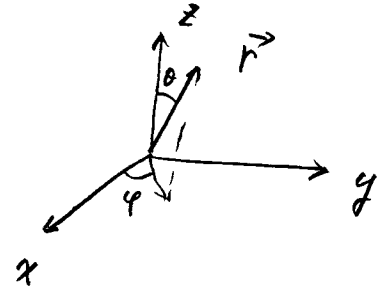


(複習) 3次元のシュレ-ディンガー-方程式 (球対称ポテンシャル)

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

極座標

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



↓

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

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

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

$$L_z = \frac{\hbar}{i} \frac{\partial}{\partial \varphi} \quad \text{「じと」}$$

■ 今日の講義

- $[L_i, L_j] = i\hbar \epsilon_{ijk} L_k$

- 球面調和関数.

$$[H, \mathbb{L}^2] = 0$$

$$\psi(r) = R(r) Y(\theta, \varphi)$$

$$\left\{ \left[T_r + \frac{\lambda \hbar^2}{2mr^2} + V(r) - E \right] R(r) \right\} Y(\theta, \varphi) = 0$$

= 0

2.2. 角運動量演算子の性質

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

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

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

同様に $[\frac{p^2}{2m}, L_z] = 0$

↑
スカラー-量

$$\begin{aligned} [p^2, L_z] &= [p_x^2 + p_y^2 + p_z^2, x p_y - y p_x] \\ &= [p_x^2, x] p_y - [p_y^2, y] p_x \\ &= -2i\hbar p_x p_y + 2i\hbar p_y p_x = 0 \end{aligned}$$

↓

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

同様に $[H, L_x] = [H, L_y] = 0$

$$\begin{aligned} \text{また, } [H, L^2] &= [H, L_x^2 + L_y^2 + L_z^2] \\ &= L_x [H, L_x] + [H, L_x] L_x + \dots \\ &= 0 \end{aligned}$$

↓ H, L_x, L_y, L_z, L^2 の同時固有状態を作れる？

→ no

↑

$$[L_i, L_j] = i\hbar \epsilon_{ijk} L_k$$

角運動量演算子は非可換。

$$\begin{aligned}
 [L_x, L_y] &= [y P_z - z P_y, z P_x - x P_z] \\
 &= y [P_z, z] P_x + x [z, P_z] P_y \\
 &= \frac{\hbar}{i} y P_x + i \hbar x P_y \\
 &= i \hbar (x P_y - y P_x) = i \hbar L_z
 \end{aligned}$$

同様にして

$$\begin{aligned}
 [L_y, L_z] &= i \hbar L_x \\
 [L_z, L_x] &= i \hbar L_y
 \end{aligned}$$

また,

$$\begin{aligned}
 [L_z, L^2] &= [L_z, L_x^2] + [L_z, L_y^2] \\
 &= i \hbar (L_x L_y + L_y L_x) \\
 &\quad - i \hbar (L_x L_y + L_y L_x) = 0 \quad \text{「だ」}
 \end{aligned}$$

↓

同時固有状態 ; $H, L^2, (L_x, L_y, L_z)$ のうち
↓
 L_z

(note)

$$\begin{aligned}
 [A, BC] &= B [A, C] + [A, B] C \\
 [AB, CD] &= C [AB, D] + [AB, C] D \\
 &= CA [B, D] + C [A, D] B \\
 &\quad + A [B, C] D + [A, C] B D
 \end{aligned}$$

2.3. 角運動量演算子の固有状態

$$l_z = \frac{1}{i} \frac{\partial}{\partial \varphi} \quad \left(= \frac{L_z}{\hbar} \right)$$

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

の同時固有状態を作る。

- l_z の固有状態:

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

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

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

φ が 1 周したとき波動関数が m だけ増える
ということをお求めすると

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

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

(note)

$$\begin{cases} \hat{l}^2 |Y\rangle = \lambda |Y\rangle \\ \hat{l}_z |Y\rangle = m |Y\rangle \end{cases}$$

とすると

$$\begin{aligned} (\hat{l}_x^2 + \hat{l}_y^2) |Y\rangle &= (\hat{l}^2 - \hat{l}_z^2) |Y\rangle \\ &= (\lambda - m^2) |Y\rangle \end{aligned}$$

$\hat{l}_x^2 + \hat{l}_y^2$ の固有値は正
($\hat{l}_x^2 + \hat{l}_y^2 = \hat{l}^2 - \hat{l}_z^2$ の「乗数」から)

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

• l^2 の固有状態.

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

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

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

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

$x = \cos\theta$ とおくと

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

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

↓

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

↓

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

解: ルジャンドル陪多項式 $P_l^m(x)$

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

$$\lambda = l(l+1), \quad l: \text{整数}, \quad -l \leq m \leq l.$$

ルジャンドル陪多項式

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

l : 整数
 $-l \leq m \leq l$

$l=0$: $P_0^0(x) = 1$

$l=1$: $P_1^0(x) = x$

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

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

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

$P_2^2(x) = 3(1-x^2)$

72 &''

$$P_l^{-m}(x) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(x)$$

$$P_l^m(-x) = (-1)^{l+m} P_l^m(x)$$

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

• 球面調和関数

以上より l^2 と l_z の 同時固有関数は

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

球面調和関数

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

l : 整数 (ゼロ 又は 正)
 $-l \leq m \leq l$

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

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

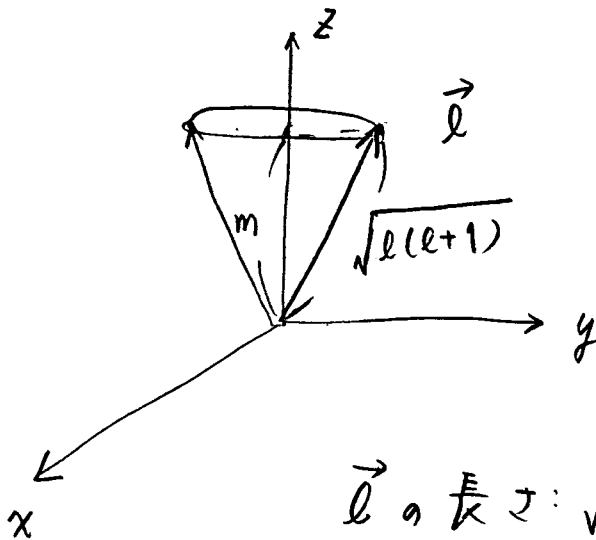
$$Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\theta$$

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

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

(note) $\hat{L}^2 |Y_{lm}\rangle = l(l+1) |Y_{lm}\rangle$
 $\hat{L}_z |Y_{lm}\rangle = m |Y_{lm}\rangle$

$$-l \leq m \leq l$$



$$\vec{l} \text{ の長さ: } \sqrt{l(l+1)} > l$$

↓ l_z を決めると l_x, l_y がい
決まらない。