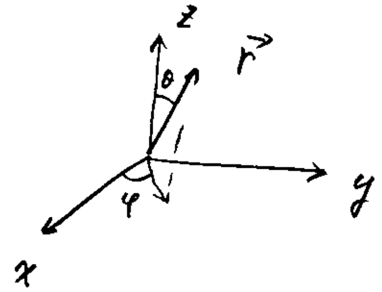
(複習) 3次元のシュレーディンガー方程式(球対称ポテンシャル)

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r) - E\right)\psi(\mathbf{r}) = 0$$

極座標

$$\begin{cases} x = r\sin\theta\cos\varphi \\ y = r\sin\theta\sin\varphi \\ z = r\cos\theta \end{cases}$$




↓

$$\left(-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\hat{\ell}^2\hbar^2}{2mr^2} + V(r) - E\right)\psi(\mathbf{r}) = 0$$

$$\hat{\ell}^2 = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$$

$$= (\mathbf{r}\times\mathbf{p})^2/\hbar^2 \equiv \mathbb{L}^2\hbar^2$$

$L_z = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}$ など

■ 今日の講義

- $[L_i, L_j] = i\hbar\,\varepsilon_{ijk}L_k$
- 球面調和関数

## 2.2. 角運動量演算子の性質

$$\hat{\mathbb{L}} = \hat{\mathbb{r}} \times \hat{\mathbb{p}}$$

(note) $[V(r), L_z] = [V(r), x p_y - y p_x]$

$$= x[V(r), p_y] - y[V(r), p_x]$$
$$= -\frac{\hbar}{i} x \frac{\partial}{\partial y} V(r) + \frac{\hbar}{i} y \frac{\partial}{\partial x} V(r)$$
$$= -\frac{\hbar}{i} x \cdot \frac{y}{r} V'(r) + \frac{\hbar}{i} y \cdot \frac{x}{r} V'(r) = 0.$$

同様に $\left[\frac{\mathbb{P}^2}{2m}, L_z\right] = 0$

↑
スカラー量

⇒ $H = \frac{\mathbb{P}^2}{2m} + V(r)$ に対し $[H, L_z] = 0$

同様に $[H, L_x] = [H, L_y] = 0$

また, $[H, \mathbb{L}^2] = [H, L_x^2 + L_y^2 + L_z^2]$
$$= L_x[H, L_x] + [H, L_x]L_x + \cdots$$
$$= 0$$

⇒ $H, L_x, L_y, L_z, \mathbb{L}^2$ の同時固有状態を作れる? → no

↑
$[L_i, L_j] = i\hbar \varepsilon_{ijk} L_k$
角運動量演算子は非可換.

$$[L_x, L_y] = [yp_z - zp_y,\ zp_x - xp_z]$$
$$= y[p_z, z]p_x + x[z, p_z]p_y$$
$$= \frac{\hbar}{i} y p_x + i\hbar x p_y$$
$$= i\hbar (x p_y - y p_x) = i\hbar L_z$$

同様に $[L_y, L_z] = i\hbar L_x$
$[L_z, L_x] = i\hbar L_y$

また，$[L_z, \mathbb{L}^2] = [L_z, L_x^2] + [L_z, L_y^2]$
$= i\hbar (L_x L_y + L_y L_x)$
$- i\hbar (L_x L_y + L_y L_x) = 0$ など.

$\Downarrow$

同時固有状態；$H, \mathbb{L}^2, (L_x, L_y, L_z)$ のうち1つ
$\downarrow$
$L_z$

(note) $[A, BC] = B[A, C] + [A, B]C$
$[AB, CD] = C[AB, D] + [AB, C]D$
$= CA[B, D] + C[A, D]B$
$+ A[B, C]D + [A, C]BD$

## 2.3. 角運動量演算子の固有状態

$$l_z = \frac{1}{i}\frac{\partial}{\partial\varphi}$$

と

$$l^2 = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin^2\theta}\underbrace{\frac{\partial^2}{\partial\varphi^2}}_{= -l_z^2}$$

