

1. 3次元球対称ポテンシャル中の運動

1次元ポテンシャル中の運動 ← 量子力学 I

$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi(x) = E \psi(x)$$

$$\text{ハミルトン} = \hat{P} \rightarrow H = \frac{P^2}{2m} + V(x)$$

$$\int_{-\infty}^{\infty} dx |\psi(x)|^2 = 1 \quad (\text{規格化条件})$$

→ 3次元ポテンシャルへの拡張

$$H = \frac{1}{2m} (P_x^2 + P_y^2 + P_z^2) + V(x, y, z) \\ = \frac{P^2}{2m} + V(r)$$

$$\text{座標表示: } \hat{P} = \frac{\hbar}{i} \nabla \quad (P_k = \frac{\hbar}{i} \frac{\partial}{\partial x_k})$$

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V(r)$$

"  $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

シムル-ティンカ'-方程式:

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

波動関数の規格化:

$$\underbrace{\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz |\psi(r)|^2}_{=} = 1$$

$$\int dr$$

ポテンシャルが変数分離型の時,

例) 3次元調和振動子

$$V(x, y, z) = \frac{1}{2} m \omega_x^2 x^2 + \frac{1}{2} m \omega_y^2 y^2 + \frac{1}{2} m \omega_z^2 z^2$$

↓

$$H = \underbrace{\frac{P_x^2}{2m} + \frac{1}{2} m \omega_x^2 x^2}_{\hbar \omega_x} + \underbrace{\frac{P_y^2}{2m} + \frac{1}{2} m \omega_y^2 y^2}_{\hbar \omega_y} + \underbrace{\frac{P_z^2}{2m} + \frac{1}{2} m \omega_z^2 z^2}_{\hbar \omega_z}$$

シュレディンガー方程式の解

$$\Psi(x, y, z) = \phi_{n_x}^{(1)}(x) \phi_{n_y}^{(2)}(y) \phi_{n_z}^{(3)}(z)$$

$$\left( \frac{P_x^2}{2m} + \frac{1}{2} m \omega_x^2 x^2 \right) \phi_{n_x}^{(1)}(x) = (n_x + \frac{1}{2}) \hbar \omega_x \times \phi_{n_x}^{(1)}(x)$$

ただし

$$E = (n_x + \frac{1}{2}) \hbar \omega_x + (n_y + \frac{1}{2}) \hbar \omega_y + (n_z + \frac{1}{2}) \hbar \omega_z$$

(note)  $\boxed{\omega_x = \omega_y = \omega_z \text{ のとき}}$   
 $\equiv \omega$

$$E = (n_x + n_y + n_z + \frac{3}{2}) \hbar \omega$$

$$V(x, y, z) = \frac{1}{2} m \omega^2 \underbrace{(x^2 + y^2 + z^2)}_{r^2}$$

→ 極座標  
を用いても解ける。

(複習) 変数分離

$$H = \underbrace{\frac{p_x^2}{2m} + V(x)}_{\hbar_x} + \underbrace{\frac{p_y^2}{2m} + V(y)}_{\hbar_y}$$

$$H \Psi(x, y) = E \Psi(x, y)$$

$$\Psi(x, y) = X(x) Y(y) \quad \text{とあ'く。}$$

$$\downarrow H \Psi = (\hbar_x X) Y + X (\hbar_y Y)$$

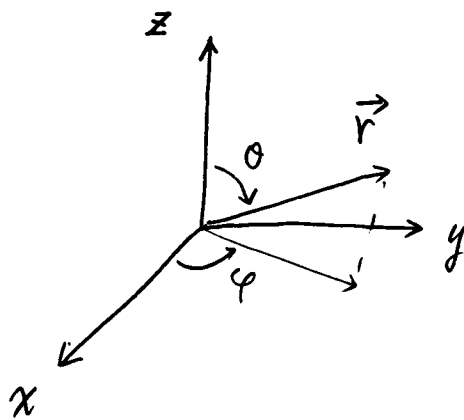
$$\begin{aligned} \leadsto \quad \hbar_x X &= E_x X \\ \hbar_y Y &= E_y Y \quad \text{の とき} \end{aligned}$$

$$H \Psi = (E_x + E_y) X \cdot Y = \underbrace{(E_x + E_y)}_E \Psi$$

ポテンシャルが球対称の時 ( $r$  の大きさ  $r = |\mathbf{r}|$  にか  
依存しない場合)

