軌道角運動量と球面調和関数

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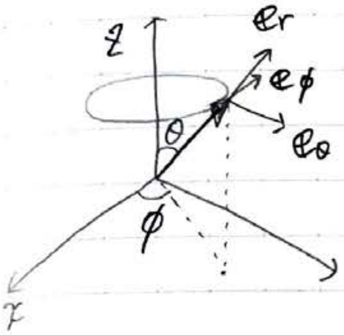
$$\mathbb{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} r\cos\phi\sin\theta \\ r\sin\phi\sin\theta \\ r\cos\theta \end{pmatrix}$$



$$(\mathbb{e}_r, \mathbb{e}_\theta, \mathbb{e}_\phi) \equiv \left(\frac{\partial_r \mathbb{r}}{h_r}, \frac{\partial_\theta \mathbb{r}}{h_\theta}, \frac{\partial_\phi \mathbb{r}}{h_\phi} \right)$$

$$\underset{1}{h_r = |\partial_\theta \mathbb{r}|}, \quad \underset{r}{h_\theta = |\partial_\theta \mathbb{r}|}, \quad \underset{r\sin\theta \geq 0}{h_\phi = |\partial_\phi \mathbb{r}|}$$

$(\mathbb{e}_r, \mathbb{e}_\theta, \mathbb{e}_\phi)$：規格直交化された右手系

$$(\mathbb{e}_r, \mathbb{e}_\theta, \mathbb{e}_\phi) \equiv \left(\frac{\partial_r \mathbb{r}}{h_r}, \frac{\partial_\theta \mathbb{r}}{h_\theta}, \frac{\partial_\phi \mathbb{r}}{h_\phi} \right) = \begin{pmatrix} \frac{1}{h_r}\frac{\partial x}{\partial r} & \frac{1}{h_\theta}\frac{\partial x}{\partial \theta} & \frac{1}{h_\phi}\frac{\partial x}{\partial \phi} \\ \frac{1}{h_r}\frac{\partial y}{\partial r} & \frac{1}{h_\theta}\frac{\partial y}{\partial \theta} & \frac{1}{h_\phi}\frac{\partial y}{\partial \phi} \\ \frac{1}{h_r}\frac{\partial z}{\partial r} & \frac{1}{h_\theta}\frac{\partial z}{\partial \theta} & \frac{1}{h_\phi}\frac{\partial z}{\partial \phi} \end{pmatrix} \equiv T$$

$$= \overset{*}{\begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} & \frac{\partial x}{\partial \phi} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} & \frac{\partial y}{\partial \phi} \\ \frac{\partial z}{\partial r} & \frac{\partial z}{\partial \theta} & \frac{\partial z}{\partial \phi} \end{pmatrix}} D^{-1} = \begin{array}{ccc} \mathbb{e}_r & \mathbb{e}_\theta & \mathbb{e}_\phi \\ \end{array}$$
$$\begin{pmatrix} \boxed{\begin{matrix} \cos\phi\sin\theta \\ \sin\phi\sin\theta \\ \cos\theta \end{matrix}} & \boxed{\begin{matrix} \cos\phi\cos\theta \\ \sin\phi\cos\theta \\ -\sin\theta \end{matrix}} & \boxed{\begin{matrix} -\sin\phi \\ \cos\phi \\ 0 \end{matrix}} \end{pmatrix}$$

$$D = \mathrm{diag}(h_r, h_\theta, h_\phi) = \mathrm{diag}(1, r, r\sin\theta)$$

$$\tilde{T}T = E_3, \quad \tilde{T} = T^{-1}$$

$* D^{-1} = T$
$* = TD$
$\tilde{*} = \widetilde{TD}$
$= D\tilde{T}$

一方、

$$\begin{pmatrix} \partial_r \\ \partial_\theta \\ \partial_\phi \end{pmatrix} = \overset{\tilde{*}}{\begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial y}{\partial r} & \frac{\partial z}{\partial r} \\ \frac{\partial x}{\partial \theta} & \frac{\partial y}{\partial \theta} & \frac{\partial z}{\partial \theta} \\ \frac{\partial x}{\partial \phi} & \frac{\partial y}{\partial \phi} & \frac{\partial z}{\partial \phi} \end{pmatrix}} \begin{pmatrix} \partial_x \\ \partial_y \\ \partial_z \end{pmatrix} = D\tilde{T} \begin{pmatrix} \partial_x \\ \partial_y \\ \partial_z \end{pmatrix}$$

