Project (2021 summer)

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A. Angular Momentum Operator in Spherical Coordinates

The angular momentum of an object is,

$$\mathbf{L} = \boldsymbol{r} \times \boldsymbol{p} \tag{1}$$

Whereas in terms of operators, $\boldsymbol{r}, \boldsymbol{p}$ are the position operator and momentum operator expressed in spherical coordinates as,

$$\boldsymbol{r} = r\hat{\boldsymbol{r}} \tag{2}$$

$$\boldsymbol{p} = -i\hbar\nabla = -i\hbar\left(\hat{\boldsymbol{r}}\frac{\partial}{\partial r} + \hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\boldsymbol{\phi}}\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\right) \tag{3}$$

Note: Eq.(3) is a result of $p_x = -i\hbar\frac{\partial}{\partial x}, \quad p_y = -i\hbar\frac{\partial}{\partial y}, \quad p_z = -i\hbar\frac{\partial}{\partial z}$. Hence,

$$\mathbf{L} = \boldsymbol{r} \times \boldsymbol{p} = \boldsymbol{r} \times (-i\hbar\nabla) = -i\hbar(\boldsymbol{r} \times \nabla) \tag{4}$$

With Eqs.(2),(3) in hand, we now express $\mathbf{L}$ in spherical coordinates as follows,

$$\mathbf{L} = -i\hbar(\boldsymbol{r} \times \nabla) = -i\hbar\begin{vmatrix} \hat{\boldsymbol{r}} & \hat{\boldsymbol{\theta}} & \hat{\boldsymbol{\phi}} \\ r & 0 & 0 \\ \frac{\partial}{\partial r} & \frac{1}{r}\frac{\partial}{\partial\theta} & \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi} \end{vmatrix} = i\hbar\left(\frac{\hat{\boldsymbol{\theta}}}{\sin\theta}\frac{\partial}{\partial\phi} - \hat{\boldsymbol{\phi}}\frac{\partial}{\partial\theta}\right) \tag{5}$$

Using the relations,

$$\hat{\boldsymbol{\theta}} = (\cos\theta\cos\phi)\hat{\boldsymbol{x}} + (\cos\theta\sin\phi)\hat{\boldsymbol{y}} - \sin\theta\hat{\boldsymbol{z}} \tag{6}$$

$$\hat{\boldsymbol{\phi}} = -\sin\phi\hat{\boldsymbol{x}} + \cos\phi\hat{\boldsymbol{y}} \tag{7}$$

$\mathbf{L}$ can be expressed in Cartesian Coordinates as,

$$\mathbf{L} = i\hbar\left((\cos\phi\cot\theta\frac{\partial}{\partial\phi} + \sin\phi\frac{\partial}{\partial\theta})\hat{\boldsymbol{x}} + (\sin\phi\cot\theta\frac{\partial}{\partial\phi} - \cos\phi\frac{\partial}{\partial\theta})\hat{\boldsymbol{y}} - (\frac{\partial}{\partial\phi})\hat{\boldsymbol{z}}\right) \tag{8}$$

Then the three components of $\mathbf{L}$ are,

$$L_x = i\hbar\left(\cos\phi\cot\theta\frac{\partial}{\partial\phi} + \sin\phi\frac{\partial}{\partial\theta}\right) \tag{9}$$

$$L_y = i\hbar\left(\sin\phi\cot\theta\frac{\partial}{\partial\phi} - \cos\phi\frac{\partial}{\partial\theta}\right) \tag{10}$$

$$L_z = -i\hbar\frac{\partial}{\partial\phi} \tag{11}$$

Since raising and lowering operators are $L_\pm = L_x \pm iL_y$, it follows that,

$$L_\pm = \hbar\left(\cot\theta(\mp\sin\phi + i\cos\phi)\frac{\partial}{\partial\phi} + (\pm\cos\phi + i\sin\phi)\frac{\partial}{\partial\theta}\right) \tag{12}$$

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with the Euler's Equation $e^{\pm i\phi} = \cos\phi \pm i\sin\phi$ and some manipulations on $\pm$ sign, the above is simplified as,

$$L_\pm = \hbar\left(i\cot\theta(\pm\sin\phi+\cos\phi)\frac{\partial}{\partial\phi} \pm (\cos\phi \pm i\sin\phi)\frac{\partial}{\partial\theta}\right) \tag{13}$$

$$L_\pm = \hbar e^{\pm i\phi}\left(i\cot\theta\frac{\partial}{\partial\phi} \pm \frac{\partial}{\partial\theta}\right) \tag{14}$$

There are several ways of computing L^2 in spherical coordinates. The following briefly introduce one way, and elaborate another way in particular. The key here is to apply each operator twice.

Since $L^2 \equiv {L_x}^2 + {L_y}^2 + {L_z}^2$, With Eqs.(9),(10),(11), L^2 can be found. The calculation might be complex, but fortunately it can be simplified by previously derived $L_\pm$ as follows[1, Eq. 4.112],

$$\begin{aligned} L_+L_- &= (L_x + iL_y)(L_x - iL_y) = {L_x}^2 + {L_y}^2 + i(L_yL_x - L_xL_y) \\ &= L^2 - {L_z}^2 + \hbar L_z \end{aligned} \tag{15}$$

So,

$$L^2 = L_+L_- + {L_z}^2 - \hbar L_z \tag{16}$$

Thus the calculation of L^2 becomes more hassle-free with what has been done above.

Now we illustrate a straightforward calculation from the beginning (Eq.5). L^2 can be treated as applying the operator $\mathbf{L}$ on a function twice.

$$L^2 \equiv \mathbf{L}\cdot\mathbf{L} = -\hbar^2\left(\frac{\hat{\boldsymbol{\theta}}}{\sin\theta}\frac{\partial}{\partial\phi} - \hat{\boldsymbol{\phi}}\frac{\partial}{\partial\theta}\right)\cdot\left(\frac{\hat{\boldsymbol{\theta}}}{\sin\theta}\frac{\partial}{\partial\phi} - \hat{\boldsymbol{\phi}}\frac{\partial}{\partial\theta}\right) \tag{17}$$

$$= -\hbar^2\left[\frac{\hat{\boldsymbol{\theta}}}{\sin\theta}\cdot\frac{\partial}{\partial\phi}\left(\frac{\hat{\boldsymbol{\theta}}}{\sin\theta}\frac{\partial}{\partial\phi}\right) + \hat{\boldsymbol{\phi}}\cdot\frac{\partial}{\partial\theta}\left(\hat{\boldsymbol{\phi}}\frac{\partial}{\partial\theta}\right) - \hat{\boldsymbol{\phi}}\cdot\frac{\partial}{\partial\theta}\left(\frac{\hat{\boldsymbol{\theta}}}{\sin\theta}\frac{\partial}{\partial\phi}\right) - \frac{\hat{\boldsymbol{\theta}}}{\sin\theta}\cdot\frac{\partial}{\partial\phi}\left(\hat{\boldsymbol{\phi}}\frac{\partial}{\partial\theta}\right)\right] \tag{18}$$

