MATH OF MULTIPOLE EXPANSION

While explaining the electrical multipole expansion in class, I have used two mathematical theorems:

- **Theorem 1:** for any 2 unit vectors $\mathbf{n}_x$ and $\mathbf{n}_y$,

$$\sum_{m=-\ell}^{+\ell} Y_{\ell,m}(\mathbf{n}_x) Y^*_{\ell,m}(\mathbf{n}_y) \;=\; \frac{2\ell+1}{4\pi}\,P_\ell(\mathbf{n}_x\cdot\mathbf{n}_y) \tag{1}$$

  where P_ℓ is the Legendre polynomial of degree ℓ.

- **Theorem 2:** for any vectors $\mathbf{x}$ and $\mathbf{y}$ such that $|\mathbf{x}|>|\mathbf{y}|$,

$$\frac{1}{|\mathbf{x}-\mathbf{y}|} \;=\; \sum_{\ell=0}^{\infty} \frac{|\mathbf{y}|^\ell}{|\mathbf{x}|^{\ell+1}}\,P_\ell(\mathbf{n}_x\cdot\mathbf{n}_y) \tag{2}$$

  where $\mathbf{n}_x=\mathbf{x}/|\mathbf{n}_x|$ and $\mathbf{n}_y=\mathbf{y}/|\mathbf{y}|$ are unit vectors in the directions of $\mathbf{x}$ and $\mathbf{y}$.

In this note I shall prove these two theorems.

Proving Theorem 1.

I am going to prove the Theorem 1 in two stages. First, let me prove the **Lemma:** *the sum on the LHS of eq.* (1) *depends only on the angle* $\Theta=\arccos(\mathbf{n}_c\cdot\mathbf{n}_y)$ *between the unit vectors* $\mathbf{x}$ *and* $\mathbf{y}$. And then I shall evaluate the sum (1)using this Lemma.

The simplest proof of the Lemma uses quantum-mechanical language in the Hilbert space of wave-functions for a particle living on a sphere. In this Hilbert space, the states of definite location $|\theta,\phi\rangle$ are labeled by the 2 coordinate on the sphere — or equivalently by the unit vectors $|\mathbf{n}\rangle$, — while the spherical harmonics $Y_{\ell,m}(\mathbf{n})\equiv Y_{\ell,m}(\theta,\phi)$ are the wave-functions of the angular momentum eigenstates $|\ell,m\rangle$. In Dirac's bracket notations,

$$Y_{\ell,m}(\mathbf{n}) \;=\; \langle\mathbf{n}|\ell,m\rangle\,. \tag{3}$$

Consequently, the sum on the LHS of eq. (1) amounts to

$$S_\ell(\mathbf{n},\mathbf{y}) \;\stackrel{\text{def}}{=}\; \sum_{m=-\ell}^{+\ell} Y_{\ell,m}(\mathbf{n}_x) Y^*_{\ell,m}(\mathbf{n}_y) \;=\; \sum_m \langle\mathbf{n}_x|\ell,m\rangle\,\langle\ell,m|\mathbf{n}_y\rangle\,, \tag{4}$$

which we may further identify as a matrix element

$$S_\ell(\mathbf{n},\mathbf{y}) \;=\; \langle\mathbf{n}_x|\,\hat{\Pi}_\ell\,|\mathbf{n}_y\rangle \tag{5}$$

of the hermitian operator

$$\hat{\Pi}_\ell \;=\; \sum_{m=-\ell}^{+\ell} |\ell,m\rangle\,\langle\ell,m|\;. \tag{6}$$

By construction, this operators is a function of the $\hat{\mathbf{L}}^2$ operator. Indeed, knowing the spectrum and all the eigenstates of the $\hat{\mathbf{L}}^2$ operator, we may construct functions of that operator as

$$F(\hat{\mathbf{L}}^2) \;=\; \sum_\ell F(\hbar^2\ell(\ell+1))\sum_m |\ell,m\rangle\,\langle\ell,m|\;. \tag{7}$$

