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Properties of the regular and irregular solid harmonics

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Abstract. Stone's Cartesian–spherical transformation formalism is shown to yield a unified, simple and concise demonstration of the properties of the regular and irregular solid harmonics.

1. Introduction

The regular and irregular solid harmonics $r^l C_{lm}(\theta, \phi)$ and $r^{-l-1}C_{lm}(\theta, \phi)$, where $C_{lm}(\theta, \phi)$ is an un-normalised spherical harmonic (Brink and Satchler 1968), are among the simplest and most familiar special functions of mathematical physics. The standard derivations of their properties are, however, lengthy exercises in algebraic manipulation (Hobson 1931, Morse and Feshbach 1953) or group theory (Talman 1968). In this paper we define, and investigate the properties of, the spherical tensorial sets of quantities

$$R_{lm}(\boldsymbol{r}) = [(2l)!/2^l]^{1/2}(l!)^{-1} \sum_{\alpha_1 \ldots \alpha_l} r_{\alpha_1} \ldots r_{\alpha_l} \langle \alpha_1 \ldots \alpha_l | 12 \ldots l; m\rangle \tag{1}$$

and

$$I_{lm}(\boldsymbol{r}) = (-1)^l [2^l/(2l)!]^{1/2} \sum_{\alpha_1 \ldots \alpha_l} \nabla_{\alpha_l} \ldots \nabla_{\alpha_1}(r^{-1}) \langle \alpha_1 \ldots \alpha_l | 12 \ldots l; m\rangle \tag{2}$$

where r_α and ∇_α are Cartesian components of the vector field $\boldsymbol{r}$ and the gradient operator ∇ respectively and $\langle \alpha_1 \ldots \alpha_l | 12 \ldots l; m\rangle$ is a Cartesian–spherical (CS) transformation coefficient as defined by Stone (1975, 1976) whose notation, within the Condon–Shortley phase convention, we use here. By exploiting the properties of these coefficients we are able to determine the differential properties of these tensors and to establish the addition theorems they obey. The defining relations (1), (2) are then shown to lead to very simple expressions for $I_{lm}(\boldsymbol{r})$ and $R_{lm}(\boldsymbol{r})$ in terms of the Cartesian derivatives of r^{-1}. When $R_{lm}(\boldsymbol{r})$ and $I_{lm}(\boldsymbol{r})$ are identified as being respectively regular and irregular solid harmonics we find that we have derived the principal properties of these functions in a straightforward and systematic fashion.

2. Differential properties

In this section we determine the forms taken by $\nabla_\mu R_{lm}(\boldsymbol{r})$ and $\nabla_\mu I_{lm}(\boldsymbol{r})$, where ∇_μ is a cyclic component of the gradient operator defined by

$$\nabla_\mu = \sum_\alpha \nabla_\alpha \langle \alpha | 1; \mu\rangle. \tag{3}$$

From (1) and (3) we have

$$\nabla_\mu R_{lm}(\boldsymbol{r})=[(2l)!/2^l]^{1/2}(l!)^{-1}\sum_{\alpha_1\ldots\alpha_l\beta}\langle\beta|1\mu\rangle\nabla_\beta(r_{\alpha_1}\ldots r_{\alpha_l})\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle.$$

Now

$$\nabla_\beta(r_{\alpha_1}\ldots r_{\alpha_l})=\sum_{j=1}^{l} r_{\alpha_1}\ldots r_{\alpha_{j-1}}r_{\alpha_{j+1}}\ldots r_{\alpha_l}\delta_{\beta\alpha_j}$$

and so we have

$$\begin{aligned}\nabla_\mu R_{lm}(\boldsymbol{r})&=[(2l)!/2^l]^{1/2}(l!)^{-1}\sum_{\alpha_1\ldots\alpha_l\beta}\sum_{j=1}^{l}\langle\beta|1\mu\rangle r_{\alpha_1}\ldots r_{\alpha_{j-1}}r_{\alpha_{j+1}}\ldots r_{\alpha_l}\delta_{\beta\alpha_j}\\&\quad\times\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle\\&=[(2l)!/2^l]^{1/2}(l!)^{-1}\sum_{\alpha_1\ldots\alpha_l}\sum_{j=1}^{l} r_{\alpha_1}\ldots r_{\alpha_{j-1}}r_{\alpha_{j+1}}\ldots r_{\alpha_l}\langle\alpha_j|1\mu\rangle\\&\quad\times\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle.\end{aligned}\tag{4}$$

