 710 6
5	11	6	6	−0.000 536 41
5	11	6	8	−0.009 926 76
5	11	6	10	−0.167 933 16
5	11	6	12	0.964 838 19
1	3	3	3	−0.258 198 89
1	3	3	5	0.856 348 84
1	3	3	9	0.195 917 94
1	4	3	4	−0.377 964 47
1	4	3	6	0.786 795 79
1	4	3	8	0.383 648 47
1	5	3	3	-0.53×10^{-15}†

† This integral is equal to zero within the accuracy of the computer we used in the calculations in accordance with the selection rules. In fact, since l is even and $n > m$ and since the selection rules are independent of the parity of k, then (21) must be satisfied.

formulae as well. The numerical value of the overlap integral of two normalised associated Legendre functions is shown in table 1 for a few cases.

4. Summary

Closed formulae have been derived for the overlap integral (1) of two normalised associated Legendre functions as well as for the definite integral given in (10). The selection rules obtained in [1] for the overlap integral of a Legendre polynomial and an associated Legendre function were found to be valid for the overlap integral of two associated Legendre functions. Interesting sum rules, (15) and (16) result from the fact that the integration (10) must lead to a real number.

Reference

[1] Salem D and Wio H S 1989 *J. Phys. A: Math. Gen.* **22** 4331-8