Some useful relations using spherical harmonics and Legendre polynomials

1973 J. Phys. A: Math. Nucl. Gen. 6 1119

(http://iopscience.iop.org/0301-0015/6/8/008)

J. Phys. A: Math., Nucl. Gen., Vol. 6, August 1973. Printed in Great Britain.

Some useful relations using spherical harmonics and Legendre polynomials

J M Dixon† and R Lacroix

Département de Chimie Physique, University of Geneva, Switzerland

Received 22 January 1973, in final form 21 March 1973

Abstract. A development of $R^l Y_l^m(\theta_R, \phi_R)$ has been established in a series of products $r_1^f Y_f^p(\theta_1, \phi_1) r_2^{l-f} Y_{l-f}^{m-p}(\theta_2, \phi_2)$ where (r_1, θ_1, ϕ_1), (r_2, θ_2, ϕ_2) and (R, θ_R, ϕ_R) are the spherical polar coordinates of the vectors $\boldsymbol{r}_1, \boldsymbol{r}_2$ and $\boldsymbol{R} = \boldsymbol{r}_1 - \boldsymbol{r}_2$. The expansion of $1/|\boldsymbol{r}_1 - \boldsymbol{r}_2|$ as a series of spherical harmonics in (θ_1, ϕ_1) and (θ_2, ϕ_2) has been generalized for the case $1/|\boldsymbol{r}_1 - \boldsymbol{r}_2|^t$, where t is an integer.

1. Introduction

There are many instances in physics where some quantity is found by evaluating an integral whose integrand contains both a Coulomb-like interaction and an entity which involves atomic orbitals with origin at different centres (Sharma 1968, Barnett and Coulson 1951). They arise in the determination of electronic energy, hyperfine coupling constants, transition probabilities, components of the electric field gradient tensor and many other quantities. One way of evaluating integrals of this type is to expand the orbitals on different centres in terms of coordinates on one centre. However, if one is particularly interested in part of the Coulomb interaction which does not appear in the multicentred part of the integrand, one must expand the Coulomb component, and one way of proceeding is to change the integration variable so that the site dependent quantity now only involves one variable. One does this however at the expense of changing the form of the Coulomb-like component of the integrand so that when one attempts to try to expand this in spherical harmonics, for example, one needs an explicit form for the coefficients. The spherical harmonics usually describe the orientation of vectors so that the latter coefficients will involve the angular momentum quantum numbers of the harmonics and the magnitudes of the vectors.

During a recent investigation into the wavevector dependence of crystalline electric fields in metals it became apparent that, although such relationships using spherical harmonics and Legendre polynomials have been given in the literature, their forms are not the most explicit and further work must be done before they can be directly applied. In particular it became necessary to expand $1/|\boldsymbol{r}_1 - \boldsymbol{r}_2 - \boldsymbol{r}_3|$ in a series whose terms are products of three harmonics with angles (θ_1, ϕ_1), (θ_2, ϕ_2) and (θ_3, ϕ_3) which represent the orientation of the vectors $\boldsymbol{r}_1, \boldsymbol{r}_2$ and $\boldsymbol{r}_3$ respectively. It is well known (Hobson 1955)

† Professeur invité on leave from the University of Warwick, Coventry, UK.

that the reciprocal distance $1/|\boldsymbol{R}-\boldsymbol{r}_3|$ may be expanded as follows:

$$\frac{1}{|\boldsymbol{R}-\boldsymbol{r}_3|} = \sum_{l,m} \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_l^m(\theta_R, \phi_R) Y_l^{m*}(\theta_3, \phi_3)$$

