



☑ シュレディンガー方程式

$$\hat{H} = \frac{1}{i\hbar} \hbar \frac{\partial}{\partial t} = \hat{p}$$

$$\hbar = \text{プランク定数} \quad \hbar = \frac{h}{2\pi} = \text{円弧定数}$$

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = \left(\underbrace{-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}}_{\text{運動エネルギー}} + \underbrace{V(x,t)}_{\text{位置エネルギー}} \right) \psi(x,t) \quad \textcircled{1} \quad \text{↑ Z' 演算を示す}$$

$\text{運動エネルギー} + \text{位置エネルギー} = E = \text{全エネルギー}$

Step up 波のエネルギー？

$$E_e = \underbrace{h\nu}_{=E} - W \quad (\text{光電効果})$$

$$E = h\nu = \hbar\omega \quad (\omega = 2\pi\nu)$$

$$\textcircled{1} \quad \psi(x,t) \sim e^{ikx - i\omega t}$$

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = E \psi(x,t)$$



↑ $\psi(x,t)$ は何を表す？



★ 波動関数

$$P(x,t) = |\psi(x,t)|^2$$

①

(x,t) に何処まで
確率を予測

○ 規格化

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 1$$

★ 定常状態 $V(x,t) \rightarrow V(x)$

$$\hat{H}\psi(x,t) = E\psi(x,t)$$

定数

$$\Rightarrow i\hbar \frac{\partial}{\partial t} \psi(x,t) = E \psi(x,t)$$

$$\therefore \psi(x,t) = \exp(-i \frac{E}{\hbar} t) \psi(x)$$

①

定数 $\psi(x)$ だけ

step up $\psi(x)$ を求めよ

$$\hat{H}\psi(x) = E\psi(x)$$

設定

①

行列の対角化のやり方

②

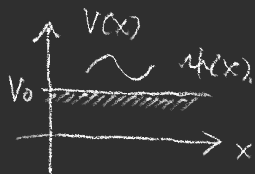
$$H\vec{u} = \lambda\vec{u}$$

③

$\psi(x)$ も $\vec{u}$ の対称性

固有値もわかるか?

(例) $V(x) = V_0$ (定数)



$$\hat{H} \psi(x) = E \psi(x)$$

$$p = \frac{h}{\lambda} = \frac{h}{2\pi} \frac{2\pi}{\lambda}$$

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_0 \right) \psi(x) = E \psi(x) = \hbar k$$

$$\frac{\partial^2}{\partial x^2} \psi(x) = -\frac{2m(E - V_0)}{\hbar^2} \psi(x)$$

$$k = \frac{2\pi}{\lambda}$$

$$\psi(x) = A \exp(ikx) + B \exp(-ikx)$$

① 一般解

$$k = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

進行波 と 逆行波 OK

Step up 運動量と運動エネルギー

$$p = \hbar k \left(= -i\hbar \frac{\partial}{\partial x} \right)$$

$$k = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

① この場合散乱を判別

$$\frac{h}{\lambda} \rightarrow \ominus \rightarrow p_0 \rightarrow \frac{h}{\lambda'}$$

$$p = \frac{h}{\lambda} = \frac{h}{2\pi} \frac{2\pi}{\lambda} = \hbar k$$

つまり $\frac{\hbar^2 k^2}{2m} = E - V_0$ ($E = \frac{\hbar^2 k^2}{2m} + V_0$)

連続スペクトル

$\psi(x) = A e^{ikx} + B e^{-ikx}$

①

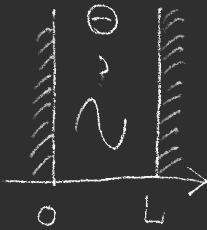
確かに1で決まる
固有関数だから

②

量子又何?!

③

$$V(x) = \begin{cases} 0 & (0 \leq x \leq L) \\ \infty & (x < 0, L < x) \end{cases} \Rightarrow \psi(x) = 0 \text{ (境界条件)}$$



$(0 \leq x \leq L)$

$\hat{H} \psi(x) = E \psi(x)$

$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \psi(x) = E \psi(x)$

同様に $\frac{\partial^2}{\partial x^2} \psi(x) = -\frac{2mE}{\hbar^2} \psi(x)$

5.2 $\psi(x) = A \exp(ikx) + B \exp(-ikx)$ (1) 一般解!