Moreover, the function $F(x)$ does not have to be well-defined for all x but only for x belonging to the spectrum of the $\hat{\mathbf{L}}^2$. In particular, for

$$F_{\tilde{\ell}}(x) \;=\; \begin{cases} 1 & \text{for } x=\hbar^2\tilde{\ell}(\tilde{\ell}+1), \\ 0 & \text{otherwise,} \end{cases} \tag{8}$$

we get

$$F_{\tilde{\ell}}(\hat{\mathbf{L}}^2) \;=\; \sum_\ell \delta_{\ell,\tilde{\ell}}\sum_m |\ell,m\rangle\,\langle\ell,m| \;=\; \sum_m \left|\tilde{\ell},m\right\rangle\left\langle\tilde{\ell},m\right| \;=\; \hat{\Pi}_{\tilde{\ell}}\,. \tag{9}$$

The point of this exercise is that $\hat{\mathbf{L}}^2$ is a scalar operator, so all functions of it — like the $\hat{\Pi}_\ell$ operators — are also scalar operators. That is, for any 3D rotation R of the sphere in question, the $\hat{\mathbf{L}}^2$ and all the $\hat{\Pi}_\ell$ operators commute with the unitary operator $\hat{\mathcal{R}}$ representing this rotation in the Hilbert space, thus

$$\hat{\mathcal{R}}^{-1}\hat{\Pi}_\ell\hat{\mathcal{R}} \;=\; \hat{\mathcal{R}}^{-1}\hat{\mathcal{R}}\hat{\Pi}_\ell \;=\; \hat{\Pi}_\ell\,. \tag{10}$$

Now consider the matrix elements of these scalar operators. Let's simultaneously rotate

$$R:\mathbf{n}_x\,to\,\mathbf{n}'_x\,,\quad R:\mathbf{n}_y\;\to\;\mathbf{n}'_y\quad\text{for the same 3D rotation } R, \tag{11}$$

then in the Hilbert space

$$\left|\mathbf{n}'_x\right\rangle \;=\; \hat{\mathcal{R}}\left|\mathbf{n}_x\right\rangle, \qquad \left|\mathbf{n}'_y\right\rangle \;=\; \hat{\mathcal{R}}\left|\mathbf{n}_y\right\rangle, \tag{12}$$

hence

$$\left\langle\mathbf{n}'_x\right| \;=\; \left\langle\mathbf{n}_x\right|\hat{\mathcal{R}}^\dagger \;=\; \left\langle\mathbf{n}_x\right|\hat{\mathcal{R}}^{-1}, \tag{13}$$

and therefore

$$\left\langle\mathbf{n}'_x\right|\hat{\Pi}_\ell\left|\mathbf{n}'_y\right\rangle \;=\; \left\langle\mathbf{n}_x\right|\hat{\mathcal{R}}^{-1}\hat{\Pi}_\ell\hat{\mathcal{R}}\left|\mathbf{n}_y\right\rangle \;=\; \left\langle\mathbf{n}_x\right|\hat{\Pi}_\ell\left|\mathbf{n}_y\right\rangle, \tag{14}$$

where the second equality follows from eq. (10).

Going back to eq. (5), eq. (14) for the matrix elements means

$$S_\ell(\mathbf{n}'_x,\mathbf{n}'_y) \;=\; S_\ell(\mathbf{n}_x,\mathbf{n}_y) \tag{15}$$

for any simultaneous rotation (11). But the only independent combination of the two unit vector that is invariant under their simultaneous rotations is the angle Θ between the two vectors, or equivalently $\cos\Theta = \mathbf{n}_x\cdot\mathbf{n}_y$. Consequently, any other rotationally-invariant function of the two unit vectors must be a function of this angle Θ, thus

$$S_\ell(\mathbf{n}_x,\mathbf{n}_y) \;=\; f_\ell(\Theta) \quad \text{for some function } f_\ell\,. \tag{16}$$

And since the $S_\ell(\mathbf{n}_x,\mathbf{n}_y)$ in this formula was defined in eq. (4) as the $\sum_m$ over spherical harmonic products on the LHS of eq. (1), we have proved that that sum must be a function of the angle Θ between the two unit vectors,

$$\sum_{m=-\ell}^{+\ell} Y_{\ell,m}(\mathbf{n}_x)Y^*_{\ell,m}(\mathbf{n}_y) \;=\; f_\ell(\Theta) \quad \text{for some function } f_\ell\,. \tag{17}$$

This completes the proof of the Lemma.

