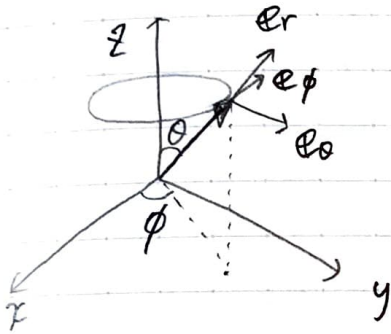


軌道角運動量と球面調和関数

201810877 林美吹

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



$$(\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_\phi) \equiv \left(\frac{\partial \mathbf{r}}{\partial r}, \frac{\partial \mathbf{r}}{\partial \theta}, \frac{\partial \mathbf{r}}{\partial \phi} \right)$$

$$h_r = \left| \frac{\partial \mathbf{r}}{\partial r} \right|, h_\theta = \left| \frac{\partial \mathbf{r}}{\partial \theta} \right|, h_\phi = \left| \frac{\partial \mathbf{r}}{\partial \phi} \right|$$

$$1 \quad r \quad r \sin \theta \geq 0$$

$(\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_\phi)$: 規格直交化した右手系

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

$$D^{-1} = \begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} & \frac{\partial x}{\partial \phi} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} & \frac{\partial y}{\partial \phi} \\ \frac{\partial z}{\partial r} & \frac{\partial z}{\partial \theta} & \frac{\partial z}{\partial \phi} \end{pmatrix} = \begin{pmatrix} \cos \phi \sin \theta & \cos \phi \cos \theta & -\sin \phi \\ \sin \phi \sin \theta & \sin \phi \cos \theta & \cos \phi \\ \cos \theta & -\sin \theta & 0 \end{pmatrix}$$

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

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

* $D^{-1} = \mathbf{T}$
 * $\tilde{\mathbf{x}} = \tilde{\mathbf{T}} \mathbf{D}$
 $\tilde{\mathbf{x}} = \tilde{\mathbf{T}} \mathbf{D}$
 $= D \tilde{\mathbf{T}}$

一方、

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

$$\left[\partial_r = \frac{\partial x}{\partial r} \partial_x + \frac{\partial y}{\partial r} \partial_y + \frac{\partial z}{\partial r} \partial_z \text{ etc.} \right]$$

逆L=角算子,

$$\nabla = \begin{pmatrix} \partial_x \\ \partial_y \\ \partial_z \end{pmatrix} = T D^{-1} \begin{pmatrix} \partial_r \\ \partial_\theta \\ \partial_\phi \end{pmatrix} = T \begin{pmatrix} \partial_r \\ \frac{1}{r} \partial_\theta \\ \frac{1}{r \sin\theta} \partial_\phi \end{pmatrix} = e_r \partial_r + e_\theta \frac{1}{r} \partial_\theta + e_\phi \frac{1}{r \sin\theta} \partial_\phi$$

$$\hbar = r e_r$$

$$\begin{aligned} \mathbb{L} &= \hbar \times \mathbb{P} = -i\hbar r e_r \times \nabla = -i\hbar r e_r \times \left(e_r \partial_r + e_\theta \frac{1}{r} \partial_\theta + e_\phi \frac{1}{r \sin\theta} \partial_\phi \right) \\ &= -i\hbar \left(e_\phi \partial_\theta - e_\theta \frac{1}{\sin\theta} \partial_\phi \right) \end{aligned}$$

↑ $r = (r, \theta, \phi)$ [球面上関数 $\Omega = (\theta, \phi)$]

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

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

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

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

$$(\partial_t = -\partial)$$

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

$$\Delta^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm}$$

$$L_z Y_{lm} = \hbar m Y_{lm}$$

$$L_+ Y_{ll} = L_- Y_{l-l} = 0$$

∴ $Y_{lm}(\Omega) = \Theta_{lm}(\theta) \Phi_m(\phi)$ と変数分離形におくと、 $L_z Y_{lm} = \hbar m Y_{lm}$ 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、 $e^{i2\pi m} = 1$ つまり m は整数である。