↑ $\partial_r = \frac{\partial x}{\partial r}\partial_x + \frac{\partial y}{\partial r}\partial_y + \frac{\partial z}{\partial r}\partial_z$ など

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逆に解いて，

$$\nabla = \begin{pmatrix} \partial_x \\ \partial_y \\ \partial_z \end{pmatrix} = TD^{-1} \begin{pmatrix} \partial_r \\ \partial_\theta \\ \partial_\phi \end{pmatrix} = T \begin{pmatrix} \partial_r \\ \frac{1}{r}\partial_\theta \\ \frac{1}{r\sin\theta}\partial_\phi \end{pmatrix} = \mathbb{e}_r \partial_r + \mathbb{e}_\theta \frac{1}{r}\partial_\theta + \mathbb{e}_\phi \frac{1}{r\sin\theta}\partial_\phi$$

$$\mathbb{r} = r\mathbb{e}_r$$

$$\mathbb{L} = \mathbb{r}\times\mathbb{p} = -i\hbar r\,\mathbb{e}_r \times \nabla = -i\hbar r\,\mathbb{e}_r \times \left(\mathbb{e}_r\partial_r + \mathbb{e}_\theta\frac{1}{r}\partial_\theta + \mathbb{e}_\phi \frac{1}{r\sin\theta}\partial_\phi\right)$$

$$= -i\hbar\left(\mathbb{e}_\phi\partial_\theta - \mathbb{e}_\theta\frac{1}{\sin\theta}\partial_\phi\right)$$

↑ rに依らない［∴球面上の関数 $\Omega=(\theta,\phi)$］

$$\begin{pmatrix} L_x \\ L_y \\ L_z \end{pmatrix} = \hbar \begin{pmatrix} i\sin\phi \\ -i\cos\phi \\ 0 \end{pmatrix}\partial_\theta + \hbar \begin{pmatrix} i\cos\phi\cot\theta \\ i\sin\phi\cot\theta \\ -i \end{pmatrix}\partial_\phi$$

$$L_+ = L_x + iL_y = \hbar(i\sin\phi + \cos\phi)\partial_\theta + \hbar(\underbrace{i\cos\phi\cot\theta - \sin\phi\cot\theta}_{i(\cos\phi+i\sin\phi)\cot\theta})\partial_\phi$$
$$= \hbar e^{i\phi}(\partial_\theta + i\cot\theta\partial_\phi)$$

$$L_- = L_x - iL_y = \hbar(i\sin\phi - \cos\phi)\partial_\theta + \hbar(\underbrace{i\cos\phi\cot\theta + \sin\phi\cot\theta}_{i(\cos\phi-i\sin\phi)\cot\theta})\partial_\phi$$
$$= \hbar e^{-i\phi}(-\partial_\theta + i\cot\theta\partial_\phi)$$

$$L_z = -i\hbar\partial_\phi$$

$$(\partial^\dagger = -\partial)$$

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球面調和関数 $Y_{\ell m}(\Omega)$ $\Omega=(\theta,\phi)$

$$\mathbb{L}^2 Y_{\ell m}=\hbar^2\ell(\ell+1)Y_{\ell m}$$
$$L_z Y_{\ell m}=\hbar m Y_{\ell m}$$
$$L_+ Y_{\ell\ell}=L_- Y_{\ell-\ell}=0$$

ここで、$Y_{\ell m}(\Omega)=\Theta_{\ell m}(\theta)\Phi_m(\phi)$ と変数分離形におくと、$L_z Y_{\ell m}=\hbar m Y_{\ell m}$より、

$$\Phi_m(\phi)=\frac{1}{\sqrt{2\pi}}e^{im\phi}$$

但し、$\int_0^{2\pi}d\phi\,|\Phi_m(\phi)|^2=1$ と規格化した。

また、この関数の一価性より、$\underbrace{e^{i2\pi m}=1}_{\Phi_m(2\pi)=\Phi_m(0)\text{より}}$ つまり mは整数である。

