(復習)

ド・ブロイ　物質波

$$\psi(\mathbf{r},t) = e^{i\mathbf{p}\cdot\mathbf{r}/\hbar - iEt/\hbar}$$

シュレーディンガー

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi$$

$$\xrightarrow[\text{拡張}]{} \quad i\hbar\frac{\partial}{\partial t}\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi$$

波動関数

$$\begin{cases} E \to i\hbar\frac{\partial}{\partial t} \\ \mathbf{p} \to \frac{\hbar}{i}\nabla \end{cases}$$

- 波動関数の意味

$$P(\mathbf{r},t)\,d\mathbf{r} = |\psi(\mathbf{r},t)|^2 d\mathbf{r}$$

粒子が点 $\mathbf{r}$ にいる確率

$$\to \quad 1 = \int d\mathbf{r}\, |\psi(\mathbf{r},t)|^2 \qquad \text{(規格化)}$$

◎ 密度とフラックス

(確率)密度 ： $\rho(\mathbf{r},t) = |\psi(\mathbf{r},t)|^2$

(確率の)流れ (流束；フラックス)

$$\mathbf{j} = \frac{\hbar}{2im}\left(\psi^* \nabla \psi - \psi \nabla \psi^*\right)$$

$$\rightarrow \quad \nabla\cdot\mathbf{j} = \frac{\hbar}{2im}\left(\cancel{\nabla\psi^*\cdot\nabla\psi} + \psi^*\nabla^2\psi - \cancel{\nabla\psi\cdot\nabla\psi^*} - \psi\nabla^2\psi^*\right)$$

$$= \frac{\hbar}{2im}\cdot\left(-\frac{2m}{\hbar^2}\right)\left(\psi^*\left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi - \psi\left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi^*\right)$$

$$= \frac{i}{\hbar}\left(\psi^*\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi - \psi\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi^*\right)$$

$$= \frac{i}{\hbar}\left(\psi^*\left(i\hbar\frac{\partial}{\partial t}\right)\psi - \psi\left(-i\hbar\frac{\partial}{\partial t}\right)\psi^*\right)$$

$$= \frac{i}{\hbar}\cdot i\hbar\frac{\partial}{\partial t}(\psi^*\psi) = -\frac{\partial}{\partial t}|\psi|^2 = -\frac{\partial\rho}{\partial t}$$

$$\downarrow \quad \boxed{\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j} = 0} \quad \text{(連続の方程式)}$$

→ 全空間で積分すると

$$\frac{\partial}{\partial t}\int d\mathbf{r}\, \rho(\mathbf{r},t) = -\int d\mathbf{r}\, \nabla\cdot\mathbf{j}(\mathbf{r},t)$$

もし $\psi(\mathbf{r},t)$ が空間のある点 $\mathbf{r}_0$ で不連続があると
この方程式は成り立たない → 非物理的

2.3. 演算子の期待値

$$P(\mathbf{r},t) = |\psi(\mathbf{r},t)|^2$$

$$\rightarrow \quad \langle \mathbf{r} \rangle = \int d\mathbf{r}\ \mathbf{r}\, P(\mathbf{r},t) = \int d\mathbf{r}\ |\psi(\mathbf{r},t)|^2 \cdot \mathbf{r}$$

$$\langle f(\mathbf{r}) \rangle = \int d\mathbf{r}\ f(\mathbf{r})\, P(\mathbf{r},t) = \int d\mathbf{r}\ |\psi(\mathbf{r},t)|^2 f(\mathbf{r})$$

$$\downarrow$$

$$\frac{d}{dt}\langle \mathbf{r} \rangle = \int d\mathbf{r}\ \mathbf{r}\,[\dot{\psi}^* \psi + \psi^* \dot{\psi}]$$

(note) $i\hbar\dot{\psi} = H\psi$
$-i\hbar\dot{\psi}^* = H\psi^*$

$$= \int d\mathbf{r}\ \mathbf{r} \cdot \frac{1}{i\hbar}\Big[+\frac{\hbar^2}{2m}(\nabla^2\psi^*)\psi - \cancel{V\psi^*\psi} - \frac{\hbar^2}{2m}\psi^*(\nabla^2\psi) + \cancel{V\psi^*\psi}\Big]$$

$$= \frac{\hbar}{2im}\int d\mathbf{r}\ [\psi^*\nabla^2(\mathbf{r}\psi) - \psi^*(\nabla^2\psi)]$$

$$= \frac{\hbar}{im}\int d\mathbf{r}\ \psi^*\nabla\psi$$

$$\rightarrow \quad \underbrace{\frac{d}{dt}\langle m\mathbf{r} \rangle}_{\updownarrow\ \langle \mathbf{p} \rangle} = \int d\mathbf{r}\ \psi^* \underbrace{\left(\frac{\hbar}{i}\nabla\right)}_{=\ \hat{\mathbf{p}}}\psi$$

