ルジャンドリアンと角運動量

0.1　ルジャンドリアン

球面調和関数 $Y = Y_\ell^m(\theta, \varphi)$ は次の微分方程式の解であった：

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2} + \ell(\ell+1)Y = 0, \tag{1}$$

ここで，ルジャンドリアン Λ を，

$$\Lambda \overset{\text{def}}{=} \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \tag{2}$$

によって定義すると，当然球面調和関数 $Y_\ell^m(\theta, \varphi)$ に対して，

$$\Lambda Y_\ell^m + \ell(\ell+1)Y_\ell^m = 0, \tag{3}$$

即ち，

$$\Lambda Y_\ell^m = -\ell(\ell+1)Y_\ell^m, \tag{4}$$

となり，球面調和関数はルジャンドリアンの固有ベクトルになる．

0.2　軌道角運動量

軌道角運動量を表す演算子 $\hat{\boldsymbol{\ell}}$ は,

$$\hat{\boldsymbol{\ell}} \overset{\text{def}}{=} \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}} = \begin{vmatrix} \boldsymbol{i} & x & \hat{p}_x \\ \boldsymbol{j} & y & \hat{p}_y \\ \boldsymbol{k} & z & \hat{p}_z \end{vmatrix} = \begin{vmatrix} \boldsymbol{i} & x & \frac{\hbar}{i}\frac{\partial}{\partial x} \\ \boldsymbol{j} & y & \frac{\hbar}{i}\frac{\partial}{\partial y} \\ \boldsymbol{k} & z & \frac{\hbar}{i}\frac{\partial}{\partial z}, \end{vmatrix} \tag{5}$$

のように表される．従って，

$$\hat{\ell}_x = +\begin{vmatrix} y & \hat{p}_y \\ z & \hat{p}_z \end{vmatrix} = +\begin{vmatrix} y & \frac{\hbar}{i}\frac{\partial}{\partial y} \\ z & \frac{\hbar}{i}\frac{\partial}{\partial z} \end{vmatrix} = y\hat{p}_z - z\hat{p}_y = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right), \tag{6}$$

$$\hat{\ell}_y = -\begin{vmatrix} x & \hat{p}_x \\ z & \hat{p}_z \end{vmatrix} = -\begin{vmatrix} x & \frac{\hbar}{i}\frac{\partial}{\partial x} \\ z & \frac{\hbar}{i}\frac{\partial}{\partial z} \end{vmatrix} = z\hat{p}_x - x\hat{p}_z = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right), \tag{7}$$

$$\hat{\ell}_z = +\begin{vmatrix} x & \hat{p}_x \\ y & \hat{p}_y \end{vmatrix} = +\begin{vmatrix} x & \frac{\hbar}{i}\frac{\partial}{\partial x} \\ y & \frac{\hbar}{i}\frac{\partial}{\partial y} \end{vmatrix} = x\hat{p}_y - y\hat{p}_x = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right), \tag{8}$$

となる．ここで，微分演算子の球座標表示より，

$$\frac{\partial}{\partial x} = \sin\theta\cos\varphi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\varphi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}, \tag{9}$$

$$\frac{\partial}{\partial y} = \sin\theta\sin\varphi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\varphi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}, \tag{10}$$

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}, \tag{11}$$

が得られているから，

$$\begin{aligned} y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} &= y\left(\cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}\right) - z\left(\sin\theta\sin\varphi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\varphi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}\right) \\ &= (y\cos\theta - z\sin\theta\sin\varphi)\frac{\partial}{\partial r} - \left(\frac{y\sin\theta}{r} + \frac{z\cos\theta\sin\varphi}{r}\right)\frac{\partial}{\partial\theta} - \frac{z\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi} \\ &= (r\sin\theta\sin\varphi\cos\theta - r\cos\theta\sin\theta\sin\varphi)\frac{\partial}{\partial r} - \left(\frac{r\sin\theta\sin\varphi\sin\theta}{r} + \frac{r\cos\theta\cos\theta\sin\varphi}{r}\right)\frac{\partial}{\partial\theta} - \frac{r\cos\theta\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi} \\ &= -\sin\varphi\frac{\partial}{\partial\theta} - \frac{\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}, \end{aligned}$$