$k = \frac{\sqrt{2mE}}{\hbar}$ 2次元連続空間 (2) 2次元連続空間

Step up 7.3.2.1a 一般解

$$u(\omega, T) \propto \frac{1}{1 - e^{-\hbar\omega/kT}}$$

$$= 1 + e^{-\hbar\omega/kT} + e^{-2\hbar\omega/kT} + \dots$$

$\hbar\omega \leftarrow E?$



(1) 一般解 $E = \hbar\omega$ (2) 一般解

量子 = 2次元連続空間

$\psi(0) = \psi(L) = 0$ (2次元)

$\psi(0) = A + B = 0 \Rightarrow B = -A$

$\psi(L) = A e^{ikL} + B e^{-ikL}$

$= 2A \sin kL = 0$

(1) $A \neq 0, L \neq 0$ 有 $k = \frac{\sqrt{2mE}}{\hbar}$

$\frac{\sqrt{2mE}}{\hbar}$

52 $k_L = 0, \pm\pi, \pm2\pi, \dots, n\pi$ ($n = 0, \pm1, \pm2, \dots$)

$$\frac{\sqrt{2mE}}{\hbar} L = n\pi \left(\frac{\sqrt{2mE}}{\hbar} = \frac{n}{2L} \right) \therefore E_n = \frac{\hbar^2 k^2}{8mL^2}$$

① 1次元-2次元化?

52 $\phi_n(x) \propto \sin k_n x$ $k_n = \frac{n\pi}{L}$ 97 1次元化

固有関数

① 規格化 $\phi_n(x) = A \sin k_n x$

$$\frac{1 - \cos 2kx}{2}$$

$$\int_0^L |\phi_n(x)|^2 dx = |A|^2 \int_0^L dx \sin^2 k_n x = |A|^2 \left(\frac{L}{2} - \frac{1}{4k_n} [\sin 2k_n x]_0^L \right)$$

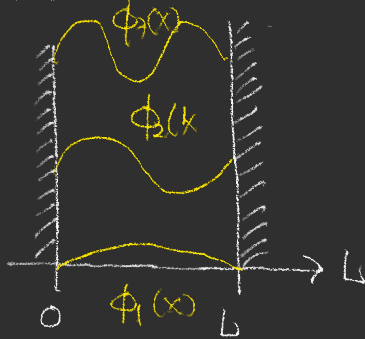
$\psi(x) = \sqrt{\frac{2}{L}} \phi_n(x)$ $\therefore A = \sqrt{\frac{2}{L}}$

① $n \neq 0$ $E_n = \frac{\hbar^2 k^2}{8mL^2}$ 2次元化

Step up 1次元化

$\psi(x) = 0$ $\psi(0) = \psi(L) = 0$
 $k_n (\Rightarrow E_n)$ 2次元化

☆ 波動関数 - 準位



$$E = \frac{9h^2}{8mL^2}$$

$$E_2 = \frac{4h^2}{8mL^2}$$

$$E_1 = \frac{h^2}{8mL^2}$$

(励起状態)

(基底状態)

①

$$\boxed{\text{エネルギー差} \quad E_m - E_n = \hbar\omega_{mn}}$$



固有振動数

②
→

ϕ_1, ϕ_2 の基底状態 - 励起状態
遷移 $\Rightarrow$ 量子化?

例1 $V(x) = 0$ 但周期 $2\pi a$ 刻



→
半径 a

$$(0 \leq x \leq 2\pi a)$$

$$\hat{H}\psi(x) = E\psi(x)$$

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}\right) \psi(x) = E\psi(x)$$

$$\text{同様} \quad \frac{\partial^2}{\partial x^2} \psi(x) = -\frac{2mE}{\hbar^2} \psi(x)$$

$$\text{よ} \quad \psi(x) = A \exp(ikx) + B \exp(-ikx) \quad \text{① 一般解!}$$

$$k = \frac{\sqrt{2mE}}{\hbar} \quad \text{② 非連続なエネルギー}$$

○ 周期境界条件

$$\psi(x + 2\pi a) = \psi(x) \quad e^{ik \cdot 2\pi a} = 1$$

$$\text{よ} \quad 2\pi k a = 2\pi n \quad (n=1, 2, \dots)$$

7-11変換と量子化

$$\hat{H}\psi(x) = E\psi(x)$$

⑪ 偏微分方程式は7-11!

