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LETTER TO THE EDITOR

Solid harmonics and their addition theorems

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Abstract. We prove the addition theorems for solid harmonics in a short, simple and novel way. The proofs use expansions in Cartesian, rather than polar, coordinates.

1. Introduction

A recent article in this journal (Tough and Stone 1977) treats solid harmonics, giving another proof of their addition theorems. We give here yet another proof of these theorems, and we believe it the simplest and shortest published so far.

The solid harmonics

$$\begin{aligned} R_l^m(\boldsymbol{r}) &= r^l P_l^m(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\phi} \qquad &\text{(regular)} \\ I_l^m(\boldsymbol{r}) &= r^{-l-1} P_l^m(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\phi} \qquad &\text{(irregular)} \end{aligned} \tag{1}$$

are both solutions of Laplace's equation $\nabla^2\Phi = 0$, and are important functions of mathematical physics. They are central to atomic problems, where $\boldsymbol{r}$ is the electron–nucleus vector.

Molecules and crystals contain more than one nucleus. In many methods used to describe their electronic properties $R_l^m(\boldsymbol{r}_1 - \boldsymbol{r}_2)$ and $I_l^m(\boldsymbol{r}_1 - \boldsymbol{r}_2)$ naturally arise, and it is a great simplification of the resultant multi-centre integrals if these solid harmonics can be expressed in terms of $R_l^m(\boldsymbol{r}_i)$ and $I_l^m(\boldsymbol{r}_i)$, $i = 1, 2$.

Several authors have treated these so called addition theorems for solid harmonics (Rose 1958, Moshinsky 1959, Seaton 1961, Sack 1964, Dahl and Barnett 1965, Talman 1968, Kay *et al* 1969, Steinborn and Ruedenberg 1973, Dixon and Lacroix 1973, Tough and Stone 1977). Their treatments are often long and/or use specialist mathematics. Our proofs are short, simple and (relatively) novel: they use the simple generating functions for solid harmonics given, for example, by Hobson (1931). These generating functions are interesting in their own right since they form a natural bridge between the polar and Cartesian forms of solid harmonics.

2. Generating functions

Consider the vector $\boldsymbol{r}$ with polar (r, θ, ϕ) and Cartesian (x, y, z) coordinates, i.e.

$$x = r\sin\theta\cos\phi \qquad y = r\sin\theta\sin\phi \qquad z = r\cos\theta. \tag{2}$$

Then the generating functions for the solid harmonics are (Hobson 1931)

$$(z+\mathrm{i}x)^l=\sum_m \mathrm{i}^m \frac{l!}{(l+m)!} R_l^m(\boldsymbol{r}) \tag{3a}$$

$$(z+\mathrm{i}x)^{-l-1}=\sum_m \mathrm{i}^{-m} \frac{(l-m)!}{l!} I_l^m(\boldsymbol{r}), \tag{3b}$$

where the associated Legendre functions are standard (Dahl and Barnett 1965, Hobson 1931).

Equation (3*a*) can easily be proved by writing

$$(z+\mathrm{i}x)^l \equiv \{z+\tfrac{1}{2}\mathrm{i}[(x+\mathrm{i}y)+(x-\mathrm{i}y)]\}^l = r^l[\cos\theta+\tfrac{1}{2}\mathrm{i}\sin\theta(\mathrm{e}^{\mathrm{i}\phi}+\mathrm{e}^{-\mathrm{i}\phi})]^l,$$

expanding the right-hand side and verifying that the coefficients of $\mathrm{e}^{\mathrm{i}m\phi}$ are the $P_l^m(\cos\theta)$. In particular, we find the following expression for $R_l^m(\boldsymbol{r})$ in Cartesian form:

$$R_l^m(\boldsymbol{r})=(l+m)!\sum_k \frac{(-1)^k(x+\mathrm{i}y)^{k+m}(x-\mathrm{i}y)^k z^{l-m-2k}}{2^{2k+m}(k+m)!k!(l-m-2k)!}, \tag{4}$$

which seems little known or used.

