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An addition theorem for spherical harmonics

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Summary. An addition theorem, expressing the spherical harmonics $Y_{lm}(\Omega_{\mathbf{r}_1-\mathbf{r}_2})$ in terms of the spherical harmonics $Y_{l_1m_1}(\Omega_{\mathbf{r}_1})$ and $Y_{l_2m_2}(\Omega_{\mathbf{r}_2})$, is derived.

1. *Introduction and résumé.* The transformation properties of spherical harmonics under rotations are well known and widely used (1). In contrast, very little is known about the behaviour of spherical harmonics under translations. In fact, all existing addition theorems describing the effect of translations, were formulated for spherical waves (of the form $[f_l(r)\,Y_{lm}(\Omega_{\mathbf{r}})]$) (2); the effect of translations on the functions $Y_{lm}(\Omega_{\mathbf{r}})$ was, apparently, not investigated. It is precisely the discussion of the last problem that forms the contents of the present paper.

Using spherical harmonics as defined by Edmonds (3), and denoting by $\Omega_{\mathbf{r}_1}$, $\Omega_{\mathbf{r}_2}$ and $\Omega_{\mathbf{r}}$ the directions of the vectors $\mathbf{r}_1$, $\mathbf{r}_2$ and $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$. the following expansion is derived:

$$Y_{lm}(\Omega_{\mathbf{r}}) = \sum_{l_1l_2} g^l_{l_1l_2}(r_1/r_2) \sum_{m_1m_2} (l_1m_1l_2m_2|lm)\,Y_{l_1m_1}(\Omega_{\mathbf{r}_1})\,Y_{l_2m_2}(\Omega_{\mathbf{r}_2}), \tag{1}$$

where

$$g^l_{l_1l_2}(x) = \left\{\begin{array}{ll} E^l_{l_1l_2}(l_10l_20|l0)\,x^{l_1}F((l_1+l_2)/2,(l_1-l_2-1)/2,(2l_1+3)/2;x^2), & x<1 \\ (-1)^l g^l_{l_1l_2}(1/x) & x>1 \end{array}\right\} \tag{2}$$

and

$$E^l_{l_1l_2} = (-1)^{\frac{1}{2}(-l_1+l_2+l)}[4\pi(2l_1+1)(2l_2+1)/(2l+1)]^{\frac{1}{2}}[(2l_1+1)!!]^{-1}\{l(l+2)(l+4)\ldots \times[l+(l_1+l_2-l-2)]\}\{(l+1)(l-1)(l-3)\ldots[(l+1)-(l_1-l_2+l-2)]\}. \tag{3}$$

In these equations, $(l_1m_1l_2m_2|lm)$ are the *V-C* (vector-coupling) coefficients (1), and $F(a,b,c;z)$ is the hypergeometric function. Due to well known properties of the *V-C* coefficients, the sum in equation (1) is limited to the values

$$l_1 = 0,1,2,\ldots, \quad m_1 = -l_1,-l_1+1,\ldots,l_1 \quad |l-l_1| \leqslant l_2 \leqslant l+l_1,$$

$$l_1+l_2+l = \text{even number}, \quad m_2 = m-m_1.$$

Equation (3) is valid for $l-l_1+2 \leqslant l_2 \leqslant l+l_1-2$. For $l_2 = l-l_1$ the first curled bracket in (3) should be replaced by 1. Similarly, for $l_2 = l+1$, the second curled bracket in (3) should be replaced by 1.

Having stated the results, we shall now outline the course of derivation. Starting with the general expansion

$$Y_{lm}(\Omega_{\mathbf{r}}) = \sum_{\substack{l_1\,m_1\\ l_2\,m_2}} A^{lm}_{l_1m_1,l_2m_2}(r_1,r_2)\,Y_{l_1m_1}(\Omega_{\mathbf{r}_1})\,Y_{l_2m_2}(\Omega_{\mathbf{r}_2}), \tag{4}$$

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we shall first apply symmetry arguments to reduce (4) to (1). Next, a differential equation for the functions $g^l_{l_1 l_2}(x)$ will be derived and solved up to multiplicative constants. Finally, these constants will be determined by solving a recursion relation.