の同時固有状態を作る。

- $\hat{l}_z$ の固有状態:

$$\hat{l}_z\,\Phi(\varphi) = \frac{1}{i}\frac{\partial}{\partial\varphi}\Phi(\varphi) = m\Phi(\varphi)$$

$$\longrightarrow \boxed{\Phi(\varphi) = \frac{1}{\sqrt{2\pi}}e^{im\varphi}}$$

(note) $\int_0^{2\pi} d\varphi\ |\Phi(\varphi)|^2 = 1.$

$\varphi$が1周したとき波動関数がもとのまま
ということを要求すると

$$\Phi(\varphi) = \Phi(\varphi + 2\pi)$$
$$= \frac{1}{\sqrt{2\pi}}e^{im\varphi}\cdot \underbrace{e^{i\cdot 2m\pi}}_{\downarrow\ 1}$$

$$\Downarrow\quad \boxed{m = 0, \pm 1, \pm 2, \cdots}$$

(note)

$$\begin{cases} \ell^2 |Y\rangle = \lambda |Y\rangle \\ \ell_z |Y\rangle = m |Y\rangle \end{cases}$$

として

$$(\hat{\ell}_x^2 + \hat{\ell}_y^2)|Y\rangle = (\hat{\ell}^2 - \hat{\ell}_z^2)|Y\rangle$$
$$= (\lambda - m^2)|Y\rangle$$

$\hat{\ell}_x^2 + \hat{\ell}_y^2$ の固有値は正

(オペレーターの2乗だから)

$\longrightarrow$ $-\sqrt{\lambda} \leq m \leq \sqrt{\lambda}$ の範囲に限定される。

- $\ell^2$ の固有状態.

$$\ell^2 Y(\theta,\varphi) = \left[-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] Y(\theta,\varphi)$$

$$= \lambda\, Y(\theta,\varphi)$$

$Y(\theta,\varphi) = \Theta(\theta)\,\Phi(\varphi)$ と変数分離すると

$$\Big[\underbrace{-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)}_{= -\frac{\partial^2}{\partial\theta^2} - \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta}} + \frac{m^2}{\sin^2\theta} - \lambda\Big]\Theta(\theta) = 0.$$

$x = \cos\theta$ とおくと

$$\frac{\partial}{\partial\theta} = \frac{\partial x}{\partial\theta}\frac{\partial}{\partial x} = -\sin\theta\frac{\partial}{\partial x}$$

$$\frac{\partial^2}{\partial\theta^2} = -\frac{\partial\sin\theta}{\partial\theta}\frac{\partial}{\partial x} - \sin\theta\cdot\frac{\partial}{\partial\theta}\frac{\partial}{\partial x}$$

$$= -\cos\theta\frac{\partial}{\partial x} + \sin^2\theta\frac{\partial^2}{\partial x^2}$$

$\Rightarrow$

$$\left[\cos\theta\frac{\partial}{\partial x} - \sin^2\theta\frac{\partial^2}{\partial x^2} + \frac{\cos\theta}{\cancel{\sin\theta}}\cdot\cancel{\sin\theta}\frac{\partial}{\partial x} + \frac{m^2}{\sin^2\theta} - \lambda\right]\Theta(\theta) = 0$$

$\Rightarrow$

$$-\left[(1-x^2)\frac{d^2}{dx^2} - 2x\frac{d}{dx} + \lambda - \frac{m^2}{1-x^2}\right]\Theta(x) = 0$$

解：ルジャンドル陪多項式 $P_\ell^m(x)$

$$\left[(1-x^2)\frac{d^2}{dx^2} - 2x\frac{d}{dx} + \ell(\ell+1) - \frac{m^2}{1-x^2}\right]P_\ell^m(x) = 0$$

$\Rightarrow$ $\boxed{\lambda = \ell(\ell+1),\quad \ell：整数,\quad -\ell \le m \le \ell.}$

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ルジャンドル陪多項式

定義： $$P_\ell^m(x) = \frac{1}{2^\ell \ell!}(1-x^2)^{\frac{m}{2}} \frac{d^{\ell+m}}{dx^{\ell+m}}(x^2-1)^\ell$$

$\ell$：整数

$-\ell \le m \le \ell$

$\ell=0$ : $P_0^0(x) = 1$

$\ell=1$ : $P_1^0(x) = x$

$P_1^1(x) = \sqrt{1-x^2}$

$\ell=2$ : $P_2^0(x) = \frac{1}{2}(3x^2-1)$

$P_2^1(x) = 3x\sqrt{1-x^2}$

$P_2^2(x) = 3(1-x^2)$ など

$$P_\ell^{-m}(x) = (-)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(x)$$

$$P_\ell^m(-x) = (-)^{\ell+m} P_\ell^m(x)$$

直交性： $$\int_{-1}^{1} P_\ell^m(x) P_{\ell'}^m(x)\,dx = \frac{2}{2\ell+1}\frac{(\ell+m)!}{(\ell-m)!} \times \delta_{\ell,\ell'}$$