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

→ 極座標表示をすることにより  
変数分離が可能



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

$$(r = \sqrt{x^2 + y^2 + z^2})$$

微分  $\nabla$  を極座標を使って書く:

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x} \frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial x} \frac{\partial}{\partial \varphi}$$

(note)  $r = \sqrt{x^2 + y^2 + z^2} \rightarrow \frac{\partial r}{\partial x} = \frac{x}{r}$

(note)  $z = r \cos \theta$  の両辺を  $x$  で微分すると

$$0 = \underbrace{\frac{\partial r}{\partial x} \cos \theta}_{= \frac{x}{r}} - r \sin \theta \frac{\partial \theta}{\partial x}$$

$$\rightarrow \frac{\partial \theta}{\partial x} = \frac{x \cos \theta}{r^2 \sin \theta} = \frac{1}{r} \cos \theta \cos \varphi$$

(note)  $y = r \sin \theta \sin \varphi$  の両辺を  $x$  で微分

↓

$$0 = \frac{\partial r}{\partial x} \sin \theta \sin \varphi + r \cos \theta \frac{\partial \theta}{\partial x} \sin \varphi + r \sin \theta \cos \varphi \frac{\partial \varphi}{\partial x}$$

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

$$= \sin \varphi \cos \varphi + r \sin \theta \cos \varphi \frac{\partial \varphi}{\partial x}$$

$$\leadsto \frac{\partial \varphi}{\partial x} = - \frac{\sin \varphi}{r \sin \theta}$$

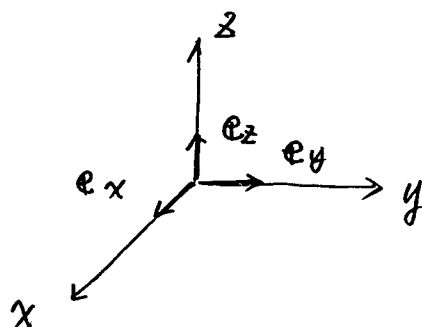
$$\leadsto \frac{\partial}{\partial x} = \sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \cos \varphi \frac{\partial}{\partial \theta} - \frac{\sin \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi}$$

$\frac{\partial}{\partial y}, \frac{\partial}{\partial z}$  も同様に求められる。

$$\nabla = \frac{\partial}{\partial x} \mathbf{e}_x + \frac{\partial}{\partial y} \mathbf{e}_y + \frac{\partial}{\partial z} \mathbf{e}_z = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$$

$$\begin{aligned} \nabla = & \left[ \sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \cos \varphi \frac{\partial}{\partial \theta} - \frac{\sin \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \right] \mathbf{e}_x \\ & + \left[ \sin \theta \sin \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \sin \varphi \frac{\partial}{\partial \theta} + \frac{\cos \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \right] \mathbf{e}_y \\ & + \left[ \cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \right] \mathbf{e}_z \end{aligned}$$

$\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$  は  $x, y, z$  方向の単位ベクトル



$$|\mathbf{e}_k| = 1$$

さらにもう一度微分演算を行えば"

$\nabla^2$  の極座標表示が得られる (うしろの A'-ジ' 参照)

↓

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}$$

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

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

↓

↔ 角運動量 (後ほど)

シュレ-ディンガー-方程式:

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

角度に関する演算子は  $\hat{L}^2$  のみ。

もし  $\hat{L}^2$  の固有状態  $\hat{L}^2 Y(\theta, \varphi) = \lambda Y(\theta, \varphi)$  がわかれば

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

と変数分離すれば

$$\left[ -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{\lambda \hbar^2}{2mr^2} + V(r) - E \right] R(r) = 0$$

