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Simple derivation of a formula for $y_{lm}(\boldsymbol{r}_1\times\boldsymbol{r}_2)$

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Abstract. A simple and straightforward derivation of an expression recently obtained by Hage Hassan *et al* for $y_{lm}(\boldsymbol{r}_1\times\boldsymbol{r}_2)$ in terms of $Y_{l_1m_1}(\theta_1,\phi_1)$ and $Y_{l_2m_2}(\theta_2,\phi_2)$ is presented.

Hage Hassan *et al* (1980) have recently obtained the interesting result

$$\begin{aligned}y_{lm}(\boldsymbol{r}_1\times\boldsymbol{r}_2)&=(-1)^{m-\frac{1}{2}l}[4\pi(2l+1)]^{1/2}(\tfrac{1}{2}r_1r_2)^l\sum_{l_1m_1l_2m_2}2^{l_1+l_2}\\&\quad\times\left[\frac{(2l_1+1)(2l_2+1)(l_1-l_2+l)!(-l_1+l_2+l)!(l_1+l_2+l+1)!}{(l_1+l_2-l)!}\right]^{1/2}\\&\quad\times\frac{[\frac{1}{2}(l_1+l)]![\frac{1}{2}(l_2+l)]!}{[\frac{1}{2}(l-l_1)]![\frac{1}{2}(l-l_2)]!}\begin{pmatrix}l_1 & l_2 & l\\ m_1 & m_2 & -m\end{pmatrix}Y_{l_1m_1}(\theta_1,\phi_1)Y_{l_2m_2}(\theta_2,\phi_2)\end{aligned}\qquad(1)$$

and used it to obtain a possibly new sum rule for the $3j$ symbols. It seems that both of their derivations are involved. We are presenting below a simple and straightforward derivation which avoids making use of various generating functions which are not so well known.

Indeed from structural considerations

$$y_{lm}(\boldsymbol{r}_1\times\boldsymbol{r}_2)=\sum_{l_1m_1l_2m_2}\langle l_1,m_1;l_2,m_2|l,m\rangle a_{l_1l_2l}Y_{l_1m_1}(\theta_1,\phi_1)Y_{l_2,m_2}(\theta_2,\phi_2)\qquad(2)$$

where $\boldsymbol{r}_1=(r_1,\theta_1,\phi_1)$, $\boldsymbol{r}_2=(r_2,\theta_2,\phi_2)$ and we need to determine the coefficients $a_{l_1l_2l}$ in the above equation. The main point of the above equation is that these coefficients do not depend upon the magnetic quantum numbers m_1, m_2, m and the angles θ_1, ϕ_1, θ_2, ϕ_2 involved in the problem.

Using the orthonormality of the spherical harmonics, we find

$$\langle l_1,m_1;l_2,m_2|l,m\rangle a_{l_1l_2l}=\int y_{lm}(\boldsymbol{r}_1\times\boldsymbol{r}_2)Y^*_{l_1m_1}(\theta_1,\phi_1)Y^*_{l_2m_2}(\theta_2,\phi_2)\,d\Omega_1\,d\Omega_2\qquad(3a)$$

where

$$d\Omega=\sin\theta\,d\theta\,d\phi.\qquad(3b)$$

We choose the special values of the magnetic quantum numbers

$$m_1=l_1,\qquad m_2=l-l_1,\qquad m=l.$$

Thus

$$\langle l_1, l_1; l_2, l-l_1|l, l\rangle a_{l_1 l_2 l} = \int y_{ll}(\boldsymbol{r}_1\times\boldsymbol{r}_2) Y^*_{l_1 l_1}(\theta_1, \phi_1) Y^*_{l_2 l-l_1}(\theta_2, \phi_2)\, \mathrm{d}\Omega_1\, \mathrm{d}\Omega_2. \tag{4}$$

In terms of the spherical polar coordinates

$$(|\boldsymbol{r}_1\times\boldsymbol{r}_2|, \theta, \phi)$$

of $\boldsymbol{r}_1\times\boldsymbol{r}_2$, we see that

$$|\boldsymbol{r}_1\times\boldsymbol{r}_2| \sin\theta \exp(\mathrm{i}\phi) = -\mathrm{i} r_1 r_2 (\sin\theta_1 \cos\theta_2 \exp(\mathrm{i}\phi_1) - \cos\theta_1 \sin\theta_2 \exp(\mathrm{i}\phi_2)). \tag{5}$$

