The coordinate-free approach to spherical harmonics

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Abstract

We present in a unified and self-contained manner the coordinate-free approach to spherical harmonics initiated in the mid 19th century by James Clerk Maxwell, William Thomson and Peter Guthrie Tait. We stress the pedagogical advantages of this approach which leads in a natural way to many physically relevant results that students find often difficult to work out using spherical coordinates and associated Legendre functions. It is shown how most physically relevant results of the theory of spherical harmonics - such as recursion relations, Legendre’s addition theorem, surface harmonics expansions, the method of images, multipolar charge distributions, partial wave expansions, Hobson’s integral theorem, rotation matrix and Gaunt’s integrals - can be efficiently derived in a coordinate free fashion from a few basic elements of the theory of solid and surface harmonics discussed in the paper.
I. INTRODUCTION

Spherical harmonics present themselves in many branches of physics and applied mathematics such as electromagnetism, quantum mechanics and gravitation theory. In most modern textbooks dealing with topics of mathematical physics\(^1\),\(^2\), the theory of spherical harmonics is built upon their representation in spherical coordinates. As is well known, in this approach one starts by expressing Laplace’s equation in spherical polar coordinates \((r, \theta, \varphi)\), where \(r\) is the distance to the origin and \(\theta\) and \(\varphi\) are the polar and azimuthal angles, respectively. One then tries a solution in separated variables that yields the spherical harmonics in the form

\[
Y_{lm}(\theta, \varphi) = C_{lm} e^{im\varphi} P_l^m(\cos \theta) \quad (l = 0, 1, \ldots, -l \leq m \leq l),
\]

where \(C_{lm}\)'s are normalization constants and the \(P_l^m(\mu)\)'s are the associated Legendre functions defined by

\[
P_l^m(\mu) \equiv (-1)^m (1 - \mu^2)^{m/2} \frac{d^l + m}{d\mu^l + m}.
\]

However, this representation often leads to cumbersome derivations of the main results needed in physical applications, so that, from a physicist’s point of view, it may be desirable to have a more compact approach in which mathematical manipulations become more direct and, perhaps, also more guided by physical insight. This is also the case with other special functions of great physical relevance such as Bessel’s functions or ellipsoidal harmonics.

The first representations of spherical harmonics freed from spherical coordinates were those given by Thomson and Tait\(^3\) in their *Treatise on Natural Philosophy* and by Maxwell\(^4\) in his *Treatise on Electricity and Magnetism*. The principle of their method is that, having given any solution of Laplace’s equation, other solutions may be obtained by differentiating the given solution any number of times in the directions of the cartesian axes \(x, y\) and \(z\) or, as Maxwell proposed, in any directions whatsoever. In particular, by applying this method to the simple solution \(1/r\), with \(r = \sqrt{x^2 + y^2 + z^2}\), all the system of spherical harmonics may be generated\(^5\). Maxwell\(^4\) also contributed with an important integral theorem which apparently has not deserved by itself much attention in the literature. In fact, after it first appeared in Maxwell’s treatise, it has almost invariably been presented as a corollary of a more general - but also more complicated - integral theorem first introduced by Niven\(^6\) and generalized afterwards by Hobson\(^5\). Nevertheless, we consider Maxwell’s theorem as an essential ingredient in our approach and, therefore, have preferred to follow here a different route that leads to Hobson’s theorem via Maxwell’s theorem.

The aim of this paper is to show how the contributions due to Maxwell and to Thomson
and Tait lead to a unified, self-consistent and spherical coordinate-free approach through which most of the properties of spherical harmonics needed in usual physical applications can easily and naturally be derived. We hope that this paper helps students and researchers to understand and work out by themselves many of the results they need when dealing with specific problems involving spherical harmonics, thus avoiding much of the trouble of constantly having to look them up in the appendices of the relevant literature or in specialized mathematical handbooks. For these purposes, we have based our presentation on the simple properties of three basic elements of the theory of solid and surface harmonics: a) the elementary solid harmonics of the form \((b \cdot r)^l l\) being a nonnegative integer and \(b\) a null vector-, b) Maxwell’s harmonics, and c) Maxwell’s integral theorem. We have introduced these basic concepts in Section II and have applied them in the rest of the paper to provide systematic, coordinate-free derivations of some physically relevant results such as the construction of the standard set of spherical harmonics \(Y_{lm}\) (Section III), recursion relations (Section IV), Legendre’s addition theorem (Section V), surface harmonics expansions (Section VI) - with applications to the method of images and multipolar charge distributions-, partial wave expansions and Hobson’s integral theorem (Section VII), rotation matrix (Section VIII) and Gaunt’s integrals (Section IX). Finally conclusions are presented in Section X.

II. GENERAL PROPERTIES OF SOLID AND SURFACE HARMONICS.

We define a solid harmonic of the type \(H_l\) or, more briefly, a \(H_l\)-harmonic, as any solution of Laplace’s equation,

\[
\nabla^2 \phi = 0,
\]

which is a homogenous polynomial of degree \(l\) in the (cartesian) variables \((x, y, z)\):

\[
H_l(x) = \sum_{\alpha+\beta+\gamma=l} C_{\alpha\beta\gamma} x^{\alpha} y^{\beta} z^{\gamma},
\]

where \(r = xe_x + ye_y + ze_z\) is the position vector and constants \(C_{\alpha\beta\gamma}\) are generally complex. As can be checked by direct substitution, to every \(H_l\)-harmonic there corresponds a second solution of (1) of the form

\[
V_l(r) = \frac{H_l(r)}{r^{2l+1}},
\]
which we will define as a solid harmonic of the type $V_l$ or, more briefly, $V_l$-harmonic. Note the following behaviors of $H_l$ and $V_l$ for small and large values of $r$

$$r \to 0: \quad H_l(r) \to 0, \quad V_l(r) \to \infty,$$

$$r \to \infty: \quad H_l(r) \to \infty, \quad V_l(r) \to 0.$$  

According to (4), $H_l$-harmonics and $V_l$-harmonics are also known as regular and irregular solid harmonics, respectively.

A surface harmonic of degree $l$, $Y_l$, is defined as the function obtained from a $H_l$-harmonic or, equivalently, a $V_l$-harmonic according to the rules

$$Y_l(r) = H_l(r)/r^l = r^{l+1}V_l(r).$$

Since $H_l$ is a homogeneous polynomial of degree $l$ in the variables $x, y$ and $z$, it is clear that the value of $Y_l$ at any point of space, $r$, is the same as that at the point of the unit sphere $e_r = r/r$: $Y_l(r) = Y_l(e_r)$. Also, note that the values of $Y_l$, $H_l$ and $V_l$ coincide on the unit sphere.

It can easily be shown\textsuperscript{3,18} that the number of independent $H_l$ - harmonics is $2l + 1$ which, of course, must also be the number of independent functions $V_l$ and $Y_l$ by (3) and (6). In effect, to a given value of the exponent $\alpha$ ($0 \leq \alpha \leq l$) in a homogeneous polynomial of degree $l$ such as (2) there correspond $l - \alpha + 1$ possible values of the exponent $\beta$, since the value of $\gamma$ is fixed by $\gamma = l - \alpha - \beta$. Thus, the maximum number of monomials of the form $x^{\alpha}y^{\beta}z^{\gamma}$ in (2) will be $\sum_{\alpha=0}^{l}(l - \alpha + 1) = (l + 1)(l + 2)/2$. Since $\nabla^2 H_l$ is a homogeneous polynomial of degree $l - 2$, it will therefore contain a maximum of $(l - 1)l/2$ terms whence the condition $\nabla^2 H_l = 0$ is equivalent $l(l - 1)/2$ equations between the constant coefficients $C_{\alpha\beta\gamma}$ in (2).

The number of independent constant remaining is thus $(l + 1)(l + 2)/2 - l(l - 1)/2$, or $2l + 1$. Therefore, any solid or surface harmonic of degree $l$ can be expressed as a linear combination of $2l + 1$ independent harmonics of the same class.

Observe that, unlike functions $H_l$ or $V_l$, surface harmonics do not satisfy Laplace’s equation, but instead

$$\nabla^2 Y_l + \frac{l(l + 1)}{r^2}Y_l = 0,$$

as is readily verified by direct substitution of (6) into (1). From (7) it is easy to obtain the orthogonality property\textsuperscript{2} for two given surface harmonics, $Y_l$ and $X_n$. In effect, if we subtract
the equation for $Y_l$ multiplied by $X_n$ from that for $X_n$ multiplied by $Y_l$ and integrate over
the volume of a sphere of radius $a$ we obtain

$$[l(l+1)-n(n+1)] \int_{r<a} dV \frac{1}{r^2} Y_l X_n = - \int_{r=a} dS \left( X_n e_r \cdot \nabla Y_l - Y_l e_r \cdot \nabla X_n \right) = 0, \quad (8)$$

where the surface integral has been obtained through Gauss’s theorem on using the identity $X_n \nabla^2 Y_l = Y_l \nabla^2 X_n = \nabla \cdot (X_n \nabla Y_l - Y_l \nabla X_n)$. Since surface harmonics do not depend on $r$, the surface integral vanishes and the volume integral in the LHS of (8) can be transformed into one on the unit sphere by writing $dV = r^2 dr d\Omega$, $d\Omega$ being the element of solid angle. Carrying out the trivial integration over the radial coordinate (8) yields

$$\int d\Omega Y_l X_n = 0 \quad \text{if} \quad l \neq n. \quad (9)$$

An interesting relation between the solid and surface harmonics satisfying (6) is obtained if one considers the function

$$\Psi \equiv \frac{1}{2l+1} \left[ a^{-l+1} H_l(r) - a^{l+2} V_l(r) \right], \quad (10)$$

where $a$ is any positive constant. On using (6) to express $V_l$ and $H_l$ in terms $Y_l$ and taking into account that $e_r \cdot \nabla Y_l = 0$ it is seen that $\Psi$ vanishes at $r = a$ and satisfies the identity

$$Y_l \equiv \left. \frac{\partial \Psi}{\partial r} \right|_{r=a} = \left[ e_r \cdot \nabla \Psi \right]_{r=a}. \quad (11)$$

The physical meaning of this identity is that $a^{-l+1} H_l(r)/(2l+1)$ and $a^{l+2} V_l(r)/(2l+1)$ yield the potential for $r \leq a$ and $r \geq a$, respectively, due to an arbitrarily thin sphere of radius $a$ with a surface charge density distribution given by $Y_l(e_r)/(4\pi)$ - the jump at the surface in the normal derivatives of the potential being represented by (11). This expression is useful when one considers the integral over the sphere $r = a$ of the product of $Y_l$ times any regular function $\Phi$ that satisfies $\nabla^2 \Phi = 0$ inside the sphere. Using the identity $\nabla \cdot (\Phi \nabla \Psi) = \nabla \cdot (\Psi \nabla \Phi) + \Phi \nabla^2 \Psi - \Psi \nabla^2 \Phi$ with $\nabla^2 \Phi = 0$, Gauss’s theorem yields

$$\int dS \Phi Y_l = \int_{r<a} dV \Phi \nabla^2 \Psi = - \frac{a^{l+2}}{2l+1} \int_{r<a} dV \Phi \nabla^2 V_l, \quad (12)$$

where we have taken into account in (10) that $H_l$ is regular for $r < a$ and $\nabla^2 H_l = 0$. In (12) $\nabla^2 V_l$ must be considered as a generalized function due to its singularity at the origin.
A. The simplest solid harmonics

The simplest \( H_l \)-harmonics are polynomials of the form \((\mathbf{b} \cdot \mathbf{r})^l\), where \( \mathbf{b} \) is any constant (complex) null vector, i.e., \( \mathbf{b} \cdot \mathbf{b} = 0 \), so that

\[
\nabla^2(\mathbf{b} \cdot \mathbf{r})^l = l \nabla \cdot [\mathbf{b} (\mathbf{b} \cdot \mathbf{r})^{l-1}] = l(l - 1)(\mathbf{b} \cdot \mathbf{r})^{l-2}\mathbf{b} \cdot \mathbf{b} = 0. \tag{13}
\]

It can be shown that any \( H_l \)-harmonic can always be written as a linear combination of the form

\[
H_l(\mathbf{r}) = A_1(\mathbf{b}_1 \cdot \mathbf{r})^l + A_2(\mathbf{b}_2 \cdot \mathbf{r})^l + ..., \tag{14}
\]

for suitable constants \( A_1, A_2, ... \) and null vectors \( \mathbf{b}_1, \mathbf{b}_2, ... \) whence any property that can be easily found out for the simplest solid harmonics can be extended by linearity to any general \( H_l \). To prove (14), let us consider the particular set of null vectors of the form \( \mathbf{b} = i \cos u \mathbf{e}_x + i \sin u \mathbf{e}_y + \mathbf{e}_z \) \((0 \leq u < 2\pi)\), or \((\mathbf{b} \cdot \mathbf{r})^l = (i x \cos u + i y \sin u + z)^l\). On expressing the trigonometric functions in polar form and binomially expanding we find for any given value \( u_s \) in \((0, 2\pi)\) that

\[
(i x \cos u_s + i y \sin u_s + z)^l = \sum_{k'=-l}^{l} h_l^{(k')}(x, y, z) e^{ik'u_s}, \tag{15}
\]

where the coefficients of the trigonometric series, i.e the homogeneous polynomials \( h_l^{(k')}(x, y, z) \), must constitute a set \( 2l + 1 \) independent solid harmonics. By taking the set of points \( u_s = 2\pi s/(2l + 1) \) \((s = 0, ... 2l)\) and using the orthogonality property

\[
\sum_{s=0}^{2l} e^{-\pi is(k-k')/(2l+1)} = (2l + 1)\delta_{kk'} \]

we can easily invert (15) to obtain

\[
h_l^{(k)}(x, y, z) = \sum_{s=0}^{2l} e^{2\pi iks/(2l+1)} \left( i x \cos \left[ \frac{2\pi iks}{2l+1} \right] + i y \sin \left[ \frac{2\pi iks}{2l+1} \right] + z \right)^l, \tag{16}
\]

whence each of the \( 2l + 1 \) independent solid harmonics \( h_l^{(k)}(x, y, z) \) can be expressed as a linear combination of solid harmonics of the form \((\mathbf{b}_j \cdot \mathbf{r})^l\). Since every \( H_l \)-harmonic is a linear combination of the \( h_l^{(k)} \)'s, equation (14) immediately follows from (16).