Given the Lemma, to complete the proof of the Theorem 1 we must evaluate the functions $f_\ell(\Theta)$ in eq. (17). So let's pick a very special direction of the unit vector $\mathbf{y}$, namely the North pole at $\theta_y = 0$. Consequently for the $\mathbf{n}_x$ pointing in some general direction with latitude θ_x and longitude ϕ_x, the angle between $\mathbf{n}_x$ and $\mathbf{n}_y$ is simply the latitude of the latter, $\Theta = \theta_x$. In terms of eq. (17), this means

$$f_\ell(\Theta) \;=\; \sum_m Y_{\ell,m}(\theta_x = \Theta, \text{any}\,\phi) \times Y^*_{\ell,m}(\theta_y = 0). \tag{18}$$

To evaluate the sum here, we use the general form of the spherical harmonics as functions of θ and ϕ:

$$Y_{\ell,m}(\theta,\phi) \;=\; \text{coefficient} \times \text{polynomial}(\cos\theta) \times (\sin\theta)^{|m|} \times e^{im\phi}. \tag{19}$$

In particular, all spherical harmonics with $m \neq 0$ vanish for $\theta = 0$, so the $Y^*_{\ell,m}(\theta_y = 0)$ factor in the sum (18) kills all the terms with $m \neq 0$. The only non-vanishing term is the $m = 0$ term, thus

$$f_\ell(\Theta) \;=\; Y_{\ell,0}(\theta_x = \Theta) \times Y^*_{\ell,0}(\theta_y = 0). \tag{20}$$

Next, for $m = 0$ the spherical harmonics are independent on the longitude ϕ while their dependence on the latitude θ is proportional to the Legendre polynomial (with same ℓ) of $\cos\theta$; specifically,

$$Y_{\ell,m}(\theta,\phi) \;=\; \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta). \tag{21}$$

Plugging this formula into eq. (20), we arrive at

$$f_\ell(\Theta) \;=\; \frac{2\ell+1}{4\pi} \times P_\ell(\cos\Theta) \times P_\ell(\cos 0). \tag{22}$$

Finally, the Legendre polynomials are normalized to $P_\ell(1) = 1$, thus $P_\ell(\cos 0) = 1$, so eq. (22) simplifies to

$$f_\ell(\Theta) \;=\; \frac{2\ell+1}{4\pi} \times P_\ell(\cos\Theta) \tag{23}$$

Now that we have calculated the functions $f_\ell(\Theta)$ using the special direction of the $\mathbf{n}_y$ vector, we may use the Lemma to apply it to all directions of the $\mathbf{n}_y$ and the $\mathbf{n}_x$. For such general directions, the Θ in eq. (17) is the angle between the $\mathbf{n}_x$ and the $\mathbf{n}_y$, hence $\cos\Theta = \mathbf{n}_x \cdot \mathbf{n}_y$ and therefore

$$\sum_{m=-\ell}^{+\ell} Y_{\ell,m}(\mathbf{n}_x) Y^*_{\ell,m}(\mathbf{n}_y) \;=\; \frac{2\ell+1}{4\pi} \times P_\ell(\mathbf{n}_x \cdot \mathbf{n}_y). \tag{24}$$

And this completes the proof of the Theorem 1.

Proving Theorem 2.

To prove Theorem 2 I am going to use integrals over contours in the complex plane and the residue methods for calculating such integrals. If you are not familiar with this kind of complex analysis, I suggest you learn it ASAP as its used in pretty much any kind of Physics. I know the Math department has an undergraduate class on functions of complex variables, and there are plenty of textbooks on the subject. For a quick-and-dirty overview (few proofs but many examples and useful formulae), I suggest *Complex Variables* in the *Schaum Outlines* series by Spiegel, Lipschutz, Schiller, and Spellman; the PMA library has a few copies.