where θ_R and ϕ_R describe the orientation of $\boldsymbol{R}$ and $r_<$ denotes R if $R < r_3$ and r_3 if $R > r_3$ with a similar definition for $r_>$. If this relation is used to attempt an expansion of $1/|\boldsymbol{r}_1-\boldsymbol{r}_2-\boldsymbol{r}_3|$ with $\boldsymbol{R} = \boldsymbol{r}_1-\boldsymbol{r}_2$ then clearly it becomes necessary to be able to express $R^l Y_l^m(\theta_R, \phi_R)$ as a series of products of harmonics one in (θ_1, ϕ_1) and the other in (θ_2, ϕ_2). Such an expansion has been given by Sack (1964) but the radial factors which enter the coefficients have been given in terms of a hypergeometric series. From the point of view of direct application, so that for example the coefficient of any one particular product of two spherical harmonics can be picked out with ease, it is obviously advantageous to have these radial factors in a more explicit form. It should be pointed out however that Sack's form is probably better if one wishes to consider the validity of such expansions near singular points or the symmetry properties of various parts of the expansion. Moreover, Sack has a very complicated way of obtaining the radial factors. He derives a differential equation for the radial factors and from considerations of dimensionality shows they must be of the form of a series in $r_{3<}/R_>$ multiplied by the product formed from a fixed power of r_3 and a power of R. The coefficients of this series, using the differential equation, can be shown to satisfy a set of recurrence relations, the solution of which can be expressed in terms of Gauss's hypergeometric function. In this paper we use a much more simple and compact proof of the expansion for $R^l Y_l^m(\theta_R, \phi_R)$ namely by induction and further the result is given in the explicit form of simple algebraic quantities which can be more readily applied to a given problem. We believe that this latter result has not been given in such a simple form before and is therefore of value.

It is conceivable that for example in a theory of screening one might also wish not only to have a formula for $1/r_{12} = 1/|\boldsymbol{r}_1-\boldsymbol{r}_2|$ in terms of spherical harmonics describing the orientations of $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, but a series of products of harmonics for $1/r_{12}^t$ where t is any integral power. Although such expansions may be written as a series of Gegenbauer polynomials in the angle between $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ it is often more convenient to expand in the orientations of $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ separately. Once again Sack has derived such expressions but in terms of hypergeometric functions. We shall derive a series for the two cases when t is an odd and when t is an even integer. Sack has previously suggested the use of Legendre functions of the second kind Q_l^μ but did not follow this train of thought because when μ is fractional there were differing conventions for the phase angles involved. In the case when t is an even integer we have used this alternative new approach to advantage since in this case no difficulties over phases arise. Whether t is odd or even our demonstrations are inherently more simple than Sack's as before and, although a few more summations are involved, the results can be applied directly without having to evaluate some other function involved (except in the case when t is even when a Legendre function of the second kind is used.)

When deriving the formulae that will be given we found it necessary to prove subsidiary relations which may also be of value.

2. A relation for $R^l Y_l^m(\theta_R, \phi_R)$

In this section we shall establish a development of $R^l Y_l^m(\theta_R, \phi_R)$ in a series of products

$r_1^f Y_f^p(\theta_1, \phi_1) r_2^{l-f} Y_{l-f}^{m-p}(\theta_2, \phi_2)$ where (r_1, θ_1, ϕ_1), (r_2, θ_2, ϕ_2) and (R, θ_R, ϕ_R) are the spherical polar coordinates of the vectors $\boldsymbol{r}_1$, $\boldsymbol{r}_2$ and $\boldsymbol{R} = \boldsymbol{r}_1 - \boldsymbol{r}_2$ respectively. A formula valid for general l and m, for $R^l Y_l^m(\theta_R, \phi_R)$ is given below:

$$|\boldsymbol{r}_1-\boldsymbol{r}_2|^l Y_l^m(\theta_R, \phi_R) = \left(\frac{4\pi(l+m)!(2l+1)!}{(2l)!(l-m)!}\right)^{1/2} \times \sum_{f=0}^{l}\sum_{w=0}^{l-m}\left(\frac{(2f)!w!(2l-2f)!(l-m-w)!}{(2f+1)!(2l-2f+1)!(2f-w)!(l-2f+m+w)!}\right)^{1/2} \times (-1)^f\, {}^{(l-m)}C_{(w)} r_1^f Y_f^{f-w}(\theta_1, \phi_1) r_2^{l-f} Y_{l-f}^{m+w-f}(\theta_2, \phi_2) \tag{1}$$

where ${}^{(l-m)}C_{(w)}$ is the binominal coefficient. f and w are integers and any particular term is considered to be zero if at least one of the relations $|f-w| \leqslant f$ and $|m+w-f| \leqslant l-f$ is violated. Note that θ_R and ϕ_R describe the orientation of the difference vector $\boldsymbol{r}_1 - \boldsymbol{r}_2$ and not, as in the addition theorem for Legendre polynomials (Jahnke and Emde 1945), the angle between the two vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$.