An important application of (14) results from the analysis of the repeated action of the differential operator \( \mathbf{b} \cdot \nabla - \mathbf{b} \) being a constant null vector - on any spherically symmetric function \( F(r) \). In effect, since

\[
\mathbf{b} \cdot \nabla F = \mathbf{b} \cdot \mathbf{e}_r \frac{dF}{dr} = \mathbf{b} \cdot \mathbf{r} \frac{1}{r} \frac{dF}{dr}, \tag{17}
\]
and
\[ b \cdot \nabla (b \cdot r)^n = n(b \cdot r)^{n-1}b \cdot \nabla (b \cdot r) = n(b \cdot r)^{n-1}b \cdot b = 0 \] (18)
for any integer \( n > 0 \), on applying \( l - 1 \) times \( l \geq 1 \) the operator \( b \cdot \nabla \) to (17) we obtain
\[ (b \cdot \nabla)^l F = (b \cdot r)^l \left( \frac{1}{r} \frac{d}{dr} \right)^l F. \] (19)
Equation (14) then implies
\[ H_l(\nabla) F(r) = H_l(r) \left( \frac{1}{r} \frac{d}{dr} \right)^l F(r), \] (20)
where \( H_l(\nabla) \) is the differential operator obtained by substituting each cartesian component of \( r \) in \( H_l(r) \) by the corresponding one of \( \nabla \).

As an illustration of (20), let us consider the integral (to be used in Section VI on partial wave expansions)
\[ \int d\Omega_q H_l(\mathbf{q}) e^{\mathbf{q} \cdot \mathbf{r}} = H_l(\nabla) \int d\Omega_q e^{\mathbf{q} \cdot \mathbf{r}}, \] (21)
where \( \mathbf{q} = q_x \mathbf{e}_x + q_y \mathbf{e}_y + q_z \mathbf{e}_z \) is a vector of the form and \( \mathbf{q} = q \mathbf{e}_q - q \) being a (possibly complex) isotropic scalar and \( \mathbf{e}_q \) a real unit vector -, and \( d\Omega_q \equiv \sin \theta_q d\theta_q d\varphi_q \) is the element of solid angle around the point \( \mathbf{e}_q \) of the unit sphere. The equality in (21) easily follows from the properties of the derivatives of the exponential function taking into account that \( H_l(\mathbf{q}) \) is a homogeneous polynomial. Introducing \( \mu_q = \cos \theta_q = \mathbf{e}_q \cdot \mathbf{e}_r \), the last integral in (21) yields
\[ \int d\Omega_q e^{\mathbf{q} \cdot \mathbf{r}} = 2\pi \int_{-1}^1 d\mu_q e^{q \mu_q} = 4\pi \frac{\sinh(q r)}{q r}, \] (22)
so that, on using (20),
\[ \int d\Omega_q H_l(\mathbf{q}) e^{\mathbf{q} \cdot \mathbf{r}} = 4\pi H_l(r) \left( \frac{1}{r} \frac{d}{dr} \right)^l \left[ \frac{\sinh(q r)}{q r} \right]. \] (23)
Defining the function
\[ s_l(\zeta) \equiv \left( \frac{1}{\zeta} \frac{d}{d\zeta} \right)^l \left( \frac{\sinh \zeta}{\zeta} \right) = \sum_{j=l}^{\infty} \frac{2^j j!}{(j-l)! (2j+1)!} \zeta^{2(j-l)} \] (24)
we can write (23) more briefly as
\[ \int d\Omega_q H_l(\mathbf{q}) e^{\mathbf{q} \cdot \mathbf{r}} = 4\pi H_l(r) q^2 s_l(q r). \] (25)
Note that the series expansion for \( s_l(\zeta) \) can be easily obtained by applying the operator \( [(1/\zeta) d/d\zeta]^l = 2^l [d/d\zeta]^l \) to the power expansion of \( \sinh \zeta/\zeta \). The fact that this series only
contains even powers of $\zeta$ makes possible to compute (21) for the case in which the vector $\mathbf{r}$ is replaced by the gradient operator $\nabla$. In effect, it is easy to convince oneself that then the result must be formally the same as (23) but with $r = \sqrt{\mathbf{r} \cdot \mathbf{r}}$ replaced by $\sqrt{\nabla \cdot \nabla} = \sqrt{\nabla^2}$:

$$\int d\Omega_q H_l(\mathbf{q}) e^{\mathbf{q} \cdot \nabla} = 4\pi H_l(\mathbf{r}) q^2 s_l \left( q \sqrt{\nabla^2} \right),$$  

(26)

where the operator on the RHS must be computed by replacing $\zeta^2$ by $(q \sqrt{\nabla^2})^2 = q^2 \nabla^2$ in the series (24) which, therefore, yields only integral powers of the operator $\nabla^2$.

### B. Maxwell’s harmonics and Maxwell’s integral theorem

Maxwell’s harmonics$^{5,11}$ are formed by taking $l$ directional derivatives of $1/r$ in any given directions defined by (generally complex) vectors $\mathbf{e}_1, \ldots, \mathbf{e}_l$. Thus the function

$$V_l(\mathbf{r}) = (\mathbf{e}_1 \cdot \nabla) \ldots (\mathbf{e}_l \cdot \nabla) (1/r) = \frac{\partial l (1/r)}{\partial h_1 \ldots \partial h_l},$$

(27)

where $\partial h_i$ ($i = 1, \ldots, l$) denotes the infinitesimal (generally complex) displacement associated to $\mathbf{e}_i$, must be a $V_l$-harmonic, since it can be seen by inspection that $r^{2l+1} V_l$ is a homogeneous polynomial of degree $l$ which satisfies Laplace’s equation (since so does $V_l$). We will illustrate this for the first few values of $l$, and then the interested reader can easily proceed by induction$^{12}$ to prove it for any $l$. For example, for $l = 1$ and $l = 2$ we have

$$\mathbf{e}_1 \cdot \nabla (1/r) = -\frac{\mathbf{e}_1 \cdot \mathbf{r}}{r^3}$$

(28)

and

$$\mathbf{e}_1 \cdot \nabla [\mathbf{e}_2 \cdot \nabla (1/r)] = \frac{3 \mathbf{e}_1 \cdot \mathbf{r} \quad \mathbf{e}_2 \cdot \mathbf{r} - r^2 \mathbf{e}_1 \cdot \mathbf{e}_2}{r^5},$$

(29)

where it can be readily checked that the homogeneous polynomials in the numerators satisfy Laplace’s equation.

Therefore, the function

$$H_l(\mathbf{r}) = r^{2l+1} \frac{\partial l (1/r)}{\partial h_1 \ldots \partial h_l}$$

(30)

is an $H_l$-harmonic, and the function

$$Y_l(\mathbf{r}) = r^{l+1} \frac{\partial l (1/r)}{\partial h_1 \ldots \partial h_l}$$

(31)

is a surface harmonic of degree $l$. Solid harmonics which, except for a constant factor, are of the form (27) and (30) will be called Maxwell’s solid harmonics of the $V_l$ and $H_l$.
types, respectively, and surface harmonics of the form (31) will be called Maxwell’s surface harmonics. The vectors $e_i$ are called the poles of the Maxwell’s harmonics, and in the particular case in which they are both unit and real, they define $l$ points on the unit sphere known as Maxwell’s poles.\textsuperscript{5,11–13}

A Maxwell’s surface harmonic in which all the $e_i$’s coincide with a given vector, say $e_1$, is called a zonal harmonic:

$$Z_l(r) = r^{l+1}(e_1 \cdot \nabla)^l (1/r) = r^{l+1} \frac{\partial^l (1/r)}{\partial h_1^l}.$$  \hspace{0.5cm} \text{(32)}

Zonal harmonics arise most naturally when one Taylor expands around $r = 0$ the potential due to a unit source localized at $r'$. For instance, the expansion valid for $r > r'$ can be written as

$$\frac{1}{|r - r'|} = \sum_{l=0}^{\infty} \frac{r^l}{r^{l+1}} \frac{(-1)^l r^{l+1}}{l!} (e'_r \cdot \nabla)^l (1/r),$$  \hspace{0.5cm} \text{(33)}

where $r' = r' e'_r$. Note that all factors $r^l/r^{l+1}$ in the series \textsuperscript{33} are multiplied by a zonal harmonic of the form \textsuperscript{32} with pole at $e'_r$. On the other hand, the well known expansion in terms of Legendre’s polynomials, $P_l$, is

$$\frac{1}{|r - r'|} = \sum_{l=0}^{\infty} \frac{r^l}{r^{l+1}} P_l(e'_r \cdot e_r),$$  \hspace{0.5cm} \text{(34)}

whence identifying terms in \textsuperscript{33}–\textsuperscript{34} we obtain:

$$P_l(e'_r \cdot e_r) = \frac{(-1)^l r^{l+1}}{l!} (e'_r \cdot \nabla)^l (1/r),$$  \hspace{0.5cm} \text{(35)}

which establishes the relation between Legendre polynomials and zonal harmonics.

Maxwell’s integral theorem results when we substitute $Y_l$ in (12) by a surface harmonic of the form (31). Then $V_l = r^{-(l+1)} Y_l$ is given by (27) and, since $\nabla^2 (1/r) = -4\pi \delta(r)$ - where $\delta(r)$ is Dirac’s delta function - we have

$$\nabla^2 V_l(r) = -4\pi \frac{\partial^l \delta(r)}{\partial h_1 \ldots \partial h_l}.$$  \hspace{0.5cm} \text{(36)}

Substituting (36) into the last integral of (12) and integrating $l$ times by parts - taking into account that $\delta(r)$ and all its partial derivatives vanish at the surface $r = a$ -, we obtain

$$\int_{r=a} dS \Phi Y_l = \frac{4\pi (-1)^l d^{l+2}}{2l + 1} \frac{\partial^l \Phi}{\partial h_1 \ldots \partial h_l} \bigg|_{r=0},$$  \hspace{0.5cm} \text{(37)}

which is Maxwell’s integral theorem. The direct proof of (37) given here is the only one we are aware of besides that given by Maxwell himself in his treatise. It seems to us than ours is
somewhat more transparent than his - which is based on the properties singular multipolar charge distributions -.

As an illustration, let us apply (37) for the case in which Φ is any solid harmonic $H_l$ and the Maxwell’s harmonic is the zonal harmonic $Z_l$ given by (32):

$$\int_{r=a} dS H_l Z_l = \frac{4\pi(-1)^l a^{l+2}}{2l + 1} [(e_1 \cdot \nabla)^l H_l]_{r=0}. \tag{38}$$

In order to compute the RHS of (38) we binomially expand the operator $(e_1 \cdot \nabla)^l$,

$$(e_1 \cdot \nabla)^l = l! \sum_{\alpha'+\beta'+\gamma'=l} \frac{e_1^{\alpha'} e_1^{\beta'} e_1^{\gamma'}}{\alpha'! \beta'! \gamma'!} \partial^{\alpha'} \partial^{\beta'} \partial^{\gamma'}, \tag{39}$$

and take into account the expression (2) for $H_l(r)$. On computing the result at $r = 0$ we obtain

$$[(e_1 \cdot \nabla)^l H_l(r)]_{r=0} = l! \sum_{\alpha+\beta+\gamma=l} C_{\alpha\beta\gamma} e_1^{\alpha} e_1^{\beta} e_1^{\gamma} = l! H_l(e_1), \tag{40}$$

which is a direct consequence of the homogeneity of $H_l$ - and therefore it remains valid if $e_1$ and $H_l(r)$ are replaced by any constant (generally complex) vector and any homogeneous polynomial of degree $l$, respectively-. Thus

$$\int_{r=a} dS H_l Z_l = \frac{4\pi(-1)^l l! a^{l+2}}{2l + 1} H_l(e_1). \tag{41}$$

III. THE STANDARD SET OF SPHERICAL HARMONICS $Y_{lm}$.  

The standard spherical harmonics of degree $l$, $Y_{lm}(r)$ $(m = -l, \ldots l)$, are $2l + 1$ independent, normalized surface harmonics such that the $m$-th one depends on the azimuthal coordinate as $e^{im\varphi}$. The normalization condition is defined as

$$\int d\Omega Y_{lm}^* Y_{lm} = \delta_{m'm}. \tag{42}$$

As already pointed out, these functions are usually given in terms of the associated Legendre functions, $P_l^m(\cos \theta)$, which can be introduced by separating variables in Laplace’s equation expressed in spherical coordinates (see also Appendix A). However, we next show how they can be generated in an almost trivial fashion by the procedure due to Thomson and Tait, who constructed Maxwell’s harmonics by taking directional derivatives of $1/r$ with respect to $z$ and with respect to the complex coordinates

$$\xi = x + iy = r \cos \theta e^{i\varphi} \quad \text{and} \quad \eta = x - iy = r \cos \theta e^{-i\varphi}. \tag{43}$$
In effect, let us assume for the moment that $m \geq 0$ and consider the $V_l$-harmonic

$$V_{lm}(r) \equiv \frac{\partial^l (1/r)}{\partial z^{l-m} \partial \eta^m} = (-1/2)^m (2m - 1)!! \xi^m \frac{\partial^{l-m} 1}{\partial z^{l-m} \eta^{2m+1}},$$  \hspace{1cm} (44)

where we have carried out $m$th-partial derivative with respect to $\eta$ of $r^{-1} = (\eta \xi + z^2)^{-1/2}$ using the notation $(2m - 1)!! \equiv (2m - 1) \times (2m - 3) \times \ldots \times 1$ with the convention $(-1)!! \equiv 1$. Observe that the presence of the factor $\xi^m$ automatically yields an azimuthal dependence of the form $e^{im\varphi}$ in (44). Therefore, the spherical harmonics $Y_{lm}$ can be obtained from the $V_{lm}$'s by just writing

$$Y_{lm} = C_{lm} r^{l+1} V_{lm},$$  \hspace{1cm} (45)

where the constants $C_{lm}$ must be determined from the normalization condition. We can readily compute the normalization integral (42) via Maxwell’s integral theorem by putting $\Phi \equiv r Y_{lm}^*, Y_l \equiv Y_{lm}$ and $a = 1$ in (37), which yields

$$\frac{4\pi (-1)^l |C_{lm}|^2 \partial(r^{2l+1} V_{lm}^*)}{2l + 1} \bigg|_{r=0} = 1.$$  \hspace{1cm} (46)