## • 球面調和関数

以上より $l^2$ と $l_z$ の同時固有関数は

$$\boxed{Y_{lm}(\theta,\varphi) = (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\; P_l^m(\cos\theta)\, e^{im\varphi}}$$

球面調和関数

$$\boxed{\begin{aligned} l^2 \,|Y_{lm}\rangle &= l(l+1)\,|Y_{lm}\rangle \\ l_z \,|Y_{lm}\rangle &= m\,|Y_{lm}\rangle \end{aligned}}$$

$l$：整数（ゼロ又は正）

$-l \le m \le l$

$l=0$ : $Y_{00} = \frac{1}{\sqrt{4\pi}}$

$l=1$ : $Y_{11} = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\varphi}$

$Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta$

$Y_{1-1} = \sqrt{\frac{3}{8\pi}}\sin\theta\, e^{-i\varphi}$

$l=2$ : $Y_{20} = \sqrt{\frac{5}{4\pi}} \cdot \frac{1}{2}(3\cos^2\theta - 1)$

(note)
$$\left[-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)-\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\left(\sin\theta\, e^{\pm i\varphi}\right)$$

$$=\left[-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\cos\theta\right)-\frac{1}{\sin^2\theta}\cdot(-1)\sin\theta\right]e^{\pm i\varphi}$$

$$=\left[-\frac{1}{\sin\theta}\left(\underbrace{\cos^2\theta-\sin^2\theta}_{\parallel \atop 1-2\sin^2\theta}\right)+\frac{1}{\sin\theta}\right]e^{\pm i\varphi}$$

$$=\left(\cancel{-\frac{1}{\sin\theta}}+2\sin\theta\cancel{+\frac{1}{\sin\theta}}\right)e^{\pm i\varphi}$$

$$=2\sin\theta\, e^{\pm i\varphi}\quad=\quad 1\cdot(1+1)\sin\theta\, e^{\pm i\varphi}$$

(note)
$$\left[-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)-\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\left(3\cos^2\theta-1\right)$$

$$=-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\cdot 6\cos\theta\cdot(-\sin\theta)\right)$$

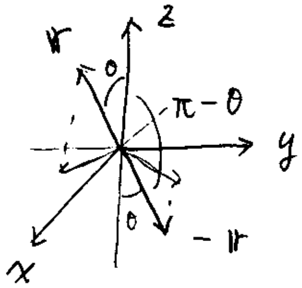
$$=\frac{6}{\sin\theta}\frac{\partial}{\partial\theta}\left(\cos\theta\underbrace{\sin^2\theta}_{\parallel \atop 1-\cos^2\theta}\right)$$

$$=\frac{6}{\sin\theta}\left(-\sin\theta-3\cos^2\theta\cdot(-\sin\theta)\right)$$

$$=6\cdot\left(3\cos^2\theta-1\right)$$

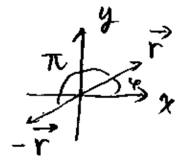
$$=2\times(2+1)\cdot\left(3\cos^2\theta-1\right)$$

## 性質




$$Y_{\ell\,-m}(\underbrace{\hat{\mathbf{r}}}_{=(\theta,\varphi)}) = (-1)^m\, Y_{\ell m}(\hat{\mathbf{r}})^*$$

$$Y_{\ell m}(-\hat{\mathbf{r}}) = Y_{\ell m}(\pi-\theta,\ \varphi+\pi) = \underbrace{(-1)^\ell}_{\text{パリティ}}\, Y_{\ell m}(\hat{\mathbf{r}})$$




## 規格化：

(note) $d\mathbf{r} = r^2 dr\, \sin\theta d\theta\, d\varphi$

$$\underbrace{\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta}_{\equiv \int d\hat{\mathbf{r}}}\ \ Y_{\ell m}^*(\theta,\varphi)\, Y_{\ell' m'}(\theta,\varphi) = \delta_{\ell,\ell'}\, \delta_{m,m'}$$

$$\langle Y_{\ell m} | Y_{\ell' m'} \rangle = \delta_{\ell\ell'}\, \delta_{m,m'}$$

## 加法定理

$$\frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_{\ell m}(\hat{\mathbf{r}}_1)\, Y_{\ell m}(\hat{\mathbf{r}}_2)^* = P_\ell(\cos\gamma)$$

$P_\ell$: ルジャンドル多項式

$\gamma$: $\hat{\mathbf{r}}_1$ と $\hat{\mathbf{r}}_2$ のなす角