・運動量表示と座標表示

波動関数のフーリエ逆変換

$$\tilde{\psi}(\mathbb{p},t)=\frac{1}{(2\pi\hbar)^{3/2}}\int d\mathbb{r}\ \psi(\mathbb{r},t)\,e^{-i\mathbb{p}\cdot\mathbb{r}/\hbar}$$

：運動量表示

$$\rightarrow\quad \psi(\mathbb{r},t)=\frac{1}{(2\pi\hbar)^{3/2}}\int d\mathbb{p}\ \tilde{\psi}(\mathbb{p},t)\,e^{i\mathbb{p}\cdot\mathbb{r}/\hbar}$$

：座標表示

(note)

$$\langle\mathbb{p}\rangle=\int d\mathbb{r}\ \psi^*(\mathbb{r},t)\left(\frac{\hbar}{i}\nabla\right)\psi(\mathbb{r},t)$$

$$=\frac{1}{(2\pi\hbar)^3}\int d\mathbb{r}\,d\mathbb{p}\,d\mathbb{p}'\ \tilde{\psi}^*(\mathbb{p},t)\cdot\left(\frac{\hbar}{i}\frac{i}{\hbar}\mathbb{p}'\right)\times\tilde{\psi}(\mathbb{p}',t)\,\underbrace{e^{i(\mathbb{p}-\mathbb{p}')\cdot\mathbb{r}/\hbar}}_{\downarrow\ \delta(\mathbb{p}-\mathbb{p}')}$$

$$=\int d\mathbb{p}\ \ \mathbb{p}\ |\tilde{\psi}(\mathbb{p},t)|^2$$

$\leadsto$ $|\tilde{\psi}(\mathbb{p},t)|^2$ は粒子が運動量 $\mathbb{p}$ を持つ確率

(note) $$i\hbar\nabla_p\tilde{\psi}(\mathbb{p},t)=\frac{1}{(2\pi\hbar)^{3/2}}\int d\mathbb{r}\ \ \mathbb{r}\ \psi(\mathbb{r},t)e^{-i\mathbb{p}\cdot\mathbb{r}/\hbar}$$

$$\leadsto\int d\mathbb{p}\ \tilde{\psi}^*(\mathbb{p},t)\left(i\hbar\nabla_p\tilde{\psi}(\mathbb{p},t)\right)$$

$$=\frac{1}{(2\pi\hbar)^3}\int d\mathbb{p}\,d\mathbb{r}\,d\mathbb{r}'\ \ \psi^*(\mathbb{r},t)\cdot\mathbb{r}'\,\psi(\mathbb{r},t)\,\underbrace{e^{i\mathbb{p}\cdot(\mathbb{r}-\mathbb{r}')/\hbar}}_{\hookrightarrow\ \delta(\mathbb{r}-\mathbb{r}')}$$

$$= \int d\mathbf{r}\ \mathbf{r}\ |\psi(\mathbf{r}, t)|^2$$

$$\leadsto \quad \boxed{\hat{\mathbf{r}} = i\hbar \nabla_p}$$

一般に：量子力学では 物理量 → 演算子の期待値

$$\langle \hat{A} \rangle = \int d\mathbf{r}\ \psi^*(\mathbf{r}, t)\, \hat{A}\, \psi(\mathbf{r}, t)$$

$$= \int d\mathbf{p}\ \tilde{\psi}^*(\mathbf{p}, t)\, \hat{A}\, \tilde{\psi}(\mathbf{p}, t).$$

$$\hat{\mathbf{r}} = i\hbar \nabla_p, \quad \hat{\mathbf{p}} = \frac{\hbar}{i} \nabla_r$$

(note) $\hat{\mathbf{r}}\, \psi(\mathbf{r}, t) = \mathbf{r}\ \psi(\mathbf{r}, t)$

$$\hat{\mathbf{p}}\, \tilde{\psi}(\mathbf{p}, t) = \mathbf{p}\ \tilde{\psi}(\mathbf{p}, t)$$

また，一般に

$$\hat{A}\, \psi_n(\mathbf{r}) = \underbrace{A_n}_{\hat{A}\text{の固有値}\ (n\text{はラベル})}\ \underbrace{\psi_n(\mathbf{r})}_{\hat{A}\text{の固有関数}}$$

を考えることができる。