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

Step up 7-11変換

$$f(x) = \int_{-\infty}^{\infty} \hat{f}(k) e^{ikx} dk$$

$$\hat{f}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$

☆ 何故7-11?

$$\frac{\partial}{\partial x} f(x)$$

⑦

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\partial}{\partial x} f(x) e^{-ikx} dx = \frac{1}{2\pi} \left[\underbrace{f(x)}_{f(\pm\infty) \rightarrow 0} e^{-ikx} \right]_{-\infty}^{\infty}$$

$$\uparrow \quad \downarrow$$

$$f(x) \quad (-ik) e^{-ikx} + (ik) \underbrace{\left[\frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \right]}_{\hat{f}(k)}$$

$$= (ik) \hat{f}(k)$$

$$\textcircled{11} \left\{ \frac{\partial}{\partial x} \rightarrow ik \right\} = \textcircled{72}$$

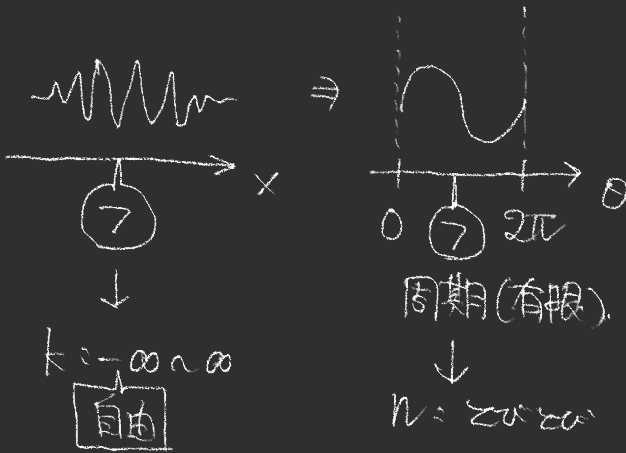
Step up 7-11 量子化

$$p = \hbar k \rightarrow -i\hbar \frac{\partial}{\partial x} \text{ (量子化)}$$

$$i\hbar \leftarrow \frac{\partial}{\partial t} \text{ (7-112)}$$

①② (古典)
 x, p 同时极小
 (量子)
 x 或 p 分别极小

★ 7-11 级数展开



Step up 7-11 级数展开

$$f(\theta) = \sum_{n=-\infty}^{\infty} A_n e^{in\theta} \quad \text{for } 0 \sim 2\pi$$

$$A_n = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) e^{-in\theta} d\theta$$

for $0 \sim L$

$$f(x) = \sum_{n=-\infty}^{\infty} A_n \exp(i \frac{2\pi}{L} nx)$$

$$A_n = \frac{1}{L} \int_0^L f(x) \exp(-i \frac{2\pi}{L} nx) dx$$

7-11 変換の定義

変換の定義 行列?

$$\begin{cases} \frac{\psi(x)}{x^2 \Delta x} = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp \frac{\psi(p)}{p^2 \Delta p} e^{i \frac{p}{\hbar} x} \\ \frac{\psi(p)}{p^2 \Delta p} = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \frac{\psi(x)}{x^2 \Delta x} e^{-i \frac{p}{\hbar} x} \end{cases} \begin{cases} p = \hbar k \\ \frac{\psi(k)}{\hbar} = \psi(p) \end{cases}$$

$\psi(x), \psi(p)$ は λ が 1 である
2つの何かからなる

(内積) $\psi(x)$?