To prove (1) we shall use induction on l and suppose the formula true for $l-1$ and prove it true for l. Hence, if the formula holds when $l = 1$ it will be true for all l. To carry out this procedure we must therefore decompose $Y_l^m(\theta_R, \phi_R)$ into harmonics of order $\bar{l} < l$ in the simplest way. We do this by writing the latter harmonic as a linear function of $Y_{l-1}^m Y_1^0$, $Y_{l-1}^{m-1} Y_1^1$ and $Y_{l-1}^{m+1} Y_1^{-1}$. It is clear that the relative magnitude of the coefficients of the latter three functions will be the same as those of the corresponding Wigner coefficients for the construction of an l manifold from those of degree $l-1$ and unity. That is (Heine 1960),

$$Y_l^m(\theta_R, \phi_R) = \alpha\left\{\left(\frac{(l-m)(l-m-1)}{(2l-1)2l}\right)^{1/2} Y_{l-1}^{m+1} Y_1^{-1} + \left(\frac{2(l+m)(l-m)}{2l(2l-1)}\right)^{1/2} Y_{l-1}^m Y_1^0 + \left(\frac{(l+m)(l+m-1)}{2l(2l-1)}\right)^{1/2} Y_{l-1}^{m-1} Y_1^1\right\}. \tag{2}$$

The value of α may be found in a number of ways. For example if we premultiply (2) by $Y_l^{m*}(\theta_R, \phi_R)$ and integrate, since the harmonics are normalized to unity we obtain α directly. We find that the constant α is given by $\alpha = \{\frac{8}{3}\pi(2l+1)/2l\}^{1/2}$.

We now decompose the right-hand side of (2) using the formula (1) assumed true for $\bar{l} \leqslant l-1$, premultiply by $|\boldsymbol{r}_1 - \boldsymbol{r}_2|^l$ and obtain

$$\left(\frac{(2l+1)4\pi}{3l}\right)^{1/2}\left[\left\{\left(\frac{4\pi(l+m)!(2l-1)!}{(2l)!(l-m)!}\right)^{1/2} \times \sum_{f=0}^{l-1}\sum_{w=0}^{l-m}\left(\frac{(2f)!w!(2l-2f-2)!(l-m-w)!}{(2f+1)!(2l-2f-1)!(2f-w)!(l-2f+m-2+w)!}\right)^{1/2} \times (-1)^f\, {}^{(l-m)}C_{(w)} r_1^f Y_f^{f-w}(\theta_1, \phi_1) r_2^{l-1-f} Y_{l-1-f}^{m-1+w-f}(\theta_2, \phi_2) \times (r_2 Y_1^1(\theta_2, \phi_2) - r_1 Y_1^1(\theta_1, \phi_1))\right\} + \left\{\left(\frac{4\pi(l+m)!(l-m)(2l-1)!2}{(2l)!(l-m-1)!}\right)^{1/2} \times \sum_{f=0}^{l-1}\sum_{w=0}^{l-m-1}\left(\frac{(2f)!w!(2l-2f-2)!(l-m-1-w)!}{(2f+1)!(2l-2f-1)!(2f-w)!(l-2f+m-1+w)!}\right)^{1/2}\right.$$

$$
\times\ (-1)^{f(l-m-1)} C_{(w)} r_1^f Y_f^{f-w}(\theta_1,\phi_1) r_2^{l-1-f} Y_{l-1-f}^{m+w-f}(\theta_2,\phi_2)
$$

$$
\left.\times\ (r_2 Y_1^0(\theta_2,\phi_2) - r_1 Y_1^0(\theta_1,\phi_1))\right\}
$$

$$
+\left\{\left(\frac{4\pi(l+m)!(l-m)(l-m-1)(2l-1)!}{(2l)!(l-m-2)!}\right)^{1/2}\right.
$$

$$
\times \sum_{f=0}^{l-1}\sum_{w=0}^{l-m-2}\left(\frac{(2f)!w!(2l-2f-2)!(l-m-2-w)!}{(2f+1)!(2l-2f-1)!(2f-w)!(l-2f+m+w)!}\right)^{1/2}
$$

$$
\times\ (-1)^{f(l-m-2)} C_{(w)} r_1^f Y_f^{f-w}(\theta_1,\phi_1) r_2^{l-1-f} Y_{l-1-f}^{m+1+w-f}(\theta_2,\phi_2)
$$

$$
\left.\left.\times\ (r_2 Y_1^{-1}(\theta_2,\phi_2) - r_1 Y_1^{-1}(\theta_1,\phi_1))\right\}\right]. \tag{3}
$$

