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

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

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

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

一般に　$\langle \hat{A}\rangle=\int d\mathbf{r}\ \psi^*(\mathbf{r},t)\underbrace{\hat{A}\ \psi(\mathbf{r},t)}_{\psi_A(\mathbf{r},t)}$

・運動量表示

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

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

$\downarrow$

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

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

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

$\rightsquigarrow$ $$\int d\mathbb{P} \; \tilde{\psi}^*(\mathbb{P},t)\,(i\hbar\nabla_p)\,\tilde{\psi}(\mathbb{P},t)$$

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

$$= \int d\mathbb{r} \; \mathbb{r}\, |\psi(\mathbb{r},t)|^2 = \langle \mathbb{r} \rangle$$

$\rightsquigarrow$ $$\hat{\mathbb{r}} = i\hbar\nabla_p \quad \leftrightarrow \quad \hat{\mathbb{P}} = \frac{\hbar}{i}\nabla$$

一般に $$\langle \hat{A} \rangle = \int d\mathbb{r} \; \psi^*(\mathbb{r},t)\, \hat{A}\, \psi(\mathbb{r},t)$$
$$= \int d\mathbb{P} \; \tilde{\psi}^*(\mathbb{P},t)\, \hat{A}\, \tilde{\psi}(\mathbb{P},t)$$

(note)
$$\langle \mathbb{r} \rangle = \int d\mathbb{r} \; \mathbb{r}\, |\psi(\mathbb{r},t)|^2$$
$$= \int d\mathbb{r} \; \psi^*(\mathbb{r},t)\, \hat{\mathbb{r}}\, \psi(\mathbb{r},t) = \int d\mathbb{P} \; \tilde{\psi}^*(\mathbb{P},t)\,(i\hbar\nabla_p) \times \tilde{\psi}(\mathbb{P},t)$$

$$\langle \mathbb{P} \rangle = \int d\mathbb{P} \; \mathbb{P}\, |\tilde{\psi}(\mathbb{P},t)|^2$$
$$= \int d\mathbb{P} \; \tilde{\psi}^*(\mathbb{P},t)\, \hat{\mathbb{P}}\, \tilde{\psi}(\mathbb{P},t) = \int d\mathbb{r} \; \psi^*(\mathbb{r},t)\left(\frac{\hbar}{i}\nabla\right) \times \psi(\mathbb{r},t)$$

$\rightsquigarrow$ $$\left.\begin{aligned} \hat{\mathbb{r}}\,\psi(\mathbb{r},t) &= \mathbb{r}\,\psi(\mathbb{r},t) \\ \hat{\mathbb{P}}\,\tilde{\psi}(\mathbb{P},t) &= \mathbb{P}\,\tilde{\psi}(\mathbb{P},t) \end{aligned}\right\} \text{とする。}$$

$$(AB)^\dagger = B^\dagger A^\dagger$$
$$[(AB)^\dagger]_{ij} = [(AB)_{ji}]^* = \sum_k A_{jk}^* B_{ki}^* = \sum_k (B^\dagger)_{ik}(A^\dagger)_{kj} = (B^\dagger A^\dagger)_{ij}$$

## 2.4. 演算子のエルミート共役とオブザーバブル

$$A_{12} \equiv \int d\mathbf{r}\, \psi_1^*(\mathbf{r},t)\hat{A}\psi_2(\mathbf{r},t) = \int d\mathbf{p}\, \tilde{\psi}_1^*(\mathbf{p},t)\hat{A}\tilde{\psi}_2(\mathbf{p},t)$$

を考える。 → $\hat{A}$ の「行列要素」

$$\begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix}\begin{pmatrix} x \\ x \\ x \end{pmatrix} = \begin{pmatrix} \cdot \\ \cdot \\ \cdot \end{pmatrix}$$
$$\hat{A}\quad \psi = \phi$$

すなわち 演算子 ⟷ 行列
（波動関数 ⟷ ベクトル）

エルミート共役 $\hat{A}^\dagger$

例） $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \rightarrow A^\dagger = \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix}$

$$(\hat{A}^\dagger)_{ij} \equiv A_{ji}^*$$

$$(A^\dagger)_{12} = \left(\int d\mathbf{r}\, \psi_2^*(\mathbf{r},t)\hat{A}\psi_1(\mathbf{r},t)\right)^*$$

エルミート演算子 $\hat{A}^\dagger = \hat{A}$ → すなわち $(A^\dagger)_{ij} = A_{ij}$

$$(A^\dagger)_{ij} = (A_{ji})^*$$

$i=j$ のとき $(A_{ii})^* = A_{ii}$

このとき $\langle \hat{A} \rangle_{11} = \int d\mathbf{r}\, \psi_1^*(\mathbf{r},t)\hat{A}\psi_1(\mathbf{r},t)$

$$\langle \hat{A}^\dagger \rangle_{11} = \int d\mathbf{r}\, \psi_1^*(\mathbf{r},t)\underbrace{\hat{A}^\dagger}_{=\hat{A}}\psi_1(\mathbf{r},t) = \langle \hat{A} \rangle_{11}$$

$A^\dagger$ の定義より

$$\left(\int d\mathbf{r}\, \psi_1^*(\mathbf{r},t)\hat{A}\psi_1(\mathbf{r},t)\right)^* = \langle \hat{A} \rangle_{11}^*$$