Note that, since $r^{2l+1} V_{lm}^*$ is a homogeneous polynomial of degree $l$ in the variables $\xi, \eta$ and $z$, only the coefficient of the term containing $\eta^m z^{l-m}$ contributes to the value at $r = 0$ of the derivative in (46). Multiplying (44) by $r^{2l+1}$ and taking complex conjugates we obtain

$$r^{2l+1} V_{lm}^* = (-1/2)^m (2m - 1)!! \eta^m r^{2l+1} \frac{\partial^{l-m} 1}{\partial z^{l-m} \eta^{2m+1}},$$  \hspace{1cm} (47)

so that in order to find the coefficient of $\eta^m z^{l-m}$ in (47) we just have to compute the value at $\eta = 0$ and $\xi = 0$ of the factor to the right of $\eta^m$, namely

$$z^{2l+1} \frac{\partial^{l-m} 1}{\partial z^{l-m} z^{2m+1}} = (-1)^{l-m} (l + m)! (2m)! z^{l-m}.$$  \hspace{1cm} (48)

Substituting (48) into (47) we obtain

$$r^{2l+1} V_{lm}^* = \frac{(-1)^l (2m - 1)!! (l + m)!}{2^m (2m)!} \eta^m z^{l-m} + \ldots,$$  \hspace{1cm} (49)

where the dots denote terms which do not contribute to the LHS of (46), whence

$$\frac{4\pi (l + m)! (l - m)! |C_{lm}|^2}{(2l + 1) 2^{2m}} = 1.$$  \hspace{1cm} (50)

The normalization constant $C_{lm}$ is determined by (50) except for a phase factor which we will choose as $(-1)^{l+m}$. This choice is motivated so that the resulting spherical harmonics
satisfy the relation (57) below, as do those used in standard references\textsuperscript{2,18}. Solving (50) for \( C_{lm} \) and substituting into (45) we finally obtain
\[
Y_{lm}(r) = \sqrt{\frac{2l+1}{4\pi}} \frac{(-1)^{l+m} 2^m r^{l+1}}{(l+m)!(l-m)!} \frac{\partial^l (1/r)}{\partial r^{l-m} \partial \eta^m}.
\] (51)
It is shown in Appendix A that (51) reproduces the standard expression\textsuperscript{14} for the \( Y_{lm} \)'s when expressed in spherical coordinates.

Until now we have assumed \( 0 \leq m \leq l \) and found a set of \( l+1 \) spherical harmonics given by (51) for \( m = 0, 1, \ldots, l \). These functions, together with their corresponding complex conjugates \( Y_{lm}^*(r) \) form a complete set of \( 2l+1 \) surface harmonics \( \{ Y_{l0}, Y_{lm}, Y_{lm}^* \mid m = 1, 2, \ldots, l \} \). However, in actual calculations it is often more convenient to work with a set of \( 2l+1 \) functions labelled by an index \( m \) running from \(-l\) to \( l \), and to arrange things so that, for negative \( m \), \( Y_{lm} \) is also given by an expression of the form (51) conveniently defined for \( m < 0 \). For this purpose, we first note the identity
\[
\nabla^2 (1/r) = 4 \frac{\partial^2 (1/r)}{\partial \eta \partial \xi} + \frac{\partial^2 (1/r)}{\partial z^2} = 0
\] (52)
obtained after expressing the Laplacian operator in coordinates \((\xi, \eta, z)\) through the chain rule. The result (52) suggests that we can give an operational meaning to symbols such as \((\partial/\partial \eta)^{-1}\) and \((\partial/\partial z)^{-2}\) when applied to \((1/r)\) by means of the relations
\[
4 \frac{\partial^2}{\partial \eta \partial \xi} = - \frac{\partial^2}{\partial z^2} \rightarrow 4 \frac{\partial}{\partial \xi} = - \left( \frac{\partial}{\partial \eta} \right)^{-1} \frac{\partial^2}{\partial z^2} \rightarrow 4 \left( \frac{\partial}{\partial z} \right)^{-2} \frac{\partial}{\partial \xi} = - \left( \frac{\partial}{\partial \eta} \right)^{-1},
\] (53)
which allow us to define \( V_{lm} \) for \( m < 0 \) in terms of \( V_{l|m|}^* \) by means of (44). In effect, according to (44) we can formally write
\[
V_{l,-|m|} \equiv \left( \frac{\partial}{\partial z} \right)^{|l+m|} \left( \frac{\partial}{\partial \eta} \right)^{|-m|} \left( \frac{1}{r} \right)
\] (54)
and, if we substitute \((\partial/\partial \eta)^{-|m|}\) by the \(|m|\)th-power of the RHS of the last operator equation in (53) we obtain
\[
V_{l,-|m|} = (-4)^{|m|} \frac{\partial^l (1/r)}{\partial z^{l-|m|} \partial \xi^{|m|}} = (-4)^{|m|} V_{l|m|}^*,
\] (55)
But it is easily seen that if we drop the absolute value sign in (55) the resulting equation,
\[
V_{l,-m} = (-1)^m 4^m V_{lm}^*,
\] (56)
remains consistent with definition (55) independently of the sign of \( m \), whence (56) can be freely used to relate the \( V_{lm} \)'s of positive and negative \( m \). This result will be of great use
in Section IV on recursion relations for spherical harmonics. The corresponding relation for the $Y_{lm}$’s can be now obtained from (45) after noticing that replacing $m$ by $-m$ in the normalization constant in (51) yields the new constant $C_{l,-m} = C_{lm}/4^m$, or

$$Y_{l,-m} = C_{l,-m}r^{l+1}V_{l,-m} = (-1)^mY_{l,m}^*.$$  \hspace{1cm} (57)

The functions $Y_{lm}$ with $-l \leq m \leq l$ defined by (51) and (57) constitute the set of standard spherical harmonics of degree $l$.

IV. RECURSION RELATIONS.

Recursion relations are of importance in calculations involving spherical harmonics, a well known application in Quantum Mechanics being the computation of the matrix elements of operators in the angular momentum representation. In classical physics the best known examples are perhaps the analysis of multipolar radiation fields and wave scattering problems solved numerically using the relatively recent Fast Multipole Method. The standard derivations of such recursion relations, i.e., using the associated Legendre functions and spherical polar coordinates, often get rather tricky and involved, yielding messy final expressions. In this section we indicate an apparently new procedure to systematically derive a whole set of useful recursion relations using the Maxwell solid harmonics $V_{lm}(r)$ defined in Section III [see (44)].

We begin by noticing the equality

$$z \frac{\partial^{-m} \partial^m}{\partial z^{-m} \partial \eta^m} \left( \frac{1}{r} \right) = \frac{\partial^{-m} \partial^m}{\partial z^{-m} \partial \eta^m} \left( \frac{z}{r} \right) - (l-m) \frac{\partial^{l-m-1} \partial^m}{\partial z^{l-m-1} \partial \eta^m} \left( \frac{1}{r} \right),$$ \hspace{1cm} (58)

where we have applied Leibnitz’s rule to the derivatives with respect to $z$ of $(z/r)$. Since $r = \sqrt{\xi \eta + z^2}$, substituting the relation

$$\frac{\partial}{\partial \eta} \left( \frac{z}{r} \right) = -\frac{\xi z}{2r^{3/2}} = \frac{\xi}{2} \frac{\partial}{\partial z} \left( \frac{1}{r} \right)$$ \hspace{1cm} (59)

into the first summand on the RHS of (58) we obtain

$$z \frac{\partial^{-m} \partial^m}{\partial z^{-m} \partial \eta^m} \left( \frac{1}{r} \right) = \frac{\xi}{2} \frac{\partial^{l-m+1} \partial^{m-1}}{\partial z^{l-m+1} \partial \eta^{m-1}} \left( \frac{1}{r} \right) - (l-m) \frac{\partial^{l-m-1} \partial^m}{\partial z^{l-m-1} \partial \eta^m} \left( \frac{1}{r} \right),$$ \hspace{1cm} (60)

or, in terms of the $V_{lm}$’s defined in (44),

$$2zV_{lm} = \xi V_{l,m-1} - 2(l-m)V_{l-1,m},$$ \hspace{1cm} (61)
which is our first recursion relation. A corresponding one for \( \eta V_{lm} \) can be obtained by replacing \( m \) by \(-m\) in (61) and taking complex conjugates using (56). This yields, after replacing \( m \) by \( m - 1 \) in the resulting equation,

\[
2\eta V_{lm} = -z V_{l,m-1} - (l + m - 1)V_{l-1,m-1}. 
\]

Also, adding (61) multiplied by \( z \) to (62) multiplied by \( \xi \) we find the relation

\[
2r^2 V_{lm} = -2(l - m)z V_{l-1,m} - (l + m - 1)\xi V_{l-1,m-1}. 
\]

Replacing \( l \) by \( l + 1 \) in (63), substituting \( z V_{lm} \) from and, finally, replacing \( m \) by \( m + 1 \) we obtain

\[
(2l + 1)\xi V_{lm} = -2r^2 V_{l+1,m+1} + 2(l - m)(l - m - 1)V_{l-1,m+1}. 
\]

Observe that the factor \( \xi \) multiplying \( V_{lm} \) in (64) depends on the angular coordinates \( \theta \) and \( \varphi \) while none of the factors multiplying the functions \( V \) on the RHS does so. Therefore, recursion relations such as (64) are very convenient to compute surface integrals (projections) of the product of the function appearing in the LHS times Maxwell’s solid or surface harmonics, since then we can use the orthogonality properties of the latter with those on the RHS. Analogous expression for \( \eta V_{lm} \) can be obtained by replacing \( m \) by \(-m\) in (64) and taking complex conjugates using (56), which yields

\[
2(2l + 1)\eta V_{lm} = r^2 V_{l+1,m-1} - (l + m)(l + m - 1)V_{l-1,m-1}, 
\]

The corresponding expression for \( z V_{lm} \), is obtained by replacing \( m \) by \( m - 1 \) in (64) and substituting into (61):

\[
(2l + 1)z V_{lm} = -r^2 V_{l+1,m} - (l - m)(l + m)V_{l-1,m}, 
\]

In some circumstances, it is convenient to express a derivative with respect to either \( z \), \( \eta \) or \( \xi \) of the product of \( V_{lm} \) times a function of \( r \), say \( B(r) \), in terms of functions \( V_{lm} \) multiplied by coefficients which only depend on \( r \). This is the case, for example, in the computation of matrix elements of the quantum momentum operator in the angular momentum representation.\(^{15}\) Since \( r = \sqrt{\xi \eta + z^2} \), applying the chain rule we obtain

\[
\frac{\partial}{\partial z} (BV_{lm}) = B'z V_{lm}/r + BV_{l+1,m}, 
\]
\[ \frac{\partial}{\partial \eta} (BV_{lm}) = B' \xi V_{lm}/(2r) + BV_{l+1,m+1}, \]  
\[ \frac{\partial}{\partial \xi} (BV_{lm}) = B' \eta V_{lm}/(2r) - BV_{l+1,m-1}/4, \]  
where we have written \( B' \equiv (dB/dr) \) and used the relations

\[ \frac{\partial V_{lm}}{\partial z} = \frac{\partial^{l-m+1}}{\partial z^{l-m+1}} \frac{\partial^{m}}{\partial \eta^{m}} \left( \frac{1}{r} \right) = V_{l+1,m}, \quad \frac{\partial V_{lm}}{\partial \eta} = \frac{\partial^{l+1-(m+1)}}{\partial z^{l+1-(m+1)}} \frac{\partial^{m+1}}{\partial \eta^{m+1}} \left( \frac{1}{r} \right) = V_{l+1,m+1}. \]

Using the recursion relations (64)-(66) in (67)-(69) we readily obtain the sought expressions.

It can be checked that the recursion relations here obtained reproduce those derived in a different way by Kramers \(^{15}\) (Ch.IV p. 178). For this, it is necessary to replace in all of them \( l \) by \( l-1 \), to make \( B(r) \equiv r^l b(r) \), and to express them in terms of the (unnormalized) surface harmonics \( \mathcal{P}_{lm} \) used by Kramers:

\[ \mathcal{P}_{lm} = (-1)^l \frac{2^{m+1} l}{(l-m)!(l+m)!} r^{l+1} V_{lm}. \]

Nevertheless, it seems to us that our derivations and expressions are simpler and more systematic than Kramer’s due to we use solid harmonics, the \( V_{lm} \)’s, instead of surface harmonics.