Each term of each double summation in (3) is composed of two parts and we take one part from each summation; that is, we pick out the parts multiplied by $r_2 Y_1^1(\theta_2,\phi_2)$, $r_2 Y_1^0(\theta_2,\phi_2)$ and $r_2 Y_1^{-1}(\theta_2,\phi_2)$. These may be regrouped by using a special case of equation (2), namely

$$
r_2^{l-f} Y_{l-f}^{m+w-f}(\theta_2,\phi_2)
$$

$$
= \left(\frac{(2l-2f+1)4\pi}{3(l-f)}\right)^{1/2}\left\{ r_2^{l-f-1} Y_{l-1-f}^{m-1+w-f}(\theta_2,\phi_2) r_2 Y_1^1(\theta_2,\phi_2)\right.
$$

$$
\times \left(\frac{(l-2f+m+w)(l-2f+m+w-1)}{(2l-2f)(2l-2f-1)}\right)^{1/2}
$$

$$
+ \left(\frac{2(l+m+w-2f)(l-m-w)}{(2l-2f)(2l-2f-1)}\right)^{1/2} r_2^{l-f-1} Y_{l-1-f}^{m+w-f}(\theta_2,\phi_2) r_2 Y_1^0(\theta_2,\phi_2)
$$

$$
\left.+ \left(\frac{(l-m-w)(l-m-w-1)}{(2l-2f)(2l-2f-1)}\right)^{1/2} r_2^{l-f-1} Y_{l-1-f}^{m+w-f+1}(\theta_2,\phi_2) r_2 Y_1^{-1}(\theta_2,\phi_2)\right\}. \tag{4}
$$

We observe also that in (3) in the second and third double summations we can extend the summation over w to $l-m$ since the additional terms will vanish because the conditions mentioned in connection with equation (1), applying to the harmonics occurring, are violated. After regrouping all the harmonics in (θ_2,ϕ_2) we obtain

$$
\left(\frac{4\pi(l+m)!(2l+1)!}{(2l)!(l-m)!}\right)^{1/2} \sum_{f=0}^{l-1}\sum_{w=0}^{l-m}\left(\frac{(2f)!w!(2l-2f)!(l-m-w)!}{(2f+1)!(2l-2f+1)!(2f-w)!(l-2f+m+w)!}\right)^{1/2}
$$

$$
\times\ (-1)^{f(l-m)} C_{(w)} r_1^f Y_f^{f-w}(\theta_1,\phi_1) r_2^{l-f} Y_{l-f}^{m+w-f}(\theta_2,\phi_2)\left(\frac{l-f}{l}\right). \tag{5}
$$

The above method is repeated by regrouping the three terms multiplied by $r_1 Y_1^1(\theta_1,\phi_1)$, $r_1 Y_1^0(\theta_1,\phi_1)$ and $r_1 Y_1^{-1}(\theta_1,\phi_1)$ using a relation involving (θ_1,ϕ_1) similar to (4) for

$r_1^{f+1}Y_{f+1}^{f+1-w}(\theta_1,\phi_1)$ instead of $r_2^{l-f}Y_{l-f}^{m+w-f}(\theta_2,\phi_2)$. The net result gives

$$\left(\frac{4\pi(l+m)!(2l+1)!}{(2l)!(l-m)!}\right)^{1/2}\sum_{f=0}^{l-1}\sum_{w=0}^{l-m}\left(\frac{(2f+2)!w!(2l-2f-2)!(l-m-w)!}{(2f+3)!(2l-2f-1)(2f-w+2)!(l-2f+m+w-2)!}\right)^{1/2}$$
$$\times(-1)^{f+1}\,{}^{(l-m)}C_{(w)}r_1^{f+1}Y_{f+1}^{f+1-w}(\theta_1,\phi_1)r_2^{l-f}Y_{l-1-f}^{m+w-1-f}(\theta_2,\phi_2)\left(\frac{f+1}{l}\right). \quad (6)$$

In (6) if f is replaced by $f-1$ each term in the double summation is the same as that in (5) except that in place of $(l-f)/l$ (at the end of each term) in (5) we have f/l. We can make this change providing we replace the summation over f in (6) by a sum from $f=1$ to $f=l$. When $f=0$ in (5) we get exactly the first term in $|r_1-r_2|^l Y_l^m(\theta_R,\phi_R)$ given in (1) since the factor $(l-f)/l$ is then equal to unity. When f (after changing f to $f-1$) in (6) is equal to l the part f/l is also equal to unity and we get the $f=l$ term in (1). If $0<f<l$ we may combine the factor $(l-f)/l$ from (5) and f/l from (6) to give unity. Thus the combination of (5) and (6) does indeed give (1) and hence the formula is true by induction since it is true for $l=1$ (which may easily be verified).