となり、 $r$  のみの 2 階の微分方程式となる。

[参考]  $\nabla^2$  の極座標表示の導出

$$\begin{aligned} \frac{\partial^2}{\partial x^2} &= \left( \sin\theta \cos\varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos\theta \cos\varphi \frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta} \frac{\partial}{\partial\varphi} \right)^2 \\ &= \sin^2\theta \cos^2\varphi \frac{\partial^2}{\partial r^2} + \frac{1}{r^2} \cos^2\theta \cos^2\varphi \frac{\partial^2}{\partial\theta^2} + \frac{\sin^2\varphi}{r^2 \sin^2\theta} \frac{\partial^2}{\partial\varphi^2} \\ &\quad + \frac{2}{r} \sin\theta \cos\theta \cos^2\varphi \frac{\partial^2}{\partial r \partial\theta} - \frac{2}{r^2} \frac{\cos\theta}{\sin\theta} \sin\varphi \cos\varphi \frac{\partial^2}{\partial\theta \partial\varphi} \\ &\quad - \frac{2}{r} \sin\varphi \cos\varphi \frac{\partial^2}{\partial r \partial\varphi} \\ &\quad - \frac{1}{r^2} \sin\theta \cos\theta \cos^2\varphi \frac{\partial^2}{\partial\theta^2} + \frac{1}{r^2} \sin\varphi \cos\varphi \frac{\partial^2}{\partial\varphi^2} \\ &\quad + \frac{1}{r} \cos^2\theta \cos^2\varphi \frac{\partial^2}{\partial r} - \frac{1}{r^2} \sin\theta \cos\theta \cos^2\varphi \frac{\partial}{\partial\theta} + \frac{\cos\theta \cos\varphi}{r} \frac{\sin\varphi}{r} \\ &\quad \times \frac{\cos\theta}{\sin^2\theta} \frac{\partial}{\partial\varphi} \\ &\quad + \frac{\sin\varphi}{r\sin\theta} \sin\theta \sin\varphi \frac{\partial}{\partial r} + \frac{\sin\varphi}{r\sin\theta} \cdot \frac{1}{r} \cos\theta \sin\varphi \frac{\partial}{\partial\theta} \\ &\quad + \frac{\sin\varphi}{r\sin\theta} \cdot \frac{\cos\varphi}{r\sin\theta} \frac{\partial}{\partial\varphi} \end{aligned}$$

$$\begin{aligned} \frac{\partial^2}{\partial y^2} &= \left( \sin\theta \sin\varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos\theta \sin\varphi \frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta} \frac{\partial}{\partial\varphi} \right)^2 \\ &= \sin^2\theta \sin^2\varphi \frac{\partial^2}{\partial r^2} + \frac{1}{r^2} \cos^2\theta \sin^2\varphi \frac{\partial^2}{\partial\theta^2} + \frac{\cos^2\varphi}{r^2 \sin^2\theta} \frac{\partial^2}{\partial\varphi^2} \\ &\quad + \frac{2}{r} \sin\theta \cos\theta \sin^2\varphi \frac{\partial^2}{\partial r \partial\theta} + \frac{2}{r^2} \frac{\cos\theta}{\sin\theta} \sin\varphi \cos\varphi \frac{\partial^2}{\partial\theta \partial\varphi} \\ &\quad + \frac{2}{r} \sin\theta \cos\varphi \frac{\partial^2}{\partial r \partial\varphi} \\ &\quad - \frac{1}{r^2} \sin\theta \cos\theta \sin^2\varphi \frac{\partial^2}{\partial\theta^2} - \frac{1}{r^2} \sin\varphi \cos\varphi \frac{\partial^2}{\partial\varphi^2} \\ &\quad + \frac{1}{r} \cos^2\theta \sin^2\varphi \frac{\partial^2}{\partial r} - \frac{1}{r^2} \sin\theta \cos\theta \sin^2\varphi \frac{\partial}{\partial\theta} + \frac{\cos\theta \sin\varphi}{r} \cdot \frac{\cos\varphi}{r} \\ &\quad \left( -\frac{\cos\theta}{\sin^2\theta} \right) \frac{\partial}{\partial\varphi} \\ &\quad + \frac{\cos\varphi}{r\sin\theta} \sin\theta \cos\varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos\theta \cos\varphi \cdot \frac{\cos\varphi}{r\sin\theta} \frac{\partial}{\partial\theta} \\ &\quad - \frac{\cos\varphi \sin\varphi}{r^2 \sin^2\theta} \frac{\partial}{\partial\varphi} \end{aligned}$$