As the CS coefficient $\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle$ is symmetric in all its Cartesian indices (Stone 1975) we have

$$\begin{aligned}\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle&=\langle\alpha_1\ldots\alpha_{j-1}\alpha_{j+1}\ldots\alpha_l\alpha_j|12\ldots l;m\rangle\\&=\sum_\nu\langle\alpha_1\ldots\alpha_{j-1}\alpha_{j+1}\ldots\alpha_l|12\ldots l-1;m-\nu\rangle\langle\alpha_j|1\nu\rangle\langle l-1\;1\;m-\nu\;\nu|l\;m\rangle\end{aligned}$$

and so (4) becomes, when we use the result

$$\sum_\alpha\langle\alpha|1;\mu\rangle\langle\alpha|1;\nu\rangle=(-1)^\mu\delta_{\mu,-\nu},$$

$$\nabla_\mu R_{lm}(\boldsymbol{r})=(-1)^\mu[l(2l-1)]^{1/2}\langle l-1\;1\;m+\mu\;-\mu\;|l\;m\rangle R_{l-1,m+\mu}(\boldsymbol{r})\tag{5}$$

$$=(-1)^{l+m+\mu}[l(2l-1)(2l+1)]^{1/2}\begin{pmatrix}l-1 & l & 1\\ m+\mu & -m & -\mu\end{pmatrix}R_{l-1,m+\mu}(\boldsymbol{r}),\tag{6}$$

where we have introduced the more symmetrical Wigner $3j$ symbol in place of the Clebsch–Gordan coefficient.

Similarly (2) and (3) give us

$$\nabla_\mu I_{lm}(\boldsymbol{r})=(-1)^l[2^l/(2l)!]^{1/2}\sum_{\substack{\alpha_1\ldots\alpha_l\\\beta}}\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle\langle\beta|1\mu\rangle\nabla_\beta\nabla_{\alpha_l}\ldots\nabla_{\alpha_1}(r^{-1}).\tag{7}$$

As the Cartesian tensor $\nabla_{\alpha_l}\ldots\nabla_{\alpha_1}(r^{-1})$ is symmetric and traceless in each pair of its indices it has only lth rank non-vanishing spherical components (see appendix). Consequently, on inverting the defining relation (2) and substituting this and the recursive definition of $\langle 12\ldots l+1;\nu|\alpha_1\ldots\alpha_l\beta\rangle$ into (7) we obtain

$$\begin{aligned}\nabla_\mu I_{lm}(\boldsymbol{r})&=-[l(2l+1)]^{1/2}\sum_{\substack{\alpha_1\ldots\alpha_l\beta\\\nu,\eta}}\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle\langle 12\ldots l;\nu-\eta|\alpha_1\ldots\alpha_l\rangle\\&\quad\times\langle\beta|1\mu\rangle\langle 1\eta|\beta\rangle\langle l\;1\;\nu-\eta\;\eta|l+1\;\nu\rangle I_{l+1,\nu}(\boldsymbol{r}).\end{aligned}$$

The unitarity of the CS transformation then gives us

$$\nabla_\mu I_{lm}(\boldsymbol{r}) = -[l(2l+1)]^{1/2}\langle l\;1\;m\;\mu|l+1\;m+\mu\rangle I_{l+1,m+\mu}(\boldsymbol{r}) \tag{8}$$

$$= (-1)^{l+m+\mu}[l(2l+1)(2l+3)]^{1/2}\begin{pmatrix} l & 1 & l+1 \\ m & \mu & -m-\mu \end{pmatrix} I_{l+1,m+\mu}(\boldsymbol{r}). \tag{9}$$

