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A formula for angular and hyperangular integration

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A formula is derived which allows angular or hyperangular integration to be performed on any function of the coordinates of a d-dimensional space, provided that it is possible to expand the function as a polynomial in the coordinates $x_1, x_2, \ldots, x_d$. The expansion need not be carried out for the formula to be applied.

1. Introduction

Since quantum chemists and physicists frequently need to perform angular integrations when calculating matrix elements, formulae for evaluating angular integrals have very general interest and utility. A number of such formulae have been discussed by the author and coworkers in previous publications [3–6,9]. In the present note, a new angular integration formula is derived, which is more general than those previously discussed.

2. Hyperangular integration in d-dimensional spaces

Let

$$\mathbf{x} = \{x_1, x_2, x_3, \ldots, x_d\} \tag{1}$$

be the Cartesian coordinates of a d-dimensional space, and let

$$r = \left(x_1^2 + x_2^2 + \cdots + x_d^2\right)^{1/2} \tag{2}$$

be the hyperradius in this space, while

$$\Delta = \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2} \tag{3}$$

is the generalized Laplacian operator. The volume element in the space can be expressed in the form [3,4]

$$\mathrm{d}x_1\,\mathrm{d}x_2 \ldots \mathrm{d}x_d = r^{d-1}\,\mathrm{d}r\,\mathrm{d}\Omega, \tag{4}$$

where $\mathrm{d}\Omega$ is the generalized solid angle element. The total solid angle in such a space can be found by noticing that

$$\int_0^\infty \mathrm{d}r\, r^{d-1}\, \mathrm{e}^{-r^2} \int \mathrm{d}\Omega = \prod_{j=1}^{d} \int_{-\infty}^{\infty} \mathrm{d}x_j\, \mathrm{e}^{-x_j^2} = \pi^{d/2} \tag{5}$$

and

$$\int_0^\infty \mathrm{d}r\, r^{d-1}\, \mathrm{e}^{-r^2} = \frac{1}{2}\Gamma\left(\frac{d}{2}\right), \tag{6}$$

and, therefore,

$$\int \mathrm{d}\Omega = \frac{2\pi^{d/2}}{\Gamma(d/2)}. \tag{7}$$

For example, when $d = 3$, this reduces to

$$\int \mathrm{d}\Omega = \frac{2\pi^{3/2}}{\Gamma(3/2)} = 4\pi, \tag{8}$$

while when $d = 4$, we have

$$\int \mathrm{d}\Omega = \frac{2\pi^{4/2}}{\Gamma(4/2)} = 2\pi^2. \tag{9}$$

The angular integration formula which will be derived in this paper states that, if $F(\mathbf{x})$ is any function which can be expanded about the origin in terms of a polynomial in $x_1, x_2, x_3, \ldots, x_d$, then

$$\int \mathrm{d}\Omega\, F(\mathbf{x}) = \frac{(d-2)!!2\pi^{d/2}}{\Gamma(d/2)} \sum_{\nu=0}^{\infty} \frac{r^{2\nu}}{(2\nu)!!(d+2\nu-2)!!} \left[\Delta^\nu F(\mathbf{x})\right]_{\mathbf{x}=0}. \tag{10}$$

When $d = 3$, this formula reduces to

$$\int \mathrm{d}\Omega\, F(\mathbf{x}) = 4\pi \sum_{\nu=0}^{\infty} \frac{r^{2\nu}}{(2\nu+1)!} \left[\Delta^\nu F(\mathbf{x})\right]_{\mathbf{x}=0}. \tag{11}$$

3. Homogeneous and harmonic polynomials

The angular integration formula shown above can be derived from the properties of homogeneous polynomials and harmonic polynomials. An homogeneous polynomial of order n is a polynomial of the form

$$f_n(\mathbf{x}) = A \prod_{j=0}^{d} x_j^{n_j} + B \prod_{j=0}^{d} x_j^{n'_j} + \cdots, \tag{12}$$

where $A, B, \ldots$ are constants and

$$\sum_{j=0}^{d} n_j = n, \qquad \sum_{j=0}^{d} n'_j = n, \qquad \text{etc.} \tag{13}$$

An harmonic polynomial, $h_n(\mathbf{x})$, is an homogeneous polynomial which, in addition to being homogeneous, also satisfies the generalized Laplace equation

$$\Delta h_n(\mathbf{x}) = 0. \tag{14}$$

Any homogeneous polynomial of order n obeys the relationship [3,4,10]

$$\left[\sum_{j=0}^{d} x_j \frac{\partial}{\partial x_j} - n\right] f_n(\mathbf{x}) = 0, \tag{15}$$

from which it follows that, for harmonic polynomials,

$$\Delta\left[r^m h_n(\mathbf{x})\right] = m(m + d + 2n - 2) r^{m-2} h_n(\mathbf{x}). \tag{16}$$