$$
\begin{aligned}
z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} &= z\left(\sin\theta\cos\varphi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\varphi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}\right) - x\left(\cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}\right)\\
&= (z\sin\theta\cos\varphi - x\cos\theta)\frac{\partial}{\partial r} + \left(\frac{z\cos\theta\cos\varphi}{r} + \frac{x\sin\theta}{r}\right)\frac{\partial}{\partial\theta} - \frac{z\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}\\
&= (r\cos\theta\sin\theta\cos\varphi - r\sin\theta\cos\varphi\cos\theta)\frac{\partial}{\partial r} + \left(\frac{r\cos\theta\cos\theta\cos\varphi}{r} + \frac{r\sin\theta\cos\varphi\sin\theta}{r}\right)\frac{\partial}{\partial\theta} - \frac{r\cos\theta\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}\\
&= \cos\varphi\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{\tan\theta}\frac{\partial}{\partial\varphi},
\end{aligned}
$$

$$
\begin{aligned}
x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} &= x\left(\sin\theta\sin\varphi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\varphi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}\right) - y\left(\sin\theta\cos\varphi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\varphi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}\right)\\
&= (x\sin\theta\sin\varphi - y\sin\theta\cos\varphi)\frac{\partial}{\partial r} + \left(\frac{x\cos\theta\sin\varphi}{r} - \frac{y\cos\theta\cos\varphi}{r}\right)\frac{\partial}{\partial\theta} + \left(\frac{x\cos\varphi}{r\sin\theta} + \frac{y\sin\varphi}{r\sin\theta}\right)\frac{\partial}{\partial\varphi}\\
&= (r\sin\theta\cos\varphi\sin\theta\sin\varphi - r\sin\theta\sin\varphi\sin\theta\cos\varphi)\frac{\partial}{\partial r} + \left(\frac{r\sin\theta\cos\varphi\cos\theta\sin\varphi}{r} - \frac{r\sin\theta\sin\varphi\cos\theta\cos\varphi}{r}\right)\frac{\partial}{\partial\theta}\\
&\quad + \left(\frac{r\sin\theta\cos\varphi\cos\varphi}{r\sin\theta} + \frac{r\sin\theta\sin\varphi\sin\varphi}{r\sin\theta}\right)\frac{\partial}{\partial\varphi}\\
&= \frac{\partial}{\partial\varphi},
\end{aligned}
$$

以上より，

$$
\hat{\ell}_x = \frac{\hbar}{i}\left(-\sin\varphi\frac{\partial}{\partial\theta} - \frac{\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right), \tag{12}
$$

$$
\hat{\ell}_y = \frac{\hbar}{i}\left(\cos\varphi\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right), \tag{13}
$$

$$
\hat{\ell}_z = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}, \tag{14}
$$

が得られた．ここで，$\hat{\boldsymbol{\ell}}\cdot\hat{\boldsymbol{\ell}} = \hat{\ell}_x^{\,2} + \hat{\ell}_y^{\,2} + \hat{\ell}_z^{\,2}$ を求めてみると，

$$
\begin{aligned}
\left(\frac{i}{\hbar}\hat{\ell}_x\right)^2 &= \left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)^2\\
&= \left(-\sin\varphi\frac{\partial}{\partial\theta} - \frac{\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)\cdot\left(-\sin\varphi\frac{\partial}{\partial\theta} - \frac{\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)\\
&= \left(-\sin\varphi\frac{\partial}{\partial\theta}\right)\cdot\left(-\sin\varphi\frac{\partial}{\partial\theta}\right) + \left(-\frac{\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)\cdot\left(-\frac{\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)\\
&\quad + \left(-\sin\varphi\frac{\partial}{\partial\theta}\right)\cdot\left(-\frac{\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right) + \left(-\frac{\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)\cdot\left(-\sin\varphi\frac{\partial}{\partial\theta}\right)\\
&= \sin^2\varphi\frac{\partial^2}{\partial\theta^2} + \frac{\cos^2\varphi}{\tan^2\theta}\frac{\partial^2}{\partial\varphi^2} + 2\frac{\sin\varphi\cos\varphi}{\tan\theta}\frac{\partial^2}{\partial\theta\partial\varphi} + \frac{\cos^2\varphi}{\tan\theta}\frac{\partial}{\partial\theta} - \frac{\sin\varphi\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi} - \frac{\sin\theta\cos\varphi}{\tan^2\theta}\cdot\frac{1}{\cos^2\theta}\frac{\partial}{\partial\varphi},\\
\left(\frac{i}{\hbar}\hat{\ell}_y\right)^2 &= \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)^2\\
&= \left(\cos\varphi\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)\cdot\left(\cos\varphi\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)\\
&= \left(\cos\varphi\frac{\partial}{\partial\theta}\right)\cdot\left(\cos\varphi\frac{\partial}{\partial\theta}\right) + \left(-\frac{\sin\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)\cdot\left(-\frac{\sin\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)\\
&\quad + \left(\cos\varphi\frac{\partial}{\partial\theta}\right)\cdot\left(-\frac{\sin\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right) + \left(-\frac{\sin\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)\cdot\left(\cos\varphi\frac{\partial}{\partial\theta}\right)\\
&= \cos^2\varphi\frac{\partial^2}{\partial\theta^2} + \frac{\sin^2\varphi}{\tan^2\theta}\frac{\partial^2}{\partial\varphi^2} - 2\frac{\sin\varphi\cos\varphi}{\tan\theta}\frac{\partial^2}{\partial\theta\partial\varphi} + \frac{\sin^2\theta}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{\sin\varphi\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi} + \frac{\sin\varphi\cos\varphi}{\tan^2\theta}\cdot\frac{1}{\cos^2\theta}\frac{\partial}{\partial\varphi},\\
\left(\frac{i}{\hbar}\hat{\ell}_z\right)^2 &= \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)^2\\
&= \left(\frac{\partial}{\partial\varphi}\right)\cdot\left(\frac{\partial}{\partial\varphi}\right)\\
&= \frac{\partial^2}{\partial\varphi^2},
\end{aligned}
$$