Finally, of special interest in Quantum Mechanics are the ladder properties of the operator \( \mathbf{r} \times \nabla \), which is proportional to the angular momentum operator, when applied to the spherical harmonics \( Y_{lm} \). Notice that, since \( \mathbf{r} \times \nabla r^{-(l+1)} = 0 \), its effect on the \( Y_{lm} \)’s will be the same as that on the functions \( V_{lm} \). In order to analyze the operator \( \mathbf{r} \times \nabla \) in a coordinate-free manner, it is convenient at this point to introduce the so-called spherical basis formed by the vector \( \mathbf{e}_z \) together with the vectors

\[ \mathbf{e}_\xi = (\mathbf{e}_x - i\mathbf{e}_y) / \sqrt{2} \quad \text{and} \quad \mathbf{e}_\eta = (\mathbf{e}_x + i\mathbf{e}_y) / \sqrt{2} = \mathbf{e}_z^*. \]

It is immediately seen that these vectors satisfy the orthogonality relations

\[ \mathbf{e}_\xi \cdot \mathbf{e}_\xi = \mathbf{e}_\eta \cdot \mathbf{e}_\eta = 0 \quad \text{and} \quad \mathbf{e}_\xi \cdot \mathbf{e}_\eta = 1 \]

and

\[ \mathbf{e}_\xi \times \mathbf{e}_\eta = i\mathbf{e}_z, \quad \mathbf{e}_\eta \times \mathbf{e}_z = i\mathbf{e}_\eta, \quad \mathbf{e}_z \times \mathbf{e}_\xi = i\mathbf{e}_\xi. \]

Note that (73) imply that \( \mathbf{e}_\xi \) and \( \mathbf{e}_\eta \) are null vectors. In terms of the spherical vectors, the cartesian vectors \( \mathbf{e}_x \) and \( \mathbf{e}_y \) are given by

\[ \mathbf{e}_x = (\mathbf{e}_\xi + \mathbf{e}_\eta) / \sqrt{2} \quad \text{and} \quad \mathbf{e}_y = i (\mathbf{e}_\xi - \mathbf{e}_\eta) / \sqrt{2}, \]
so that any vector $\mathbf{u}$ can be written as

$$
\mathbf{u} = u_x \mathbf{e}_x + u_y \mathbf{e}_y + u_z \mathbf{e}_z = u_\xi \mathbf{e}_\xi + u_\eta \mathbf{e}_\eta + u_z \mathbf{e}_z,
$$

(76)

with the components $u_\xi$ and $u_\eta$ given by

$$
\mathbf{u} \cdot \mathbf{e}_\eta = u_\xi = (u_x + iu_y)/\sqrt{2} \quad \text{and} \quad \mathbf{u} \cdot \mathbf{e}_\xi = u_\eta = (u_x - iu_y)/\sqrt{2}.
$$

(77)

In particular, for the position vector we have

$$
\mathbf{r} = \xi \mathbf{e}_\xi/\sqrt{2} + \eta \mathbf{e}_\eta/\sqrt{2} + z \mathbf{e}_z,
$$

(78)

and the gradient operator is

$$
\nabla = \mathbf{e}_x \frac{\partial}{\partial x} + \mathbf{e}_y \frac{\partial}{\partial y} + \mathbf{e}_z \frac{\partial}{\partial z} = \sqrt{2} \mathbf{e}_\xi \frac{\partial}{\partial \eta} + \sqrt{2} \mathbf{e}_\eta \frac{\partial}{\partial \xi} + \mathbf{e}_z \frac{\partial}{\partial z},
$$

(79)

where we have used (75) together with the relations between the partial derivatives with respect to the cartesian and the complex coordinates - obtained via the chain rule using (43) - :

$$
\frac{\partial}{\partial x} = \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta} \quad \text{and} \quad \frac{\partial}{\partial y} = i \frac{\partial}{\partial \xi} - i \frac{\partial}{\partial \eta}.
$$

(80)

Using the recursion relations and the properties of the spherical basis derived above, it is easy to show that the operator $\mathbf{e}_\eta \cdot (\mathbf{r} \times \nabla)$ rises the index $m$ of functions $V_{lm}$ ($m = -l, -l + 1, \ldots, l - 1, l$) on which it acts, while the operator $\mathbf{e}_\xi \cdot (\mathbf{r} \times \nabla)$ lowers it. In effect, taking into account that

$$
\mathbf{e}_\eta \times \mathbf{r} = \xi \mathbf{e}_\eta \times \mathbf{e}_\xi/\sqrt{2} + z \mathbf{e}_\eta \times \mathbf{e}_z = -i \xi \mathbf{e}_z/\sqrt{2} + iz \mathbf{e}_\eta
$$

(81)

and that $\mathbf{e}_\eta \cdot \nabla = \sqrt{2} \partial/\partial \eta$ [see (79)], we find

$$
\mathbf{e}_\eta \cdot (\mathbf{r} \times \nabla V_{lm}) = (\mathbf{e}_\eta \times \mathbf{r}) \cdot \nabla V_{lm} = -i \xi / \sqrt{2} V_{l+1,m} + \sqrt{2} i z V_{l+1,m+1},
$$

(82)

or, using recursion relation (61),

$$
\mathbf{e}_\eta \cdot (\mathbf{r} \times \nabla V_{lm}) = -\sqrt{2} i (l - m) V_{l,m+1}.
$$

(83)

The corresponding property for the operator $\mathbf{e}_\xi \cdot (\mathbf{r} \times \nabla)$ can be obtained by replacing $m$ by $-m$ in (83) and taking the complex conjugate of the resulting expression. Thus relations (56) and (61) lead to

$$
\mathbf{e}_\xi \cdot (\mathbf{r} \times \nabla V_{lm}) = -i (l + m) V_{l,m-1}/\sqrt{2}.
$$

(84)
In terms of the spherical harmonics (45) equations (83) and (84) read

\[ \mathbf{e}_\eta \cdot (\mathbf{r} \times \nabla Y_{lm}) = i \sqrt{(l - m)(l + m + 1)} Y_{l,m+1}/\sqrt{2}. \] (85)

\[ \mathbf{e}_\xi \cdot (\mathbf{r} \times \nabla Y_{lm}) = i \sqrt{(l + m)(l - m + 1)} Y_{l,m-1}/\sqrt{2}. \] (86)

Relations (85) and (86) are usually expressed in terms of spherical polar coordinates \( r \) and \( \theta \) and \( \varphi \). To do this, we first obtain the cartesian components of the operator

\[ \mathbf{r} \times \nabla = \mathbf{e}_\varphi \frac{\partial}{\partial \theta} - \mathbf{e}_\theta \frac{\partial}{\sin \theta \, \partial \varphi} \] (87)

by recalling that \( \mathbf{e}_\varphi = -\sin \varphi \mathbf{e}_x + \cos \varphi \mathbf{e}_y \) and \( \mathbf{e}_\theta = \mathbf{e}_x \times \mathbf{e}_r \), which, in turn, imply \( \mathbf{e}_x \cdot \mathbf{e}_\theta = (\mathbf{e}_x \times \mathbf{e}_\varphi) \cdot \mathbf{e}_r = \cos \varphi \cos \theta \) and \( \mathbf{e}_y \cdot \mathbf{e}_\theta = \sin \varphi \cos \theta \). Thus

\[ \mathbf{r} \times \nabla = - (\mathbf{e}_x \sin \varphi - \mathbf{e}_y \cos \varphi) \frac{\partial}{\partial \theta} - (\mathbf{e}_x \cos \varphi + \mathbf{e}_y \sin \varphi) \cot \theta \frac{\partial}{\partial \varphi}, \] (88)

and taking into account that \( \mathbf{e}_\eta \cdot \mathbf{e}_x = 2^{-1/2} \) and \( \mathbf{e}_\eta \cdot \mathbf{e}_y = i 2^{-1/2} \) (85)-(86) can be written in compact form as

\[ e^{\pm im\varphi} \left( \pm \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \varphi} \right) Y_{lm} = \sqrt{(l \mp m)(l \pm m + 1)} Y_{l,m \pm 1}. \] (89)

V. LEGENDRE’S ADDITION THEOREM.

Maxwell’s integral theorem leads to a very simple derivation of the well known - and physically very useful - Legendre’s addition theorem. In effect, if we restrict \( \mathbf{e}_l \) in (38) to be a real, unit vector then \( H_l(\mathbf{e}_l) = Y_l(\mathbf{e}_l) \) - where \( Y_l \equiv H_l/r^l \) - and, after dividing (38) by \( a^l \), we obtain

\[ \int_{r=a} dS Y_l Z_l = \frac{4\pi (-1)^l l! a^2}{2l + 1} Y_l(\mathbf{e}_l), \] (90)

which must hold for any surface harmonic \( Y_l \). Therefore, if we take any set of \( 2l + 1 \) orthonormal surface harmonics of degree \( l \), \( \{ X_{ln}(\mathbf{r}) : \int d\Omega X_{ln} X_{ln'}^* = \delta_{nn'} (n = 1, ... 2l + 1) \} \), the coefficients in the expansion

\[ Z_l(\mathbf{r}) = \sum_{n=1}^{2l+1} A_n X_{ln}(\mathbf{r}) \] (91)

are given by

\[ A_n = \int d\Omega X_{ln}^* Z_l = \frac{4\pi (-1)^l l!}{2l + 1} X_{ln}^*(\mathbf{e}_l), \] (92)
where we have used (90) with $a = 1$. Thus

$$Z_l(r) = \frac{4\pi(-1)^l l!}{2l + 1} \sum_{n=1}^{2l+1} X_n^l(e_1)X_n(r),$$

and using the relation (35) to express $Z_l = (-1)^l l! P_l(e_1 \cdot e_r)$ we finally obtain the celebrated Legendre’s addition theorem:

$$P_l(e_1 \cdot e_r) = \frac{4\pi}{2l + 1} \sum_{n=1}^{2l+1} X_n^l(e_1)X_n(e_r),$$

where we have taken into account that $X_n^l(r) = X_n^l(e_r)$ since the $X_n^l$’s are surface harmonics. Notice that (94) reproduces the familiar form of the addition theorem\(^{1, 2}\) for the particular case in which the set $X_n^l (n = 0, ..., 2l + 1)$ is chosen to be the set of standard spherical harmonics, $Y_{lm}(r)$ ($m = -l, ..., 0, ..., +l$), introduced in the Section III.

VI. SURFACE HARMONICS EXPANSIONS AND THE COMPLETENESS RELATION.

Let us consider an arbitrarily thin sphere of radius $a$ charged with a given surface charge density distribution $f(\theta, \varphi)$. If $r' = ae_r'$ denotes the generic point on the sphere, the electric potential at any point $r$ of space is

$$\phi(r) = \int_{r' = a} dS' f(\theta', \varphi') \frac{1}{|r - r'|}.$$  

(95)

Inserting the expansion (34) into (95) we obtain

$$\phi(r) = \sum_{l=0}^{\infty} \frac{a^l}{r^{l+1}} \int_{r' = a} dS' P_l(e_r' \cdot e_r) f(\theta', \varphi')$$

(96)

for $r > a$ and, on using the expansion analogous to (34) but with the roles of $r$ and $r'$ interchanged - i.e., the expansion valid for $r < r'$ - we obtain

$$\phi(r) = \sum_{l=0}^{\infty} \frac{r^l}{a^{l+1}} \int_{r' = a} dS' P_l(e_r' \cdot e_r) f(\theta', \varphi')$$

(97)

for $r < a$. Using (96) and (97), the jump condition for the normal derivative of the potential at any point of the surface $r = ae_r(\theta, \varphi)$, $4\pi f(\theta, \varphi) = [-\partial \phi / \partial r]_a^+ - [-\partial \phi / \partial r]_a^-$, writes

$$f(\theta, \varphi) = \sum_{l=0}^{\infty} \frac{2l + 1}{4\pi} \int d\Omega' P_l(e_r' \cdot e_r) f(\theta', \varphi'),$$

(98)
where we have set \( dS' = a^2 d\Omega' \).

Observe that if we replace each \( P_l(e'_r \cdot e_r) \) in the RHS of (98) by its expression as the second term of (35) and carry out the integrals in the primed quantities, we obtain an expansion of \( f(\theta, \varphi) \) in terms of (Maxwell’s) surface harmonics. Therefore, any finite, physically admissible, function defined on the unit sphere admits an expansion in surface harmonics. The completeness of any system of orthonormal surface harmonics of the form \( [X_{ln}(e_r) : l = 0, 1, 2... \text{and } n = 1, 2...2l + 1] \) now follows by combining the results (98) and (94) as

\[
f(\theta, \varphi) = \sum_{l=0}^{\infty} \sum_{n=1}^{\infty} \int d\Omega' f(\theta', \varphi') X^*_{ln}(e'_r) X_{ln}(e_r).
\]

(99)

Since \( d\Omega' = \sin \theta' d\varphi' d\theta' \), equality of both sides in (99) demands the so-called completeness relation:

\[
\frac{\delta(\varphi - \varphi') \delta(\theta - \theta')}{\sin \theta} = \sum_{l=0}^{\infty} \sum_{n=1}^{\infty} X^*_{ln}(e'_r) X_{ln}(e_r).
\]

(100)

If in (99) and (100) we replace the generic \( X_{ln}' \)'s by the standard \( Y_{lm} \)'s we obtain the familiar results

\[
f(\theta, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} A_{lm} Y_{lm}(e_r) \rightarrow A_{lm} = \int d\Omega' f(\theta', \varphi') Y^*_{lm}(e'_r)
\]

(101)

and

\[
\frac{\delta(\varphi - \varphi') \delta(\theta - \theta')}{\sin \theta} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y^*_{lm}(e'_r) Y_{lm}(e_r).
\]

(102)

Note that if \( f \) is independent of \( \varphi \) only the \( A_{lm} \)'s with \( m = 0 \) survive in (101) (since \( Y_{lm} \sim e^{im\varphi} \)), and therefore in this particular case we can write the expansion in terms of Legendre’s polynomials. In effect, using (51) and replacing \( e'_r \) by \( e_z \) in (35), we find that the functions \( Y_{l0} P_l(\cos \theta) \) are proportional:

\[
Y_{l0}(r) = \sqrt{\frac{2l+1}{4\pi}} \frac{(-1)^l r^{l+1}}{l!} \frac{\partial^l}{\partial z^l} \frac{1}{r} = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos \theta),
\]