We can now establish that both $R_{lm}(\boldsymbol{r})$ and $I_{lm}(\boldsymbol{r})$ are harmonic functions; that is, that they are solutions of Laplace's equation

$$\nabla^2\psi = 0.$$

This follows immediately in the case of $I_{lm}(\boldsymbol{r})$ since r^{-1} is itself an harmonic function. Two applications of (5) give us

$$\nabla^2 R_{lm}(\boldsymbol{r}) = \sum_\mu (-1)^\mu \nabla_\mu \nabla_{-\mu} R_{lm}(\boldsymbol{r})$$

$$= [l(l-1)(2l+1)(2l-1)]^{1/2} R_{l-2,m}(\boldsymbol{r})$$

$$\times \sum_\mu (-1)^\mu \langle l-1\;1\;m+\mu\;-\mu|lm\rangle\langle l-2\;1\;m\;\mu|l-1\;m+\mu\rangle$$

from which $\nabla^2 R_{lm}(\boldsymbol{r}) = 0$ follows by the orthogonality of the Clebsch–Gordan coefficients.

3. Addition theorems

We will now determine the forms taken by $R_{lm}(\boldsymbol{r}')$ and $I_{lm}(\boldsymbol{r}')$, where $\boldsymbol{r}' = \boldsymbol{r} + \boldsymbol{a}$. From the defining relation (1) we have

$$R_{lm}(r') = [(2l)!/2^l]^{1/2}(l!)^{-1} \sum_{\alpha_1\ldots\alpha_l} r'_{\alpha_1}\ldots r'_{\alpha_l}\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle \tag{1a}$$

where $r'_\alpha = r_\alpha + a_\alpha$. By direct expansion we have

$$r'_{\alpha_1}\ldots r'_{\alpha_l} = a_{\alpha_1}\ldots a_{\alpha_l} + \sum_i a_{\alpha_1}\ldots a_{\alpha_{i-1}} a_{\alpha_{i+1}}\ldots a_{\alpha_l} r_{\alpha_i}$$

$$+ \sum_{i,j} a_{\alpha_1}\ldots a_{\alpha_{i-1}} a_{\alpha_{i+1}}\ldots a_{\alpha_{j-1}} a_{\alpha_{j+1}}\ldots a_{\alpha_l} r_{\alpha_i} r_{\alpha_j} + \ldots + r_{\alpha_1}\ldots r_{\alpha_l}$$

which gives us, on substitution into ($1a$),

$$R_{lm}(r') = [(2l)!/2^l]^{1/2} \sum_{\alpha_1\ldots\alpha_l}\sum_{s=0}^{l} [s!(l-s)!]^{-1} r_{\alpha_1}\ldots r_{\alpha_s} a_{\alpha_{s+1}}\ldots a_{\alpha_l}\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle$$

where we have again exploited the symmetry of $\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle$ in its Cartesian indices. A standard Cartesian–spherical transformation (Stone 1976) enables us to evaluate

$$\sum_{\alpha_1\ldots\alpha_l} r_{\alpha_1}\ldots r_{\alpha_s} a_{\alpha_{s+1}}\ldots a_{\alpha_l}\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle.$$

Explicitly we have

$$\sum_{\alpha_1\ldots\alpha_l} r_{\alpha_1}\ldots r_{\alpha_s} a_{\alpha_{s+1}}\ldots a_{\alpha_l}\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle$$

$$=\prod_{\sigma=1}^{s}[(2l+2\sigma-2s-1)(2\sigma+1)]^{1/2}W(\sigma-1\,1\,l-s\,l-s+\sigma;\sigma\,l-s+\sigma-1)$$

$$\times\sum_{\substack{\alpha_1\ldots\alpha_l\\ t}} r_{\alpha_1}\ldots r_{\alpha_s}\langle\alpha_1\ldots\alpha_s|12\ldots s;t\rangle a_{\alpha_{s+1}}\ldots a_{\alpha_l}$$

$$\times\langle\alpha_{s+1}\ldots\alpha_l|12\ldots l-s;m-t\rangle\langle l-s\,s\,m-t\,t|l\,m\rangle.$$