3. A formula for $1/r_{12}^t$ when t is odd

In this section we first give below a formula for differentiating the Legendre polynomial

$$P_n(x)=\frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^2-1)^n$$

with respect to x, s times:

$$\frac{\mathrm{d}^s}{\mathrm{d}x^s}P_n(x)=\sum_{p=0}^{\frac{1}{2}(n-s),\frac{1}{2}(n-s-1)}{}^{(s+p-1)}C_{(p)}(2n-2s-4p+1)\prod_{k=0}^{s-2}(2n-1-2p-2k)P_{n-s-2p}(x). \quad (7)$$

The two upper limits on the sum p are for the cases when $n-s$ is even or odd.

Now let us prove (7) by induction on s. When $s=1$ we obtain

$$\frac{\mathrm{d}}{\mathrm{d}x}P_n(x)=(2n-1)P_{n-1}(x)+(2n-5)P_{n-3}(x)+(2n-9)P_{n-5}(x)+\cdots\begin{cases}+P_0 & \text{if } n \text{ is odd}\\ +3P_1 & \text{if } n \text{ is even}\end{cases}$$

which is a relation given in many elementary texts (Copson 1935).

Assume now that (7) is true for $s-1$, thus

$$\frac{\mathrm{d}^{s-1}}{\mathrm{d}x^{s-1}}P_n(x)=\sum_{p=0}^{\frac{1}{2}(n-s+1),\frac{1}{2}(n-s)}{}^{(s+p-2)}C_{(p)}(2n-2s-4p+3)$$
$$\times\prod_{k=0}^{s-3}(2n-1-2p-2k)P_{n-s+1-2p}(x). \quad (9)$$

If h is an integer, then we use the well known relation for Legendre functions (see Jahnke and Emde 1945, to be referred to as I)

$$(2h+1)P_h=\frac{\mathrm{d}}{\mathrm{d}x}P_{h+1}-\frac{\mathrm{d}}{\mathrm{d}x}P_{h-1}.$$

Using the above relation the right-hand side of (7) becomes, with $h = n-s-2p$,

$$\frac{\mathrm{d}}{\mathrm{d}x}\sum_{p=0}^{\frac{1}{2}(n-s),\frac{1}{2}(n-s-1)} {}^{(s+p-1)}C_{(p)}\prod_{k=0}^{s-2}(2n-1-2p-2k)(P_{n-s-2p+1}(x)-P_{n-s-2p-1}(x))$$

$$= \frac{\mathrm{d}}{\mathrm{d}x}F(x) \qquad (10)$$

where $F(x)$ is defined by equation (10). Thus, if we can show that $F(x)$ is equal to the right-hand side of (9), then

$$\frac{\mathrm{d}}{\mathrm{d}x}F(x) = \frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}^{s-1}}{\mathrm{d}x^{s-1}}P_n(x)$$

and we shall have proved the result for any s assuming it to be true for $s-1$. In order to simplify the comparison with (9) we rewrite $F(x)$ as

$$F(x) = \sum_{p=0}^{\frac{1}{2}(n-s),\frac{1}{2}(n-s-1)} {}^{(s+p-1)}C_{(p)}\prod_{k=0}^{s-2}(2n-1-2p-2k)P_{n-s-2p+1}(x)$$
$$- \sum_{p=1}^{\frac{1}{2}(n-s+1),\frac{1}{2}(n-s)} {}^{(s+p-2)}C_{(p-1)}\prod_{k=0}^{s-2}(2n+1-2p-2k)P_{n-s-2p+1}(x). \qquad (11)$$

The term with $p = 0$ in the summation of (9) equals

$$(2n-2s+3)(2n-1)(2n-3)(2n-5)\dots(2n-2s+7)(2n-2s+5)$$

whereas the same term in the first summation of (11) equals

$$(2n-1)(2n-3)(2n-5)\dots(2n-2s+5)(2n-2s+3)$$

so the $p = 0$ term is the same in (11) and (9). For $p \geqslant 1$ the coefficients of $P_{n-s-2p+1}(x)$ in (11) may be rewritten as

$$\{{}^{(s+p-1)}C_{(p)}(2n-2p-2s+3) - {}^{(s+p-2)}C_{(p-1)}(2n+1-2p)\}$$
$$\times(2n-1-2p)(2n-3-2p)\dots(2n-2p-2s+7)(2n-2p-2s+5)$$
$$= {}^{(s+p-2)}C_{(p)}(2n-2s-4p+3)\prod_{k=0}^{s-3}(2n-1-2p-2k)$$

which is exactly the pth term of (9). Therefore (7) is proved by induction.