2. *Symmetry considerations.* (*a*) A *rotation* R of the coordinate system transforms each $Y_{kq}(\Omega)$ into the linear combination

$$Y_{kq}(\Omega') = \sum_{q'} [D^{(k)}(R)]^\dagger_{q'q} Y_{kq'}(\Omega), \tag{5}$$

where Ω' is the new direction and $D^{(k)}(R)$ are the Wigner rotation matrices (1). ($[D^{(k)}(R)]^\dagger$ denotes the adjoint of $D^{(k)}(R)$.) Applying the transformation (5) to (4) and utilizing the orthogonality properties of the D and Y functions, we obtain

$$A^{lm}_{l_1 m_1, l_2 m_2}(r_1, r_2) = (l_1 m_1 l_2 m_2 | lm) [\sum_{\mu_1 \mu_2} A^{l\mu}_{l_1 \mu_1 l_2 \mu_2}(r_1, r_2) \cdot (l_1 \mu_1 l_2 \mu_2 | l\mu)]$$
$$\equiv (l_1 m_1 l_2 m_2 | lm) B^l_{l_1 l_2}(r_1, r_2). \tag{6}$$

The last equation is just the familiar Wigner-Eckart theorem (4), as applied to the integral

$$\iint Y^*_{l_1 m_1}(\Omega_{\mathbf{r}_1}) Y_{lm}(\Omega_{\mathbf{r}}) Y^*_{l_2 m_2}(\Omega_{\mathbf{r}_2}) \, d\Omega_{\mathbf{r}_1} d\Omega_{\mathbf{r}_2}.$$

(*b*) A *dilatation* $\mathbf{r}_1 \to \alpha \mathbf{r}_1$, $\mathbf{r}_2 \to \alpha \mathbf{r}_2$, $(\mathbf{r} \to \alpha \mathbf{r}), \alpha > 0$ leaves the spherical harmonics invariant. Hence, $B^l_{l_1 l_2}(r_1, r_2) = B^l_{l_1 l_2}(\alpha r_1, \alpha r_2)$. In particular, for $\alpha = 1/r_2$ we have

$$B^l_{l_1 l_2}(r_1, r_2) = B^l_{l_1 l_2}(r_1/r_2, 1) \equiv g^l_{l_1 l_2}(r_1/r_2) \tag{7}$$

and (4) reduces to (1).

(*c*) A *reflection* in the origin transforms each $Y_{kq}(\Omega)$ into $(-1)^k Y_{kq}(\Omega)$ and leads to the parity condition

$$g^l_{l_1 l_2}(r_1/r_2) = (-1)^{l_1 + l_2 + l} g^l_{l_1 l_2}(r_1/r_2). \tag{8}$$

(*d*) Finally, by applying the *permutation* $\mathbf{r}_1 \to \mathbf{r}_2$, $\mathbf{r}_2 \to \mathbf{r}_1$ and using the parity condition (8) together with the symmetry relation

$$(l_1 m_1 l_2 m_2 | lm) = (-1)^{l_1 + l_2 - l} (l_2 m_2 l_1 m_1 | lm)$$

we obtain

$$g^l_{l_1 l_2}(r_1/r_2) = (-1)^l g^l_{l_2 l_1}(r_2/r_2). \tag{9}$$

3. *Differential equation for* $g^l_{l_1 l_2}(x)$. The Laplacian operators with respect to $\mathbf{r}, \mathbf{r}_1$ and $\mathbf{r}_2$ satisfy identically

$$\Delta_{\mathbf{r}} f(\mathbf{r}) = \Delta_{\mathbf{r}_1} f(\mathbf{r}) = \Delta_{\mathbf{r}_2} f(\mathbf{r}),$$

where $f(\mathbf{r})$ is any (twice differentiable) function of the variable $\mathbf{r}$. In particular, for $f(\mathbf{r}) = Y_{lm}(\Omega_{\mathbf{r}})$ we have

$$\Delta_{\mathbf{r}} Y_{lm}(\Omega_{\mathbf{r}}) = \Delta_{\mathbf{r}_1} Y_{lm}(\Omega_{\mathbf{r}}) = \Delta_{\mathbf{r}_2} Y_{lm}(\Omega_{\mathbf{r}}). \tag{10}$$