Be aware of the order in which the partial derivative is applied in expanding the equation. They are NOT commutative. Changing the order would ultimately change the expression.
Continue expanding the above with chain rule and simplify. Notice that we have

$$\hat{\boldsymbol{\theta}}\cdot\hat{\boldsymbol{\theta}} = \hat{\boldsymbol{\phi}}\cdot\hat{\boldsymbol{\phi}} = 1 \tag{19}$$

$$\hat{\boldsymbol{\theta}}\cdot\hat{\boldsymbol{\phi}} = 0 \tag{20}$$

$$\hat{\boldsymbol{\theta}}\cdot\frac{\partial\hat{\boldsymbol{\theta}}}{\partial\phi} = \hat{\boldsymbol{\phi}}\cdot\frac{\partial\hat{\boldsymbol{\phi}}}{\partial\theta} = \hat{\boldsymbol{\phi}}\cdot\frac{\partial\hat{\boldsymbol{\theta}}}{\partial\theta} = 0 \tag{21}$$

$$\hat{\boldsymbol{\theta}}\cdot\frac{\partial\hat{\boldsymbol{\phi}}}{\partial\phi} = -\cos\theta \tag{22}$$

Eqs.(21),(22) are proved by transforming $\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\phi}}$ into xyz-coordinates. So Eq.(18) becomes,

$$L^2 = -\hbar^2\left(\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta}\right) \tag{23}$$

This is more commonly written as

$$L^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right) \tag{24}$$

Now,

$$\begin{aligned} [L^2, L_z] &= L^2L_z - L_zL^2 \\ &= i\hbar^3\left[\left(\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta}\right)\frac{\partial}{\partial\phi} - \frac{\partial}{\partial\phi}\left(\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta}\right)\right] = 0 \end{aligned} \tag{25}$$

B. Spherical Harmonics

The spherical harmonics $Y_l^m(\theta, \phi)$ are defined as[1, p. 137],

$$Y_l^m(\theta,\phi) = \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}e^{im\phi}P_l^m(\cos\theta) \tag{26}$$

where P_l^m is called the associated Legendre function($|m| < l$). Y_l^m are augular parts of solutions to the Time-Independent Schrodinger Equation of the form:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi = E\psi \tag{27}$$

where $\psi = \psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$.

First few examples of spherical harmonics are illustrated here ($l = 0, 1, 2$).

$$\begin{aligned}
Y_0^0 &= \frac{1}{2}\sqrt{\frac{1}{\pi}} & Y_1^{-1} &= \frac{1}{2}\sqrt{\frac{3}{2\pi}}e^{-i\phi}\sin\theta & Y_1^0 &= \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta \\
Y_1^1 &= -\frac{1}{2}\sqrt{\frac{3}{2\pi}}e^{i\phi}\sin\theta & Y_2^{-2} &= \frac{1}{4}\sqrt{\frac{15}{2\pi}}e^{-2i\phi}\sin^2\theta & Y_2^{-1} &= \frac{1}{2}\sqrt{\frac{15}{2\pi}}e^{-i\phi}\sin\theta\cos\theta \\
Y_2^0 &= \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta - 1) & Y_2^1 &= -\frac{1}{2}\sqrt{\frac{15}{2\pi}}e^{i\phi}\sin\theta\cos\theta & Y_2^2 &= -\frac{1}{4}\sqrt{\frac{15}{2\pi}}e^{2i\phi}\sin^2\theta
\end{aligned}$$

Apparently, spherical harmonics are complex. To visualize, we plot their real and imaginary parts separately on a sphere in Fig. 1.

1. *Vector spherical harmonics*

The three vectors spherical harmonics are,

$$\mathbf{U}_{lm}(\theta,\phi) = |\mathbf{r}|\nabla Y_{lm}(\theta,\phi), \tag{28}$$

$$\mathbf{V}_{lm}(\theta,\phi) = \mathbf{r} \times \nabla Y_{lm}(\theta,\phi), \tag{29}$$

$$\mathbf{Y}_{lm}(\theta,\phi) = \frac{\mathbf{r}}{|\mathbf{r}|}Y_{lm}(\theta,\phi). \tag{30}$$

We'll make a vector plot to visualize their real and imaginary parts separately on a sphere in the same manner as the density plot.