よって、ℓも0以上の整数となる。（$m:-\ell,\dots,\ell$であるので）

ここで、θの関数 $f(\theta)$ に対して、

$$\underset{\hbar e^{i\phi}(\partial_\theta+i\cot\theta\partial_\phi)}{\underline{\underline{L_+}}}[e^{im\phi}f(\theta)]=e^{im\phi}\hbar e^{i\phi}\left[\frac{df}{d\theta}-mf\cot\theta\right]$$

$$\underset{\hbar e^{-i\phi}(-\partial_\theta+i\cot\theta\partial_\phi)}{\underline{\underline{L_-}}}[e^{im\phi}f(\theta)]=-e^{im\phi}\hbar e^{-i\phi}\left[\frac{df}{d\theta}+mf\cot\theta\right]$$

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$$\begin{cases} \dfrac{d}{d\theta} = \dfrac{d\cos\theta}{d\theta}\dfrac{d}{d\cos\theta} = -\sin\theta\dfrac{d}{d\cos\theta} \ , \ \dfrac{d}{d\cos\theta} = -\sin^{-1}\theta\dfrac{d}{d\theta} \\ \dfrac{d\sin\theta}{d\cos\theta} = \dfrac{d(1-\cos^2\theta)^{\frac{1}{2}}}{d\cos\theta} = \dfrac{1}{2}(1-\cos^2\theta)^{-\frac{1}{2}}(-2\cos\theta) = -\cot\theta \end{cases}$$

これらを用いて書き直すと、

$$L_+[e^{im\phi}f(\theta)] = -\hbar e^{i(m+1)\phi}\sin^{m+1}\theta\frac{d}{d\cos\theta}[\sin^{-m}\theta f(\theta)] \quad \text{—①}$$

$$L_-[e^{im\phi}f(\theta)] = \hbar e^{i(m-1)\phi}\sin^{-(m-1)}\theta\frac{d}{d\cos\theta}[\sin^{m}\theta f(\theta)] \quad \text{—②}$$

確認

① の $\dfrac{d}{d\cos\theta}[\sin^{-m}\theta f(\theta)] = -m\sin^{-m-1}\theta\dfrac{d\sin\theta}{d\cos\theta}f + \sin^{-m}\theta\dfrac{df}{d\cos\theta}$

$$= -m\sin^{-(m+1)}\theta(-\cot\theta)f + \sin^{-m}\theta\left(-\sin^{-1}\theta\frac{df}{d\theta}\right)$$

$$= -\sin^{-(m+1)}\theta\left[\frac{df}{d\theta} - mf\cot\theta\right]$$

$$\rightarrow -\sin^{m+1}\theta\frac{d}{d\cos\theta}[\sin^{-m}\theta f(\theta)] = \frac{df}{d\theta} - mf\cot\theta \quad \rightarrow \text{ok}$$

② の $\dfrac{d}{d\cos\theta}[\sin^{m}\theta f(\theta)] = m\sin^{m-1}\theta\dfrac{d\sin\theta}{d\cos\theta}f + \sin^{m}\theta\dfrac{df}{d\cos\theta}$

$$= m\sin^{m-1}\theta(-\cot\theta)f + \sin^{m}\theta\left(-\sin^{-1}\theta\frac{df}{d\theta}\right)$$

$$= -\sin^{(m-1)}\theta\left[\frac{df}{d\theta} + mf\cot\theta\right]$$

$$\rightarrow \sin^{-(m-1)}\theta\frac{d}{d\cos\theta}[\sin^{m}\theta f(\theta)] = -\left[\frac{df}{d\theta} + mf\cot\theta\right] \rightarrow \text{ok}$$

$$L_+[e^{im\phi}f(\theta)] = -\hbar e^{i(m+1)\phi} \underbrace{\sin^{m+1}\theta \frac{d}{d\cos\theta}[\sin^{-m}\theta f(\theta)]}_{f\text{とみる}}$$

