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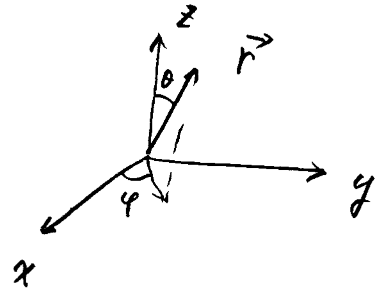
(複習)　3次元のシュレーディンガー方程式 (球対称ポテンシャル)

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

極座標

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



$$\downarrow$$

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

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

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

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

▨ 今日の講義

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

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

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

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

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2.2. 角運動量演算子の性質

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

(note) $[V(r), L_z] = [V(r), xP_y - yP_x]$

$= [V(r), \frac{\hbar}{i}\frac{\partial}{\partial\varphi}]$

$= -\frac{\hbar}{i}\frac{\partial V}{\partial \varphi} = 0$

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

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

↑
スカラー量

$$\left(\begin{aligned} [\mathbb{P}^2, L_z] &= [P_x^2 + P_y^2 + P_z^2, xP_y - yP_x] \\ &= [P_x^2, x]P_y - [P_y^2, y]P_x \\ &= -2i\hbar P_x P_y + 2i\hbar P_y P_x = 0 \end{aligned} \right)$$

↓

$H = \frac{\mathbb{P}^2}{2m} + V(r)$ 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.

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

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

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

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

と

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

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

φ 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。

● ℓ^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

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

$x = \cos\theta$ とおくと

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

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

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

$\to$

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

$\to$

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

解：ルジャンドル陪多項式 $P_\ell^m(x)$

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

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

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ルジャンドル陪多項式

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

ℓ : 整数

$-\ell \leq m \leq \ell$

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

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

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

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

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

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

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

球面調和関数

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

ℓ：整数（ゼロ又は正）
$-\ell \le m \le \ell$

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

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

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

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

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

※ 位相の $(-1)^m$ は慣習 (convention)

$(-1)^m$ がある場合

$$e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right)Y_{\ell m} = \pm\sqrt{(\ell-m)(\ell+m+1)}\; Y_{\ell\, m+1}$$

$(-1)^m$ がない場合

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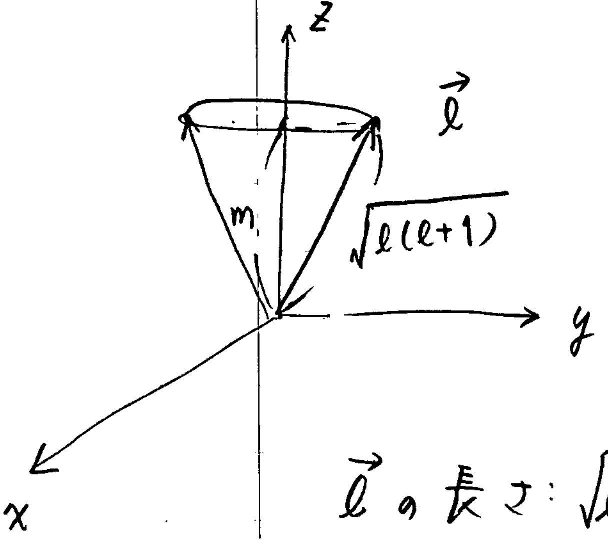
(note) $\hat{\ell}^2 |Y_{\ell m}\rangle = \ell(\ell+1)|Y_{\ell m}\rangle$

$\hat{\ell}_z |Y_{\ell m}\rangle = m |Y_{\ell m}\rangle$

$-\ell \leq m \leq \ell$



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

⇕ ℓ_zを決めると ℓ_x, ℓ_yが決まらない。