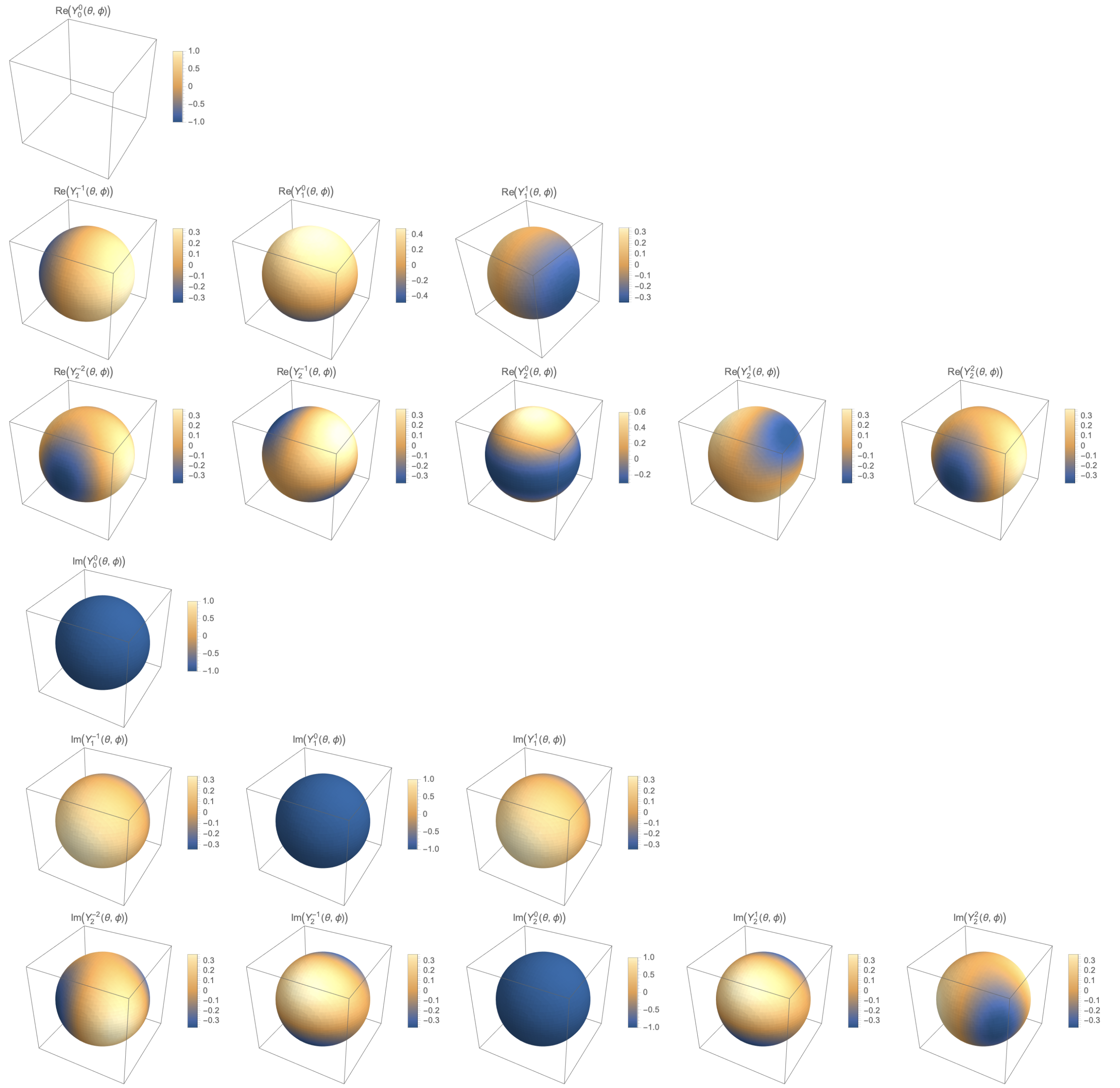
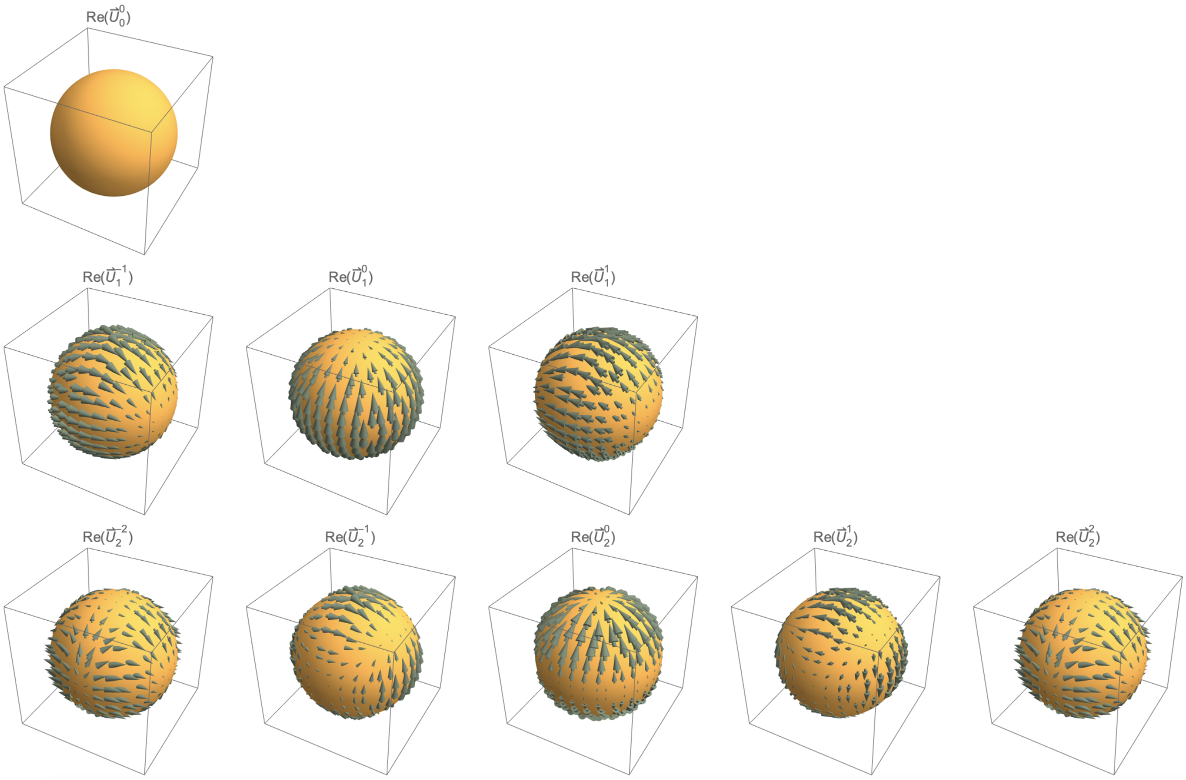