As the Racah W function has a value given by

$$W(\sigma-1\,1\,l-s\,l-s+\sigma;\sigma\,l-s+\sigma-1)=[(2l-2s+2\sigma-1)(2\sigma+1)]^{-1/2}$$

we have, after identifying $R_{st}(\boldsymbol{r})$ and $R_{l-s,m-t}(\boldsymbol{a})$

$$R_{lm}(\boldsymbol{r}')=\sum_{\substack{s=0\\|t|\leqslant s}}^{l}[(2l)!/(2s)!(2l-2s)!]^{1/2}R_{st}(\boldsymbol{r})R_{l-s,m-t}(\boldsymbol{a})\langle s\,l-s\,t\,m-t|l\,m\rangle \tag{10}$$

$$=\sum_{\substack{s=0\\|t|\leqslant s}}^{l}(-1)^{l+m}\left(\frac{(2l+1)!}{(2s)!(2l-2s)!}\right)^{1/2}R_{st}(\boldsymbol{r})R_{l-s,m-t}(\boldsymbol{a})\begin{pmatrix}l-s & s & l\\ m-t & t & -m\end{pmatrix}. \tag{11}$$

$I_{lm}(\boldsymbol{r}')$ can be found by transforming the Taylor series expansion

$$\nabla_{\alpha_l}\ldots\nabla_{\alpha_1}(R^{-1})_{\boldsymbol{R}=\boldsymbol{r}+\boldsymbol{a}}=\sum_{\substack{s\\ \beta_1\ldots\beta_s}}(s!)^{-1}r_{\beta_1}\ldots r_{\beta_s}\nabla_{\beta_s}\ldots\nabla_{\beta_1}\nabla_{\alpha_l}\ldots\nabla_{\alpha_1}(R^{-1})_{\boldsymbol{R}=\boldsymbol{a}},$$

$$|\boldsymbol{r}|<|\boldsymbol{a}|,$$

from Cartesian to spherical tensorial form. Standard methods give us

$$\sum_{\substack{\alpha_1\ldots\alpha_l\\ \beta_1\ldots\beta_s}}\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle r_{\beta_1}\ldots r_{\beta_s}\nabla_{\beta_s}\ldots\nabla_{\beta_1}\nabla_{\alpha_l}\ldots\nabla_{\alpha_1}(R^{-1})_{\boldsymbol{R}=\boldsymbol{a}}$$

$$=(-1)^s[(2l+2s+1)/(2l+1)]^{1/2}\prod_{\sigma=1}^{s}[(2l+2\sigma-1)(2\sigma+1)]^{1/2}$$

$$\times W(\sigma-1\,1\,l\,l+\sigma;\sigma\,l+\sigma-1)\sum_{\substack{\alpha_1\ldots\alpha_l\\ \beta_1\ldots\beta_s\\ t}}\langle\beta_1\ldots\beta_s|1\ldots s;t\rangle r_{\beta_1}\ldots r_{\beta_s}$$

$$\times\langle\beta_1\ldots\beta_s\,\alpha_1\ldots\alpha_l|12\ldots l+s,m-t\rangle$$

$$\times\nabla_{\beta_s}\ldots\nabla_{\beta_1}\nabla_{\alpha_l}\ldots\nabla_{\alpha_1}(R^{-1})_{\boldsymbol{R}=\boldsymbol{a}}\langle l+s\,s\,m-t\,t|l\,m\rangle.$$

Evaluation of the Racah W functions simplifies this to

$$(-1)^s[(2l+2s+1)/(2l+1)]^{1/2}\sum_{\substack{\alpha_1\ldots\alpha_l\\ \beta_1\ldots\beta_s\\ t}}\langle\beta_1\ldots\beta_s|12\ldots s;t\rangle r_{\beta_1}\ldots r_{\beta_s}$$

$$\times\langle\beta_1\ldots\beta_s\alpha_1\ldots\alpha_l|12\ldots l+s;m-t\rangle$$

$$\times\nabla_{\beta_s}\ldots\nabla_{\beta_1}\nabla_{\alpha_l}\ldots\nabla_{\alpha_1}(R^{-1})_{\boldsymbol{R}=\boldsymbol{a}}\langle l+s\,s\,m-t\,t|l\,m\rangle$$