ブラケット記法

$$\langle x | \psi \rangle = \int_{-\infty}^{\infty} dp \frac{1}{\sqrt{2\pi\hbar}} e^{i \frac{p}{\hbar} x} \langle x | p \rangle \langle p | \psi \rangle$$

$$\langle p | \psi \rangle = \int_{-\infty}^{\infty} dx \frac{1}{\sqrt{2\pi\hbar}} e^{-i \frac{p}{\hbar} x} \langle p | x \rangle \langle x | \psi \rangle$$

I = 恒等変換

Step up ブラケット表記

$$\begin{aligned} \psi(x) &\equiv \langle x | \psi \rangle \quad (x \text{ 表示}) \\ \psi(p) &\equiv \langle p | \psi \rangle \quad (p \text{ 表示}) \end{aligned}$$

Step up) 恒等演算

$$\int_{-\infty}^{\infty} dx |x\rangle\langle x| = I$$

$$\int_{-\infty}^{\infty} dp |p\rangle\langle p| = I$$

正しく代入すれば共役

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x}$$

(共役)

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-i\frac{p}{\hbar}x}$$

★演算子 $\frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x}$

$$-i\hbar \frac{\partial}{\partial x} \langle x|p\rangle = p \langle x|p\rangle$$

① $\langle x|p\rangle$ が固有...

$$\hat{p} \langle x|p\rangle = p \langle x|p\rangle$$

何故? 確か!

$$\hat{p} |p\rangle = p |p\rangle$$

行方! 何処! 確か!

① 運動量 p の状態 (固有)
 $\hat{p} |p\rangle = p |p\rangle$

左から $\langle x|$

$$\langle x| \hat{p} |p\rangle = p \langle x|p\rangle$$

比較

$$[-i\hbar \frac{\partial}{\partial x} \langle x|p\rangle = p \langle x|p\rangle]$$

x は変数 (E-1)

① $\hat{p} \rightarrow -i\hbar \frac{\partial}{\partial x}$, 確か?
 p は x の関数

$$\hat{x} |x\rangle = x |x\rangle \text{ 確か}$$

$$\langle p| \hat{x} |x\rangle = x \langle p|x\rangle$$

$$i\hbar \frac{\partial}{\partial p} \langle p|x\rangle = x \langle p|x\rangle$$

p は変数 (E-1)

Step up $\hat{X}$ の p 表示 $\hat{p}$ の x 表示

$$\langle x | \hat{p} = -i\hbar \frac{\partial}{\partial x} \langle x | \cdot$$

x の関数

$$[\hat{p}^\dagger | x \rangle = i\hbar \frac{\partial}{\partial x} | x \rangle]$$

$$\langle p | \hat{X} = i\hbar \frac{\partial}{\partial p} \langle p | \cdot$$

p の関数

$$[\hat{X}^\dagger | p \rangle = -i\hbar \frac{\partial}{\partial p} | p \rangle]$$

Step up 共役 + 転置 = 随伴

$$\hat{X}^\dagger | x \rangle = X | x \rangle$$

$\downarrow$ $\dagger$ = 随伴 (随伴)

$$\langle x | \hat{X}^\dagger = \langle x | X$$

(物理量の共役)

$$= \langle x | X$$

$$\textcircled{上} \langle x | \hat{X} | x \rangle = X \langle x | x \rangle$$

$$\textcircled{下} \langle x | \hat{X}^\dagger | x \rangle = X \langle x | x \rangle$$

Step up 物理量 (実数) は エルミート

$$\hat{X} = \hat{X}^\dagger \quad \text{同様} \quad \hat{p} = \hat{p}^\dagger$$

★ シュレディンガー方程式

$$\hat{H} | \psi \rangle = E | \psi \rangle$$

$\langle x | \psi \rangle$ $\langle x | \psi \rangle$

実数

$$\Rightarrow \hat{H} | \psi \rangle = E | \psi \rangle$$

行列 ハミルトニアン スカラー

$$\langle x | \hat{H} | \psi \rangle = E \langle x | \psi \rangle$$

$$\langle x | \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) | \psi \rangle = E \langle x | \psi \rangle$$

$\Downarrow$ 第1量子化 [$\langle x | \psi \rangle$ 変数]

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)\right) \langle x | \psi \rangle = E \langle x | \psi \rangle \quad (\text{波動方程式})$$

① ② $\left[\begin{array}{l} \psi(x) \text{ 波動関数} \quad |\psi\rangle \text{ 状態ベクトル} \\ \text{微分方程式} \quad \text{線型代数} \end{array} \right]$