FIG. 1: Density 3D plots of the real and imaginary parts of spherical harmonics $Y_l^m(\theta, \phi)$ when $l = 0, 1, 2$ and $-l \leq m \leq l$. Lighter represents a higher value(density).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$\mathrm{Re}(\vec{U}_1^{-1})$
$\mathrm{Re}(\vec{U}_1^0)$
$\mathrm{Re}(\vec{U}_1^1)$
$\mathrm{Re}(\vec{U}_2^{-2})$
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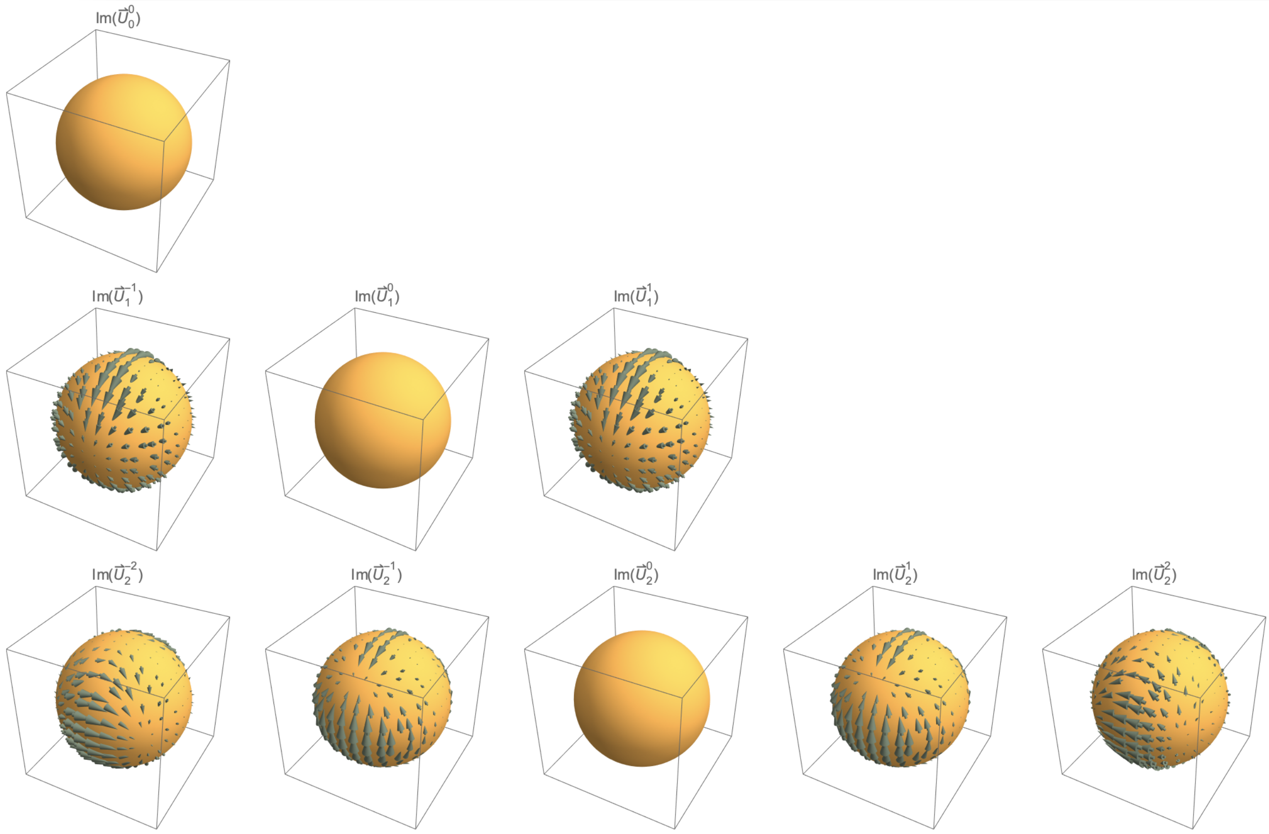
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$\mathrm{Im}(\vec{U}_1^0)$
$\mathrm{Im}(\vec{U}_1^1)$
$\mathrm{Im}(\vec{U}_2^{-2})$
$\mathrm{Im}(\vec{U}_2^{-1})$
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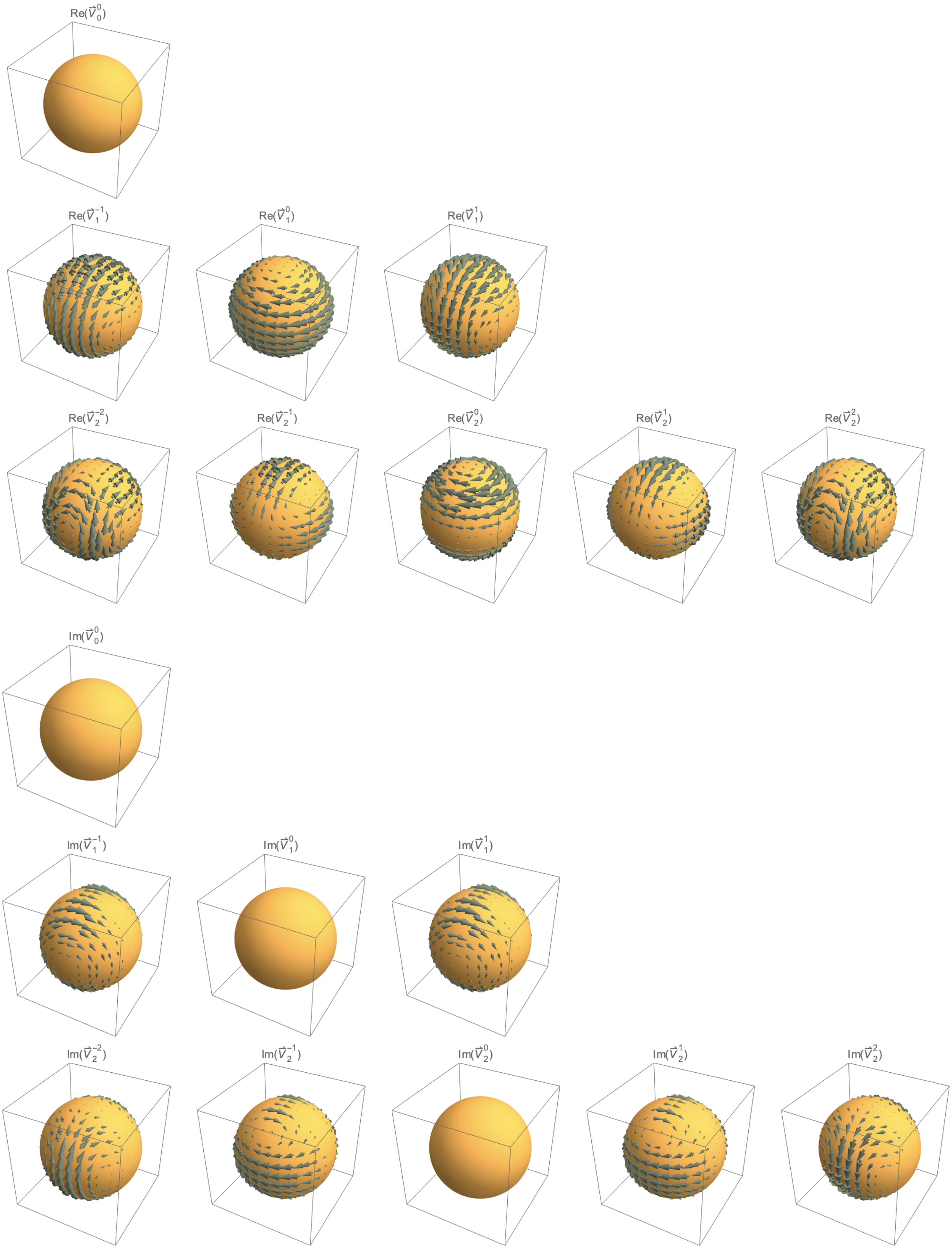
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Re($\vec{V}_1^{-1}$)
Re($\vec{V}_1^0$)
Re($\vec{V}_1^1$)
Re($\vec{V}_2^{-2}$)
Re($\vec{V}_2^{-1}$)
Re($\vec{V}_2^0$)
Re($\vec{V}_2^1$)
Re($\vec{V}_2^2$)
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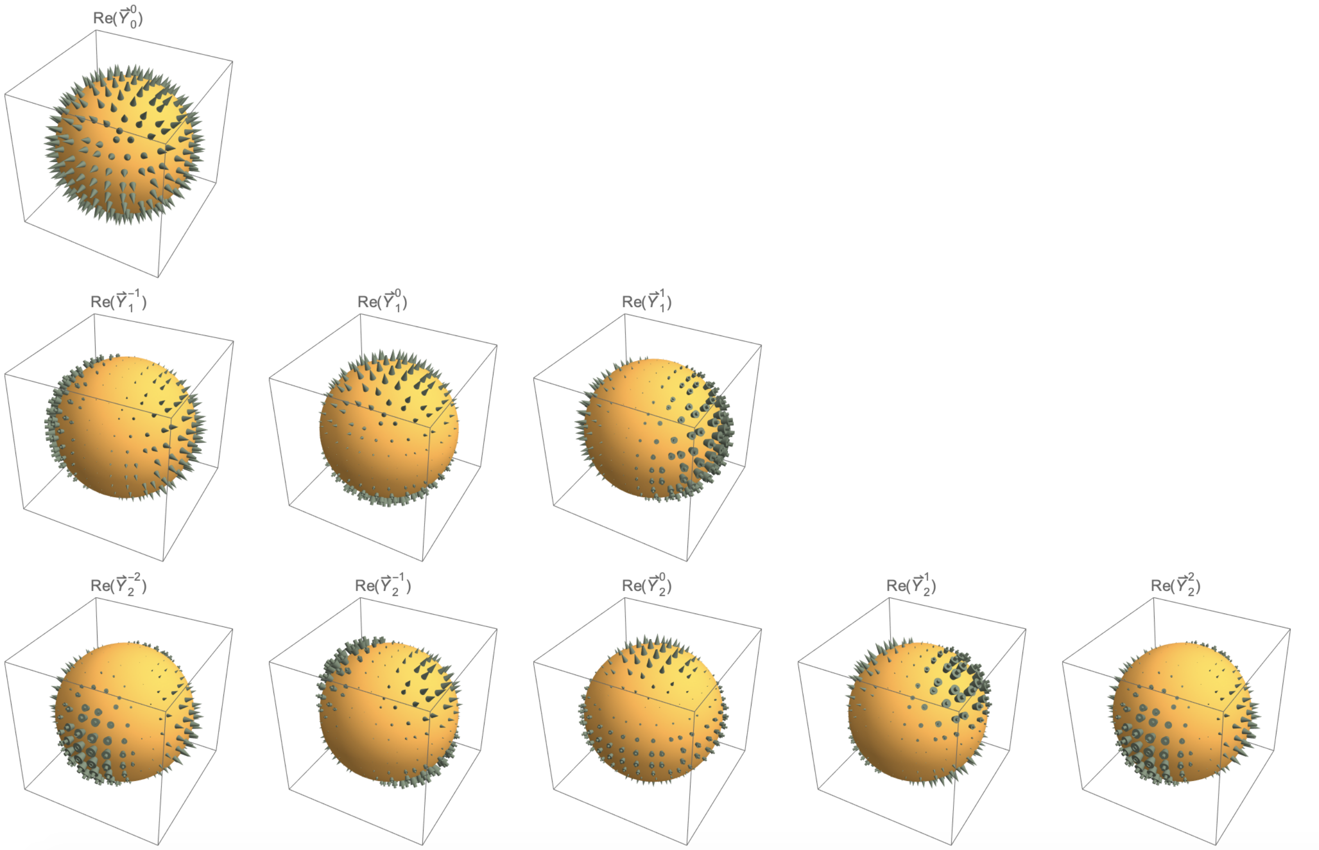
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$\mathrm{Re}(\vec{Y}_1^{-1})$
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$\mathrm{Re}(\vec{Y}_1^1)$
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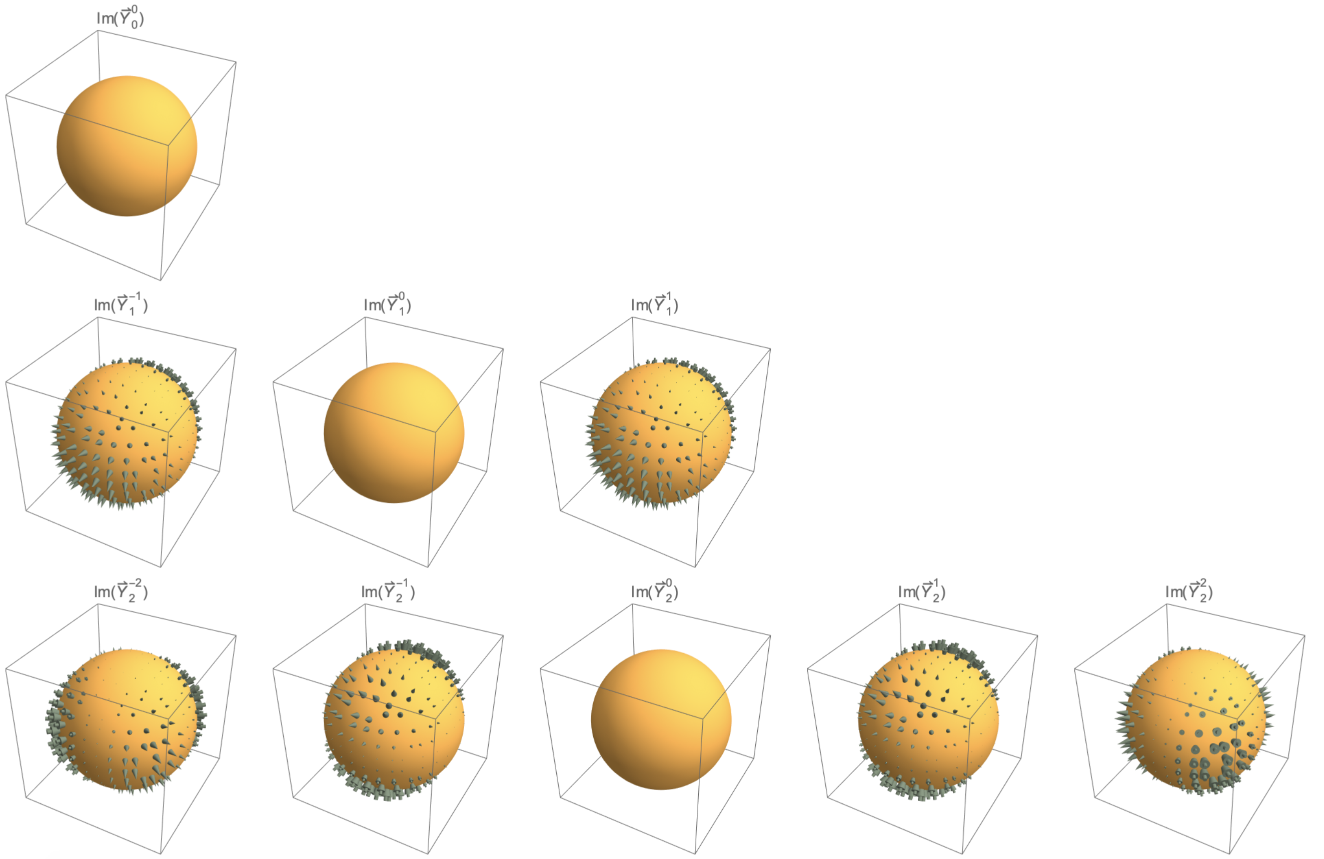
$\mathrm{Im}(\vec{Y}_0^0)$
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$\mathrm{Im}(\vec{Y}_2^2)$