(103)

equation (101) can be written as

\[
f(\theta) = \sum_{l=0}^{\infty} B_l P_l(\cos \theta) \rightarrow B_l = \frac{2l+1}{2} \int_0^{\pi} d\theta' \sin \theta' f(\theta') P_l(\cos \theta'),
\]

(104)

where we have used the result

\[
\int_0^{\pi} d\theta' \sin \theta' P^2_l(\cos \theta') = \frac{1}{2\pi} \frac{4\pi}{2l+1} \int d\Omega' Y^2_{l0}(e'_r) = \frac{2}{2l+1}.
\]

(105)
As a first illustration of surface harmonics expansions, let us consider the electrostatic field due a point charge $q$ located at a point $\mathbf{R}$ external to an arbitrarily thin conducting sphere of radius $a$ and grounded at zero potential. This problem illustrates well the relation between the method of images\textsuperscript{2} and that of surface harmonics expansions\textsuperscript{18}. The potential at any point $\mathbf{r}$ external to the sphere is

$$\phi(\mathbf{r}) = \frac{q}{|\mathbf{r} - \mathbf{R}|} + \int_{r' = a} dS' \frac{\sigma(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, \quad (106)$$

where $\sigma(\mathbf{r}')$ is the a priori unknown surface charge distribution on the sphere. To determine it, we substitute the expansions $\sigma = \sum_{lm} \sigma_{lm} Y_{lm}(\mathbf{e}_r)$, $|\mathbf{r} - \mathbf{r}'|^{-1} = 4\pi/(2l + 1) \sum_{lm} r'^l/r^{l+1} Y_{lm}(\mathbf{e}_r)Y_{lm}(\mathbf{e}'_r)$ and $|\mathbf{r} - \mathbf{R}|^{-1} = 4\pi/(2l + 1) \sum_{lm} r^l/R^{l+1} Y_{lm}(\mathbf{e}_r)Y_{lm}(\mathbf{e}_R)$ into (106) and carry out the surface integral using the orthogonality properties of the spherical harmonics, which yields:

$$\phi(\mathbf{r}) = \frac{4\pi q}{2l + 1} \sum_{lm} \frac{r^l}{R^{l+1}} Y_{lm}(\mathbf{e}_r)Y_{lm}(\mathbf{e}_R) + \frac{4\pi}{2l + 1} \sum_{lm} \frac{a^{l+2}}{r^{l+1}} \sigma_{lm} Y_{lm}(\mathbf{e}_r). \quad (107)$$

Since $\phi = 0$ at the sphere’s surface, particularizing (107) for $r = a$ we obtain

$$\sigma_{lm} = -\frac{q}{a^2} \left(\frac{a}{R}\right)^{l+1} Y_{lm}(\mathbf{e}_R), \quad (108)$$

and (107) can be written as:

$$\phi(\mathbf{r}) = \frac{q}{|\mathbf{r} - \mathbf{R}|} - \frac{4\pi(a/R)q}{2l + 1} \sum_{lm} \frac{(a^2/R)^l}{r^{l+1}} Y_{lm}(\mathbf{e}_r)Y_{lm}(\mathbf{e}_R) = \frac{q}{|\mathbf{r} - \mathbf{R}|} - \frac{(a/R)q}{|\mathbf{r} - \mathbf{e}_R a^2/R|}, \quad (109)$$

Equation (109) expresses the solution to the original problem for potential at any point external to the sphere as the superposition of those due to $q$ and an image (fictitious) charge of magnitude $(a/R)q$ located inside the sphere at the point $\mathbf{e}_R a^2/R$. Of course, if instead of a point charge we have a charge density distribution $\rho(\mathbf{R})$ within a region $V$ external to the sphere, we must replace $q$ by $\rho(\mathbf{R}) d^3R$ in (109) and integrate over $V$.

As a second illustration, let us compute the electrostatic interaction energy of two charge density distributions $\rho_1$ and $\rho_2$ occupying non-overlapping regions $V_1$ and $V_2$, respectively. Taking two points $O_1$ and $O_2$ within $V_1$ and $V_2$, respectively, and denoting by $\mathbf{r}_1$ ($\mathbf{r}_2$) the position vectors with respect to $O_1$ ($O_2$) of a generic point of $V_1$ ($V_2$), the interaction energy is

$$E = \int_{V_1} \int_{V_2} dV_1 dV_2 \frac{\rho_1(\mathbf{r}_1)\rho_2(\mathbf{r}_2)}{|\mathbf{r} + \mathbf{r}_2 - \mathbf{r}_1|}, \quad (110)$$
where \( \mathbf{r} \) is the position vector of \( O_2 \) with respect to \( O_1 \). Since \( |\mathbf{r}_1| \) and \( |\mathbf{r}_2| \) are less than \( |\mathbf{r}| \) we can expand \( |\mathbf{r} + \mathbf{r}_2 - \mathbf{r}_1|^{-1} \) independently in \( \mathbf{r}_1 \) and in \( \mathbf{r}_2 \) by means of the double Taylor series:

\[
\frac{1}{|\mathbf{r} + \mathbf{r}_2 - \mathbf{r}_1|} = \sum_{l_1 l_2} (-1)^{l_1} r_2^{l_1} \frac{(\mathbf{e}_2 \cdot \nabla)^{l_1}}{l_1!} \frac{(\mathbf{e}_1 \cdot \nabla)^{l_2}}{l_2!} \frac{1}{r}.
\]

(111)

But

\[
\frac{(-1)^{l_1} (\mathbf{e}_1 \cdot \nabla)^{l_1}}{l_1!} \frac{1}{r} = \frac{P_{l_1} (\mathbf{e}_1 \cdot \mathbf{r})}{r^{l_1 + 1}} = \frac{4\pi}{2l_1 + 1} \sum_{m_1 = -l_1}^{l_1} C_{l_1 m_1} Y_{l_1 m_1}^{*}(\mathbf{e}_1) \frac{\partial^{l_1} (1/r)}{\partial z_{l_1 - m_1} \partial \eta^{m_1}},
\]

(112)

where we have used the addition theorem (94) and expressed \( Y_{l_1 m_1}^{*}(\mathbf{e}_r) \) in terms of \( V_{l_1 m_1} \) using (45) and (44). Analogously,

\[
\frac{(-1)^{l_2} (\mathbf{e}_2 \cdot \nabla)^{l_2}}{l_2!} \frac{1}{r} = \frac{4\pi}{2l_2 + 1} \sum_{m_2 = -l_2}^{l_2} C_{l_2 m_2} Y_{l_2 m_2}^{*}(\mathbf{e}_2) \frac{\partial^{l_2} (1/r)}{\partial z_{l_2 - m_2} \partial \eta^{m_2}},
\]

(113)

whence applying the operator \( (\mathbf{e}_2 \cdot \nabla)^{l_2} / l_2! \) to (112) and commuting it with the derivatives in the last term we obtain, on using (113),

\[
\frac{(-1)^{l_1} (\mathbf{e}_2 \cdot \nabla)^{l_2}}{l_2!} \frac{(\mathbf{e}_1 \cdot \nabla)^{l_1}}{l_1!} \frac{1}{r} = \frac{4^2 \pi^2 (-1)^{l_2}}{(2l_2 + 1)(2l_1 + 1)} \sum_{m_2 m_1} C_{l_1 m_1} C_{l_2 m_2} Y_{l_1 m_1}^{*}(\mathbf{e}_1) Y_{l_2 m_2}^{*}(\mathbf{e}_2) \frac{\partial^L (1/r)}{\partial z^{L-M} \partial \eta^M},
\]

(114)

where \( L \equiv l_1 + l_2 \) and \( M \equiv m_1 + m_2 \). If we now substitute (114) into (111) taking into account that \( Y_{LM} = C_{LM} r^{L+1} V_{LM} \) and defining \( A_{LM} \equiv [4^2 \pi^2 (-1)^{l_2} C_{l_1 m_1} C_{l_2 m_2}] / [(2l_2 + 1)(2l_1 + 1) C_{LM}] \), or

\[
A_{LM} = \frac{4^2 \pi^2 (-1)^{l_2}}{(2l_2 + 1)(2l_1 + 1)} \left[ \frac{(2l_2 + 1)(2l_1 + 1)(L + M)!(L - M)!}{(2L + 1)(l_1 + m_1)!(l_1 - m_1)!(l_2 + m_2)!(l_2 - m_2)!} \right]^{1/2},
\]

(115)

we finally obtain

\[
E = \sum_{l_1 l_2 m_1 m_2} \frac{A_{LM}}{r^{L+1}} (\rho_1)_{l_1 m_1} Y_{LM}(\mathbf{e}_r) (\rho_2)_{l_2 m_2},
\]

(116)

where we have defined the multipole moment, \( \rho_{lm} \), of a charge density distribution occupying a region \( V \) as

\[
\rho_{lm} = \int_V dV' r'^n \rho(r') Y_{lm}^*(r').
\]

(117)

Except for a factor of \( \sqrt{4\pi} \), expression (116) was obtained by Schwinger at al.\cite{kn:5} using a different reasoning.
VII. PARTIAL WAVE EXPANSIONS AND HOBSON’S INTEGRAL THEOREM

Partial wave expansions are of fundamental importance in scattering problems in both classical and quantum physics. In this section we consider the expansions in any orthonormal basis of surface or solid harmonics of the function \( e^{q \cdot r} \) - which leads to the partial wave expansion of a plane wave, or Rayleigh’s expansion, and for the translation operator \( e^{q \cdot \nabla} \), where \( q \) is a constant vector. We will see that the latter expansion immediately leads to a proof of Hobson’s integral theorem mentioned in the introduction. Let us first consider the case in which \( q \) is a vector of the form \( a = qe_q \), where \( e_q \) is a real unit vector and the scalar \( q \) may be complex. Then \( q \cdot r = qr \cos \theta \), where \( \cos \theta \equiv e_q \cdot e_r \), and we can use (104) to expand \( e^{a \cdot r} \) in terms of Legendre polynomials in the form

\[
e^{q \cdot r} = \sum_{l=0}^{\infty} f_l(qr) P_l(\cos \theta).
\] (118)

In order to determine the functions \( f_l \) it is first convenient to rewrite (118) using Legendre’s addition theorem (94) as

\[
e^{q \cdot r} = \sum_{l=0}^{\infty} \frac{4\pi f_l(qr)}{2l + 1} \sum_{n=1}^{2l+1} X^*_{ln}(e_q)X_{ln}(e_r),
\] (119)

where the \( X_{ln} \)'s are the members of any given orthonormal basis of surface harmonics of degree \( l \). In terms of the regular solid harmonics \( H_{ln} = r^lX_{ln} \) (119) writes

\[
e^{q \cdot r} = \sum_{l=0}^{\infty} \frac{4\pi f_l(qr)}{2l + 1} \sum_{n=1}^{2l+1} H^*_{ln}(q)H_{ln}(r)
\] (120)

If we multiply (120) by \( H_{ln}(q)d\Omega_q \) and integrate over the unit sphere using (25) and taking into account that \( \int d\Omega_q H_{ln}H_{ln'}^* = q^lq^{l'} \int d\Omega X_{ln}X_{ln'}^* = q^{2l} \delta_{ll'} \delta_{nn'} \) we obtain

\[
\frac{4\pi f_l(qr)}{2l + 1} H_{ln}(r) = 4\pi H_{ln}(r)q^l q^l s_l(qr),
\] (121)

where the function \( s_l \) is defined in (24). Hence (119) takes the form

\[
e^{q \cdot r} = 4\pi \sum_{l=0}^{\infty} q^l q^l s_l(qr) \sum_{n=1}^{2l+1} X^*_{ln}(e_q)X_{ln}(e_r).
\] (122)

In particular, for a plane wave one has \( q = ik \), where \( k \) is a real vector, \( qr = ikr \) and, since \( \sinh(ikr) = i \sin(kr) \), it is customary to rewrite (122) in terms of the spherical Bessel
function of order \( l \) defined as \( j_l(\zeta) \equiv \zeta^l s_l(i\zeta) \) or, using (24),

\[
j_l(\zeta) \equiv (-1)^l \zeta^l \left( \frac{1}{\zeta} \frac{d}{d\zeta} \right)^l \left( \frac{\sin \zeta}{\zeta} \right)
\]  

(123)

Then the expansion (122) yields the well known Rayleigh's expansion for a plane wave:

\[
e^{ikr} = \sum_{l=0}^{\infty} (2l + 1) j_l(kr) P_l(e_k \cdot e_r),
\]

(124)

where we have replaced the sum over \( n \) in (122) using Legendre's theorem (94).

On the other hand, (122) writes in terms of the solid harmonics \( H_{ln} \) as

\[
e^{qr} = 4\pi \sum_{l=0}^{\infty} \sum_{n=1}^{2l+1} H_{ln}^*(q) H_{ln}(r) s_l(q\sqrt{\nabla^2}),
\]

(125)

which is a good starting point to obtain the expansion for the translation operator \( e^{q \nabla} \). In effect, by formally replacing \( r \) in (125) by the operator \( \nabla \) and \( qr = q\sqrt{r \cdot r} \) by \( q\sqrt{\nabla^2} \) (see Section II) we obtain

\[
e^{q \nabla} = 4\pi \sum_{l=0}^{\infty} \sum_{n=1}^{2l+1} H_{ln}^*(q) H_{ln}(\nabla) s_l(q\sqrt{\nabla^2}),
\]

(126)

where we have used the fact that the operators \( H_{ln}(\nabla) \) and \( s_l(q\sqrt{\nabla^2}) \) obviously commute.