繰り返して、

$$L_+^2[e^{im\phi}f(\theta)] = -\hbar L_+[e^{i(m+1)\phi} \overbrace{\sin^{m+1}\theta \frac{d}{d\cos\theta}[\sin^{-m}\theta f(\theta)]}^{f}]$$

$$= (-\hbar)^2 e^{i(m+2)\phi} \sin^{m+2}\theta \frac{d}{d\cos\theta}[\sin^{-m-1}\theta \sin^{m+1}\theta \frac{d}{d\cos\theta}[\sin^{-m}\theta f(\theta)]]$$

$$= (-\hbar)^2 e^{i(m+2)\phi} \underbrace{\sin^{m+2}\theta \left[\frac{d}{d\cos\theta}\right]^2 [\sin^{-m}\theta f(\theta)]}_{f\text{とみる}}$$

$$L_+^3[e^{im\phi}f(\theta)] = (-\hbar)^2 L_+[e^{i(m+2)\phi} \sin^{m+2}\theta \left[\frac{d}{d\cos\theta}\right]^2 [\sin^{-m}\theta f(\theta)]]$$

$$= (-\hbar)^3 e^{i(m+3)\phi} \sin^{m+3}\theta \frac{d}{d\cos\theta} [\sin^{-m-2}\theta \sin^{m+2}\theta \left[\frac{d}{d\cos\theta}\right]^2 [\sin^{-m}\theta f(\theta)]$$

$$= (-\hbar)^3 e^{i(m+3)\phi} \sin^{m+3}\theta \left[\frac{d}{d\cos\theta}\right]^3 [\sin^{-m}\theta f(\theta)]$$

k回繰り返すと、

$$L_+^k[e^{im\phi}f(\theta)] = (-\hbar)^k e^{i(m+k)\phi} \sin^{m+k}\theta \left[\frac{d}{d\cos\theta}\right]^k [\sin^{-m}\theta f(\theta)]$$

L_+同様にL_-についても考える。

$$L_-[e^{im\phi}f(\theta)]=\hbar e^{i(m-1)\phi}\sin^{-(m-1)}\theta\frac{d}{d\cos\theta}[\sin^m\theta f(\theta)]$$

繰り返して、

$$L_-^2[e^{im\phi}f(\theta)]=\hbar L_-[e^{i(m-1)\phi}\overbrace{\sin^{-(m-1)}\theta\frac{d}{d\cos\theta}[\sin^m\theta f(\theta)]}^{f}]$$

$$=\hbar^2 e^{i(m-2)\phi}\sin^{-(m-2)}\theta\frac{d}{d\cos\theta}[\sin^{m-1}\theta\sin^{-(m-1)}\theta\frac{d}{d\cos\theta}[\sin^m\theta f(\theta)]]$$

$$=\hbar^2 e^{i(m-2)\phi}\sin^{-(m-2)}\theta\left[\frac{d}{d\cos\theta}\right]^2[\sin^m\theta f(\theta)]$$

$$L_-^3[e^{im\phi}f(\theta)]=\hbar^2 L_-[e^{i(m-2)\phi}\overbrace{\sin^{-(m-2)}\theta\left[\frac{d}{d\cos\theta}\right]^2[\sin^m\theta f(\theta)]}^{f}]$$

$$=\hbar^3 e^{i(m-3)\phi}\sin^{-(m-3)}\theta\frac{d}{d\cos\theta}[\sin^{m-2}\theta\sin^{-(m-2)}\left[\frac{d}{d\cos\theta}\right]^2[\sin^m\theta f(\theta)]]$$

$$=\hbar^3 e^{i(m-3)\phi}\sin^{-(m-3)}\theta\left[\frac{d}{d\cos\theta}\right]^3[\sin^m\theta f(\theta)]$$

k回繰り返して、

$$L_-^k[e^{im\phi}f(\theta)]=\hbar^k e^{i(m-k)\phi}\sin^{-(m-k)}\theta\left[\frac{d}{d\cos\theta}\right]^k[\sin^m\theta f(\theta)]$$

まとめて、

$$\begin{cases} L_+^k[e^{im\phi}f(\theta)]=(-\hbar)^k e^{i(m+k)\phi}\sin^{m+k}\theta\left[\frac{d}{d\cos\theta}\right]^k[\sin^{-m}\theta f(\theta)] \\ L_-^k[e^{im\phi}f(\theta)]=\hbar^k e^{i(m-k)\phi}\sin^{-(m-k)}\theta\left[\frac{d}{d\cos\theta}\right]^k[\sin^m\theta f(\theta)] \end{cases}$$