Applying the last identity to (1) we obtain, using spherical coordinates,

$$\left[\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1} - \frac{l_1(l_1+1)}{r_1^2}\right] g^l_{l_1 l_2}(r_1/r_2) = \left[\frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial}{\partial r_2} - \frac{l_2(l_2+1)}{r_2^2}\right] g^l_{l_1 l_2}(r_1/r_2),$$

from which we deduce

$$x^2(1-x^2) g'' + 2x g' + [l_2(l_2+1) x^2 - l_1(l_1+1)] g = 0, \tag{11}$$

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where $x_1 = r_1/r_2$. Substituting

$$g(x) = x^{l_1}.f(z) \quad (z = x^2),$$

we find that $f(z)$ satisfies the hypergeometric equation

$$z(1-z)\frac{d^2f}{\partial z^2}+\left[\frac{2l_1+3}{2}-\frac{2l_1+1}{2}z\right]\frac{df}{dz}-\left[\frac{l_1(l_1-1)}{4}-\frac{l_2(l_2+1)}{4}\right]f=0 \tag{12}$$

with parameters

$$a = \tfrac{1}{2}(l_1+l_2), \quad b = \tfrac{1}{2}(l_1-l_2-1), \quad \text{and} \quad c = \tfrac{1}{2}(2l_1+3) = a+b+2.$$

Two independent solutions of (12) in the neighbourhood of $z = 0$ are (5)

$$f_1(z) = F(a,b,c,;z)$$

and

$$f_2(z) = z^{1-c}F(a+1-c, b+1-c, 2-c; z),$$

where $F(a,b,c;z)$ is the hypergeometric function. Hence, the general solution of (11), which is regular at $x=0$, is

$$g^l_{l_1l_2}(x) = C^l_{l_1l_2}x^{l_1}F(\tfrac{1}{2}(l_1+l_2), \tfrac{1}{2}(l_1-l_2-1), \tfrac{1}{2}(2l_1+3); x^2), x<1. \tag{13}$$

The numerical coefficients $C^l_{l_1l_2}$ are yet to be determined.

4. *Recursion relation for* $C^l_{l_1l_2}$. The first identity in (10) reads in spherical coordinates

$$-l(l+1)Y_{lm}(\Omega_r) = (r_1^2+r_2^2-2r_1r_2\cos\theta_{12})\Delta_{r_1}Y_{lm}(\Omega_r).$$

Introducing for $Y_{lm}(\Omega_r)$ the expansion (1) and using the addition theorem (6)

$$\cos\theta_{12} = \tfrac{4}{3}\pi\sum_{M=-1}^{1}(-1)^MY_{1M}(\Omega_{r_1})Y_{1-M}(\Omega_{r_2})$$

we obtain after somewhat tedious yet straightforward calculation

$$\begin{aligned}-l(l+1)g^l_{\lambda_1\lambda_2}-(1+x^2)\left[\frac{d^2}{dx^2}g^l_{\lambda_1\lambda_2}+\frac{2}{x}\frac{d}{dx}g^l_{\lambda_1\lambda_2}-\frac{\lambda_1(\lambda_1+1)}{x^2}g^l_{\lambda_1\lambda_2}\right]\\ = 2x[(2\lambda_1+1)(2\lambda_2+1)]^{\frac{1}{2}}\sum_{l_1l_2}(10\lambda_10|l_10)(10\lambda_20|l_20)\begin{Bmatrix}l_2 & l_1 & l\\ \lambda_1 & \lambda_2 & 1\end{Bmatrix}\\ \times\left[\frac{d^2}{dx^2}g^l_{l_1l_2}+\frac{2}{x}\frac{d}{dx}g^l_{l_1l_2}-\frac{l_1(l_1+1)}{x^2}g^l_{l_1l_2}\right],\end{aligned} \tag{14}$$