As a first illustration of (126), let us consider the expansion of a function of the form \( \phi(|r - r'|) \). If, for concreteness, we assume \( r > r' \), Taylor’s expansion around \( r = 0 \) can be written in the well known form \( \phi(|r - r'|) = e^{-r' \nabla} \phi(r) \), whence

\[
\phi(|r - r'|) = 4\pi \sum_{l=0}^{\infty} \sum_{n=1}^{2l+1} (-1)^l H_{ln}^*(r') \left[ H_{ln}(\nabla) s_l(r'\sqrt{\nabla^2}) \right] \phi(r),
\]

(127)

where we have taken into account that \( H_{ln}^*(r') = (-1)^l H_{ln}^*(r') \) An important particular case of (127) is that of a spherical wave due to a point source located at \( r' \), \( e^{ik|r-r'|/|r-r'|} \), where \( k \) is the wave number. In this case

\[
\nabla^2 \left( \frac{e^{ikr}}{r} \right) = -k^2 \frac{e^{ikr}}{r},
\]

(128)

whence \( s_l(r'\sqrt{\nabla^2}) (e^{ikr}/r) = s_l(r'\sqrt{-k^2}) (e^{ikr}/r) = s_l(ikr') (e^{ikr}/r) \). Thus (127) can be written as

\[
\frac{e^{ik|r-r'|}}{|r-r'|} = 4\pi \sum_{l=0}^{\infty} \sum_{n=1}^{2l+1} (-1)^l s_l(ikr') H_{ln}^*(r') H_{ln}(\nabla) \left( \frac{e^{ikr}}{r} \right)
\]

(129)
or, using \( (20) \),
\[
e^{ik|\mathbf{r}-\mathbf{r}'|} = 4\pi \sum_{l=0}^{\infty} \sum_{n=1}^{2l+1} (-1)^l s_l(ikr') H_{ln}^*(\mathbf{r}') H_{ln}(\mathbf{r}) \left( \frac{1}{r} \frac{d}{dr} \right)^l \left( \frac{e^{ikr}}{r} \right).
\]
(130)

It is customary to write \( (130) \) in terms of the spherical Hankel function of the first kind and of order \( l \) defined as
\[
h_l^{(1)}(\zeta) \equiv \left. \frac{(-1)^l \zeta^l}{i} \left( \frac{d}{d\zeta} \right)^l \left( \frac{e^{i\zeta}}{\zeta} \right) \right|_{\zeta=kr},
\]
(131)
in which case, using the definition \( j_l(\zeta) = k^l r^l s_l(ikr) \), substituting \( H_{ln}^*(\mathbf{r}') H_{ln}(\mathbf{r}) = r^{d-1} r^l X_{ln}^*(\mathbf{e}_r') X_{ln}(\mathbf{e}_r) \) and taking account that for \( r < r' \) an analysis entirely analogous to the one carried out above leads to an expression of the same form as \( (130) \) but with the roles of \( \mathbf{r} \) and \( \mathbf{r}' \) interchanged, the result \( (130) \) can be expressed in the more familiar form
\[
e^{ik|\mathbf{r}-\mathbf{r}'|} = 4\pi i k \sum_{l=0}^{\infty} \sum_{n=2l+1}^{n=2l+1} j_l(\zeta) h_l^{(1)}(\zeta) X_{ln}^*(\mathbf{r}_<) X_{ln}(\mathbf{r}>).
\]
(132)
The result \( (132) \) constitutes the general expression for the expansion of a spherical wave in any basis of orthonormal surface harmonics.

As a second application of \( (126) \) we will provide an apparently new proof of Hobson’s theorem\(^\circ\) for the integral over a sphere of radius \( R \) of the product of a surface harmonic, \( Y_k(\mathbf{r}) \), and any function \( F(\mathbf{r}) \) which is analytic for \( r \leq R \). In effect, by replacing in \( (126) \) vector \( \mathbf{a} \) by \( \mathbf{r} \) and \( a^2 \) by \( R^2 \), Taylor’s expansion around the origin for \( F(\mathbf{r}) \) can be written as,
\[
F(\mathbf{r}) = e^{\mathbf{r} \cdot \nabla_o} F = 4\pi \sum_{l=0}^{\infty} \sum_{n=1}^{2l+1} H_{ln}^*(\mathbf{r}) \left[ H_{ln}(\nabla) s_l(R\sqrt{\nabla^2}) \right]_o F,
\]
(133)
where subscript \( o \) means that the derivatives of \( F \) must be particularized at the origin. Now, if we normalize the surface harmonic \( Y_k \) by dividing it by \( \sqrt{C} \) - where \( C \equiv \int d\Omega Y_k Y_k^* \) - then \( Y_k/\sqrt{C} \) can always be taken as one of the elements of the generic basis \( X_{ln} \), in which case \( r^k Y_k/\sqrt{C} \) replaces one of the \( H_{ln} \) in \( (133) \). The rest of the basis elements could be obtained, for example, via Gram-Schmidt orthogonalization. Therefore, since \( Y_k \) is orthogonal to all solid harmonics in \( (133) \) except to \( H_k/\sqrt{C} \) and \( \int d\Omega Y_k H_k^* = R^{k+2} C \), we obtain
\[
\int_{r=R} d\Omega Y_k F(\mathbf{r}) = 4\pi R^{k+2} \left[ s_k(R\sqrt{\nabla^2}) H_k(\nabla) \right]_o F,
\]
(134)
which is Hobson’s integral theorem.
VIII. THE ROTATION MATRIX FOR THE SPHERICAL HARMONICS.

It is well known\(^\text{22,23}\) that if a given rotation brings the position vector \( \mathbf{r} \) into the vector \( \mathbf{r}' \) - the *image* of \( \mathbf{r} \), then the value at \( \mathbf{r}' \) of any spherical harmonic of degree \( l \), \( Y_{lm}(\mathbf{r}') \), is a linear combination of the values at \( \mathbf{r} \) of all \( 2l + 1 \) spherical harmonics of the set of degree \( l \), i.e. \( Y_{lm}(\mathbf{r}') = \sum_{m=-l}^{l} D_{m'm}^{l} Y_{lm}(\mathbf{r}) \) \((m' = -l, \ldots l)\), where the elements of the rotation matrix, \( D_{m'm}^{l} \), are uniquely determined by the rotation. In this section we will carry out an analysis of the rotational properties of the spherical harmonics based on the invariance under rotations of the scalar product, that is, if \( \mathbf{r}' \) and \( \mathbf{b}' \) are the images of vectors \( \mathbf{r} \) and \( \mathbf{b} \), then \((\mathbf{b} \cdot \mathbf{r})' = (\mathbf{b} \cdot \mathbf{r})'\) or, since \( r = r' \), \((\mathbf{b} \cdot \mathbf{e}_r)' = (\mathbf{b} \cdot \mathbf{e}_r)'\). Thus if \( \mathbf{b} \) is a null vector, so is its image \( \mathbf{b}' \) \((\mathbf{b}^2 = 0)\) and \((\mathbf{b} \cdot \mathbf{r})'\) and \((\mathbf{b}' \cdot \mathbf{r})'\) are solid harmonics whose values at \( \mathbf{e}_r \) and \( \mathbf{e}_r' \) can be expanded in terms of the \( Y_{lm}(\mathbf{e}_r) \) and \( Y_{lm}(\mathbf{e}_r') \) \((m = -l, \ldots l)\), respectively. Then the elements of the rotation matrix are obtained after equating corresponding terms in both expansions.

According to \((101)\) we can write \[
(b \cdot e_r)' = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm}(e_r) \int d\Omega'' (b \cdot e_r'' Y_{lm}^*(e_r''), \tag{135}

\]
where the double prime denotes the generic point on the unit sphere. Since, on the unit sphere \((b \cdot r)' = (b \cdot e_r)'\), the integrals on the RHS of \((135)\) can be computed using Maxwell’s theorem \((37)\) with

\[
a \equiv 1, \quad \Phi \equiv (b \cdot r)' \quad \text{and} \quad Y_l \equiv Y_{lm}^* = \sqrt{\frac{2l+1}{4\pi}} \frac{(-1)^{l+m} 2^m r^{l+1}}{(l+m)! (l-m)!} \frac{\partial (1/r)}{\partial z^{-m} \partial \xi^m} \tag{136}
\]
which yields \[
\int d\Omega'' (b \cdot e_r'' Y_{lm}^*(e_r'')) = \sqrt{\frac{4\pi}{2l+1}} \frac{(-1)^{m+1} 2^m}{(l+m)! (l-m)!} \frac{\partial (b \cdot r)'}{\partial z^{-m} \partial \xi^m} \bigg|_{r=0}. \tag{137}
\]

In order to compute the RHS of \((137)\), we express \( \mathbf{b} \) in the spherical basis, \[
\mathbf{b} = b_\xi \mathbf{e}_\xi + b_\eta \mathbf{e}_\eta + b_z \mathbf{e}_z, \tag{138}
\]
and dot it with \( \mathbf{r} = (\xi \mathbf{e}_\xi + \eta \mathbf{e}_\eta)/\sqrt{2} + z \mathbf{e}_z \), which yields \[
(b \cdot r)' = \left[ (b_\xi \eta + b_\eta \xi) / \sqrt{2} + zb_z \right]' = \sum_{j=0}^{l} \frac{l! 2^{-j/2}}{(l-j)! j!} (b_\xi \eta + b_\eta \xi)^j z^{l-j} b_z^{l-j}. \tag{139}
\]
Thus, since the only term in the binomial expansion of \((\mathbf{b} \cdot \mathbf{r})^l\) which contributes to the derivative in the RHS of (137) is that containing the product \(z^{l-m} \xi^m\) - whose coefficient is readily found from (139) to be \(l! 2^{-m/2} b^m \eta^{l-m}/[(l - m)! m!]\) - we have

\[
\frac{\partial^l (\mathbf{b} \cdot \mathbf{r})^l}{\partial z^{l-m} \partial \xi^m} \bigg|_{r=0} = l! 2^{-m/2} b^m \eta^{l-m} \frac{(l-m)!}{2^{l/2-m} \eta^{(l-m)/2} \eta^{(l+m)/2}},
\]

where we have used the fact that

\[
b^2 = 0 \Rightarrow b_z = i \sqrt{2b^x_b^y} \quad \text{or} \quad \mathbf{b} \cdot \mathbf{e}_z = i \sqrt{2b^x_b^y b \cdot \mathbf{e}_z}.
\]

Substituting (140) into (137) we finally obtain the expansion

\[
(b \cdot r/r)^l = 2^{l/2} i^l l! \sqrt{\frac{4\pi}{2l + 1}} \sum_{m=-l}^{m=l} \frac{i^m b^m \xi^{(l-m)/2} \eta^{(l+m)/2} Y_{lm}(e_r)}{\sqrt{(l + m)! (l - m)!}},
\]

which was introduced by Kramers\(^{15}\) and, later, by Schwinger\(^{18}\) as a generating function for defining the spherical harmonics on the LHS. Here, we have preferred to proceed instead by expanding \((b \cdot r/r)^l\) into the already known [see (11)] \(Y_{lm}\)'s and, then, finding the expansion coefficients using Maxwell’s integral theorem.

The invariance under rotations of (142) makes it a suitable expression to analyze the rotational transformation properties of the spherical harmonics. In effect, let there be given two orthonormal, righthanded sets of vectors, \((\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z = \mathbf{e}_x \times \mathbf{e}_y)\) and \((\mathbf{e'}_x, \mathbf{e'}_y, \mathbf{e'}_z = \mathbf{e'}_x \times \mathbf{e'}_y)\), and consider the rotation about the origin of coordinates defined as that bringing the vector \(\mathbf{e}_x\) into \(\mathbf{e'}_x\) and the vector \(\mathbf{e}_y\) into \(\mathbf{e'}_y\). Then, any vector which rotates rigidly with the unprimed system will be brought by the rotation into another vector - the image - that has the same components with respect to the primed system as has the former with respect to the primed one. Hence if with respect to the spherical basis associated with the unprimed set a vector \(\mathbf{b}\) has components \(b_\xi, b_\eta\) and \(b_z\) and its image, \(\mathbf{b'}\), has components \(b'_\xi, b'_\eta\) and \(b'_z\), we have

\[
\mathbf{b'} = b'_\xi \mathbf{e}_\xi + b'_\eta \mathbf{e}_\eta + b'_z \mathbf{e}_z = b_\xi \mathbf{e}_\xi' + b_\eta \mathbf{e}_\eta' + b_z \mathbf{e}_z',
\]

where \(\mathbf{e'}_\xi, \mathbf{e'}_\eta\) and \(\mathbf{e'}_z\) are the vectors of the spherical basis associated with the primed set. On taking the scalar product of both sides of the last equality in (143) by \(\mathbf{e'}_\eta\) and \(\mathbf{e'}_\xi\), respectively, we obtain

\[
b_\xi = b'_\xi \mathbf{e}_\eta' \cdot \mathbf{e}_\xi + b'_\eta \mathbf{e}_\eta' \cdot \mathbf{e}_\eta + b'_z \mathbf{e}_\eta' \cdot \mathbf{e}_z,
\]

\(26\)
and
\[ b_\eta = b'_\xi e'_\xi \cdot e_\xi + b'_\eta e'_\eta \cdot e_\eta + b'_z e'_z \cdot e_z. \]  
(145)

Now, if \( \mathbf{b} \) is a null vector, so is its image under rotation, \( \mathbf{b}' \), whence
\[ b'_z = i \sqrt{2b'_\xi b'_\eta} \]  
(146)

and, since \( e'_\eta \) and \( e'_\xi \) are null vectors, (141) yields
\[ e'_\eta \cdot e_z = i \sqrt{2} b'_\xi e'_\xi \cdot e_z \]  
(147)

where we have taken different branches for the square root in order to satisfy the condition \( e'_\eta \cdot e_z = (e'_\eta \cdot e_z)^* \). Introducing (146) and (147) into (144) and (145) it is easily seen that the transformation laws for the \( \xi \) and \( \eta \) components of a null vector can be written as the perfect squares
\[ b_\xi = \left( b^{1/2}_\xi \sqrt{e'_\eta \cdot e_\xi} - b^{1/2}_\eta \sqrt{e'_\xi \cdot e_\eta} \right)^2 \]  
(148)

and
\[ b_\eta = \left( b^{1/2}_\xi \sqrt{e'_\xi \cdot e_\xi} + b^{1/2}_\eta \sqrt{e'_\eta \cdot e_\eta} \right)^2. \]  
(149)

Thus, defining the quantities \( s \equiv b^{1/2}_\xi, t \equiv b^{1/2}_\eta, c \equiv \sqrt{e'_\eta \cdot e_\xi} \) and \( d \equiv \sqrt{e'_\xi \cdot e_\xi} \), we can write (148)-(149) more compactly as
\[ s = cs' - dt', \]  
(150)
\[ t = ds' + c^*t'. \]  
(151)

It is easy to show that (150)-(151) is an unitary transformation with unit determinant - i.e. it belongs to the group SU2-, so that the quantities \( b^{1/2}_\xi \) and \( b^{1/2}_\eta \) transform as the components of a two-spinor\(^{13,15}\). In effect, from the definitions of \( c \) and \( d \), and according to (147) we have \( cc^* + dd^* = e'_\xi \cdot e_\eta e'_\eta \cdot e_\xi = e'_\eta \cdot e_z e'_z = \mathbf{I} \cdot e'_\xi = 1 \),
(152)

where
\[ \mathbf{I} = e_x e_x + e_y e_y + e_z e_z = e_\xi e_\xi + e_\eta e_\eta + e_z e_z \]
(153)
is the unit dyadic. Since we assume that no reflections are involved in the transformation of the coordinate system we take the positive root in (153) and obtain \( cc^* + dd^* = 1 \), whence the transformation (150)-(151) is unimodular.