Any homogeneous polynomial, $f_n(\mathbf{x})$, can be decomposed into a series of harmonic polynomials multiplied by appropriate powers of the hyperradius [10]:

$$f_n(\mathbf{x}) = h_n(\mathbf{x}) + r^2 h_{n-2}(\mathbf{x}) + r^4 h_{n-4}(\mathbf{x}) + \cdots. \tag{17}$$

For even n, the final term in this decomposition is $r^n h_0$, where h_0 is a constant. If we apply the generalized Laplacian operator $n/2$ times to both sides of equation (17), making use of (16) we obtain, for even n,

$$\Delta^{n/2} f_n(\mathbf{x}) = \frac{n!!(d + n - 2)!!}{(d - 2)!!} h_0. \tag{18}$$

Thus the constant h_0 which occurs in (17) when n is even is given by

$$h_0 = \frac{(d - 2)!!}{n!!(d + n - 2)!!} \Delta^{n/2} f_n(\mathbf{x}). \tag{19}$$

4. Grand angular momentum

The generalized Laplacian operator can be written in the form [3,4]

$$\Delta = \frac{1}{r^{d-1}} \frac{\partial}{\partial r} r^{d-1} \frac{\partial}{\partial r} - \frac{\Lambda^2}{r^2}, \tag{20}$$

where

$$\Lambda^2 = -\sum_{i>j}^{d} \left(x_i \frac{\partial}{\partial x_j} - x_j \frac{\partial}{\partial x_i} \right)^2 \tag{21}$$

is the generalized or grand angular momentum operator. From (14) and (20) we have, for any harmonic polynomial,

$$\left(\frac{1}{r^{d-1}}\frac{\partial}{\partial r}r^{d-1}\frac{\partial}{\partial r} - \frac{\Lambda^2}{r^2}\right)h_n(\mathbf{x}). \tag{22}$$

If we let

$$Y_n(\Omega) \equiv r^{-n}h_n(\mathbf{x}), \tag{23}$$

then (22) yields

$$\left[n(n+d-2) - \Lambda^2\right]r^n Y_n(\Omega) = 0, \tag{24}$$

because $Y_n(\Omega)$ is a pure function of the hyperangles and is independent of r. We can rewrite (24) in the form

$$\Lambda^2 h_n(\mathbf{x}) = n(n+d-2)h_n(\mathbf{x}). \tag{25}$$

In other words, every harmonic polynomial of order n is an eigenfunction of the grand angular momentum operator Λ^2. The decomposition of an homogeneous polynomial into harmonic polynomials multiplied by powers of the hyperradius (equation (17)) can thus be interpreted as a decomposition of the homogeneous polynomial into eigenfunctions of Λ^2. Since eigenfunctions of Λ^2 corresponding to different eigenvalues are orthogonal when integrated over the generalized solid angle [3], we have

$$\int \mathrm{d}\Omega\, h_{n'}(\mathbf{x})h_n(\mathbf{x}) = 0 \quad \text{if } n' \neq n. \tag{26}$$

If we let $n' = 0$ and if we remember that h_0 is a constant, (26) implies that

$$\int \mathrm{d}\Omega\, h_n(\mathbf{x}) = 0 \quad \text{if } n \neq 0. \tag{27}$$

Making use of (17) and (27) for the case of even n, we obtain

$$\int \mathrm{d}\Omega\, f_n(\mathbf{x}) = \int \mathrm{d}\Omega\left[h_n(\mathbf{x}) + r^2 h_{n-2}(\mathbf{x}) + \cdots + r^n h_0\right] = r^n h_0 \frac{2\pi^{d/2}}{\Gamma(d/2)}. \tag{28}$$

With the help of (19), we can rewrite (28) in the form

$$\int \mathrm{d}\Omega\, f_n(\mathbf{x}) = \frac{(d-2)!!2\pi^{d/2}r^n}{\Gamma(d/2)n!!(n+d-2)!!}\Delta^{n/2} f_n(\mathbf{x}). \tag{29}$$