which, upon identification of $R_{st}(\boldsymbol{r})$ and $I_{l+s,m-t}(\boldsymbol{a})$, yields the addition theorem

$$I_{lm}(\boldsymbol{r}+\boldsymbol{a})=\sum_{\substack{s=0\\|t|\leq s}}^{\infty}[(2l+2s+1)!/(2l+1)!(2s)!]^{1/2}R_{st}(\boldsymbol{r})I_{l+s,m-t}(\boldsymbol{a})\langle l+s\,s\,m-t\,t|l\,m\rangle,$$

$$|\boldsymbol{r}|<|\boldsymbol{a}| \tag{12}$$

$$=\sum_{\substack{s=0\\|t|\leq s}}^{\infty}(-1)^{l+m}\left(\frac{(2l+2s+1)!}{(2l)!(2s)!}\right)^{1/2}R_{st}(\boldsymbol{r})I_{l+s,m-t}(\boldsymbol{a})\begin{pmatrix}l+s & s & l\\ m-t & t & -m\end{pmatrix},$$

$$|\boldsymbol{r}|<|\boldsymbol{a}|. \tag{13}$$

When $l=m=0$ this result reduces to an expansion of $|\boldsymbol{r}+\boldsymbol{a}|^{-1}$:

$$|\boldsymbol{r}+\boldsymbol{a}|^{-1}=\sum_{\substack{s=0\\|t|\leq s}}^{\infty}(-1)^{s+t}R_{st}(\boldsymbol{r})I_{s,-t}(\boldsymbol{a}),\qquad |\boldsymbol{r}|<|\boldsymbol{a}|. \tag{14}$$

4. Explicit expressions for $I_{lm}(r)$ and $R_{lm}(r)$

The defining relation (2), along with the recursive definition of the CS coefficient $\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle$, gives us the result

$$I_{lm}(\boldsymbol{r})=-[l(2l-1)]^{-1/2}\sum_{\mu}\nabla_{\mu}I_{l-1,m-\mu}(\boldsymbol{r})\langle l-1\,1\,m-\mu\,\mu|l\,m\rangle. \tag{15}$$

We will now prove, by induction, that this implies the following expression for $I_{lm}(\boldsymbol{r})$ in terms of Cartesian derivatives of r^{-1}:

$$I_{lm}(\boldsymbol{r})=\frac{(-1)^{l+m}}{[(l+m)!(l-m)!]^{1/2}}\left(\frac{\partial}{\partial x}+\mathrm{i}\frac{\partial}{\partial y}\right)^{m}\frac{\partial^{l-m}}{\partial z^{l-m}}\left(\frac{1}{r}\right),\qquad m\geq 0 \tag{16}$$

or, in terms of the spherical components of the gradient operator,

$$I_{lm}(\boldsymbol{r})=(-1)^{l}2^{m/2}[(l+m)!(l-m)!]^{-1/2}\nabla_1^m\nabla_0^{l-m}(r^{-1}),\qquad m\geq 0. \tag{17}$$

To do this we substitute in (15) an expression of the form of (17) for $I_{l-1,m-\mu}(\boldsymbol{r})$, and the algebraic expression (Rose 1957) for the Clebsch–Gordan coefficient, and making use of the result

$$\nabla_{-1}\nabla_1(r^{-1})=\tfrac{1}{2}\nabla_0^2(r^{-1}),\qquad \boldsymbol{r}\neq 0,$$

we find that some straightforward algebra leads to (17). This establishes the induction. As (17) holds trivially when $l=0$ we now see that it holds for all l, $m\geq 0$.

