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A single-sum expression for the overlap integral of two associated Legendre polynomials

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Abstract. A single-sum expression is given for the overlap integral of two associated Legendre polynomials. This is compared with recently reported double-sum expressions for this integral.

1. Introduction

In a recent paper by Wong [1], a derivation is given for a definite integral over two associated Legendre polynomials (that is of interest in mathematical physics), namely:

$$I(l_1, m_1; l_2, m_2) = \int_{-1}^{1} P_{l_1}^{m_1}(x) P_{l_2}^{m_2}(x) \,\mathrm{d}x.$$
⁽¹⁾

Wong's expression for this integral is a generalization of the result of Salem *et al* [2] (that treats this integral in the special case $m_1 = 0$), is less cumbersome than the expression for the same integral given by Szalay [3], and involves a double sum. For the case $m_1 = m_2$, Wong's expression does not, however, simplify analytically to the usual orthogonality condition:

$$I(l_1, m; l_2, m) = \int_{-1}^{1} P_{l_1}^m(x) P_{l_2}^m(x) \, \mathrm{d}x = \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \delta_{l_1, l_2 = l}.$$
 (2)

Wong mentions that this condition is satisfied numerically for all the cases he considered.

In this paper we derive an alternative expression for this integral which differs formally from the above expression in that it involves a *single* sum. Moreover, this alternative expression reduces to equation (2) when $m_1 = m_2$.

2. Alternative derivation

The definite integral of a single (unnormalized) associated Legendre polynomial (where *n*, *m* are integers, and $m \le n$) may be written as [4]:

$$\int_{0}^{1} P_{n}^{m}(x) dx = \frac{(-1)^{m} \pi (m+n)!}{2^{2m+1} \Gamma(\frac{m+1}{2}) \Gamma(\frac{m+3}{2})(n-m)!} {}_{3}F_{2} \left[\frac{m+n+1}{2}, \frac{m-n}{2}, \frac{m}{2} + 1; \right]$$

$$m+1, \frac{3+m}{2}; 1 \right]$$
(3)

where ${}_{3}F_{2}(\alpha, \beta, \gamma; \delta, \epsilon; 1)$ is a generalized hypergeometric function. This generalized hypergeometric is not necessarily a terminating series. However, if one considers the integral

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in equation (3) between the limits -1 to 1, rather than 0 to 1, for these symmetric limits, this integral vanishes if the integrand $P_n^m(x)$, i.e. n+m is odd. For this case the ${}_3F_2(\alpha, \beta, \gamma; \delta, \epsilon; 1)$ is Saalschutzian [5] since n+m = n-m+2m, hence n-m must be even. Since additionally $m \le n$, this makes the fraction (m-n)/2 in the ${}_3F_2$ a negative integer or zero, while additionally $1 + \alpha + \beta + \gamma = \delta + \epsilon$. Hence, for these limits

$${}_{3}F_{2}\left[\frac{m+n+1}{2},\frac{m-n}{2},\frac{m}{2}+1;m+1,\frac{3+m}{2};1\right] = \frac{\Gamma(\frac{n}{2})m!\Gamma(\frac{n-m+1}{2})\Gamma(\frac{m+3}{2})}{\sqrt{\pi}\Gamma(\frac{m}{2})\Gamma(\frac{n+3}{2})(\frac{n+m}{2})!}.$$
(4)

Using the duplication formula for the Gamma function [6], one can write the resulting integral as follows:

$$\int_{-1}^{1} P_n^m(x) \,\mathrm{d}x = \frac{((-1)^m + (-1)^n)2^{m-2}m\Gamma(\frac{n}{2})\Gamma(\frac{n+m+1}{2})}{(\frac{n-m}{2})!\Gamma(\frac{n+3}{2})}.$$
(5)

This expression is zero, as it should be for m = 0, unless *n* is also zero, in which case, since $P_0^0(x) = 1$, it equals 2, and for the special case m = 2 it reduces directly to 4, independent of the (even) value of *n* (where $n \ge 2$):

$$\int_{-1}^{1} P_n^2(x) \, \mathrm{d}x = 2(1 + (-1)^n).$$

If m = n equation (5) reduces to:

$$\int_{-1}^{1} P_n^n(x) \, \mathrm{d}x = \frac{(-1)^n \pi(2n)!}{2^{2n} \Gamma(\frac{n+1}{2}) \Gamma(\frac{n+3}{2})}.$$