となるので，

$$
\begin{aligned}
\left(\frac{i}{\hbar}\hat{\ell}_x\right)^2+\left(\frac{i}{\hbar}\hat{\ell}_y\right)^2+\left(\frac{i}{\hbar}\hat{\ell}_z\right)^2 &= \frac{\partial^2}{\partial\theta^2}+\left(1+\frac{1}{\tan^2\theta}\right)\frac{\partial^2}{\partial\varphi^2}+\frac{1}{\tan\theta}\frac{\partial}{\partial\theta} \\
&= \frac{\partial^2}{\partial\theta^2}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}+\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta} \\
&= \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \\
&= \Lambda,
\end{aligned}
$$

即ち，

$$
\begin{aligned}
\hat{\boldsymbol{\ell}}\cdot\hat{\boldsymbol{\ell}} &= {\hat{\ell}_x}^{\,2}+{\hat{\ell}_y}^{\,2}+{\hat{\ell}_z}^{\,2} \\
&= -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] \\
&= -\hbar^2\Lambda,
\end{aligned}
$$

が得られた．

さて，以上の結果より，

$$
\hat{\boldsymbol{\ell}}\cdot\hat{\boldsymbol{\ell}}Y_\ell^m(\theta,\ \varphi)=-\hbar^2\Lambda Y_\ell^m(\theta,\ \varphi)=-\hbar^2[-\ell(\ell+1)Y_\ell^m(\theta,\ \varphi)]=\ell(\ell+1)\hbar^2Y_\ell^m(\theta,\ \varphi) \tag{15}
$$

が分かったわけだが，球面調和関数が，

$$
Y_\ell^m(\theta,\ \varphi)=\Theta(\theta)\mathit{\Phi}(\varphi)=(-1)^{\frac{m+|m|}{2}}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}P_\ell^{|m|}(\cos\theta)e^{im\varphi} \tag{16}
$$

と表され，φ 方向の成分が $e^{im\varphi}$ であることより，

$$
\hat{\ell}_zY_\ell^m(\theta,\ \varphi)=\frac{\hbar}{i}\frac{\partial}{\partial\varphi}Y_\ell^m(\theta,\ \varphi)=\frac{\hbar}{i}(im)Y_\ell^m(\theta,\ \varphi)=m\hbar Y_\ell^m(\theta,\ \varphi) \tag{17}
$$

となり，$Y_\ell^m(\theta,\ \varphi)$ は，$\hat{\boldsymbol{\ell}}\cdot\hat{\boldsymbol{\ell}}$ と $\hat{\ell}_z$ の同時固有関数になっている．一方，$\hat{\ell}_x$ 及び $\hat{\ell}_\mathrm{y}$ に対しては固有関数にならない．このような結果になると，まるで z 軸方向が特別な方向のように思えるが，そもそも元の微分方程式は球対称なポテンシャルに対するシュレディンガー方程式であったのだから，z 軸方向だけを特別扱いするのは不自然である．この結果はむしろ，球座標を

$$
x=r\sin\theta\cos\varphi, \tag{18}
$$

$$
y=r\sin\theta\sin\varphi, \tag{19}
$$

$$
z=r\cos\theta, \tag{20}
$$

と取った瞬間に，実は z 軸方向を固有関数になるように”定めてしまっていた”と見るべきであって，一般にどの方向を z 軸にとるかは自由であると考えるべきであろう．このように考えると，ある方向に角運動量を測定して”定めると”それに直交する方向の角運動量は未確定になってしまうことが分かる．