Let me start the proof with the Rodriguez formula for the Legendre polynomials:

$$P_\ell(c) \;=\; \frac{1}{2^\ell\,\ell!}\,\frac{d^\ell}{dc^\ell}\big((c^2-1)^\ell\big)^\ell. \tag{25}$$

The ℓ^{th} derivative here can be identified as the residue

$$\text{Residue}\left[\frac{(z^2-1)^\ell}{(z-c)^\ell+1}\right]_{@z=c} \;=\; \frac{1}{\ell!}\,\frac{d^\ell}{dc^\ell}\big((c^2-1)^\ell\big)^\ell \tag{26}$$

and hence as a contour integral in the complex plane

$$\oint\limits_\Gamma \frac{dz}{2\pi i}\,\frac{(z^2-1)^\ell}{(z-c)^\ell+1} \;=\; \text{Residue}\left[\frac{(z^2-1)^\ell}{(z-c)^\ell+1}\right]_{@z=c} \;=\; \frac{1}{\ell!}\,\frac{d^\ell}{dc^\ell}\big((c^2-1)^\ell\big)^\ell, \tag{27}$$

provided the contour Γ circles in the complex plane around the point c. For our purposes, we are interested in $P_\ell(c)$ for $c = \cos\Theta$ hence $-1 \le c \le +1$, so to circle all such points (but not much more than that) let Γ be the circle of radius just a tiny bit larger than 1 and centered at 0. For this choice of a contour, we have

$$P_\ell(c) = \frac{1}{2^\ell} \oint\limits_\Gamma \frac{dz}{2\pi i} \frac{(z^2-1)^\ell}{(z-c)^\ell+1} \quad \forall c \text{ with } |c| \leq 1. \tag{28}$$

Given this integral formula for the Legendre polynomials, let's sum the series

$$I = \sum_{\ell=0}^{\infty} t^\ell \times P_\ell(c). \tag{29}$$

Note that for real c between -1 and $+1$ — which assures $|P_\ell(c)| \leq 1$ — and t with $|t| < 1$, this series converges absolutely. Also, the countour integrals (28) for the Legendre polynomials converge absolutely, so once we plug them into the series (29), we are allowed to change the order of summation and integration. Thus,

$$\begin{aligned} I &= \sum_{\ell=0}^{\infty} \frac{t^\ell}{2^\ell} \times \oint\limits_\Gamma \frac{dz}{2\pi i} \frac{(z^2-1)^\ell}{(z-c)^\ell+1} \\ &= \oint\limits_\Gamma \frac{dz}{2\pi i} \sum_{\ell=0}^{\infty} \frac{t^\ell}{2^\ell} \times \frac{(z^2-1)^\ell}{(z-c)^\ell+1} \end{aligned} \tag{30}$$

where

$$\begin{aligned} \sum_{\ell=0}^{\infty} \frac{t^\ell}{2^\ell} \times \frac{(z^2-1)^\ell}{(z-c)^\ell+1} &= \frac{1}{z-c} \sum_{\ell=0}^{\infty} \left(\frac{t(z^2-1)}{2(z-c)} \right)^\ell \\ &= \frac{1}{z-c} \times \left[1 - \frac{t(z^2-1)}{2(z-c)} \right]^{-1} \\ &= \frac{2}{2(z-c) - t(z^2-1)}, \end{aligned} \tag{31}$$

hence

$$I = \oint\limits_\Gamma \frac{dz}{2\pi i} \frac{2}{2(z-c) - t(z^2-1)}. \tag{32}$$

Now let's rewrite the quadratic polynomial in the denominator here as

$$2(z-c)\;-\;t(z^2-1)\;=\;\frac{-1}{t}\left(z^2\,-\,\frac{2}{t}\,z\,+\,\frac{2c}{t}\,-\,1\right)\;=\;\frac{-1}{t}\,(z-z_1)(z-z_2) \tag{33}$$

where z_1 and z_2 are the roots of this polynomial,

$$z_{1,2}\;=\;\frac{1}{t}\;\pm\;\sqrt{\frac{1}{t^2}\,-\,\frac{2c}{t}\,+\,1}\;=\;\frac{1\pm\sqrt{1-2tc+t^2}}{t} \tag{34}$$

Consequently,

$$I\;=\;\frac{-2}{t}\oint\limits_{\Gamma}\frac{dz}{2\pi i}\,\frac{1}{(z-z_1)(z-z_2)}\,, \tag{35}$$

and we may easily evaluate this integral by the residue method. The integrand here has two simple poles at z_1 and at z_2 and there are no other singularities, so all we need to know is whether each pole lies inside our outside the integration contour Γ.