C. Maxwell's Equations in Spherical Coordinates

1. Derivatives of unit bases

$$\frac{\partial \hat{\boldsymbol{r}}}{\partial r} = 0 \qquad \frac{\partial \hat{\boldsymbol{\theta}}}{\partial r} = 0 \qquad \frac{\partial \hat{\boldsymbol{\phi}}}{\partial r} = 0 \tag{31}$$

$$\frac{\partial \hat{\boldsymbol{r}}}{\partial \theta} = \hat{\boldsymbol{\theta}} \qquad \frac{\partial \hat{\boldsymbol{\theta}}}{\partial \theta} = -\hat{\boldsymbol{r}} \qquad \frac{\partial \hat{\boldsymbol{\phi}}}{\partial \theta} = 0 \tag{32}$$

$$\frac{\partial \hat{\boldsymbol{r}}}{\partial \phi} = \hat{\boldsymbol{\phi}} \sin\theta \qquad \frac{\partial \hat{\boldsymbol{\theta}}}{\partial \phi} = \hat{\boldsymbol{\phi}} \cos\theta \qquad \frac{\partial \hat{\boldsymbol{\phi}}}{\partial \phi} = -(\hat{\boldsymbol{r}} \sin\theta + \hat{\boldsymbol{\theta}} \cos\theta) \tag{33}$$

Either by transforming unit bases into Cartesian coordinates plus some substitution or, by a geometric approach, we can get the above results.