The result

$$\langle\alpha_1\ldots\alpha_l|12\ldots l;m\rangle^*=(-1)^m\langle\alpha_1\ldots\alpha_l|12\ldots l;\ -m\rangle$$

then gives us

$$I_{l,-m}(\boldsymbol{r})=(-1)^m I_{lm}(\boldsymbol{r})^*$$

and so we can write

$$I_{l,\pm m}(\boldsymbol{r})=(-1)^l 2^{m/2}[(l+m)!(l-m)!]^{-1/2}\nabla_{\pm 1}^m\nabla_0^{l-m}(r^{-1}),\qquad m\geq 0. \tag{18}$$

We will now show that

$$I_{lm}(\boldsymbol{r}) = r^{-2l-1} R_{lm}(\boldsymbol{r}). \tag{19}$$

The proof is again by induction. Firstly though, we find it convenient to introduce the spherical tensorial set of quantities

$$\mathscr{C}_{lm}(\hat{\boldsymbol{r}}) = R_{lm}(\hat{\boldsymbol{r}}) = r^{-l} R_{lm}(\boldsymbol{r}) \tag{20}$$

where $\hat{\boldsymbol{r}} = |\boldsymbol{r}|^{-1}\boldsymbol{r}$. $\mathscr{C}_{lm}(\hat{\boldsymbol{r}})$ is thus a function only of the direction of $\boldsymbol{r}$ and not of its magnitude. The Lth rank spherical tensor

$$\sum_{mm'} \mathscr{C}_{lm}(\hat{\boldsymbol{r}}) \mathscr{C}_{l'm'}(\hat{\boldsymbol{r}}) \langle l\, l'\, m\, m' | L\, M \rangle$$

is again a function only of the direction of $\boldsymbol{r}$; consequently we can write

$$\sum_{mm'} \mathscr{C}_{lm}(\hat{\boldsymbol{r}}) \mathscr{C}_{l'm'}(\hat{\boldsymbol{r}}) \langle l\, l'\, m\, m' | L\, M \rangle = A_{ll'L} \mathscr{C}_{LM}(\hat{\boldsymbol{r}}). \tag{21}$$

To identify the constant $A_{ll'L}$ we consider the special case in which $\hat{\boldsymbol{r}}$ is $\boldsymbol{e}_z$, the unit vector in the z direction. It is readily shown from the definitions (20), (1) that $\mathscr{C}_{lm}(\boldsymbol{e}_z) = \delta_{m,0}$. From this we see that $A_{ll'L} = \langle l\, l'\, 0\, 0 | L\, 0 \rangle$, while inversion of (21) gives us

$$\mathscr{C}_{lm}(\hat{\boldsymbol{r}}) \mathscr{C}_{l'm'}(\hat{\boldsymbol{r}}) = \sum_{LM} \langle l\, l'\, 0\, 0 | L\, 0 \rangle \langle l\, l'\, m\, m' | L\, M \rangle \mathscr{C}_{LM}(\hat{\boldsymbol{r}}). \tag{22}$$

To establish (19) we substitute an expression of this form for $I_{l-1,m-\mu}(\boldsymbol{r})$ into (15). This then gives us

$$I_{lm}(\boldsymbol{r}) = -[l(2l-1)]^{1/2} \sum_{\mu} \langle l-1\; 1\; m-\mu\; \mu | l\, m \rangle \nabla_\mu (r^{-2l+1} R_{l-1,m-\mu}(\boldsymbol{r})).$$

Now

$$\nabla_\mu (r^{-2l+1} R_{l-1,m-\mu}(\boldsymbol{r})) = r^{-2l+1} \nabla_\mu R_{l-1,m-\mu}(\boldsymbol{r}) - (2l-1) r^{-2l-1} r_\mu R_{l-1,m-\mu}(\boldsymbol{r}). \tag{23}$$

The first term in this expression is readily obtained from (5); to evaluate the second term we note that

$$\begin{aligned} r_\mu R_{l-1,m-\mu}(\boldsymbol{r}) &= r^l \mathscr{C}_{1\mu}(\hat{\boldsymbol{r}}) \mathscr{C}_{l-1,m-\mu}(\hat{\boldsymbol{r}}) \\ &= r^l \{[l/(2l-1)]^{1/2} \langle 1\; l-1\; \mu\; m-\mu | l\, m \rangle \mathscr{C}_{lm}(\hat{\boldsymbol{r}}) + (-1)^\mu (2l-1)^{-1} \\ &\quad \times [(l-1)(2l-3)]^{1/2} \langle 1\; l-2-\mu\; m | l-1\; m-\mu \rangle \mathscr{C}_{l-2,m-\mu}(\hat{\boldsymbol{r}})\} \end{aligned}$$