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Now, if the images under the rotation of the null vector \( \mathbf{b} \) and of the position vector \( \mathbf{r} \) are \( \mathbf{b}' \) and \( \mathbf{r}' \), respectively, an expansion analogous to \((132)\) must hold for \((\mathbf{b}' \cdot \mathbf{r}'/r')^l \) where \( b_\xi, b_\eta \) and \( \mathbf{e}_r \) are replaced by \( b'_\xi, b'_\eta \) and \( \mathbf{e}'_r \). Thus, equating both expressions we obtain

\[
\sum_{m'=-l}^l i^{m'} s^{l-m'} t^{l+m'} Y_{lm'}(\mathbf{e}'_r) = \sum_{m=-l}^l i^m s^{l-m} t^{l+m} Y_{lm}(\mathbf{e}_r)
\]

(154)

To find \( Y_{lm'}(\mathbf{e}'_r) \) in terms of the \( Y_{lm}(\mathbf{e}_r) \)'s we just have to substitute the transformation \((150)-(151)\) into the RHS of \((154)\) and, for each \( m \), find the term containing \( s^{l-m'} t^{l+m'} \). The factor multiplying \( s^{l-m'} t^{l+m'} \) in the \( m \)-th summand can be computed as

\[
\frac{1}{(l-m')!(l+m')!} \frac{\partial^{l-m'}}{\partial s^{l-m'} \partial t^{l+m'}} \left[ (cs' - d^* t')^{l-m} (ds' + c^* t')^{l+m} \right]_{(s', t')=(0,0)},
\]

(155)

or, applying Leibnitz rule to the \((l+m')\)-th partial derivative with respect to \( t' \) of the product in \((155)\) and evaluating the result at \( t' = 0 \),

\[
\frac{1}{(l-m')!(l+m')!} \sum_{k=0}^{l+m'} \frac{(l-m)! (l+m)! (-1)^k d^* e^* t^{l+m'-k} e^{l-m-k} d^{m-m'+k} s^{l-m'}}{k! (l+m'-k)! (l-m-k)! (m-m'+k)!},
\]

(156)

with the convention that the factorial of a negative number is infinity. Carrying out now the derivative with respect to \( s' \) in \((156)\) and substituting the result in \((154)\) we readily obtain

\[
Y_{lm'}(\theta', \varphi') = \sum_{m=-l}^l D^l_{m'm}(\mathbf{e}'_\eta,\mathbf{e}_\eta) Y_{lm}(\theta, \varphi),
\]

(157)

where \( (\theta', \varphi') \) and \( (\theta, \varphi) \) are the spherical coordinates of the points \( \mathbf{e}'_\eta \) and \( \mathbf{e}_\eta \), respectively, and we have set

\[
D^l_{m'm}(\mathbf{e}'_\eta,\mathbf{e}_\eta) \equiv i^{m-m'} \sqrt{\frac{(l-m)!(l+m)!}{(l-m')!(l+m')!}} \times \sum_{k=0}^{l+m'} \binom{l-m'}{m-m'+k} \binom{l+m'}{k} (-1)^k d^* e^* t^{l+m'-k} e^{l-m-k} d^{m-m'+k}
\]

(158)

with

\[
c \equiv \sqrt{\mathbf{e}'_\eta \cdot \mathbf{e}_\xi} = \sqrt{\mathbf{e}_\eta \cdot \mathbf{e}_\eta^*}, \quad \text{and} \quad d \equiv \sqrt{\mathbf{e}'_\xi \cdot \mathbf{e}_\xi} = \sqrt{\mathbf{e}_\eta \cdot \mathbf{e}_\eta^*},
\]

(159)

Expression \((158)\) yields the elements of the rotation matrix, \( D^l_{m'm}(\mathbf{e}'_\eta,\mathbf{e}_\eta) \), for the rotation of the coordinate system defined as that bringing the spherical vector \( \mathbf{e}_\eta \) into \( \mathbf{e}'_\eta \) - or, equivalently, the vector \( \mathbf{e}_x \) into \( \mathbf{e}'_x \) and the vector \( \mathbf{e}_y \) into \( \mathbf{e}'_y \). Notice that \((158)-(159)\) are independent of the particular parametrization chosen to describe the rotation, and that \((159)\)
provides with a direct geometrical meaning for parameters \( c \) and \( d \) of the SU2 transformation \( (150)-(151) \). In particular, it is easy to show that for the usual Euler angles employed in Quantum Mechanics\(^{22}\) to parametrize a rotation, namely: a) a rotation by an angle \( \alpha \) around the z-axis, b) a rotation by an angle \( \beta \) around the new y-axis and c) a rotation by an angle \( \gamma \) around the new z-axis, one obtains (by expressing the vectors \([e'_x, e'_y] \) in terms of \([e_x, e_y] \) and the Euler angles)

\[
(e'_{\eta} \cdot e^*_{\eta})^{1/2} = e^{-i(\alpha+\gamma)/2} \cos(\beta/2), \quad (e'^*_{\eta} \cdot e^*_{\eta})^{1/2} = e^{i(\gamma-\alpha)/2} \sin(\beta/2), \tag{160}
\]

and (158) goes into the standard form of the rotation matrix elements\(^{23}\).

Finally, note that we have considered here only the case of rotation matrices of integer rank. However, in the theory of quantum angular momentum\(^{22}\) both integer and half-integer ranks are, of course, of importance. A very complete presentation of compact, parametrization-free representations of finite rotation matrices of arbitrary rank using invariant tensor forms and spinor operators can be found in the works by Manakov et al.\(^{24-26}\), where they also give some applications such as photo-emission by polarized atoms or reduction formulae for some tensor constructions characterizing photoprocesses.

\section*{IX. GAUNT INTEGRALS AND WIGNER COEFFICIENTS.}

In this section we will apply Hobson’s integral theorem \((134)\) to obtain a generating function for integrals of products of three spherical harmonics - the so-called Gaunt integrals\(^{27}\) and provide their expressions in terms of the well known Wigner coefficients\(^{22}\). For this purpose, let us first use \((142)\) to express the regular solid harmonic associated to the spherical harmonic \(Y_{lm}\), \(H_{lm} = r^l Y_{lm}\), as

\[
H_{lm}(r) = \sqrt{\frac{(2l+1)(l+m)!(l-m)!}{4\pi(-1)^l m 2^l l!^2}} \left[ (b \cdot r)^l \right]_{l-m l+m}, \tag{161}
\]

where the subscript on the RHS means the coefficient of \(s^{l-m l+m} \equiv \hat{b}^{(l-m)/2} \hat{b}^{(l+m)/2}\) in the binomial expansion of \((b \cdot r)^l\). Thus we have

\[
\int_{r=R} dSH_{l_{mb} m c} H_{l_{mc} d} = \sqrt{\frac{(2b + 1)(2l_c + 1)(2l_d + 1)\mu_b \mu_c \mu_d \nu_b \nu_c \nu_d}{4\pi(-1)^{M} 2^L l!^2 l!^2}} I_{l_{mc} l_{mc}}, \tag{162}
\]

where

\[
I \equiv \int d\Omega (b \cdot r)^l (c \cdot r)^l (d \cdot r)^l, \tag{163}
\]

29
and, to simplify notation, we have written
\[
\mu \equiv l - m, \quad \nu \equiv l + m, \quad \rho \equiv s^{l-m}l^{l+m},
\]
\[
L \equiv l_b + l_c + l_d \quad \text{and} \quad M \equiv m_b + m_c + m_d.
\tag{164}
\]

In order to compute (163) we apply Hobson’s integral theorem (13) with \( R = 1, Y_k = H_k \equiv (\mathbf{b} \cdot \mathbf{r})^l_b \) and \( F(r) \equiv (\mathbf{c} \cdot \mathbf{r})^{l_c} (\mathbf{d} \cdot \mathbf{r})^{l_d} \), whence
\[
I = 4\pi \left[ s_{l_b}(\sqrt{\nabla^2})(\mathbf{b} \cdot \nabla)^{l_b} \right]_o \left[ (\mathbf{c} \cdot \mathbf{r})^{l_c} (\mathbf{d} \cdot \mathbf{r})^{l_d} \right].
\tag{165}
\]
Since \((\mathbf{c} \cdot \mathbf{r})^{l_c} (\mathbf{d} \cdot \mathbf{r})^{l_d}\) is a homogeneous polynomial of degree \( l_c + l_d \), it is clear that the RHS of (165) vanishes unless \( \lambda_b \equiv l_c + l_d - l_b \) is zero or a positive even integer. Therefore, the only term in the power series (24) for \( S_{l_b}(\nabla^2) \) which contributes to (165) is that containing \( (\nabla^2)^{\lambda_b/2} \), which corresponds to \( j = L/2 \), where \( L \equiv l_c + l_d + l_b \). Thus, taking into account (24), (165) yields
\[
I = \frac{4\pi 2^{l_b}(L/2)!}{(L + 1)! (\lambda_b/2)!} \left[ (\nabla^2)^{\lambda_b/2} (\mathbf{b} \cdot \nabla)^{l_b} \right]_o \left[ (\mathbf{c} \cdot \mathbf{r})^{l_c} (\mathbf{d} \cdot \mathbf{r})^{l_d} \right].
\tag{166}
\]
Now, since \( \nabla^2 (\mathbf{c} \cdot \mathbf{r})^{l_c} = \nabla^2 (\mathbf{d} \cdot \mathbf{r})^{l_d} = 0 \) we have
\[
\nabla^2 \left[ (\mathbf{c} \cdot \mathbf{r})^{l_c} (\mathbf{d} \cdot \mathbf{r})^{l_d} \right] = 2\nabla (\mathbf{c} \cdot \mathbf{r})^{l_c} \cdot \nabla (\mathbf{d} \cdot \mathbf{r})^{l_d} = 2l_c l_d \mathbf{c} \cdot \mathbf{d} (\mathbf{c} \cdot \mathbf{r})^{l_c-1} (\mathbf{d} \cdot \mathbf{r})^{l_d-1},
\tag{167}
\]
and repeating the process \( \lambda_b/2 \) times we easily obtain
\[
(\nabla^2)^{\lambda_b/2} \left[ (\mathbf{c} \cdot \mathbf{r})^{l_c} (\mathbf{d} \cdot \mathbf{r})^{l_d} \right] = \frac{2\lambda_b/2! l_c! l_d! (\mathbf{c} \cdot \mathbf{d})^{\lambda_b/2}}{(\lambda_c/2)! (\lambda_d/2)!} (\mathbf{c} \cdot \mathbf{r})^{\lambda_c/2} (\mathbf{d} \cdot \mathbf{r})^{\lambda_d/2},
\tag{168}
\]
where we have written \( \lambda_c \equiv l_b + l_c - l_d \) and \( \lambda_d \equiv l_b + l_c - l_d \). Thus,
\[
I = \frac{4\pi 2^{L/2}(L/2)! l_c! l_d!}{(L + 1)! (\lambda_b/2)! (\lambda_c/2)! (\lambda_d/2)!} \left[ (\mathbf{b} \cdot \nabla)^{l_b} \right]_o \left[ (\mathbf{c} \cdot \mathbf{r})^{\lambda_c/2} (\mathbf{d} \cdot \mathbf{r})^{\lambda_d/2} \right].
\tag{169}
\]
Also, Leibnitz’s rule yields
\[
(\mathbf{b} \cdot \nabla)^{l_b} \left[ (\mathbf{c} \cdot \mathbf{r})^{\lambda_d/2} (\mathbf{d} \cdot \mathbf{r})^{\lambda_c/2} \right] = \sum_{j=0}^{l_b} \frac{l_b!}{j!(l_b - j)!} \left[ (\mathbf{b} \cdot \nabla)^{j} (\mathbf{c} \cdot \mathbf{r})^{\lambda_d/2} \right] (\mathbf{b} \cdot \nabla)^{l_b-j} (\mathbf{d} \cdot \mathbf{r})^{\lambda_c/2},
\tag{170}
\]
and the only term in the series in the LHS that gives non zero contribution at \( \mathbf{r} = \mathbf{0} \) corresponds to \( j = \lambda_d/2 \), which also makes \( l_b - j = \lambda_c/2 \). Thus
\[
\left[ (\mathbf{b} \cdot \nabla)^{l_b} \right]_o \left[ (\mathbf{c} \cdot \mathbf{r})^{\lambda_d/2} (\mathbf{d} \cdot \mathbf{r})^{\lambda_c/2} \right] = l_b! (\mathbf{b} \cdot \mathbf{c})^{\lambda_d/2} (\mathbf{b} \cdot \mathbf{d})^{\lambda_c/2},
\tag{171}
\]
30
and inserting (171) and (169) into (166) we finally obtain
\[
I = \frac{4\pi^2 L^2 (L/2)! b_c d_c! (c \cdot d)^{\lambda_b/2} (b \cdot c)^{\lambda_d/2} (b \cdot d)^{\lambda_c/2}}{(L + 1)! (\lambda_b/2)! (\lambda_c/2)! (\lambda_d/2)!}. \tag{172}
\]

Notice that (172) vanishes if \( \lambda_b \) is odd or if any of the parameters \( \lambda_b, \lambda_c \) or \( \lambda_d \). Thus, given the values of \( l_c \) and \( l_d \), \( I \neq 0 \) only if the value \( l_b \) is one of the set
\[
l_c + l_d, \quad l_c + l_d - 2, \quad \ldots \quad |l_c - l_d|. \tag{173}
\]

The reader familiar with group theory might have noticed that this set of integers is the same as that in the Clebsch-Gordan series for the decomposition into irreducible representations of the tensor product of two irreducible representations. Also, observe that the foregoing procedure based on Hobson’s integral theorem can be extended, in principle, to compute integrals of products of any number of simple solid harmonics \((b \cdot r)^{l_b}(c \cdot r)^{l_c}(q \cdot r)^{l_q}\) but, of course, the result of applying the operator \([\nabla^2 (l_c + l_q - l_b)/2 (b \cdot \nabla)]_a\) gets more involved as the number of factors increases.