2. Del, div, curl

First we define del operator ∇ with scalar field $u = u(r, \theta, \phi)$ as

$$du = \nabla u \cdot d\boldsymbol{r} \tag{34}$$

where

$$du = \frac{\partial u}{\partial r} dr + \frac{\partial u}{\partial \theta} d\theta + \frac{\partial u}{\partial \phi} d\phi \tag{35}$$

$$d\boldsymbol{r} = \hat{\boldsymbol{r}} dr + \hat{\boldsymbol{\theta}} r d\theta + \hat{\boldsymbol{\phi}} r \sin\theta d\phi \tag{36}$$

Plug the above two expressions into Eq.(34), then we get the vector ∇u expressed as

$$\nabla u = \hat{\boldsymbol{r}} \frac{\partial u}{\partial r} + \frac{\hat{\boldsymbol{\theta}}}{r} \frac{\partial u}{\partial \theta} + \frac{\hat{\boldsymbol{\phi}}}{r \sin\theta} \frac{\partial u}{\partial \phi} \tag{37}$$

Hence,

$$\nabla = \hat{\boldsymbol{r}} \frac{\partial}{\partial r} + \frac{\hat{\boldsymbol{\theta}}}{r} \frac{\partial}{\partial \theta} + \frac{\hat{\boldsymbol{\phi}}}{r \sin\theta} \frac{\partial}{\partial \phi} \tag{38}$$

If $\boldsymbol{V}$ is a vector field such that $\boldsymbol{V} = V_r \hat{\boldsymbol{r}} + V_\theta \hat{\boldsymbol{\theta}} + V_\phi \hat{\boldsymbol{\phi}}$,then

$$\nabla \cdot \boldsymbol{V} = \left(\hat{\boldsymbol{r}} \frac{\partial}{\partial r} + \frac{\hat{\boldsymbol{\theta}}}{r} \frac{\partial}{\partial \theta} + \frac{\hat{\boldsymbol{\phi}}}{r \sin\theta} \frac{\partial}{\partial \phi} \right) \cdot (V_r \hat{\boldsymbol{r}} + V_\theta \hat{\boldsymbol{\theta}} + V_\phi \hat{\boldsymbol{\phi}}) \tag{39}$$

$$\nabla \times \boldsymbol{V} = \left(\hat{\boldsymbol{r}} \frac{\partial}{\partial r} + \frac{\hat{\boldsymbol{\theta}}}{r} \frac{\partial}{\partial \theta} + \frac{\hat{\boldsymbol{\phi}}}{r \sin\theta} \frac{\partial}{\partial \phi} \right) \times (V_r \hat{\boldsymbol{r}} + V_\theta \hat{\boldsymbol{\theta}} + V_\phi \hat{\boldsymbol{\phi}}) \tag{40}$$

expanding, rearranging, with the derivatives summarized in Section C 1 (similar to the process in Eq.(18)) we found,

$$\nabla \cdot \boldsymbol{V} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 V_r \right) + \frac{1}{r \sin\theta} \frac{\partial}{\partial \theta} \left(V_\theta \sin\theta \right) + \frac{1}{r \sin\theta} \frac{\partial V_\phi}{\partial \phi} \tag{41}$$

$$\nabla \times \boldsymbol{V} = \frac{\hat{\boldsymbol{r}}}{r \sin\theta} \left[\frac{\partial}{\partial \theta} \left(V_\phi \sin\theta \right) - \frac{\partial V_\theta}{\partial \phi} \right] + \frac{\hat{\boldsymbol{\theta}}}{r \sin\theta} \left[\frac{\partial V_r}{\partial \phi} - \sin\theta \frac{\partial}{\partial r} \left(r V_\phi \right) \right] + \frac{\hat{\boldsymbol{\phi}}}{r} \left[\frac{\partial}{\partial r} \left(r V_\theta \right) - \frac{\partial V_r}{\partial \theta} \right] \tag{42}$$

3. Maxwell's equations

Maxwell's equations in vacuum with Lorentz–Heaviside unit are:

$$\nabla\cdot\mathbf{E}=0 \tag{43}$$
$$\nabla\cdot\mathbf{B}=0 \tag{44}$$
$$\nabla\times\mathbf{E}=-\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t} \tag{45}$$
$$\nabla\times\mathbf{B}=\frac{1}{c}\frac{\partial\mathbf{E}}{\partial t} \tag{46}$$

If $\mathbf{E}=E_r\hat{\boldsymbol{r}}+E_\theta\hat{\boldsymbol{\theta}}+E_\phi\hat{\boldsymbol{\phi}}$ and $\mathbf{B}=B_r\hat{\boldsymbol{r}}+B_\theta\hat{\boldsymbol{\theta}}+B_\phi\hat{\boldsymbol{\phi}}$, with Eq.(41), we re-express Maxwell's equations in spherical coordinates. The first two Eqs. are saclar,

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2E_r\right)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(E_\theta\sin\theta\right)+\frac{1}{r\sin\theta}\frac{\partial E_\phi}{\partial\phi}=0 \tag{47}$$
$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2B_r\right)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(B_\theta\sin\theta\right)+\frac{1}{r\sin\theta}\frac{\partial B_\phi}{\partial\phi}=0 \tag{48}$$

The latter two are vector Eqs. and thus having three scalar Eqs. to express each.

we have to find the time derivatives of $\mathbf{E},\mathbf{B}$. For $\mathbf{E}$,

$$\frac{\partial\mathbf{E}}{\partial t}=\frac{\partial}{\partial t}\left(E_r\hat{\boldsymbol{r}}+E_\theta\hat{\boldsymbol{\theta}}+E_\phi\hat{\boldsymbol{\phi}}\right) \tag{49}$$

and

$$\dot{\hat{\boldsymbol{r}}}=\dot\theta\hat{\boldsymbol{\theta}}+\sin\theta\dot\phi\hat{\boldsymbol{\phi}} \tag{50}$$
$$\dot{\hat{\boldsymbol{\theta}}}=-\dot\theta\hat{\boldsymbol{r}}+\cos\theta\dot\phi\hat{\boldsymbol{\phi}} \tag{51}$$
$$\dot{\hat{\boldsymbol{\phi}}}=-\sin\theta\dot\phi\hat{\boldsymbol{r}}-\cos\theta\dot\phi\hat{\boldsymbol{\theta}} \tag{52}$$

Using the above and combine Eqs.(42)(45)(46), we have the remaining two Maxwell's equations (two vector Eqs. = six scalar Eqs.),

$$\begin{aligned}
\frac{c}{r\sin\theta}\left[\frac{\partial}{\partial\theta}\left(E_\phi\sin\theta\right)-\frac{\partial E_\theta}{\partial\phi}\right]&=-\dot B_r+\dot\theta B_\theta+\sin\theta\dot\phi B_\phi\\
\frac{c}{r\sin\theta}\left[\frac{\partial E_r}{\partial\phi}-\sin\theta\frac{\partial}{\partial r}\left(rE_\phi\right)\right]&=-\dot B_\theta-\dot\theta B_r+\cos\theta\dot\phi B_\phi\\
\frac{c}{r}\left[\frac{\partial}{\partial r}\left(rE_\phi\right)-\frac{\partial E_r}{\partial\theta}\right]&=-\dot B_\phi-\sin\theta\dot\phi B_r-\cos\theta\dot\phi B_\theta
\end{aligned} \tag{53}$$

$$\begin{aligned}
\frac{c}{r\sin\theta}\left[\frac{\partial}{\partial\theta}\left(B_\phi\sin\theta\right)-\frac{\partial B_\theta}{\partial\phi}\right]&=\dot E_r-\dot\theta E_\theta-\sin\theta\dot\phi E_\phi\\
\frac{c}{r\sin\theta}\left[\frac{\partial B_r}{\partial\phi}-\sin\theta\frac{\partial}{\partial r}\left(rB_\phi\right)\right]&=\dot E_\theta+\dot\theta E_r-\cos\theta\dot\phi E_\phi\\
\frac{c}{r}\left[\frac{\partial}{\partial r}\left(rB_\phi\right)-\frac{\partial B_r}{\partial\theta}\right]&=\dot E_\phi+\sin\theta\dot\phi E_r+\cos\theta\dot\phi E_\theta
\end{aligned} \tag{54}$$

