The Overlap Integral of Three Associated Legendre Polynomials

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Abstract—A closed formula with a double sum is obtained for the overlap integral of three associated Legendre polynomials (ALPs). The result is applicable to integral involving the ALP with arbitrary degree $l$ and order $m$. Special overlap integrals, including the cases $m_3 = m_1 + m_2$ or $|m_1 - m_2|$, are presented. A general formula for the overlap integral of an arbitrary number of ALPs is also developed. © 2002 Elsevier Science Ltd. All rights reserved.

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1. INTRODUCTION

It is well known that the overlap integral of three ALPs

\[ I(l_1, m_1; l_2, m_2; l_3, m_3) = \int_{-1}^{1} P_{l_1}^{m_1}(x)P_{l_2}^{m_2}(x)P_{l_3}^{m_3}(x) \, dx \]  

cannot be found in the common literature. The integral of type (1) appears, for example, in the study of the effect of a fluid over bodies of various axisymmetric shapes such as sphere and spheroid [1], and in the multiple scattering formalism [2,3] through the form of Gaunt numbers [4, p. 57]. Recently, this overlap integral has been derived in closed form [1]. The approach is based on the previous result of the overlap integral of two ALPs presented by Mavromatis [5], which presented a phase flaw, a problem of increasing importance when equation (1) is considered. In this work, we address again the derivation of equation (1) in order to point out such a mistake, as well as to develop a general formula for the integral involving a product of an arbitrary number of ALPs.

We start by presenting the result on which the derivation of equation (1) is based. The following expression for the product of two ALPs was given in [1]:

\[ P_{l_1}^{m_1}(x)P_{l_2}^{m_2}(x) = (-1)^{m_1} \sqrt{(l_1 + m_1)!(l_2 + m_2)!} \sum_l G \sqrt{(l - m_2 + m_1)!(l + m_2 - m_1)!} P_{l}^{-m_1+m_2}(x), \]
with
\[ G = (-1)^{-m_1+m_2}(2l+1) \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ -m_1 & m_2 & m_1-m_2 \end{pmatrix} \tag{3} \]
and \(|l_1-l_2| \leq l \leq l_1+l_2, l \geq |m_1-m_2|,\) and \(l+l_1+l_2\) is even, which is determined by the property of \(3-j\) symbols [6]. Equation (2) is deduced by using the relation [7, p. 235]
\[ P_l^{-m}(x) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(x), \tag{4} \]
in the expansion of two spherical harmonics [8]. The overlap integral of two ALPs, obtained directly from (2), is then given by a sum of integral involving one ALP. The integral of a single ALP is obtained from [9, p. 807], where we take \(c = 0,\)
\[ \int_0^1 P_n^m dx = \frac{(-1)^m \pi (m+n)!2^{(-1-2m)}}{\Gamma((1+m)/2)\Gamma((3+m)/2)(n-m)!} {_3F_2}[\alpha, \beta, \gamma; \delta, \epsilon; 1], \quad m = 0, 1, 2, \ldots, \tag{5} \]
where
\[ \alpha = \frac{m+n+1}{2}, \quad \beta = \frac{m-n}{2}, \quad \gamma = \frac{m}{2} + 1, \quad \delta = m+1, \quad \epsilon = \frac{3+m}{2}, \tag{6} \]
and \(_3F_2[\alpha, \beta, \gamma; \delta, \epsilon; 1]\) is the generalized hypergeometric function. Equation (5) requires \(m \geq 0.\) This means that it cannot be applied for arbitrary \(m_1\) and \(m_2\) in (2), e.g., for negative \(-m_1+m_2\). The correct overlap integral of two ALPs is given in [10]
\[ I(l_1, m_1; l_2, m_2) = C(l_1, m_1; l_2, m_2) \sum_l D(|m_2-m_1|, l)(2l+1) \]
\[ \cdot \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ -m_1 & m_2 & m_1-m_2 \end{pmatrix}, \tag{7} \]
where
\[ C(l_1, m_1; l_2, m_2) = (-1)^l |m_2-m_1|^2 |m_2-m_1|^{-2} \sqrt{\frac{(l_1+m_1)!(l_2+m_2)!}{(l_1-m_1)!(l_2-m_2)!}}, \tag{8} \]
\[ D(|m_2-m_1|, l) = \left[ 1 + (-1)^l |m_2-m_1| \right] \sqrt{\frac{(l-|m_2-m_1|)!\Gamma((l+|m_2-m_1|+1)/2)}{(l+|m_2-m_1|)!\Gamma((l-|m_2-m_1|)/2)!\Gamma((l+3)/2)}, \tag{9} \]
with the phase
\[ \delta = \begin{cases} m_1, \text{ when } m_2 \geq m_1, \\ m_2, \text{ when } m_2 < m_1, \end{cases} \tag{10} \]
\(\delta\) is taken to be \(m_2\) in [1], while in [5] the particular case \(\delta = m_1\) is chosen. From another point of view, we note that \(\int_0^1 P_n^m(x)P_n^m(x) dx\) is symmetrical with respect to interchange of indices 1,2. This symmetry is satisfied in (7), but not in the expressions given in [1,5].