↓

$$\begin{aligned} \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} &= \sin^2 \theta \frac{\partial^2}{\partial r^2} + \frac{1}{r^2} \cos^2 \theta \frac{\partial^2}{\partial \theta^2} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \\ &+ \frac{2}{r} \sin \theta \cos \theta \frac{\partial^2}{\partial r \partial \theta} - \frac{1}{r^2} \sin \theta \cos \theta \frac{\partial}{\partial \theta} \\ &+ \frac{1}{r} \cos^2 \theta \frac{\partial}{\partial r} - \frac{1}{r^2} \sin \theta \cos \theta \frac{\partial}{\partial \theta} + \frac{1}{r} \frac{\partial}{\partial r} \\ &+ \frac{\cos \theta}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \end{aligned}$$

U

$$\begin{aligned} \frac{\partial^2}{\partial z^2} &= \left( \cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \right)^2 \\ &= \cos^2 \theta \frac{\partial^2}{\partial r^2} + \frac{\sin^2 \theta}{r^2} \frac{\partial^2}{\partial \theta^2} - \frac{2 \sin \theta \cos \theta}{r} \frac{\partial^2}{\partial r \partial \theta} \\ &+ \frac{1}{r^2} \sin \theta \cos \theta \frac{\partial}{\partial \theta} + \frac{\sin^2 \theta}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \sin \theta \cos \theta \frac{\partial}{\partial \theta} \end{aligned}$$

↓

$$\begin{aligned} \nabla^2 &= \frac{\partial^2}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} + \frac{2}{r} \frac{\partial}{\partial r} \\ &+ \frac{\cos \theta}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \end{aligned}$$

U

$$= \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}$$



## 2. 角運動量

### 2.1. 角運動量演算子の極座標表示

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

は角運動量の2乗を  $\hbar^2 l(l+1)$  "割" ったもの:

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

○ (note)  $L_z = x p_y - y p_x = \frac{\hbar}{i} (x \partial_y - y \partial_x)$

$$= \frac{\hbar}{i} \left\{ r \sin\theta \cos\varphi \left( \cancel{\sin\theta \sin\varphi \partial_r} + \frac{1}{r} \cancel{\cos\theta \sin\varphi \partial_\theta} + \frac{\cos\varphi}{r \sin\theta} \partial_\varphi \right) - r \sin\theta \sin\varphi \left( \cancel{\sin\theta \cos\varphi \partial_r} + \frac{1}{r} \cancel{\cos\theta \cos\varphi \partial_\theta} - \frac{\sin\varphi}{r \sin\theta} \partial_\varphi \right) \right\}$$

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

○ 同様に

$$L_x = \frac{\hbar}{i} (-\sin\varphi \partial_\theta - \frac{\cos\theta}{\sin\theta} \cos\varphi \partial_\varphi)$$

$$L_y = \frac{\hbar}{i} (\cos\varphi \partial_\theta - \frac{\cos\theta}{\sin\theta} \sin\varphi \partial_\varphi)$$