→ 期待値は常に実数（$\langle \hat{A} \rangle_{11} = \langle \hat{A} \rangle_{11}^*$）

観測可能量（オブザーバブル）
→ エルミート演算子を用いて記述

$A = A^\dagger \rightarrow$ $a = a^*$, $d = d^*$, $b = c^*$

(note)

$$(\hat{p}^{\dagger})_{12} = \left[ \int d\mathbf{r} \; \psi_2^*(\mathbf{r},t) \left(\frac{\hbar}{i}\nabla\right) \psi_1(\mathbf{r},t) \right]^*$$

$$= \int d\mathbf{r} \; \psi_2(\mathbf{r},t) \left(-\frac{\hbar}{i}\nabla\right) \psi_1^*(\mathbf{r},t)$$

$$= \int d\mathbf{r} \; \psi_1^*(\mathbf{r},t) \underbrace{\left(\frac{\hbar}{i}\nabla\right)}_{=\left(\frac{\hbar}{i}\nabla\right)^{\dagger}} \psi_2(\mathbf{r},t) = \hat{p}_{12}$$

部分積分

すなわち $\hat{p}^{\dagger} = \hat{p}$ : $\hat{p}$ はエルミート演算子

同様に $\hat{\mathbf{r}}^{\dagger} = \hat{\mathbf{r}}$

## 2.5. 演算子の交換関係

演算子の積も演算子 $\hat{C} \equiv \hat{A}\hat{B}$

$$\hat{C}\psi = \hat{A}\hat{B}\psi = \hat{A}\underbrace{(\hat{B}\psi)}_{=\phi} = \hat{A}\phi$$

一般に $\hat{A}\hat{B} \neq \hat{B}\hat{A}$

(例えば) $\hat{p}_x \hat{x}\, \psi(\mathbf{r}) = \hat{p}_x \cdot (x\,\psi(\mathbf{r})) = \frac{\hbar}{i}\frac{\partial}{\partial x}(x\,\psi(\mathbf{r}))$

$$= \frac{\hbar}{i}\left(\psi(\mathbf{r}) + x\frac{\partial}{\partial x}\psi(\mathbf{r})\right)$$

$$\hat{x}\,\hat{p}_x\,\psi(\mathbf{r}) = \hat{x}\cdot\frac{\hbar}{i}\left(\frac{\partial}{\partial x}\psi(\mathbf{r})\right) = \frac{\hbar}{i}\,x\frac{\partial}{\partial x}\psi(\mathbf{r})$$

$$[\hat{p}_x\hat{x} - \hat{x}\hat{p}_x]\,\psi(\mathbf{r}) = \frac{\hbar}{i}\psi(\mathbf{r})$$

$$[\hat{x}\hat{p}_x - \hat{p}_x\hat{x}]\,\psi(\mathbf{r}) = i\hbar\,\psi(\mathbf{r})$$

$$(\hat{A}+\hat{B})^2 = (\hat{A}+\hat{B})(\hat{A}+\hat{B})$$
$$= \hat{A}^2 + \hat{A}\hat{B} + \hat{B}\hat{A} + \hat{B}^2 \neq \hat{A}^2 + 2\hat{A}\hat{B} + \hat{B}^2$$

## 交換関係

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$$

(note) $[\hat{B}, \hat{A}] = -[\hat{A}, \hat{B}]$

例) $[\hat{x}_i, \hat{p}_j]\psi(\mathbf{r}, t) = (\hat{x}_i \hat{p}_j - \hat{p}_j \hat{x}_i)\psi(\mathbf{r}, t)$

$$= (\hat{x}_i \cdot \frac{\hbar}{i}\partial_j - \frac{\hbar}{i}\partial_j \hat{x}_i)\psi$$
$$= \frac{\hbar}{i} x_i (\partial_j \psi) - \frac{\hbar}{i}\partial_j (x_i \psi)$$
$$= \cancel{\frac{\hbar}{i} x_i (\partial_j \psi)} - \frac{\hbar}{i}(\delta_{i,j}\psi + \cancel{x_i \partial_j \psi})$$
$$= i\hbar \delta_{i,j}\psi$$

任意の波動関数 $\psi$ に対してこれが成り立つので

$$[\hat{x}_i, \hat{p}_j] = i\hbar \delta_{i,j}$$
$$[\hat{p}_i, \hat{x}_j] = \frac{\hbar}{i}\delta_{i,j}$$

「正準交換関係」

(note) $[\hat{A}, \hat{B}\hat{C}] = ABC - BCA$

$$= (AB - \underset{\sim}{BA})C - B(CA - \underset{\sim}{AC})$$

$$= [A, B]C + B[A, C]$$

$$[\hat{p}, \hat{x}^2] = \hat{x}[\hat{p}, \hat{x}] + [\hat{p}, \hat{x}]\hat{x} = \frac{2\hbar}{i}\hat{x}$$

$$[\hat{p}, \hat{x}^3] = \hat{x}^2[\hat{p}, \hat{x}] + [\hat{p}, \hat{x}^2]\hat{x} = \frac{3\hbar}{i}\hat{x}^2$$

$$[\hat{p}, \hat{x}^n] = \frac{\hbar}{i} n \hat{x}^{n-1}$$

(note) $[\hat{p}, \hat{x}^n]\psi = \frac{\hbar}{i}\frac{\partial}{\partial x}(\hat{x}^n\psi) - \hat{x}^n\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\psi\right)$

$$= \frac{\hbar}{i} \cdot n\hat{x}^{n-1}\psi$$

$$[\hat{p}, f(\hat{x})] = [\hat{p}, \sum_n \frac{1}{n!} f^{(n)}(0)\hat{x}^n]$$

$$= \frac{\hbar}{i}\sum_n \frac{f^{(n)}(0)}{n!} \cdot n\hat{x}^{n-1}$$

$$= \frac{\hbar}{i} f'(\hat{x})$$

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}]}$$

ベイカー・キャンベル・ハウスドルフの公式

→ レポート問題