Let's focus on real c between -1 and $+1$ and real t strictly between 0 and 1. In this case, $(1-2tc+t^2)>0$, so both roots z_1 and z_2 are real; moreover

$$|z_2|\;\le\;1\quad\text{while } z_1\;>\;1. \tag{36}$$

Indeed, for $-1\le c\le+1$ we have

$$(1-t)^2\;\le\;1\,-\,2ct\,+\,t^2\;\le\;(1+t)^2\quad\Longrightarrow\quad 1\,-\,t\;\le\;\sqrt{1-2ct+t^2}\;\le\;1\,+\,t, \tag{37}$$

hence

$$z_1\;=\;\frac{1+\sqrt{1-2ct+t^2}}{t}\;\ge\;\frac{1+1-t}{t}\;>\;1\quad\text{for } t<1 \tag{38}$$

while

$$-1\;=\;\frac{1-(1+t)}{t}\;\le\;z_2\;=\;\frac{1-\sqrt{1-2ct+t^2}}{t}\;\le\;\frac{1-(1-t)}{t}\;=\;+1. \tag{39}$$

Consequently, for the contour Γ being the unit circle (or just a tiny bit larger than that) we have z_2 lying inside Γ while z_1 lies outside Γ.

Therefore, the integral in eq. (35) obtains from the residue of the integrand at the z_2 pole inside the integration contour, while the residue at the other pole z_1 does not contribute since it lies outside the contour. Thus,

$$\oint\limits_{\Gamma} \frac{dz}{2\pi i} \frac{1}{(z-z_1)(z-z_2)} = \text{Residue}\left[\frac{1}{(z-z_1)(z-z_2)}\right]_{@z=z_2} \\ = \left[\frac{1}{z-z_1}\right]_{@z=z_2} = \frac{1}{z_2-z_1} \\ = \frac{-t}{2\sqrt{1-2ct+t^2}} \tag{40}$$

and consequently

$$I = \frac{1}{\sqrt{1-2ct+t^2}}. \tag{41}$$

This completes our summing up the series (29). To summarize,

$$\sum_{\ell=0}^{\infty} t^\ell \times P_\ell(c) = \frac{1}{\sqrt{1-2ct+t^2}}. \tag{42}$$

Finally, let's relate the abstract variables t and c in eq. (42) to the two radius-vectors $\mathbf{x}$ and $\mathbf{y}$:

$$c = \mathbf{n}_x \cdot \mathbf{n}_y = \cos(\text{angle between } \mathbf{x} \text{ and } \mathbf{y}), \tag{43}$$

$$t = \frac{r_y = |\mathbf{y}|}{r_x = |\mathbf{x}|}, \tag{44}$$

where we assume $r_y < r_x$ and hence $t < 1$. In terms of $\mathbf{x}$ and $\mathbf{y}$,

$$1 - 2ct + t^2 = \frac{r_x^2 - 2cr_xr_y + r_y^2}{r_x^2} = \frac{|\mathbf{x}-\mathbf{y}|^2}{r_x^2}, \tag{45}$$

so the RHS of eq. (42) is

$$\frac{1}{\sqrt{1-2ct+t^2}} = \frac{r_x}{|\mathbf{x}-\mathbf{y}|}, \tag{46}$$

while the LHS amounts to

$$\sum_{\ell=0}^{\infty} t^{\ell} \times P_{\ell}(c) \;=\; \sum_{\ell=0}^{\infty} \frac{r_y^{\ell}}{r_x^{\ell}} \times P_{\ell}(\mathbf{n}_x \cdot \mathbf{n}_y). \tag{47}$$

Hence, dividing both sides of eq. (42) by the r_x and swapping the two sides gives us

$$\frac{1}{|\mathbf{x} - \mathbf{y}|} \;=\; \sum_{\ell=0}^{\infty} \frac{r_y^{\ell}}{r_x^{\ell+1}} \times P_{\ell}(\mathbf{n}_x \cdot \mathbf{n}_y). \tag{48}$$

And this completes the proof of the Theorem 2.