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

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」

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

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

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

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

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

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

(note)

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

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

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

部分積分

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

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

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) $\hat{P}_x \hat{x}\, \psi(\mathbb{r}) = \hat{P}_x \cdot (x\, \psi(\mathbb{r})) = \frac{\hbar}{i}\frac{\partial}{\partial x}(x\, \psi(\mathbb{r}))$

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

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

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

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

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

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

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

$$= (\hat{x}_i \cdot \frac{\hbar}{i}\partial_j - \frac{\hbar}{i}\partial_j \hat{x}_i)\psi$$

$$= \frac{\hbar}{i} x_i (\partial_j \psi) - \frac{\hbar}{i}\partial_j (x_i \psi)$$

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

$$= i\hbar\, \delta_{i,j}\psi$$

任意の波動関数 ψ 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」

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

$$= (AB - BA)C - B(CA - AC)$$

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

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

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

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

(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

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2.6. 不確定性関係

$$\begin{cases} \langle x \rangle = \int d\mathbf{r}\ \psi^*(\mathbf{r},t)\ x\ \psi(\mathbf{r},t) \\ \langle p_x \rangle = \int d\mathbf{r}\ \psi^*(\mathbf{r},t) \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \psi(\mathbf{r},t) \end{cases}$$

$$\psi_x(\mathbf{r},t) \equiv (\hat{x} - \langle x \rangle)\psi(\mathbf{r},t)$$

$$= (x - \langle x \rangle)\psi(\mathbf{r},t)$$

$$\psi_p(\mathbf{r},t) \equiv (\hat{p}_x - \langle p_x \rangle)\psi(\mathbf{r},t)$$

$$= \left(\frac{\hbar}{i}\frac{\partial}{\partial x} - \langle p_x \rangle\right)\psi(\mathbf{r},t)$$

とする。ただし、$\int d\mathbf{r}\ \psi^*(\mathbf{r},t)\psi(\mathbf{r},t) = 1.$

$$\int d\mathbf{r}\ \psi_x^*(\mathbf{r},t)\psi_x(\mathbf{r},t)$$

$$= \int d\mathbf{r}\ \psi(\mathbf{r},t)\ \underbrace{(x - \langle x \rangle)^2}_{= x^2 - 2x\langle x \rangle + \langle x \rangle^2}\ \psi(\mathbf{r},t)$$

$$= \langle x^2 \rangle - \langle x \rangle^2 = (\Delta x)^2$$

x の分散

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$$\int d\mathbf{r}\ \psi_p^*(\mathbf{r},t)\,\psi_p(\mathbf{r},t)$$

$$= \int d\mathbf{r}\ \left(-\frac{\hbar}{i}\left(\frac{\partial}{\partial x}\psi^*(\mathbf{r},t)\right) - \langle p_x\rangle \psi^*(\mathbf{r},t)\right)\left(\frac{\hbar}{i}\left(\frac{\partial \psi}{\partial x}\right) - \langle p_x\rangle \psi\right)$$

$$= \int d\mathbf{r}\ \Big[\hbar^2\left(\frac{\partial}{\partial x}\psi^*\right)\left(\frac{\partial}{\partial x}\psi\right) - \langle p_x\rangle \psi^*\left(\frac{\hbar}{i}\frac{\partial \psi}{\partial x}\right)$$

$$+ \langle p_x\rangle \psi\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\psi^*\right) + \langle p_x\rangle^2 \psi^*\psi\Big]$$

$$\xrightarrow[\text{部分積分}]{} \int d\mathbf{r}\ \left[-\hbar^2\psi^*\frac{\partial^2}{\partial x^2}\psi - 2\langle p_x\rangle\psi^*\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\psi\right)\right] + \langle p_x\rangle^2$$

$\psi(x=\pm\infty)=0$

$$= \langle p_x^2\rangle - \langle p_x\rangle^2 = (\Delta p_x)^2$$

$$\hat{p}_x^2 = \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 = -\hbar^2\frac{\partial^2}{\partial x^2}$$