A second problem presented in [1] is concerned with the expression used for the hypergeometric function \(_3F_2[\alpha, \beta, \gamma; \delta, \epsilon; 1]\), which is obtained directly from the summation formula of Saalschutzian series [5, p. 191]
\[ _3F_2[\alpha, \beta, \gamma; \delta, \epsilon; 1] = \frac{\Gamma(\delta)\Gamma(1+\alpha-\epsilon)\Gamma(1+\beta-\epsilon)\Gamma(1+\gamma-\epsilon)}{\Gamma(1-\epsilon)\Gamma(\delta-\alpha)\Gamma(\delta-\beta)\Gamma(\delta-\gamma)}, \tag{11} \]
where \(\beta\) is a negative integer or zero and \(\delta + \epsilon = \alpha + \beta + \gamma + 1.\) From the variables of the relevant problem, equation (11) takes the form [1]
\[ _3F_2[\alpha, \beta, \gamma; \delta, \epsilon; 1] = \frac{\Gamma(1/2)\Gamma(n/2)\Gamma(m+1)\Gamma(-n+1/2)}{\Gamma((m-n+1)/2)\Gamma((m+1)/2)\Gamma((n+m)/2+1)\Gamma(-(m+1)/2)}. \tag{12} \]
This result cannot be applied directly because the some gamma functions present negative arguments simultaneously. However, using the following formula [7, p. 991]:

$$\Gamma(z)\Gamma(1 - z) = \frac{\pi}{\sin(\pi z)},$$  \hspace{1cm} (13)

we can obtain the practical result:

$$3F_2[\alpha, \beta; \gamma; \delta, \epsilon; 1] = \frac{\Gamma(n/2)m!\Gamma((n - m + 1)/2)\Gamma((n + 3)/2)}{\sqrt{\pi}\Gamma(m/2)\Gamma((n + 3)/2)(n + m)/2)!}. \hspace{1cm} (14)$$

The results for (1) presented by Mavromatis and Alassar are based on equations (8) and (9) given in [1], which, as we have shown, present the wrong phase as well as a problem of applicability. It is thus convenient to restudy this problem in order to present the correct overlap integral of three ALPs, which is the aim of this paper.

2. EVALUATION OF $I(l_1, m_1; l_2, m_2; l_3, m_3)$

In this section, we shall express the overlap integral of three ALPs in terms of integrals of a single ALP. Substituting equation (14) into equation (5) allows to obtain

$$\int_{-1}^{1} P^m_n(x) dx = \frac{\Gamma(n/2)m!\Gamma((n - m + 1)/2)\Gamma((n + 3)/2)}{(n - m)/2)!\Gamma((n + 3)/2)}.$$  \hspace{1cm} (15)

We now express two ALPs as a sum over a single ALP directly from the product of two spherical harmonics. The relation between ALP and the spherical harmonic can be expressed as [11]

$$Y_l^m(\theta, \varphi) = (-1)^m \sqrt{\frac{2l + 1}{4\pi}} \frac{(l - m)!}{(l + m)!} P_l^m(\cos \theta)e^{im\varphi}, \hspace{1cm} m \geq 0. \hspace{1cm} (16)$$

On the other hand, the product of two spherical harmonics is given by [8]

$$Y_{l_1}^{m_1}(\theta, \varphi)Y_{l_2}^{m_2}(\theta, \varphi) = \sum_{l} \left[ \frac{(2l_1 + 1)(2l_2 + 1)}{4\pi(2l_1 + 1)} \right]^{1/2} C^{l_1}_{m_1} C^{l_2}_{m_2} Y_{l_1 l_2}(\theta, \varphi), \hspace{1cm} (17)$$

where $m_{12} = \sum_{i=1}^{2} m_i$ and $C^{l_1}_{m_1} C^{l_2}_{m_2}$, $C^{l_1 l_2}_{m_1 m_2}$ are Clebsch-Gordan coefficients. Introducing the notation $\cos \theta = x$, it is shown from equations (16) and (17) that

$$P_{l_1}^{m_1}(x)P_{l_2}^{m_2}(x) = \sqrt{\frac{(l_1 + m_1)!(l_2 + m_2)!}{(l_1 - m_1)!(l_2 - m_2)!}} \sum_{l_{12}} \sqrt{\frac{(l_1 - m_{12})!}{(l_2 + m_{12})!}} C^{l_{12}}_{m_1 m_2 m_{12}} C^{l_{12}}_{0 0} P_{l_{12}}^{m_{12}}(x). \hspace{1cm} (18)$$