★ 交換関係 (行列形式)

Step up 交換関係

$$[\hat{a}, \hat{b}] = \hat{a}\hat{b} - \hat{b}\hat{a}$$

① ② $[\hat{x}, \hat{p}] = i\hbar$ ③ ④ ⑤ ⑥ ⑦ ⑧ ⑨ ⑩ ⑪ ⑫ ⑬ ⑭ ⑮ ⑯ ⑰ ⑱ ⑲ ⑳ ㉑ ㉒ ㉓ ㉔ ㉕ ㉖ ㉗ ㉘ ㉙ ㉚ ㉛ ㉜ ㉝ ㉞ ㉟ ㊱ ㊲ ㊳ ㊴ ㊵ ㊶ ㊷ ㊸ ㊹ ㊺ ㊻ ㊼ ㊽ ㊾ ㊿

$$\langle x | \hat{x} \hat{p} | \psi \rangle = x \langle x | \hat{p} | \psi \rangle = x (-i\hbar \frac{\partial}{\partial x}) \langle x | \psi \rangle$$

$$\langle x | \hat{p} \hat{x} | \psi \rangle = (-i\hbar \frac{\partial}{\partial x}) \langle x | \hat{x} | \psi \rangle = (-i\hbar \frac{\partial}{\partial x}) x \langle x | \psi \rangle$$

→

$$= -i\hbar \langle x | \psi \rangle + x (-i\hbar \frac{\partial}{\partial x}) \langle x | \psi \rangle$$

$$\langle x | [\hat{x}, \hat{p}] | \psi \rangle = i\hbar \langle x | \psi \rangle \quad \text{① ② ③ ④ ⑤ ⑥ ⑦ ⑧ ⑨ ⑩ ⑪ ⑫ ⑬ ⑭ ⑮ ⑯ ⑰ ⑱ ⑲ ⑳ ㉑ ㉒ ㉓ ㉔ ㉕ ㉖ ㉗ ㉘ ㉙ ㉚ ㉛ ㉜ ㉝ ㉞ ㉟ ㊱ ㊲ ㊳ ㊴ ㊵ ㊶ ㊷ ㊸ ㊹ ㊺ ㊻ ㊼ ㊽ ㊾ ㊿}$$

Step up 反交換関係

$$\{\hat{a}, \hat{b}\} = \hat{a}\hat{b} + \hat{b}\hat{a}$$

$$[\hat{a}, \hat{b}]^\dagger = (\hat{a}\hat{b})^\dagger - (\hat{b}\hat{a})^\dagger = \hat{b}\hat{a} - \hat{a}\hat{b} = -[\hat{a}, \hat{b}]$$

$$\{\hat{a}, \hat{b}\}^\dagger = (\hat{a}\hat{b})^\dagger + (\hat{b}\hat{a})^\dagger = \hat{b}\hat{a} + \hat{a}\hat{b} = \{\hat{a}, \hat{b}\}$$

$$[\hat{a}, \hat{b}] = i0$$

$$\{\hat{a}, \hat{b}\} = \Delta$$

☆ 期待値

$$P(x) = |\psi(x)|^2 = \langle \psi | x \rangle \langle x | \psi \rangle$$

$$\int_{-\infty}^{\infty} dx P(x) = \int_{-\infty}^{\infty} \underline{dx} \langle \psi | \underline{x} \rangle \langle \underline{x} | \psi \rangle \overset{I}{=} 1 \quad \therefore \langle \psi | \psi \rangle = 1.$$

$$\begin{aligned} \circ \langle f(x) \rangle &= \int_{-\infty}^{\infty} dx f(x) \cdot P(x) \quad (\text{期待値}) \\ &= \int_{-\infty}^{\infty} dx f(x) \langle \psi | x \rangle \langle x | \psi \rangle = \int_{-\infty}^{\infty} \underline{dx} \langle \psi | f(x) \rangle \underline{\langle x | \psi \rangle} \overset{I}{=} \\ &= \langle \psi | f(x) | \psi \rangle \end{aligned}$$

[step up] 期待値

$$\langle f(x) \rangle = \langle \psi | f(x) | \psi \rangle$$

$$\text{一般に } \langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle \text{ ok!}$$