We now continue with the relation for $1/r_{12}^t$. When $x = \cos\theta$ and $r < 1$ (see I) we expand as follows:

$$(1-2rx+r^2)^{-\frac{1}{2}} = \sum_{u=0}^{\infty} r^u P_u(x). \qquad (12)$$

Differentiating both sides of (12) q times with respect to x, we obtain:

$$(-\tfrac{1}{2}).(-\tfrac{3}{2}).(-\tfrac{5}{2})\dots\{-\tfrac{1}{2}(2q-1)\}(-2r)^q(1-2rx+r^2)^{-\frac{1}{2}-q}$$
$$= 1.3.5.7\dots(2q-1)r^q(1-2rx+r^2)^{-\frac{1}{2}-q}$$
$$= \bar{f}(q)r^q(1-2rx+r^2)^{-\frac{1}{2}-q} \qquad (13)$$

where $\bar{f}(q) = 1.3.5.7\ldots(2q-1) = (2q-1)!!$ (13) is therefore equal to

$$\sum_{u=0}^{\infty} r^u \frac{d^q}{dx^q} P_u(x)$$

and using (7) this becomes

$$\sum_{u=0}^{\infty} \sum_{v=0}^{\frac{1}{2}(u-q),\frac{1}{2}(u-q-1)} r^{u(q+v-1)} C_{(v)}(2u-2q-4v+1) \prod_{k=0}^{q-2} (2u-1-2v-2k) P_{u-q-2v}(x). \tag{14}$$

$1/|\boldsymbol{r}_1 - \boldsymbol{r}_2|^t$ may be written as

$$\frac{\{1+(\bar{r}_</\bar{r}_>)^2 - 2(\bar{r}_</\bar{r}_>)\cos\theta\}^{-t/2}}{\bar{r}^t}$$

where θ is the angle between the two vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ and $\bar{r}_<$ and $\bar{r}_>$ are defined to be the smallest and the greatest of r_1 and r_2 respectively. x in (12), (13) and (14) is now identified with $\cos\theta$, $\bar{r}_</\bar{r}_>$ with r and $2q+1$ with t. Thus

$$\begin{aligned}\frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|^t} = \sum_{u=0}^{\infty} &\sum_{v=0}^{\frac{1}{2}(2u-t+1),\frac{1}{2}(2u-t-1)} \frac{1}{\bar{r}^t_>} \frac{1}{r^{(t-1)/2}\bar{f}((t-1)/2)} \\ &\times r^{u(\frac{1}{2}(t+2v-3))} C_{(v)}(2u-4v-t+2) \\ &\times \prod_{k=0}^{\frac{1}{2}(t-1)-2} (2u-1-2v-2k) P_{u-2v-\frac{1}{2}(t-1)}(\cos\theta).\end{aligned}$$

It is convenient now to use the addition theorem for Legendre functions which may be stated as

$$P_l(\cos\theta) = \sum_{m=-l}^{l} \frac{(l-|m|)!}{(l+|m|)!} P_l^{|m|}(\cos\theta_1) P_l^{|m|}(\cos\theta_2) \exp\{\mathrm{i}\, m(\phi_1 - \phi_2)\}$$

where (θ_1, ϕ_1) and (θ_2, ϕ_2) denote the orientation of the vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ and the sum contains products of associated Legendre polynomials. Finally, we get the following relation:

$$\begin{aligned}\frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|^t} = \sum_{u=0}^{\infty} &\sum_{v=0}^{\frac{1}{2}(2u-t+1),\frac{1}{2}(2u-t-1)} \sum_{m=-\{u-2v-\frac{1}{2}(t-1)\}}^{u-2v-\frac{1}{2}(t-1)} \frac{1}{\bar{r}^t_>} \frac{1}{\bar{f}((t-1)/2)} \\ &\times r^{u-\frac{1}{2}(t-1)(\frac{1}{2}(t+2v-3))} C_{(v)}(2u-4v-t+2) \\ &\times \prod_{k=0}^{\frac{1}{2}(t-1)-2} (2u-1-2v-2k) \frac{(u-2v-\frac{1}{2}(t-1)-|m|)!}{(u-2v-\frac{1}{2}(t-1)+|m|)!} \\ &\times P^{|m|}_{u-2v-\frac{1}{2}(t-1)}(\cos\theta_1) P^{|m|}_{u-2v-\frac{1}{2}(t-1)}(\cos\theta_2) \exp \mathrm{i}\, m(\phi_1 - \phi_2) \\ = 4\pi \sum_{u=0}^{\infty} &\sum_{v=0}^{\frac{1}{2}(2u-t+1),\frac{1}{2}(2u-t-1)} \sum_{m=-\{u-2v-\frac{1}{2}(t-1)\}}^{u-2v-\frac{1}{2}(t-1)} \frac{1}{\bar{r}^t_>} \frac{1}{\bar{f}((t-1)/2)} \\ &\times r^{u-\frac{1}{2}(t-1)(\frac{1}{2}(t+2v-3))} C_{(v)} \\ &\times \prod_{k=0}^{\frac{1}{2}(t-1)-2} (2u-1-2v-2k) Y^m_{u-2v-\frac{1}{2}(t-1)}(\theta_1, \phi_1) Y^{m*}_{u-2v-\frac{1}{2}(t-1)}(\theta_2, \phi_2)\end{aligned} \tag{15}$$

4. A formula for $1/r_{12}^t$ when t is even

When t is even we shall make use of formula (7) for the derivative with respect to x performed s times on a Legendre polynomial. We first find a formula for $(1-2rx+r^2)^{-1}$ and then extend this using (7) to the case $(1-2rx+r^2)^{-t/2}$ for even t. It is supposed that the former may be expanded in Legendre polynomials as

$$(1-2rx+r^2)^{-1} = \sum_{d=0}^{\infty} b_d(r)P_d(x). \tag{16}$$

Multiplying (16) through by $P_z(x)$ and integrating we obtain

$$b_z\frac{2}{2z+1} = \frac{1}{2r}\int_{-1}^{1}\frac{P_z(x)}{\{(1+r^2)/2r\}-x}\,\mathrm{d}x. \tag{17}$$

By a relation due to Neumann (see I) (17) becomes

$$b_z = \frac{2z+1}{2r}Q_z\left(\frac{1+r^2}{2r}\right)$$

and

$$(1-2rx+r^2)^{-1} = \sum_{d=0}^{\infty}\frac{2d+1}{2r}Q_d\left(\frac{1+r^2}{2r}\right)P_d(x) \tag{18}$$

where $Q_z(y)$ is a Legendre polynomial of the second kind of the zth order which may be expanded for $|y|>1$ (a condition which always holds in (18)) as follows:

$$Q_z(y) = \frac{z!}{1.3.5\ldots(2z+1)}\left(\frac{1}{y^{z+1}}+\frac{(z+1)(z+2)}{2(2z+3)}\frac{1}{y^{z+3}} + \frac{(z+1)(z+2)(z+3)(z+4)}{2.4.(2z+3)(2z+5)}\frac{1}{y^{z+5}}+\ldots\right). \tag{19}$$

If we differentiate $(1-2rx+r^2)^{-1}$, μ times with respect to x, we get

$$\frac{\mathrm{d}^\mu}{\mathrm{d}x^\mu}(1-2rx+r^2)^{-1} = 2^\mu r^\mu(\mu!)(1-2rx+r^2)^{-1-\mu}\ldots. \tag{20}$$

To find the expansion for $1/|\boldsymbol{r}_1-\boldsymbol{r}_2|^t$ we identify $\cos\theta$ with x again, $\bar{r}_</\bar{r}_>$ with r and $\mu+1$ with $t/2$. We deduce from (20), (18) and (7) that

$$\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|^t} = \sum_{d=0}^{\infty}\frac{2d+1}{2r}Q_d\left(\frac{1+r^2}{2r}\right)\frac{1}{2^{\frac{1}{2}t-1}}\frac{1}{r^{\frac{1}{2}t-1}}\frac{1}{(\frac{1}{2}t-1)!}\frac{1}{\bar{r}_>^t} \times\sum_{v=0}^{\frac{1}{2}(2d-t+2),\frac{1}{2}(2d-t)} {}^{\frac{1}{2}(t+2v-4)}C_{(v)}(2d-4v-t+3) \times\prod_{k=0}^{\frac{1}{2}t-3}(2d-1-2v-2k)P_{\frac{1}{2}(2d-t+2-4v)}(x). \tag{21}$$