I. REAL REPRESENTATION AND ELECTROSTATIC FIELD

The complex spherical harmonics $Y_l^m(\theta,\phi)$ are defined as[1, p. 137],

$$Y_l^m(\theta,\phi)=\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}e^{im\phi}\,P_l^m(\cos\theta) \tag{55}$$

where P_l^m is called the associated Legendre function($|m| < l$). Let us define the real spherical harmonics $Y_{lm}(\theta, \phi)$:

$$Y_{lm} = \begin{cases} \frac{(-1)^m}{\sqrt{2}\mathrm{i}}\left(Y_l^{|m|} - Y_l^{|m|*}\right) & \text{if } m < 0 \\ Y_l^0 & \text{if } m = 0 \\ \frac{(-1)^m}{\sqrt{2}}\left(Y_l^m + Y_l^{m*}\right) & \text{if } m > 0 \end{cases} \tag{56}$$

$$= \begin{cases} \sqrt{2}(-1)^m \Im\left[Y_l^{|m|}\right] & \text{if } m < 0 \\ Y_l^0 & \text{if } m = 0 \\ \sqrt{2}(-1)^m \Re\left[Y_l^m\right] & \text{if } m > 0 \end{cases} \tag{57}$$

$$= \begin{cases} (-1)^m\sqrt{2}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}P_\ell^{|m|}(\cos\theta)\sin(|m|\varphi) & \text{if } m < 0 \\ \sqrt{\frac{2\ell+1}{4\pi}}P_\ell(\cos\theta) & \text{if } m = 0 \\ (-1)^m\sqrt{2}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}P_\ell^{m}(\cos\theta)\cos(m\varphi) & \text{if } m > 0 \end{cases} . \tag{58}$$

The corresponding normalization relations for these real spherical harmonics are

$$\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} Y_{lm}Y_{l'm'}\mathrm{d}\Omega = \delta_{ll'}\delta_{mm'} \tag{59}$$

The three vectors spherical harmonics are,

$$\mathbf{U}_{lm}(\theta,\phi) = r\nabla Y_{lm}(\theta,\phi) \tag{60}$$

$$\mathbf{V}_{lm}(\theta,\phi) = \mathbf{r}\times\nabla Y_{lm}(\theta,\phi) \tag{61}$$

$$\mathbf{Y}_{lm}(\theta,\phi) = Y_{lm}(\theta,\phi)\hat{\mathbf{r}} \tag{62}$$

The additional theorem for spherical harmonics does not change:

$$\sum_{m=-l}^{l}\frac{4\pi}{2l+1}Y_{lm}(\theta,\phi)Y_{lm}(\theta',\phi') = P_l(\cos\gamma). \tag{63}$$

Among the above equation, γ is the included angle between the two points (θ,ϕ) and (θ',ϕ') on a sphere. Thus we have the expression for the Coulomb potential as follow

$$\sum_{lm}\frac{4\pi}{2l+1}\frac{r'^l}{r^{l+1}}Y_{lm}(\theta,\phi)Y_{lm}(\theta',\phi') = \frac{1}{|\mathbf{r}-\mathbf{r}'|}, \quad r' < r. \tag{64}$$

The potential for an electrostatic field in the spherical coordinate can be expressed by an integral

$$\Phi(\mathbf{r}) = \frac{1}{4\pi}\int\frac{\rho(\mathbf{r}')}{|\mathbf{r}'-\mathbf{r}|}\mathrm{d}V' \tag{65}$$

Using the following formula

$$-\nabla^2\frac{1}{|\mathbf{r}'-\mathbf{r}|} = 4\pi\delta^3(\mathbf{r}'-\mathbf{r}), \tag{66}$$

we can see Eq. (65) can give the Poisson equation

$$-\nabla^2\Phi(\mathbf{r}) = \rho(\mathbf{r}), \tag{67}$$

which is just the result of Gaussian theorem

$$\nabla\cdot\mathbf{E}(\mathbf{r}) = \rho(\mathbf{r}) \tag{68}$$

under the curl-free condition for the electrostatic field.

Now, if we apply the multi-pole expansion to the electric potential function, we can obtain

$$\Phi(\mathbf{r}) = \sum_{lm}\frac{Y_{lm}(\theta,\phi)}{(2l+1)r^{l+1}}q_{lm}, \tag{69}$$

$$q_{lm} = \int\rho(\mathbf{r}')r'^lY_{lm}(\theta',\phi')dV'. \tag{70}$$

Note that we should restrict $\rho(\mathbf{r}')$ to distribute in the region $r' < r$. The electric field is the gradient of the potential function:

$$\mathbf{E}(\mathbf{r}) = -\nabla\Phi(\mathbf{r}), \tag{71}$$

$$= \sum_{lm} \frac{q_{lm}}{(2l+1)r^{l+2}}[(l+1)\mathbf{Y}_{lm} - \mathbf{U}_{lm}], \tag{72}$$

$$q_{lm} = \int \rho(\mathbf{r}')r'^{l} Y_{lm}(\theta', \phi')dV'. \tag{73}$$

We define the spherical multi-pole field as

$$\mathbf{E}_{lm}(\mathbf{r}) = (l+1)\mathbf{Y}_{lm} - \mathbf{U}_{lm}. \tag{74}$$

Based on physics, we should know $\mathbf{E}(\mathbf{r})$ and $\mathbf{E}_{lm}(\mathbf{r})$ do not contain any zeros at far field places. Therefore, we are able to define a winding number of a multi-pole field over an origin-centered sphere.

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[1] D. J. Griffiths and D. F. Schroeter, *Introduction to quantum mechanics* (Cambridge University Press, 2018).

Spherical electromagnetic field

I. MAXWELL EQUATION IN VACUUM

The aim of us is to study the spherical electromagnetic field in vacuum. Firstly, we should write down the Maxwell's equations in Lorentz–Heaviside units:

$$\nabla \cdot \vec{E}(\vec{r}, t) = 0, \tag{1}$$
$$\nabla \cdot \vec{B}(\vec{r}, t) = 0, \tag{2}$$
$$\nabla \times \vec{E}(\vec{r}, t) = -\frac{1}{c}\frac{\partial \vec{B}(\vec{r}, t)}{\partial t}, \tag{3}$$
$$\nabla \times \vec{B}(\vec{r}, t) = \frac{1}{c}\frac{\partial \vec{E}(\vec{r}, t)}{\partial t}. \tag{4}$$

If we consider the electromagnetic oscillation at a constant frequency ω ($\omega = 0$ corresponds to the electrostatic and magnetostatics), the time variable among the Maxwell's equations can be removed:

$$\nabla \cdot \vec{E}(\vec{r}) = 0, \tag{5}$$
$$\nabla \cdot \vec{B}(\vec{r}) = 0, \tag{6}$$
$$\nabla \times \vec{E}(\vec{r}) = ik\vec{B}(\vec{r}), \tag{7}$$
$$\nabla \times \vec{B}(\vec{r}) = -ik\vec{E}(\vec{r}). \tag{8}$$