不確定性関係

Step up コーシー・シュワルツの不等式

$$\|\vec{a}\|^2 \|\vec{b}\|^2 \geq (\vec{a} \cdot \vec{b})^2$$

①
②

類似度は1以上

$$\frac{\vec{a} \cdot \vec{b}}{\|\vec{a}\| \|\vec{b}\|} = \cos \theta$$

$$\Rightarrow \langle \varphi | \varphi \rangle \langle \phi | \phi \rangle \geq \langle \varphi | \phi \rangle \langle \phi | \varphi \rangle$$

(*)

(*)

$$|\varphi\rangle = (\hat{A} - \langle \hat{A} \rangle) |\psi\rangle$$

$$|\phi\rangle = (\hat{B} - \langle \hat{B} \rangle) |\psi\rangle$$

① ② 期待値の差

①
②

期待値の差

$$\langle \Delta A^2 \rangle \langle \Delta B^2 \rangle \geq \langle (\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle) \rangle \langle (\hat{B} - \langle \hat{B} \rangle)(\hat{A} - \langle \hat{A} \rangle) \rangle$$

$$(*) = \langle \hat{A}\hat{B} \rangle - \langle \hat{A} \times \hat{B} \rangle = \frac{1}{2} \left(\langle [\hat{A}, \hat{B}] \rangle + \langle [\hat{A}, \hat{B}] \rangle \right) - \langle \hat{A} \times \hat{B} \rangle = 2$$

$$(*)^* = \langle \hat{B}\hat{A} \rangle - \langle \hat{A} \times \hat{B} \rangle = \frac{1}{2} \left(\langle [\hat{A}, \hat{B}] \rangle - \langle [\hat{A}, \hat{B}] \rangle \right) - \langle \hat{A} \times \hat{B} \rangle = 2^*$$

$$(*) (*)^* = |2|^2 = \left(\frac{1}{2} \langle [\hat{A}, \hat{B}] \rangle - \langle \hat{A} \times \hat{B} \rangle \right)^2 + \frac{1}{4} |\langle [\hat{A}, \hat{B}] \rangle|^2$$

$$\geq \frac{1}{4} |\langle [\hat{A}, \hat{B}] \rangle|^2$$

Step up ケーブル・ディラックの不等式

$$\langle \Delta A^2 \rangle \langle \Delta B^2 \rangle \geq \frac{1}{4} |\langle [\hat{A}, \hat{B}] \rangle|^2$$

$$⑬ \langle \Delta x^2 \rangle \langle \Delta p^2 \rangle \geq \frac{\hbar^2}{4} \quad (\text{ケール})$$

[1927]

同じ $|\psi\rangle \geq 100\%$

$\langle \Delta x^2 \rangle \geq 50\%$ 同様に

$\langle \Delta p^2 \rangle \geq 50\%$ 同様に

$$\langle \Delta x^2 \rangle \langle \Delta p^2 \rangle \geq \frac{\hbar^2}{4}$$

①
②

$|\psi\rangle$ 自体に不確定性

①
②

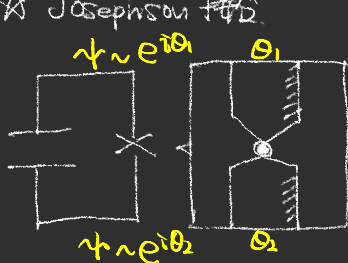
測定の結果 z なら

量子セルの作り方

☆ $[\hat{x}, \hat{p}] = i\hbar$ は力学

$\text{---} \bigcirc \Rightarrow \frac{1}{2}mv^2 + \frac{1}{2}kx^2 = E \Rightarrow \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2 = \hat{H} \quad (\hat{H}|\psi\rangle = E|\psi\rangle)$
 $\text{---} \bigcirc \Rightarrow \frac{1}{2}L\dot{\varphi}^2 + \frac{q^2}{2C} = E \Rightarrow \frac{\hat{\phi}^2}{2L} + \frac{\hat{q}^2}{2C} = \hat{H}$
 $\text{---} \bigcirc \Rightarrow \frac{1}{2}L\dot{\varphi}^2 + \frac{q^2}{2C} = E \Rightarrow \frac{\hat{\phi}^2}{2L} + \frac{\hat{q}^2}{2C} = \hat{H}$
 $\text{---} \bigcirc \Rightarrow \frac{1}{2}L\dot{\varphi}^2 + \frac{q^2}{2C} = E \Rightarrow \frac{\hat{\phi}^2}{2L} + \frac{\hat{q}^2}{2C} = \hat{H}$