$$\Phi_m(2\pi) = \Phi_m(0) \text{ より}$$

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

∴ θ の関数 $f(\theta)$ に対し、

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

$$\hbar e^{i\phi} (-\partial_\theta + i \cot \theta \partial_\phi)$$

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

$$\hbar e^{i\phi} (-\partial_\theta + i \cot \theta \partial_\phi)$$

$$\left\{ \begin{array}{l} \frac{d}{d\theta} = \frac{d \cos \theta}{d\theta} \frac{d}{d \cos \theta} = -\sin \theta \frac{d}{d \cos \theta}, \quad \frac{d}{d \cos \theta} = -\sin^{-1} \theta \frac{d}{d\theta} \\ \frac{d \sin \theta}{d \cos \theta} = \frac{d(1 - \cos^2 \theta)^{\frac{1}{2}}}{d \cos \theta} = \frac{1}{2} (1 - \cos^2 \theta)^{-\frac{1}{2}} (-2 \cos \theta) = -\cot \theta \end{array} \right.$$

二つ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

$$\begin{aligned} \textcircled{1} \text{ の } \frac{d}{d \cos \theta} [\sin^{-m} \theta f(\theta)] &= -m \sin^{-m-1} \theta \frac{d \sin \theta}{d \cos \theta} f + \sin^{-m} \theta \frac{df}{d \cos \theta} \\ &= -m \sin^{-(m+1)} \theta (-\cot \theta) f + \sin^{-m} \theta \left(-\sin^{-1} \theta \frac{df}{d\theta} \right) \\ &= -\sin^{-(m+1)} \theta \left[\frac{df}{d\theta} - m f \cot \theta \right] \end{aligned}$$

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

$$\begin{aligned} \textcircled{2} \text{ の } \frac{d}{d \cos \theta} [\sin^m \theta f(\theta)] &= m \sin^{m-1} \theta \frac{d \sin \theta}{d \cos \theta} f + \sin^m \theta \frac{df}{d \cos \theta} \\ &= m \sin^{m-1} \theta (-\cot \theta) f + \sin^m \theta \left(-\sin^{-1} \theta \frac{df}{d\theta} \right) \\ &= -\sin^{(m-1)} \theta \left[\frac{df}{d\theta} + m f \cot \theta \right] \end{aligned}$$

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

$$L_+[e^{im\phi} f(\theta)] = -\hbar e^{i(m+1)\phi} \underbrace{\sin^{m+1}\theta \frac{d}{d\cos\theta} [\sin^{-m}\theta f(\theta)]}_{f \text{ かつ } 3}$$

繰り返して、

$$\begin{aligned} L_+^2[e^{im\phi} f(\theta)] &= -\hbar L_+[e^{i(m+1)\phi} \underbrace{\sin^{m+1}\theta \frac{d}{d\cos\theta} [\sin^{-m}\theta f(\theta)]}_f] \\ &= (-\hbar)^2 e^{i(m+2)\phi} \sin^{m+2}\theta \frac{d}{d\cos\theta} [\sin^{-m-1}\theta \sin^{m+1}\theta \frac{d}{d\cos\theta} [\sin^{-m}\theta f(\theta)]] \\ &= (-\hbar)^2 e^{i(m+2)\phi} \sin^{m+2}\theta \underbrace{\left[\frac{d}{d\cos\theta}\right]^2 [\sin^{-m}\theta f(\theta)]}_{f \text{ かつ } 3} \end{aligned}$$

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

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 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、

$$\begin{aligned} L_-^2 [e^{im\phi} f(\theta)] &= \hbar L_- [e^{i(m-1)\phi} \sin^{-(m-1)} \theta \frac{d}{d\cos\theta} [\sin^m \theta f(\theta)]] \\ &= \hbar^2 e^{i(m-2)\phi} \sin^{-(m-2)} \theta \frac{d}{d\cos\theta} [\sin^{m-1} \theta \sin^{-(m-1)} \theta \frac{d}{d\cos\theta} [\sin^m \theta f(\theta)]] \\ &= \hbar^2 e^{i(m-2)\phi} \sin^{-(m-2)} \theta \left[\frac{d}{d\cos\theta} \right]^2 [\sin^m \theta f(\theta)] \end{aligned}$$

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

k 回繰り返して、

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

まとめると、

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