where we have used (22) and the symmetry properties of the Clebsch–Gordan coefficients. Thus from (23) and (5) we see that

$$\begin{aligned} I_{lm}(\boldsymbol{r}) &= r^{-l-1} \mathscr{C}_{lm}(\hat{\boldsymbol{r}}) \sum_{\mu} \langle 1\; l-1\; \mu\; m-\mu | l\, m \rangle \langle l-1\; 1\; m-\mu\; \mu | l\, m \rangle \\ &= r^{-l-1} \mathscr{C}_{lm}(\hat{\boldsymbol{r}}) = r^{-2l-1} R_{lm}(\boldsymbol{r}). \end{aligned}$$

This establishes the induction. As the result holds trivially for $l = 0$ we see that it holds for all l, m. We now have an explicit expression for $R_{lm}(\boldsymbol{r})$:

$$\begin{aligned} R_{l,\pm m}(\boldsymbol{r}) &= r^{2l+1} I_{l,\pm m}(\boldsymbol{r}) \\ &= (-1)^l 2^{m/2} [(l+m)!(l-m)!]^{-1/2} r^{2l+1} \nabla_{\pm 1}^m \nabla_0^{l-m} (r^{-1}), \qquad m \geqslant 0. \end{aligned}$$

5. Discussion

The quantities $R_{lm}(\boldsymbol{r})$ and $I_{lm}(\boldsymbol{r})$ are respectively the regular and irregular solid harmonics $r^l C_{lm}(\theta, \phi)$ and $r^{-l-1} C_{lm}(\theta, \phi)$. This identification is made most readily through the results (17) and (19) derived in § 3. We note the result (Hobson 1931, p 134)

$$(-1)^{l-m}(l-m)!\,\frac{P_l^m(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\phi}}{r^{l+1}} = \left(\frac{\partial}{\partial x}+\mathrm{i}\frac{\partial}{\partial y}\right)^m \frac{\partial^{l-m}}{\partial z^{l-m}}\left(\frac{1}{r}\right), \qquad m \geqslant 0, \qquad (24)$$

where $P_l^m(z)$ is an associated Legendre function with argument z; the identification

$$I_{lm}(\boldsymbol{r}) = r^{-l-1} C_{lm}(\theta, \phi)$$

then follows immediately. From (19) we obtain

$$R_{lm}(\boldsymbol{r}) = r^{2l+1} I_{lm}(\boldsymbol{r}) = r^l C_{lm}(\theta, \phi).$$

The quantities $\mathscr{C}_{lm}(\hat{\boldsymbol{r}})$ of (20) can be identified with the spherical harmonics $C_{lm}(\theta, \phi)$, where θ, ϕ are the polar angles defining the direction of $\hat{\boldsymbol{r}}$.

Having identified the regular and irregular solid harmonics we see that, while no new results have been obtained, our CS transformation formalism, which combines the conceptual simplicity of the Taylor series expansion methods of the classical approach described by Hobson (1931) with the more powerful algebraic methods of the representation theory of the rotation group, has allowed us to derive the principal properties of these functions in a concise and elegant fashion. The differential properties of § 2 have previously been obtained both as special cases of the gradient formula, conventionally derived by dint of some fairly heavy Racah algebra (Rose 1957) and by classical methods in which the Clebsch–Gordan coefficients are carried throughout in their explicit algebraic forms (Hobson 1931). The addition theorems of § 3 have been obtained both by classical methods (Hobson 1931) and by the use of sophisticated group theoretical techniques (Talman 1968); the analysis involved in both these derivations is much more complicated than is that of our procedure. The demonstration of even the special case (14) from a Taylor series expansion is achieved by classical methods only 'after considerable algebraic drudgery' (Morse and Feshbach 1953). Finally, we note that of the derivation of (17) and Hobson's demonstration of (24) our proof is much the more compact.