↷

$$L_x^2 + L_y^2 + L_z^2 = -\hbar^2 \left( -\sin\varphi \partial_\theta - \frac{\cos\theta}{\sin\theta} \cos\varphi \partial_\varphi \right)^2 \\ - \hbar^2 \left( \cos\varphi \partial_\theta - \frac{\cos\theta}{\sin\theta} \sin\varphi \partial_\varphi \right)^2 \\ - \hbar^2 \partial_\varphi^2$$

$$= -\hbar^2 \left\{ \partial_\theta^2 + \frac{\cos^2\theta}{\sin^2\theta} \partial_\varphi^2 + \partial_\varphi^2 \right.$$

$$+ \cancel{\sin\varphi \cos\varphi \left( \frac{-\sin\theta}{\sin\theta} - \frac{\cos^2\theta}{\sin^2\theta} \right) \partial_\varphi}$$

$$- \cancel{\sin\varphi \cos\varphi \left( \frac{-\sin\theta}{\sin\theta} - \frac{\cos^2\theta}{\sin^2\theta} \right) \partial_\varphi}$$

$$+ \frac{\cos\theta}{\sin\theta} \cos^2\varphi \partial_\theta + \frac{\cos\theta}{\sin\theta} \sin^2\varphi \partial_\theta \left. \right\}$$

$$= -\hbar^2 \left( \partial_\theta^2 + \frac{\cos\theta}{\sin\theta} \partial_\theta + \frac{1}{\sin^2\theta} \partial_\varphi^2 \right)$$

$$= \ell^2 \hbar^2$$

U

U

(note)

$$\begin{aligned}
 & \left( -\sin\varphi \partial_\theta - \frac{\cos\theta}{\sin\theta} \cos\varphi \partial_\varphi \right)^2 \\
 &= \left( -\sin\varphi \partial_\theta - \frac{\cos\theta}{\sin\theta} \cos\varphi \partial_\varphi \right) \left( -\sin\varphi \partial_\theta - \frac{\cos\theta}{\sin\theta} \cos\varphi \partial_\varphi \right) \\
 &= \sin^2\varphi \partial_\theta^2 + \sin\varphi \cos\varphi \underbrace{\left( \partial_\theta \frac{\cos\theta}{\sin\theta} \right)}_{\substack{= \\ -\frac{\sin\theta}{\sin^2\theta} - \frac{\cos^2\theta}{\sin^2\theta}} \partial_\varphi} + \frac{\cos\theta}{\sin\theta} \sin\varphi \cos\varphi \partial_\varphi \partial_\theta \\
 &\quad + \frac{\cos\theta}{\sin\theta} \cos^2\varphi \partial_\theta + \frac{\cos\theta}{\sin\theta} \sin\varphi \cos\varphi \partial_\theta \partial_\varphi \\
 &\quad + \frac{\cos^2\theta}{\sin^2\theta} \cos\varphi \underbrace{\partial_\varphi (\cos\varphi \partial_\varphi)}_{=} \\
 &\quad \quad \quad - \sin\varphi \partial_\varphi + \cos\varphi \partial_\varphi^2
 \end{aligned}$$

同様にして

$$\begin{aligned}
 & \left( \cos\varphi \partial_\theta - \frac{\cos\theta}{\sin\theta} \sin\varphi \partial_\varphi \right)^2 \\
 &= \left( \cos\varphi \partial_\theta - \frac{\cos\theta}{\sin\theta} \sin\varphi \partial_\varphi \right) \left( \cos\varphi \partial_\theta - \frac{\cos\theta}{\sin\theta} \sin\varphi \partial_\varphi \right) \\
 &= \cos^2\varphi \partial_\theta^2 - \sin\varphi \cos\varphi \left( \partial_\theta \frac{\cos\theta}{\sin\theta} \right) \partial_\varphi - \frac{\cos\theta}{\sin\theta} \sin\varphi \cos\varphi \partial_\varphi \partial_\theta \\
 &\quad + \frac{\cos\theta}{\sin\theta} \sin^2\varphi \partial_\theta - \frac{\cos\theta}{\sin\theta} \sin\varphi \cos\varphi \partial_\theta \partial_\varphi \\
 &\quad + \frac{\cos^2\theta}{\sin^2\theta} \sin\varphi \underbrace{\partial_\varphi (\sin\varphi \partial_\varphi)}_{=} \\
 &\quad \quad \quad \cos\varphi \partial_\varphi + \sin\varphi \partial_\varphi^2
 \end{aligned}$$