Using the addition theorem for Legendre functions and the definition of spherical harmonics given by Condon and Shortley (1964) (21) becomes

$$\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|^t}=4\pi\sum_{d=0}^{\infty}\sum_{v=0}^{\frac{1}{2}(2d-t+2),\frac{1}{2}(2d-t)}\sum_{m=-\frac{1}{2}(2d-t+2-4v)}^{\frac{1}{2}(2d-t+2-4v)}\frac{2d+1}{2r}Q_d\left(\frac{1+r^2}{2r}\right)$$
$$\times\frac{1}{2^{\frac{1}{2}t-1}}\frac{1}{r^{\frac{1}{2}t-1}}\frac{1}{(\frac{1}{2}t-1)!}\frac{1}{\bar{r}_>^t}\,{}^{\frac{1}{2}(t+2v-4)}C_{(v)}$$
$$\times\prod_{k=0}^{\frac{1}{2}t-3}(2d-1-2v-2k)Y^m_{\frac{1}{2}(2d-t+2-4v)}(\theta_1,\phi_1)Y^{m*}_{\frac{1}{2}(2d-t+2-4v)}(\theta_2,\phi_2). \quad (22)$$

5. Conclusions

In this paper we have studied the spherical harmonic which describes the orientation of the vector difference $\boldsymbol{r}_1-\boldsymbol{r}_2$. We have proved a formula for the expansion of this harmonic in a series of products of spherical harmonics in the orientation of $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ separately. There are many areas of physics, we believe, where such a formula would prove to be of value. Further, it is easy to see how our formula could be generalized to generate a harmonic expansion for $|\boldsymbol{r}_1-\boldsymbol{r}_2-\boldsymbol{r}_3-\boldsymbol{r}_4\ldots-\boldsymbol{r}_n|^l Y_l^m(\bar{\theta},\bar{\phi})$ by repeated use of the relation we have given ($\bar{\theta}$ and $\bar{\phi}$ here represent the orientation of the vector inside the moduli signs).

A second relation has been given for a Legendre polynomial P_n differentiated s times. This was expanded in terms of Legendre polynomials and was used in conjunction with other relationships to write $1/|\boldsymbol{r}_1-\boldsymbol{r}_2|^t$ as a series of products of spherical harmonics, one in the orientation of $\boldsymbol{r}_1$ and the other in the orientation of $\boldsymbol{r}_2$, where t is an integer. We have in fact investigated the cases when t is odd and even separately. One obvious example where such an expansion would prove useful is in the use of a Thomas–Fermi screened Coulomb interaction of the form $e^2\exp(-L/r_{12})/r_{12}$ where L is the screening length.

These formulae are particularly useful when collected together in one place. The utility of the expansions we have given, particularly that for $Y_l^m(\theta_R,\phi_R)$, becomes clear if we wish to pick out a given spherical harmonic, for example $Y_{\bar{l}}^{\bar{m}}(\theta,\phi)$, from the series. Our expansions enable us to pick out the contributions to the coefficient of such a harmonic and to readily assess their magnitude and importance in any particular physical application. A further generalization is possible if we use our formulae to generate a harmonic expansion for $1/|\boldsymbol{r}_1-\boldsymbol{r}_2-\boldsymbol{r}_3-\ldots-\boldsymbol{r}_n|^t$.

Acknowledgments

This work was performed as part of research supported by the Swiss National Foundation for Scientific Research.

References

Barnett M P and Coulson C A 1951 *Phil. Trans. R. Soc.* A **243** 221
Condon E U and Shortley G H 1964 *The Theory of Atomic Spectra* (London: Cambridge University Press)

Copson E T 1935 *Theory of Functions of a Complex Variable* (Oxford: Clarendon Press)
Heine V 1960 *Group Theory in Quantum Mechanics* (Oxford: Pergamon) appendix 1
Hobson E W 1955 *The Theory of Spherical and Ellipsoidal Harmonics* (New York: Chelsea)
Jahnke E and Emde F 1945 *Tables of Functions with Formulae and Curves* (New York: Dover)
Sack R A 1964 *J. math. Phys.* **5** 245–51, 252–9
Sharma R R 1968 *J. math. Phys.* **9** 505–9