Now

$$y_{ll}(\boldsymbol{r}_1\times\boldsymbol{r}_2) = (-1)^l \frac{1}{2^l l!}\left(\frac{(2l+1)!}{4\pi}\right)^{1/2} (|\boldsymbol{r}_1\times\boldsymbol{r}_2| \sin\theta \exp(\mathrm{i}\phi))^l \tag{6a}$$

$$Y^*_{l_1 l_1}(\theta_1, \phi_1) = (-1)^{l_1} \frac{1}{2^{l_1} l_1!}\left(\frac{(2l_1+1)!}{4\pi}\right)^{1/2} (\sin\theta_1 \exp(-\mathrm{i}\phi_1))^{l_1} \tag{6b}$$

and

$$Y^*_{l_2 l-l_1}(\theta_2, \phi_2) = (-1)^{l-l_1}\left(\frac{(2l_2+1)(l_1+l_2-l)!}{4\pi(-l_1+l_2+l)!}\right)^{1/2} P^{l-l_1}_{l_2}(\cos\theta_2) \exp[-\mathrm{i}(l-l_1)\phi_2] \tag{6c}$$

where we have used equations (2.5.17) and (2.5.29) in Edmonds (1960).

On making use of the equations (4)–(6) above and performing the trivial ϕ_1, ϕ_2 integrations after expanding

$$(\sin\theta_1 \cos\theta_2 \exp(\mathrm{i}\phi_1) - \cos\theta_1 \sin\theta_2 \exp(\mathrm{i}\phi_2))^l$$

in a binomial series, we arrive at

$$\begin{aligned}\langle l_1, l_1; l_2, l-l_1|l, l\rangle a_{l_1 l_2 l} &= h(l-l_1)\left(\frac{(2l_2+1)(2l_1+1)!(2l+1)!(l_1+l_2-l)!}{(-l_1+l_2+l)!}\right)^{1/2} \\ &\quad\times \pi^{1/2}(\mathrm{i} r_1 r_2)^l (-1)^{l_1} \frac{1}{2^{l_1+l_2+1} l_1! l_1! (l-l_1)!} \\ &\quad\times \int_0^\pi \sin^{(2l_1+1)}\theta_1 \cos^{(l-l_1)}\theta_1\, \mathrm{d}\theta_1 \int_0^\pi \sin^{(l-l_1+1)}\theta_2 \cos^{l_1}\theta_2 P^{l-l_1}_{l_2}(\cos\theta_2)\, \mathrm{d}\theta_2\end{aligned} \tag{7}$$

where the function h is defined by

$$\begin{aligned} h(n) &= 1 \qquad \text{if } n \text{ is a non-negative integer} \\ &= 0 \qquad \text{otherwise.}\end{aligned} \tag{8}$$

Now

$$h(l-l_1)\int_0^\pi \sin^{(2l_1+1)}\theta_1 \cos^{(l-l_1)}\theta_1\, \mathrm{d}\theta_1 = h[\tfrac{1}{2}(l-l_1)] \frac{l_1!\,\Gamma[\frac{1}{2}(l-l_1+1)]}{\Gamma[\frac{1}{2}(l+l_1+3)]} \tag{9a}$$

whereas

$$h[\tfrac{1}{2}(l-l_1)]\int_0^{\pi}\sin^{(l-l_1+1)}\theta_2\cos^{l_1}\theta_2 P_{l_2}^{l-l_1}(\cos\theta_2)\,d\theta_2$$

$$=h[\tfrac{1}{2}(l-l_1)]\int_{-1}^{1}x^{l_1}(1-x^2)^{\frac{1}{2}(l-l_1)}P_{l_2}^{l-l_1}(x)\,dx$$

$$=(-1)^{l-l_1}2^{-l+l_1}h[\tfrac{1}{2}(l-l_2)]$$

$$\times\frac{\Gamma(\frac{1}{2}l_1+\frac{1}{2})\Gamma(\frac{1}{2}l_1+1)(-l_1+l_2+l)!}{[\frac{1}{2}(l-l_2)]!\,(l_1+l_2-l)!\,\Gamma[\frac{1}{2}(l+l_2+3)]} \tag{9b}$$

(equation (7.132(5)) in Gradshteyn and Ryzhik (1965)).

Combining equations (7) and (9), using the duplication formula

$$\Gamma(2z)=\frac{1}{\pi^{1/2}}2^{2z-1}\Gamma(z)\Gamma(z+\tfrac{1}{2}) \tag{10}$$

for the gamma function and

$$\langle l_1, l_1; l_2, l-l_1|l, l\rangle=\left(\frac{(2l_1)!\,(2l+1)!}{(l_1-l_2+l)!\,(l_1+l_2+l+1)!}\right)^{1/2} \tag{11}$$

(equation (3.6.13) in Edmonds 1960), we finally arrive at equation (1) above on noting the relationship

$$\langle l_1, m_1; l_2, m_2|l, m\rangle=(-1)^{l_1-l_2+m}(2l+1)^{1/2}\begin{pmatrix} l_1 & l_2 & l\\ m_1 & m_2 & -m\end{pmatrix}$$

between the Clebsch–Gordan coefficients and the Wigner 3*j* symbols (Edmonds 1960, equation (3.7.3)).

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