Considering the relation between Clebsch-Gordan coefficient and 3 - $j$ symbol

$$C^{j_1 j_2 j_3}_{m_1 m_2 m_3} = (-1)^{m_1 + j_1 - j_2} \sqrt{2j_3 + 1} \binom{j_1}{m_1} \binom{j_2}{m_2} \binom{j_3}{-m_3}, \hspace{1cm} (19)$$

we can rewrite equation (18) as

$$P_{l_1}^{m_1}(x)P_{l_2}^{m_2}(x) = \sqrt{\frac{(l_1 + m_1)!(l_2 + m_2)!}{(l_1 - m_1)!(l_2 - m_2)!}} \sum_{l_{12}} G_{12} \sqrt{\frac{(l_1 - m_{12})!}{(l_2 + m_{12})!}} P_{l_{12}}^{m_{12}}(x), \hspace{1cm} (20)$$

with

$$G_{12} = (-1)^{m_{12}} (2l_{12} + 1) \begin{pmatrix} l_{12} & l_{12} & \cr l_{1} & l_{2} & l_{12} \cr 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_{1} & l_{2} & l_{12} \cr m_{1} & m_{2} & -m_{12} \end{pmatrix}, \hspace{1cm} (21)$$

where $|l_1 - l_2| \leq l_{12} \leq l_1 + l_2$, $l_{12} \geq m_{12}$, and $l_{12} + l_1 + l_2$ is even.
Let us now consider the overlap integral (1). Substituting equation (20) into equation (1), this overlap integral can be taken as

\[ I(l_1, m_1; l_2, m_2; l_3, m_3) = \sqrt{\frac{(l_1 + m_1)!(l_2 + m_2)!(l_3 + m_3)!}{(l_1 - m_1)!(l_2 - m_2)!(l_3 - m_3)!}} \sum_{l_{12}} \int_{-1}^{1} P_{l_{12}}^{m_12}(x)P_{l_3}^{m_3}(x) \, dx, \]  

with \( G_{12} \) defined by equation (21). If we proceed to use equation (18) in equation (22), we obtain

\[ I(l_1, m_1; l_2, m_2; l_3, m_3) = \sqrt{\frac{(l_{123} + m_{123})!}{(l_{123} - m_{123})!}} \cdot I(l_{123}, m_{123}), \]

with

\[ G_{123} = (-1)^{m_{123}}(2l_{123} + 1) \begin{pmatrix} l_{12} & l_{123} & l_{123} \\ 0 & 0 & 0 \\ m_{12} & m_{3} & -m_{123} \end{pmatrix}, \]

where \( |l_{12} - l_3| \leq l_{123} \leq l_{12} + l_3, l_{123} \geq m_{123} = \sum_{i=1}^{3} m_i, \) and \( l_{12} + l_3 + l_{123} \) is even, and

\[ I(l_{123}, m_{123}) = \int_{-1}^{1} P_{l_{123}}^{m_{123}}(x) \, dx = \frac{[(-1)^{m_{123}} + (-1)^{l_{123}}] 2^{m_{123}} - 2m_{123} \Gamma((l_{123} + 1)/2) \Gamma((l_{123} + m_{123} + 1)/2)}{(l_{123} - m_{123})/2! \Gamma((l_{123} + 3)/2)}. \]

The \( m's \) in (23) are supposed to be positive. In case we were interested in calculating an overlap integral involving a negative \( m, \) we could use equation (4).

A remarkable property of result (23) is that no phase is involved. This fact suggests that we apply successively (18) to obtain a general formula for the overlap integral of any number of ALPs. We obtain for \( i \) ALPs

\[ I(l_1, m_1; \ldots; l_i, m_i) = \sqrt{\frac{(l_1 + m_1)! \cdots (l_i + m_i)!}{(l_1 - m_1)! \cdots (l_i - m_i)!}} \sum_{l_{12} \ldots l_{i-1}} \sum_{l_{i} \ldots l_{i+1}} \cdots \sum_{l_{i} \ldots l_{i+1}} \]

\[ G_{12} G_{123} \ldots G_{12i} \sqrt{\frac{(l_{12 \ldots i} - m_{12 \ldots i})!}{(l_{12 \ldots i} + m_{12 \ldots i})!}} \cdot I(l_{12 \ldots i}, m_{12 \ldots i}), \]