A formula that expresses two associated Legendre polynomials as a sum over a single associated Legendre polynomial is:

$$P_{l_1}^{m_1}(x)P_{l_2}^{m_2}(x) = (-1)^{m_1}\sqrt{\frac{(l_1+m_1)!(l_2+m_2)!}{(l_1-m_1)!(l_2-m_2)!}} \sum_k G\sqrt{\frac{(k-m_2+m_1)!}{(k+m_2-m_1)!}} P_k^{-m_1+m_2}(x)$$
(6)

where

$$G = (-1)^{-m_1+m_2}(2k+1) \begin{pmatrix} l_1 & l_2 & k \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & k \\ -m_1 & m_2 & m_1 - m_2 \end{pmatrix}$$

$$|l_1 - l_2| \leq k \leq l_1 + l_2, \ k \geq |m_1 - m_2|, \ k + l_1 + l_2 \text{ is even and } \begin{pmatrix} l_1 & l_2 & k \\ 0 & 0 & 0 \end{pmatrix},$$

$$\begin{pmatrix} l_1 & l_2 & k \\ -m_1 & m_2 & m_1 - m_2 \end{pmatrix}, \ \text{are } 3 \text{-} j \text{ symbols. The } 3 \text{-} j \text{ symbol: } \begin{pmatrix} l_1 & l_2 & k \\ 0 & 0 & 0 \end{pmatrix} \text{ imposes the last of these three conditions on k since this } 3 \text{-} j \text{ vanishes if } l_1 + l_2 + k \text{ is odd. The result of equation (6) can be obtained by expressing the product of two spherical harmonics in terms of a sum over one spherical harmonic, and then writing out the spherical harmonics in terms of associated Legendre polynomials [7]. Combining equations (5) and (6) one finally obtains:$$

Combining equations (5) and (6) one finally obtains:

$$I(l_1, m_1; l_2, m_2) = C(l_1, m_1; l_2, m_2) \sum_k D(|m_2 - m_1|, k)(2k+1) \begin{pmatrix} l_1 & l_2 & k \\ 0 & 0 & 0 \end{pmatrix} \times \begin{pmatrix} l_1 & l_2 & k \\ -m_1 & m_2 & m_1 - m_2 \end{pmatrix}$$
(7)

where, because of equation (5) one has the additional constraint that $k + m_2 - m_1$ is even and

$$C(l_1, m_1; l_2, m_2) = (-1)^{m_1} |m_2 - m_1| 2^{|m_2 - m_1| - 2} \sqrt{\frac{(l_1 + m_1)!(l_2 + m_2)!}{(l_1 - m_1)!(l_2 - m_2)!}}$$

$$D(|m_2 - m_1|, k) = (1 + (-1)^{k + |m_2 - m_1|}) \sqrt{\frac{(k - |m_2 - m_1|)!}{(k + |m_2 - m_1|)!}} \frac{\Gamma(\frac{k}{2})\Gamma(\frac{k + |m_2 - m_1| + 1}{2})}{(\frac{k - |m_2 - m_1|}{2})!\Gamma(\frac{k + 3}{2})}.$$

If $m_1 = m_2 = m$ equation (7) is zero because of the $|m_2 - m_1|$ term in the expression $C(l_1, m_1; l_2, m_2)$, unless additionally k = 0, in which case the integral over $P_k^{|m_2 - m_1|}$ equals 2. For k = 0 the 3-*j* symbol: $\begin{pmatrix} l_1 & l_2 & k \\ 0 & 0 & 0 \end{pmatrix}$ is zero unless $l_1 = l_2 = l$, and $I(l_1, m_1; l_2, m_2) = (-1)^m \frac{(l+m)!}{(l-m)!} 2 \begin{pmatrix} l & l & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l & 0 \\ -m & m & 0 \end{pmatrix}$ $= (-1)^m \frac{(l+m)!}{(l-m)!} \frac{2(-1)^m}{2l+1} \delta_{l_1, l_2=l} = \frac{(l+m)!}{(l-m)!} \frac{2}{2l+1} \delta_{l_1, l_2=l}$

i.e. equation (7) reduces to equation (2). The integral over three associated Legendre polynomials can be treated by similar methods [9].

3. Conclusions

A single-sum expression for the integral over two associated Legendre polynomials is given. If the *m* are identical this expression reduces to the usual two associated Legendre polynomial orthonormality condition.

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