where $\{\begin{smallmatrix}a & b & c\\ d & e & f\end{smallmatrix}\}$ is the 6-j-symbol (1). Due to the triangular and parity conditions on the V-C coefficients, the sum in (14) is limited to four terms at most, namely, the terms with $l_1 = \lambda_1 \pm 1$ and $l_2 = \lambda_2 \pm 1$. Dividing both sides of (14) by x^{λ_1} and letting x go to zero, we obtain, using (11) and (13),

$$\begin{aligned}C^l_{\lambda_1\lambda_2}[\lambda_2(\lambda_{2+1})-\lambda_1(\lambda_1-1)-l(l+1)] = 2(10\,\lambda_10|\lambda_1-1,0)[(2\lambda_1+1)(2\lambda_2+1)]^{\frac{1}{2}}\\ \times\sum_{l_2}C^l_{\lambda_1-1,l_2}[(\lambda_1-1)(\lambda_1-2)-l_2(l_2+1)](10\lambda_20|l_20)\begin{Bmatrix}l_2 & \lambda_1-1 & l\\ \lambda_1 & \lambda_2 & 1\end{Bmatrix},\end{aligned} \tag{15}$$

where l_2 assumes the values $\lambda_2 \pm 1$ at most. Equation (15) constitutes a recursion relation for the coefficients $C^l_{\lambda_1\lambda_2}$. The starting coefficient C^l_{0l} can be easily calculated from (1) and (13) by letting x go to zero, with the result

$$C^l_{0l} = (-1)^l\sqrt{4\pi}. \tag{16}$$

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Equations (15) and (16) provide a stepwise procedure for calculating all the coefficients $C^l_{\lambda_1\lambda_2}$ of interest. (By (1), (8) and (13), only those coefficients enter the expansion (1), for which the V-C coefficient $(\lambda_1 0 \lambda_2 0|l0)$ does not vanish.)

Fortunately, the recursion system (15) and (16) can be solved explicitly. Introducing

$$C^l_{\lambda_1\lambda_2} = (\lambda_1 0 \lambda_2 0|l0)\, E^l_{\lambda_1\lambda_2} \tag{17}$$

and using the explicit expressions for the V-C coefficients and the 6-j-symbols (1), we obtain from (15) and (16)

$$\begin{aligned} E^l_{\lambda_1\lambda_2}[\lambda_2(\lambda_2+1)-\lambda_1(\lambda_1-1)-l(l+1)] &= -[(2\lambda_1-1)(2\lambda_1+1)(2\lambda_2+1)]^{-\frac{1}{2}} \\ &\times \{E^l_{\lambda_1-1,\lambda_2-1}(l+\lambda_1+\lambda_2+1)(-l+\lambda_1+\lambda_2)[(\lambda_1-1)(\lambda_1-2)-\lambda_2(\lambda_2-1)](2\lambda_2-1)^{-\frac{1}{2}} \\ &+ E^l_{\lambda_1-1,\lambda_2+1}(l+\lambda_1-\lambda_2)(l-\lambda_1+\lambda_2+1)[(\lambda_1-1)(\lambda_1-2)-(\lambda_2+1)(\lambda_2+2)](2\lambda_2+3)^{-\frac{1}{2}}\} \end{aligned} \tag{18}$$

together with

$$E^l_{0l} = (-1)^l\sqrt{4\pi}. \tag{19}$$

It is easy to check that (3) is a solution of the system (18) and (19).

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