with the definition

\[ G_{12 \ldots i} = (-1)^{m_{12 \ldots i}}(2l_{12 \ldots i} + 1) \begin{pmatrix} l_{12 \ldots i-1} & l_{i} & l_{12 \ldots i} \\ 0 & 0 & 0 \\ m_{12 \ldots i-1} & m_{i} & -m_{12 \ldots i} \end{pmatrix}, \]

where \( l_{12 \ldots i} \geq m_{12 \ldots i} = \sum_{j=1}^{i} m_j \) and \( l_{12 \ldots i-1} + l_i + l_{12 \ldots i} \) is even. The relation between \( l_{12 \ldots i-1} \) and \( l_i \) as well as \( l_{12 \ldots i} \) can be determined by the selection rule of \( 3 - j \) symbols. The corresponding integral \( I(l_{12 \ldots i}, m_{12 \ldots i}) \) can be expressed as

\[ I(l_{12 \ldots i}, m_{12 \ldots i}) = \int_{-1}^{1} P_{l_{12 \ldots i}}^{m_{12 \ldots i}}(x) \, dx \]

\[ = \frac{[(-1)^{m_{12 \ldots i}} + (-1)^{l_{12 \ldots i}}] 2^{m_{12 \ldots i}} - 2m_{12 \ldots i} \Gamma((l_{12 \ldots i} + 1)/2) \Gamma((l_{12 \ldots i} + m_{12 \ldots i} + 1)/2)}{(l_{12 \ldots i} - m_{12 \ldots i})/2! \Gamma((l_{12 \ldots i} + 3)/2)}. \]
Let us turn our attention to the special case \( m_3 = m_1 + m_2 \). First, we recall the overlap integral of two ALPs for the special case \( m_1 = m_2 \) [5,7,9,10]

\[
I(l_1, m_1; l_2, m_1) = \frac{(l_1 + m_1)!}{(l_1 - m_1)!} \frac{2}{2l_1 + 1} \delta_{l_1, l_2}.
\] (29)

When this expression is used in equation (22), we obtain

\[
I(l_1, m_1; l_1, m_2, l_3, m_3) = 2(-1)^{m_3} \sqrt{\frac{(l_1 + m_1)!(l_2 + m_2)!(l_3 + m_3)!}{(l_1 - m_1)!(l_2 - m_2)!(l_3 - m_3)!}} \cdot \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & -m_3 \end{pmatrix}.
\] (30)

This result can be obtained directly from the Gaunt numbers [4, p. 57]. An additional special case is obtained by using (2), repeatedly. When \( m_3 = |m_1 - m_2| \), we have

\[
I(l_1, m_1; l_1, m_2, l_3, m_3) = 2(-1)^{\delta - m_1 + m_2} \sqrt{\frac{(l_1 + m_1)!(l_2 + m_2)!(l_3 + m_3)!}{(l_1 - m_1)!(l_2 - m_2)!(l_3 - m_3)!}} \cdot \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ -m_1 & m_2 & m_1 - m_2 \end{pmatrix},
\] (31)

with \( \delta \) given in equation (10).

As pointed out in [1], it is interesting to note that some integrals of the type

\[
\int_{-1}^{1} F(x)P_{l_1}^{m_1}(x)P_{l_2}^{m_2}(x)P_{l_3}^{m_3}(x) \, dx,
\] (32)
can be easily obtained with the aid of equation (23). For example, for \( F(x) \) taken as \( F(x) = x/\sqrt{1 - x^2}, x, \sqrt{1 - x^2} \), the recursion relations [9, p. 1022] will first be used and then apply result (26).

The importance of this method to determine the overlap integrals relies on the accuracy of the results, which contrasts with the numerical calculation, where finer and finer mesh points are required due to the numerous zeros as the order \( m \) and degree \( l \) increases.

**3. CONCLUDING REMARKS**

In this paper, we have restudied the overlap integral of three ALPs. The result is given in closed form in terms of a double sum. This approach is different from that used in [1]. We have also generalized this problem to the corresponding overlap integral of an arbitrary number of ALPs. The case of negative \( m_3 \) has been also analyzed. If this is case, we should make use of equation (4) to make the \( m_3 \) positive, and then we can derive the overlap integral following the method as indicated above. On the other hand, it has been emphasized that some related integrals involving ALPs can be obtained by means of the recursion relations. The special cases \( m_3 = m_1 + m_2, |m_1 - m_2| \) for three ALPs are also discussed.

**REFERENCES**