(note) $\int d\mathbf{r}\ \psi_p^*(\mathbf{r},t)\,\psi_p(\mathbf{r},t)$

$$= \int d\mathbf{r}\ \psi^*(\mathbf{r},t)\,(\hat{p}_x - \langle p_x\rangle)^\dagger(\hat{p}_x - \langle p_x\rangle)\,\psi(\mathbf{r},t)$$

$$= \int d\mathbf{r}\ \psi^*(\mathbf{r},t)\,(\hat{p}_x^2 - 2\langle p_x\rangle\hat{p}_x + \langle p_x\rangle^2)\,\psi(\mathbf{r},t)$$

$$= \langle p_x^2\rangle - \langle p_x\rangle^2$$

$\hat{A}\,\Psi$

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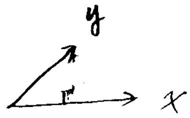
行列　ベクトル



$\vec{x}\cdot\vec{y} = xy\cos\theta$

$$(\Delta x)^2(\Delta p_x)^2 = \left[\int d\mathbf{r}\ \psi_x^*(\mathbf{r},t)\psi_x(\mathbf{r},t)\right]\left[\int d\mathbf{r}\ \psi_p^*(\mathbf{r},t)\psi_p(\mathbf{r},t)\right]$$

(note)　コーシー・シュワルツの不等式

$$\langle\vec{x},\vec{x}\rangle\cdot\langle\vec{y},\vec{y}\rangle \geq |\langle\vec{x},\vec{y}\rangle|^2$$

$$(\Delta x)^2(\Delta p_x)^2 \geq \left|\int d\mathbf{r}\ \psi_x^*(\mathbf{r},t)\psi_p(\mathbf{r},t)\right|^2$$

(note)　$|z|^2 = (\mathrm{Re}\,z)^2 + (\mathrm{Im}\,z)^2 \geq (\mathrm{Im}\,z)^2 = \left(\frac{z-z^*}{2i}\right)^2$

複素数

$$(\Delta x)^2(\Delta p_x)^2 \geq \left[\frac{1}{2i}\int d\mathbf{r}\ \psi_x^*(\mathbf{r},t)\psi_p(\mathbf{r},t) - \frac{1}{2i}\int d\mathbf{r}\ \psi_p^*(\mathbf{r},t)\psi_x(\mathbf{r},t)\right]^2$$

(note)
$$\int \psi_x^*(\mathbf{r},t)\psi_p(\mathbf{r},t)\,d\mathbf{r} = \int d\mathbf{r}\ \psi^*(\mathbf{r},t)(x-\langle x\rangle)(\hat{p}_x-\langle p_x\rangle)\psi$$
$$= \langle x p_x\rangle - \langle x\rangle\langle p_x\rangle$$
$$\int \psi_p^*(\mathbf{r},t)\psi_x(\mathbf{r},t)\,d\mathbf{r} = \langle p_x x\rangle - \langle x\rangle\langle p_x\rangle$$

$$(\Delta x)^2(\Delta p_x)^2 \geq \left(\frac{1}{2i}\left(\langle x p_x\rangle - \langle p_x x\rangle\right)\right)^2 = \left(\frac{1}{2i}\langle[x, p_x]\rangle\right)^2$$
$$= \left(\frac{i\hbar}{2i}\right)^2 = \left(\frac{\hbar}{2}\right)^2$$

$$\boxed{(\Delta x)(\Delta p_x) \geq \frac{\hbar}{2}}$$ 「不確定性関係」

位置と運動量を同時に決めることはできない。

例) $\psi(x,t) = e^{ipx/\hbar - iEt/\hbar}$

$$\hat{p}\,\psi(x,t) = p\,\psi(x,t)$$
$$\hat{p}^2\psi(x,t) = p^2\psi(x,t)$$

$\rightarrow \Delta p_x = 0$

$e^{ipx/\hbar}$ は $-\infty \leq x \leq \infty$ の範囲で広がっている。

一般化: $[\hat{A}, \hat{B}] = i\hat{C}$ のとき

$$(\Delta A)(\Delta B) \geq \frac{|\langle \hat{C} \rangle|}{2}$$

四 $[\hat{A}, \hat{B}] = 0$ のとき $(\Delta A)(\Delta B) = 0$

$\rightarrow$ A と B を同時に決めることができる。

$\leftrightarrow$ 演算子 $\hat{A}$, $\hat{B}$ の両方の固有状態

$$\hat{A}\,\psi_{AB}(\mathbf{r},t) = A\,\psi_{AB}(\mathbf{r},t)$$
$$\hat{B}\,\psi_{AB}(\mathbf{r},t) = B\,\psi_{AB}(\mathbf{r},t)$$

「同時固有状態」

cf. ハミルトニアンの対称性