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Appendix

It will be shown that a Cartesian tensor $A_{\alpha_1 \ldots \alpha_l}$ of rank l which is symmetrical and traceless in each pair of indices has only $(2l+1)$ independent components, which form a rotationally irreducible set.

The CS coefficient projecting out the spherical component $A_{j_1 \ldots j_l, m}$ from the tensor $A_{\alpha_1 \ldots \alpha_l}$ is

$$\langle \alpha_1 \ldots \alpha_l | j_1 \ldots j_l ; m \rangle.$$

This coefficient will be, like the tensor itself, traceless in every pair of adjacent Cartesian indices. Therefore we have

$$\sum_{\alpha_r, \alpha_{r+1}} \delta_{\alpha_r, \alpha_{r+1}} \langle \alpha_1 \ldots \alpha_l | j_1 \ldots j_l ; m \rangle$$

$$= \delta_{j_{r+1}, j_{r-1}} (-1)^{j_r + j_{r-1}} \langle \alpha_1 \ldots \alpha_{r-1} \alpha_{r+2} \ldots \alpha_l | j_1 \ldots j_{r-1} j_{r+2} \ldots j_l ; m \rangle$$

$$= 0$$

which implies that $j_{r-1} \neq j_{r+1}$. Consequently $j_{r+1} = j_{r-1} \pm 1, j_{r-1} \pm 2$, these being the only values allowed by the triangle conditions on the coupling of the constituent ($j = 1$) units to form the polyadic or archetypal tensor.

The CS coefficient must also be invariant under the interchange of adjacent Cartesian indices. Therefore we have

$$(r, r+1) \langle \alpha_1 \ldots \alpha_l | j_1 \ldots j_l ; m \rangle$$

$$= \sum_f (-1)^{j_r + f} [(2j_r + 1)(2f + 1)]^{1/2} \begin{Bmatrix} 1 & j_{r-1} & j_r \\ 1 & j_{r+1} & f \end{Bmatrix}$$

$$\times \langle \alpha_1 \ldots \alpha_l | j_1 \ldots j_{r-1} f j_{r+1} \ldots j_l ; m \rangle$$

$$= \langle \alpha_1 \ldots \alpha_l | j_1 \ldots j_l ; m \rangle.$$

It is readily verified that only those CS coefficients for which $j_{r+1} = j_{r-1} \pm 2$ have this property. Now $j_1 = 1$ and therefore $j_3 = 3$. The $(1, j_2, j_3)$ triangle condition requires that $j_2 = 2$; the $(j_3, 1, j_4)$ triangle condition requires that $j_4 = 4$. Similarly $j_r = r$. Consequently the only CS coefficients with the requisite properties have the form $\langle \alpha_1 \ldots \alpha_l | 12 \ldots l ; m \rangle$; this proves the theorem.

We note that the fact that the tensor $A_{\alpha_1 \ldots \alpha_l}$ has only $(2l + 1)$ independent components can also be proved quite simply by counting. A totally symmetrical rank l Cartesian tensor has $\frac{1}{2}(l+1)(l+2)$ independent components; the $\frac{1}{2}l(l-1)$ constraints implicit in the tracelessness property of the tensor reduce this number of independent components to

$$\tfrac{1}{2}(l+1)(l+2) - \tfrac{1}{2}l(l-1) = \tfrac{1}{2}(4l+2) = 2l + 1.$$

An example of a Cartesian tensor with these properties which is of considerable importance in physical applications is the interaction tensor (Buckingham 1965) $T_{\alpha_1 \ldots \alpha_l}(\boldsymbol{r}) = \nabla_{\alpha_l} \ldots \nabla_{\alpha_1}(r^{-1})$. We now see that the only non-vanishing spherical components of this tensor are proportional to the irregular solid harmonics:

$$T_{j_1 \ldots j_l, m}(\boldsymbol{r}) = (-1)^l [(2l)!/2^l]^{1/2} \prod_{\sigma=1}^{l} \delta_{\sigma, j_\sigma} r^{-l-1} C_{lm}(\theta, \phi).$$

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