In order to compute \(I_{\rho_c \rho_q \rho_b}\) we must find the coefficient of the term \(s_{b_c}^{\mu_b} t_{b_c}^{\nu_b} s_{c_c}^{\mu_c} t_{c_c}^{\nu_c} s_{d_c}^{\mu_d} t_{d_c}^{\nu_d}\) in the expansion of the product \((c \cdot d)^{\lambda_b/2} (b \cdot c)^{\lambda_d/2} (b \cdot d)^{\lambda_c/2}\) where \(\lambda_b = l_c + l_d - l_b, \lambda_c = l_d + l_b - l_c\) and \(\lambda_d = l_b + l_c - l_d\). Note that if we write \(b = b_\xi e_\xi + b_\eta e_\eta + b_\zeta e_\zeta, \quad s_b \equiv b_\xi^{1/2}, \quad t_b \equiv b_\eta^{1/2}\) and \(b_z \equiv i \sqrt{2} s_b t_b \) (\(b\) null vector), with corresponding definitions for \(s_c, t_c, s_d\) and \(t_d\), we have
\[
b \cdot c = s_b^2 t_c^2 + t_b^2 s_c^2 - 2s_b t_b s_c t_c = (s_b t_c - t_b s_c)^2 \tag{174}
\]
and, analogously,
\[
b \cdot d = (s_b t_d - t_b s_d)^2 \quad \text{and} \quad c \cdot d = (s_c t_d - t_c s_d)^2, \tag{175}
\]
whence
\[
(c \cdot d)^{\lambda_b/2} (b \cdot c)^{\lambda_d/2} (b \cdot d)^{\lambda_c/2} = (s_c t_d - t_c s_d)^{\lambda_b} (s_b t_c - t_b s_c)^{\lambda_d} (s_d t_d - t_d s_d)^{\lambda_c}. \tag{176}
\]

By binomially expanding \((s_b t_c - t_b s_c)^{\lambda_d}\),
\[
(s_b t_c - t_b s_c)^{\lambda_d} = \sum_{j=0}^{\lambda_d} \frac{(-1)^{\lambda_d - j} \lambda_d!}{(\lambda_d - j)! j!} s_b^{\lambda_d - j} t_b^j s_c^{\lambda_d - j}, \tag{177}
\]
we see that the only term in the binomial expansion of \((s_b t_d - t_b s_d)^{\lambda_c}\) which multiplied by \(s_b^{\lambda_d - j}\) in (177) yields \(s_b^{\mu_b} t_{b_c}^{\nu_b}\) or \(p_b\) is that containing \(s_b^{k_b} t_b^{\lambda_b - k}\) with \(k = - j + \mu_b\) which, in
addition, also makes $\lambda_c - k + \lambda_d - j = \lambda_c + \lambda_d - \mu_b = \nu_b$. Therefore,

$$
[(s_b t_d - t_b s_d)_{179}(s_b t_c - t_b s_c)_{180}]_{\mu_b \equiv s_b t_b} = \sum_{j=0}^{\lambda_d} \frac{(-1)^{l_b-m_b} \lambda_d! \lambda_c! \mu_j^{s_c} \lambda_{s_d}^{l_d} \mu_{l_d}^{j} \nu_b + j}{(\lambda_d - j)! j!(\mu_b - j)!(\nu_b - \lambda_d + j)!}. \tag{178}
$$

Also, the term containing $s_c^{k} l_c^{s_d} s_d^{k} \lambda_{s_d}^{l_d}$ with $k = j - \lambda_d + \mu_c$ is the only one in the binomial expansion of $(s_c t_d - t_c s_d)_{180}$ which can yield $s_c^{\mu_c} l_c^{\mu_c} s_d^{\mu_d} t_d^{\mu_d} \equiv \rho_c \rho_d$ when multiplied by $t_c^{\lambda_j} l_c^{\mu_j} s_d^{\lambda_{s_d}^{l_d} \mu_{l_d}^{j} \nu_b + j}$ in (178). It is clear that such a value of $k$ also makes $\lambda_b - k + j = \lambda_b + \lambda_d - \mu_c = \nu_c$ and, since we must also have that $\nu_d = k + \mu_b - j = \mu_b - \lambda_d + \mu_c$, the $m$-indexes must satisfy the condition

$$M = m_b + m_c + m_d = 0. \tag{179}
$$

That relation (179) must be satisfied for (162) to be non vanishing becomes obvious if we express the integral on the LHS in spherical coordinates, since it assures the independence of the azimuthal coordinate of the integrand. Observe that (179) also implies that the exponent of $s_d$ is $\lambda_b - k - \lambda_d + \nu_b + j = \lambda_b + \nu_b - \mu_c = \mu_d$, as it should be. Therefore,

$$
[(c \cdot d)^{\lambda_b/2}(b \cdot c)^{\lambda_d/2}(b \cdot d)^{\lambda_c/2}]_{\rho_c \rho_d \rho_d} = \sum_{j=0}^{\lambda_d} \frac{(-1)^{l_c + l_d + m_b + j} \lambda_b! \lambda_c! \lambda_d!}{j!(\lambda_d - j)!(\mu_b - j)!(\nu_b - \lambda_d + j)!(\mu_c - \lambda_d)!(\nu_c - j)!}. \tag{180}
$$

where the sum in (180) is over all integers $j$ for which the factorials all have nonnegative arguments.Inserting (180) into the RHS of (172) and the later into (162) we finally obtain, after dividing by $R^{L+2}$,

$$
\int d\Omega \frac{H_b m_a Y_{b m_a} Y_{c m_c} Y_{d m_d}}{4\pi} \left( \begin{array}{c} l_b \ l_c \ l_d \\ m_b \ m_c \ m_d \end{array} \right) = \frac{(2l_b + 1)(2l_c + 1)(2l_d + 1)}{(2l_b + 1)(2l_c + 1)(2l_d + 1)} \left( \begin{array}{ccc} l_b & l_c & l_d \\ 0 & 0 & 0 \\ m_b & m_c & m_d \end{array} \right) \tag{181}
$$

where the integral in the LHS vanishes unless

$$m_b + m_c + m_d = 0, \quad l_b + l_c \geq l_d, \quad l_c + l_d \geq l_b \quad \text{and} \quad l_d + l_b \geq l_c, \tag{182}
$$

and we introduced the standard Wigner 3j-symbols defined as

$$
\left( \begin{array}{ccc} l_b & l_c & l_d \\ m_b & m_c & m_d \end{array} \right) \equiv \sum_{j=0}^{\Delta(l_b, l_c, l_d)} \frac{(-1)^{l_b + l_c - m_d} \Delta(l_b, l_c, l_d) \sqrt{\Delta(l_b, l_c, l_d) \mu_b \mu_c \mu_d \nu_b \nu_c \nu_d}}{j!(\lambda_d - j)!(\mu_b - j)!(\nu_b - \lambda_d + j)!(\mu_c - \lambda_d + j)!}. \tag{183}
$$

where

$$\Delta(l_b, l_c, l_d) \equiv \frac{\lambda_b! \lambda_c! \lambda_d!}{(L + 1)!}, \tag{184}
$$

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and

\[
\begin{pmatrix}
l_b & l_c & l_d \\
0 & 0 & 0
\end{pmatrix} = \frac{(-1)^{L/2} \sqrt{\Delta(l_b, l_c, l_d)} (L/2)!}{(\lambda_b/2)! (\lambda_c/2)! (\lambda_d/2)!} \cdot
\]

(185)

X. CONCLUSIONS.

We have presented the coordinate-free approach to spherical harmonics based on the contributions by Maxwell, Thomson and Tait. It has been shown that many results of the theory of spherical harmonics needed in physical applications can straightforwardly and systematically derived from the simple properties of elementary solid harmonics \((\mathbf{b} \cdot \mathbf{r})^l\) (\(\mathbf{b}\) null vector), Maxwell’s harmonics and Maxwell’s integral theorem. In particular, we have provided simple and apparently new proofs of known results such as Maxwell’s integral theorem and Legendre’s addition theorem, the latter being obtained in terms of a general basis of orthonormal surface harmonics. Also, it has been shown how the derivation of recursions relations can be made simpler and more systematic using Maxwell’s solid \(V_l\)-harmonics than - as is conventionally done - using surface harmonics and spherical coordinates. Surface harmonics expansion have been discussed and their relation with the method of images illustrated and, also, they have been used to efficiently compute the interaction energy of non-overlapping charge distributions. We have reviewed in a unified manner partial wave expansions and provided a seemingly new proof of Hobson’s integral theorem. A procedure based on compact vector methods has been given to express the elements of the rotation matrix in a form which is independent of the parametrization of the rotation. Finally, we have shown how Hobson’s integral theorem can be used to find integrals involving products of three (or more) spherical harmonics.

Appendix A: Derivation of the expression for \(Y_{lm}\) in spherical coordinates.

The \(V_l\)-harmonic \(V_{lm}\) defined by (44) can be easily expressed in spherical coordinates through the familiar Legendre polynomials as follows. First, consider the well known Legendre’s expansion

\[
\frac{1}{\sqrt{1 - 2s\mu + s^2}} = \sum_{j=0}^{\infty} s^j P_j(\mu),
\]

(A1)
where \( P_j(\mu) \) is the Legendre polynomial of degree \( j \),

\[
P_j(\mu) = \frac{1}{2^j j!} \frac{d^j}{d\mu^j} (\mu^2 - 1)^j.
\] (A2)

Taking \( m \) times the derivative with respect to \( \mu \) in both sides of (A1) we get

\[
\frac{1}{(1 - 2s\mu + s^2)^{m+1/2}} = \frac{1}{(2m + 1)!!} \sum_{j=m}^{\infty} s^{j-m} \frac{d^m P_j}{d\mu^m} = \frac{1}{(2m + 1)!!} \sum_{j=0}^{\infty} s^{j} \frac{d^m P_{j+m}}{d\mu^m},
\] (A3)

where we have taken into account that \( \frac{d^m P_j}{d\mu^m} = 0 \) for \( j < m \). Making \( s = h/r \) and \( \mu = z/r = e_z \cdot r/r \), with \( r = (x^2 + y^2 + z^2)^{1/2} \), we can write (A3) as

\[
\frac{1}{[x^2 + y^2 + (z - h)^2]^{m+1/2}} = \frac{r^{-2m}}{(2m + 1)!!} \sum_{j=0}^{\infty} \frac{h^j}{r^{j+1}} \frac{d^m P_{j+m}}{d\mu^m},
\] (A4)

Now, it is readily seen that we can compute \( \partial^{l-m} (1/r^{2m+1})/\partial z^{l-m} \) as \((-1)^{l-m}\) times the \((l-m)\)-th derivative of (A4) with respect to \( h \) evaluated at \( h = 0 \), or

\[
\frac{\partial^{l-m}}{\partial z^{l-m}} \frac{1}{r^{2m+1}} = (-1)^{l-m} \frac{(l-m)!}{(2m + 1)!!} r^{-(l+m+1)} \frac{d^m P_l}{d\mu^m}.
\] (A5)

Therefore,

\[
V_{lm}(r) = \frac{(-1)^l(l-m)!}{2^{m+l+m+1}} \xi^m \frac{d^m P_l}{d\mu^m} = \frac{(-1)^l(l-m)!}{2^{m+l+1}} \sin^m \theta e^{im\phi} \frac{d^m P_l}{d\mu^m}.
\] (A6)

Substituting (A6) into (51) and using (A2) we obtain the familiar\(^{1,2,8}\) expression for \( Y_{lm} \)

\[
Y_{lm}(r) = \sqrt{\frac{2l+1}{4\pi}} \sqrt{\frac{(l-m)!}{(l+m)!}} (-1)^m \frac{1}{2^l l!} \sin^m \theta e^{im\phi} \frac{d^m P_l}{d\mu^m},
\] (A7)

which is valid also for \( m < 0 \).

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