☆ Josephson 接合



BEC の 1.4 節

超伝導の超伝導体では

"Josephson 接合"

$$I = I_0 \sin \theta = I_0 \sin 2\pi \left(\frac{\phi}{\phi_0} \right) \quad [\theta = \theta_1 - \theta_2]$$

$$V = \frac{d\phi}{dt} = L \frac{dI}{dt} \quad \text{より} \quad \frac{dI}{dt} = \frac{2\pi I_0}{\phi_0} \cos 2\pi \left(\frac{\phi}{\phi_0} \right) \frac{d\phi}{dt}$$

$$L = \frac{d\phi/dt}{dI/dt} = \frac{\phi_0}{2\pi I_0} \frac{1}{\cos 2\pi (\phi/\phi_0)} \quad \text{L の 非線形性}$$

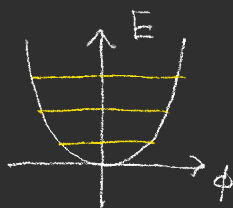
また

$$E_{JNL} = \int L i \frac{d\phi}{dt} dt = \frac{1}{2} L \dot{\phi}^2$$

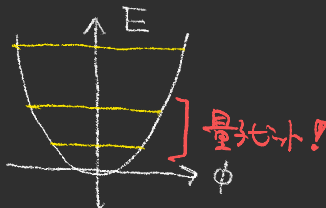
$$= \int \frac{d\phi}{dt} I_0 \sin 2\pi \left(\frac{\phi}{\phi_0} \right) dt = I_0 \frac{\phi_0}{2\pi} \left(1 - \cos 2\pi \left(\frac{\phi}{\phi_0} \right) \right)$$

$$\approx \frac{I_0 \phi_0}{2\pi} \left[\frac{1}{2} \left(\frac{2\pi \phi}{\phi_0} \right)^2 - \frac{1}{4!} \left(\frac{2\pi \phi}{\phi_0} \right)^4 + \dots \right]$$

非調和振動子



$\Rightarrow$

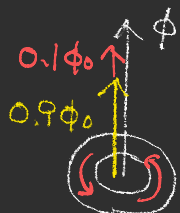


低エネルギー帯を利用

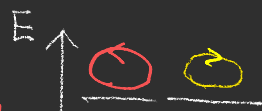
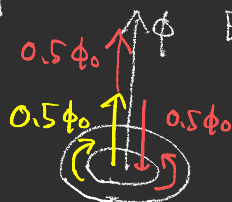
★ 磁束の量子化



「超伝導リング」



0.1 ϕ_0 の電流が流れる



$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$$

量子力学

★ Pauli 行列

$$|\psi\rangle = a|0\rangle + b|1\rangle$$

① 基底の2状態

$$\hat{H} = \begin{pmatrix} H_{00} & H_{01} \\ H_{10} & H_{11} \end{pmatrix}$$

$$\hat{H} = \hat{H}^\dagger \left\{ \begin{array}{l} H_{00} = H_{00}^* \\ H_{01} = H_{10}^* \\ H_{10} = H_{01}^* \\ H_{11} = H_{11}^* \end{array} \right. \begin{array}{l} H_{10} = a+ib \\ H_{01} = a-ib \end{array}$$

$$\hat{H} = \begin{pmatrix} c+d & a-ib \\ a+ib & -c+d \end{pmatrix} = a\hat{\sigma}_x + b\hat{\sigma}_y + c\hat{\sigma}_z + d\hat{I}$$

$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Step up Pauli 行列

② 4つの代表?