Among the above equations, $\vec{E}(\vec{r}, t) = \vec{E}(\vec{r})e^{-i\omega t}$, $\vec{B}(\vec{r}, t) = \vec{B}(\vec{r})e^{-i\omega t}$, and $k = \omega/c$. $\vec{E}(\vec{r})$ and $\vec{B}(\vec{r})$ are the amplitude field. However, for convenience we still call them as electric field and magnetic field. Through the among first-order partial differential equations, we can obtain the decoupled second-order equation:

$$(\nabla^2 + k^2)\vec{E}(\vec{r}) = 0, \tag{9}$$
$$(\nabla^2 + k^2)\vec{B}(\vec{r}) = 0. \tag{10}$$

Furthermore, it can be proved that [1]

$$(\nabla^2 + k^2)\vec{r} \cdot \vec{E}(\vec{r}) = 0, \tag{11}$$
$$(\nabla^2 + k^2)\vec{r} \cdot \vec{B}(\vec{r}) = 0. \tag{12}$$

To solve these partial differential equations in spherical coordinate, we expand the field by vector spherical harmonic functions:

$$\vec{U}_{lm}(\theta, \phi) = |\vec{r}|\nabla Y_{lm}(\theta, \phi), \tag{13}$$
$$\vec{V}_{lm}(\theta, \phi) = \vec{r} \times \nabla Y_{lm}(\theta, \phi), \tag{14}$$
$$\vec{Y}_{lm}(\theta, \phi) = \frac{\vec{r}}{|\vec{r}|}Y_{lm}(\theta, \phi). \tag{15}$$

Vector spherical harmonic functions are complete bases for the vector field in spherical coordinate[2, 3]. Note that $\vec{U}_{lm}$ and $\vec{V}_{lm}$ are tangent vector fields on a sphere while $\vec{Y}_{lm}$ is along the radial direction. The complete spherical expansion for any vector field $\vec{\Psi}(\vec{r})$ is

$$\vec{\Psi}(\vec{r}) = \sum_{lm} A_{lm}(r)\vec{U}_{lm}(\theta, \phi) + B_{lm}(r)\vec{V}_{lm}(\theta, \phi) + C_{lm}(r)\vec{Y}_{lm}(\theta, \phi). \tag{16}$$

The divergence and curl of $\vec{\Psi}(\vec{r})$ can be calculated as

$$\nabla\cdot\vec{\Psi}(\vec{r})=\sum_{lm}[\frac{dC_{lm}(r)}{dr}+\frac{2}{r}C_{lm}(r)-\frac{l(l+1)}{r}A_{lm}(r)]Y(\theta,\phi), \tag{17}$$

$$\begin{aligned}\nabla\times\vec{\Psi}(\vec{r})=&\sum_{lm}-[\frac{dB_{lm}(r)}{dr}+\frac{1}{r}B_{lm}(r)]\vec{U}_{lm}(\theta,\phi)+[\frac{dA_{lm}(r)}{dr}+\frac{1}{r}A_{lm}(r)-\frac{1}{r}C_{lm}(r)]\vec{V}_{lm}(\theta,\phi)\\&-\frac{l(l+1)}{r}B_{lm}(r)\vec{Y}_{lm}(\theta,\phi).\end{aligned} \tag{18}$$

If we consider TE modes which means $\vec{r}\cdot\vec{E}(\vec{r})=0$, $\vec{E}(\vec{r})$ can be simplified as:

$$\vec{E}(\vec{r})=\sum_{lm}E_{lm}(r)\vec{V}_{lm}(\theta,\phi). \tag{19}$$

Eq. (12) gives

$$\vec{r}\cdot\vec{B}(\vec{r})=\sum_{lm}ie_{lm}\frac{l(l+1)h_l^{(1)}(kr)}{k}Y_{lm}(\theta,\phi), \tag{20}$$

where $h_l^{(1)}(kr)$ is the first type spherical Hankel function and e_{lm} is the corresponding coefficient. Since $\vec{B}$ is related with $\vec{E}$ through Maxwell's equations, we have

$$\begin{aligned}\vec{E}&=\sum_{lm}e_{lm}h_l^{(1)}(kr)\vec{V}_{lm}(\theta,\phi)\\&=(\vec{r}\times\nabla)\Phi(\vec{r}),\end{aligned} \tag{21}$$

$$\Phi(\vec{r})=\sum_{lm}e_{lm}h_l^{(1)}(kr)Y_{lm}(\theta,\phi), \tag{22}$$

$$\begin{aligned}\vec{B}&=-\frac{i}{k}\nabla\times\vec{E}\\&=-\frac{i}{k}\nabla\times(\vec{r}\times\nabla\Phi(\vec{r}))\\&=\frac{i}{k}\sum_{lm}e_{lm}\{(\frac{h_l^{(1)}(kr)}{r}+\frac{dh_l^{(1)}(kr)}{dr})\vec{U}_{lm}(\theta,\phi)+\frac{l(l+1)}{r}h_l^{(1)}(kr)\vec{Y}_{lm}(\theta,\phi)\}.\end{aligned} \tag{23}$$

$\Phi(\vec{r})$ obeys the scalar Helmholtz equation.

Then we concern the TM modes. Similarly, we have

$$\begin{aligned}\vec{B}&=\sum_{lm}b_{lm}h_l^{(1)}(kr)\vec{V}_{lm}(\theta,\phi)\\&=(\vec{r}\times\nabla)\Psi(\vec{r}),\end{aligned} \tag{24}$$

$$\Psi(\vec{r})=\sum_{lm}b_{lm}h_l^{(1)}(kr)Y_{lm}(\theta,\phi), \tag{25}$$

$$\begin{aligned}\vec{E}&=\frac{i}{k}\nabla\times\vec{B}\\&=\frac{i}{k}\nabla\times(\vec{r}\times\nabla\Psi(\vec{r}))\\&=-\frac{i}{k}\sum_{lm}b_{lm}\{(\frac{h_l^{(1)}(kr)}{r}+\frac{dh_l^{(1)}(kr)}{dr})\vec{U}_{lm}(\theta,\phi)+\frac{l(l+1)}{r}h_l^{(1)}(kr)\vec{Y}_{lm}(\theta,\phi)\}.\end{aligned} \tag{26}$$

Overall, the general spherical electromagnetic field should be combined by TE and TM modes:

$$\vec{E}(\vec{r})=(\vec{r}\times\nabla)\Phi(\vec{r})+\frac{i}{k}\nabla\times(\vec{r}\times\nabla\Psi(\vec{r})), \tag{27}$$

$$\vec{B}(\vec{r})=(\vec{r}\times\nabla)\Psi(\vec{r})-\frac{i}{k}\nabla\times(\vec{r}\times\nabla\Phi(\vec{r})), \tag{28}$$

where $\Phi(\vec{r})$ and $\Psi(\vec{r})$ are all the solutions of scalar Helmholtz equation. In fact, the above expressions are actually originated from the Poloidal–toroidal decomposition theorem.

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