We have assumed that it is possible to expand $F(\mathbf{x})$ about the origin in terms of a polynomial in the coordinates $x_1, x_2, \ldots, x_d$, and thus we can write

$$F(\mathbf{x}) = \sum_{n=0}^{\infty} f_n(\mathbf{x}), \tag{30}$$

where the functions $f_n(\mathbf{x})$ are homogeneous polynomials. Combining (30) and (29), we obtain

$$\int \mathrm{d}\Omega\, F(\mathbf{x}) = \frac{(d-2)!!2\pi^{d/2}}{\Gamma(d/2)} \sum_{n=0,2,\ldots}^{\infty} \frac{r^n}{n!!(n+d-2)!!} \Delta^{n/2} f_n(\mathbf{x}), \tag{31}$$

where the odd terms have been omitted because, as a consequence of (17) and (27), they cannot contribute to the angular integral. From (30) it follows that

$$\left[\Delta^{n/2} F(\mathbf{x})\right]_{\mathbf{x}=0} = \Delta^{n/2} f_n(\mathbf{x}), \tag{32}$$

since the operation of setting $\mathbf{x} = 0$ eliminates all parts of a polynomial in $x_1, x_2, \ldots, x_d$ except the constant term. Finally, if we let $n = 2\nu$, making use of (32), we can see that (31) will take on the form shown in equation (10).

5. Some illustrative examples

To illustrate the angular integration formula discussed above, we can consider the case where $F(\mathbf{x})$ is a d-dimensional plane wave

$$F(\mathbf{x}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} = \mathrm{e}^{\mathrm{i}(k_1 x_1 + k_2 x_2 + \cdots + k_d x_d)}. \tag{33}$$

Then

$$\left[\Delta^{\nu} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\right]_{\mathbf{x}=0} = (-1)^{\nu} k^{2\nu}, \tag{34}$$

so that (10) yields

$$\int \mathrm{d}\Omega\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} = \frac{(d-2)!!2\pi^{d/2}}{\Gamma(d/2)} \sum_{\nu=0}^{\infty} \frac{(-1)^{\nu}(kr)^{2\nu}}{(2\nu)!!(d+2\nu-2)!!}. \tag{35}$$

When $d = 3$, this reduces to

$$\int \mathrm{d}\Omega\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} = 4\pi \sum_{\nu=0}^{\infty} \frac{(-1)^{\nu}(kr)^{2\nu}}{(2\nu+1)!} = 4\pi j_0(kr), \tag{36}$$

where $j_0(kr)$ is a spherical Bessel function of order zero.

As a second example, let us consider the angular integral of a product of three spherical harmonics in a 3-dimensional space, i.e., the case where

$$F(\mathbf{x}) = Y^*_{l,m}(\theta,\phi) Y_{l',m'}(\theta,\phi) Y_{l'',m''}(\theta,\phi). \tag{37}$$

Since equations (10) and (11) are really designed for the angular integration of polynomials, we begin the calculation by converting the spherical harmonics into harmonic polynomials in Cartesian coordinates x_1, x_2 and x_3:

$$Y_{l,m}(\theta,\phi) \equiv r^{-l} h_{l,m}(\mathbf{x}). \tag{38}$$

Then

$$\int \mathrm{d}\Omega\, Y^*_{l,m} Y_{l',m'} Y_{l'',m''} = \frac{1}{r^n} \int \mathrm{d}\Omega\, f_n(\mathbf{x}), \tag{39}$$

where $n = l + l' + l''$ and

$$f_n(\mathbf{x}) \equiv h^*_{l,m}(\mathbf{x}) h_{l',m'}(\mathbf{x}) h_{l'',m''}(\mathbf{x}). \tag{40}$$

Since $f_n(\mathbf{x})$ is an homogeneous polynomial of order n, the integral vanishes if $n = l + l' + l''$ is odd (as a consequence of equations (17) and (27)). When n is even, the integral is given by a single term in the series shown in equation (11), the term where $\nu = n/2$. Thus we have

$$\int \mathrm{d}\Omega\, Y^*_{l,m} Y_{l',m'} Y_{l'',m''} = \frac{4\pi}{(l + l' + l'' + 1)!} \Delta^{(l+l'+l'')/2} h^*_{l,m}(\mathbf{x}) h_{l',m'}(\mathbf{x}) h_{l'',m''}(\mathbf{x}), \tag{41}$$

where the harmonic polynomials $h_{l,m}(\mathbf{x})$ are defined by (38). It is unnecessary to set $\mathbf{x} = 0$ in this case, since $\Delta^{n/2} f_n(\mathbf{x})$ is a constant. Integrals involving hyperspherical harmonics (such as the integrals needed in the Shibuya–Wulfman method [10,12], or in molecular dynamics [1,2], or in dimensional scaling [7,8]) can, of course, be calculated with equal ease from equation (10) using systems such as *Mathematica* or *Maple*, within which differentiation of polynomials is an easily-performed operation.

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