3. Addition theorems

Since $\boldsymbol{r}=\boldsymbol{r}_1-\boldsymbol{r}_2$ we have

$$(z+\mathrm{i}x)^l=[(z_1+\mathrm{i}x_1)-(z_2+\mathrm{i}x_2)]^l$$

which, expanding by the binomial theorem, is

$$(z+\mathrm{i}x)^l=\sum_{l'}\binom{l}{l'}(-1)^{l-l'}(z_1+\mathrm{i}x_1)^{l'}(z_2+\mathrm{i}x_2)^{l-l'}. \tag{5}$$

Substituting (3*a*) into (5) gives

$$\sum_m \mathrm{i}^m \frac{l!}{(l+m)!}R_l^m(\boldsymbol{r})$$

$$=\sum_{l',m_1,m_2}\binom{l}{l'}(-1)^{l-l'}\mathrm{i}^{m_1+m_2}\frac{l'!}{(l'+m_1)!}\frac{(l-l')!}{(l-l'+m_2)!}R_{l'}^{m_1}(\boldsymbol{r}_1)R_{l-l'}^{m_2}(\boldsymbol{r}_2). \tag{6}$$

Identifying coefficients of terms with equal azimuthal numbers $m=m_1+m_2$ in (6) and simplifying finally leaves

$$R_l^m(\boldsymbol{r}_1-\boldsymbol{r}_2)=\sum_{l',m'}(-1)^{l-l'}\binom{l+m}{l'+m'}R_{l'}^{m'}(\boldsymbol{r}_1)R_{l-l'}^{m-m'}(\boldsymbol{r}_2) \tag{7}$$

which is the addition theorem for regular solid harmonics.

For irregular harmonics (3*b*), assume $|z_1+\mathrm{i}x_1|>|z_2+\mathrm{i}x_2|$ and expand

$$(z+\mathrm{i}x)^{-l-1}=(z_1+\mathrm{i}x_1)^{-l-1}\left(1-\frac{z_2+\mathrm{i}x_2}{z_1+\mathrm{i}x_1}\right)^{-l-1}$$

by the binomial theorem, giving

$$(z+\mathrm{i}x)^{-l-1}=\sum_{l'}(-1)^{l'}\binom{-l-1}{l'}(z_2+\mathrm{i}x_2)^{l'}(z_1+\mathrm{i}x_1)^{-l'-l-1}. \tag{8}$$

We now substitute (3) in (8),

$$\sum_m \mathrm{i}^{-m}\frac{(l-m)!}{l!}I_l^m(\boldsymbol{r})$$

$$=\sum_{l',m_1,m_2}(-1)^{l'}\binom{-l-1}{l'}\mathrm{i}^{m_2-m_1}\frac{l'!}{(l'+m_2)!}\frac{(l+l'-m_1)!}{(l+l')!}R_{l'}^{m_2}(\boldsymbol{r}_2)I_{l+l'}^{m_1}(\boldsymbol{r}_1), \tag{9}$$

identify $m=m_1+m_2$ in (9) and simplify; the result is

$$I_l^m(\boldsymbol{r}_1-\boldsymbol{r}_2)=\sum_{l',m'}(-1)^{m-m'}\binom{l+l'-m'}{l-m}R_{l'}^{m-m'}(\boldsymbol{r}_2)I_{l+l'}^{m'}(\boldsymbol{r}_1), \tag{10}$$

which is the addition theorem for irregular harmonics.

4. Discussion

Addition theorems (7) and (10) result from generating functions (3), using only the binomial theorem: we believe this proof to be the simplest and shortest yet published. The simplicity derives from treating $\boldsymbol{r}$ in its Cartesian form $\boldsymbol{r}(x, y, z)$ rather than its polar one $\boldsymbol{r}(r, \theta, \phi)$. We suggest that (3) and (4) afford a natural transition between solid harmonics in Cartesian and polar forms, and that they could facilitate the analysis of more general addition theorems (e.g. of $f(r)P_l^m(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\phi}$).

We now comment on (3*b*). The complete expansion needs all integral m, whereas the P_l^m in (1) are non-zero only for $|m|\leq l$. However, Hobson (1931) defines his P_l^m for all m by means of a hypergeometric function which is identical to the P_l^m of (1) for $|m|\leq l$. Thus we may take $m=l, l-1, \ldots, -l$ in (3*b*) which is what we have implicitly done.

A word on the literature. Rose (1958), Moshinsky (1959), Seaton (1961) and Dahl and Barnett (1965) all treat the expansions considered here, but several later authors seem unaware of this and proceed to the same end with longer and more involved analysis.

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