$$\hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$[\hat{\sigma}_x, \hat{\sigma}_y] = \hat{\sigma}_x \hat{\sigma}_y - \hat{\sigma}_y \hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$\begin{matrix} y & z \\ z & x \end{matrix}$

$$= \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = 2i\hat{\sigma}_z$$

$\begin{matrix} x \\ y \end{matrix}$

Step up 交換関係

$$[\hat{\sigma}_1, \hat{\sigma}_2] = 2i\hat{\sigma}_3 \quad \{\hat{\sigma}_1, \hat{\sigma}_2\} = 0$$

★ 有効モデル

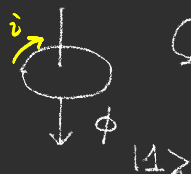
$$\hat{H} = -\hbar \hat{G}_z - \Gamma \hat{G}_x \quad \boxed{\Gamma \neq 0}$$

縦磁場 横磁場

$$= \begin{pmatrix} -\hbar & -\Gamma \\ -\Gamma & +\hbar \end{pmatrix} = \begin{pmatrix} -\hbar & 0 \\ 0 & \hbar \end{pmatrix}$$

$$\begin{cases} \hat{H} |0\rangle = -\hbar |0\rangle \\ \hat{H} |1\rangle = +\hbar |1\rangle \end{cases} \quad (|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix})$$

(例)



$\hat{H} |0\rangle = -\hbar |0\rangle$
 $\hat{H} |1\rangle = +\hbar |1\rangle$

$\boxed{\hbar=0}$

$$\hat{H} = \begin{pmatrix} 0 & -\Gamma \\ -\Gamma & 0 \end{pmatrix} \quad \hat{H} |\psi\rangle = E |\psi\rangle \quad \det(E\hat{I} - \hat{H})$$

$$= \begin{vmatrix} E & \Gamma \\ \Gamma & E \end{vmatrix} = E^2 - \Gamma^2 = 0$$

$\therefore E = \pm \Gamma$

$$\hat{H} |\psi\rangle = \pm \Gamma |\psi\rangle \quad \exists \text{ 非零 } |\psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix} \quad \text{とある}$$

$$\begin{pmatrix} 0 & -\Gamma \\ -\Gamma & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \pm \Gamma \begin{pmatrix} a \\ b \end{pmatrix} \quad \begin{cases} -\Gamma b = \pm \Gamma a \\ -\Gamma a = \pm \Gamma b \end{cases} \quad \begin{matrix} \oplus a=1, b=-1 \\ \ominus a=b=1 \end{matrix}$$

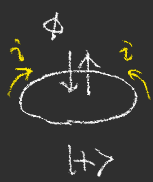
$a, b \neq 0$

$$|\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \equiv |+\rangle$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \equiv |-\rangle$$

$\boxed{\text{重ね合わせの状態}}$

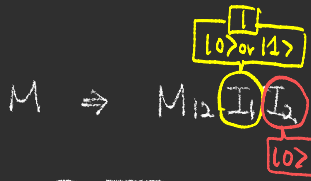
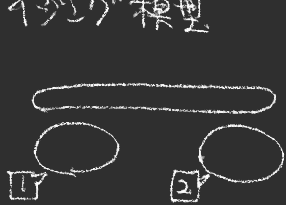
⑬①



-見方はない

12を10, 11, 14, 2, 7

イジング模型



相互作用?

この2つの量子ビットを表現する空間は42

00, 01, 10, 11

テンソル積

$$\begin{pmatrix} a \\ b \end{pmatrix} \otimes \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} ac \\ ad \\ bc \\ bd \end{pmatrix} = ac|00\rangle + ad|01\rangle + bc|10\rangle + bd|11\rangle$$

$$\hat{H} = -\mu_1 \hat{\sigma}_1^z - \mu_2 \hat{\sigma}_2^z - J_1 \hat{\sigma}_1^x - J_2 \hat{\sigma}_2^x - J \hat{\sigma}_1^z \hat{\sigma}_2^z$$

$\hat{\sigma}_1^z \otimes \hat{I}_2$ $\hat{I}_1 \otimes \hat{\sigma}_2^z$ $\hat{\sigma}_1^x \otimes \hat{\sigma}_2^x$ 相互作用

⑬①

$$\hat{\sigma}_1^z \otimes \hat{I}_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\hat{I}_1 \otimes \hat{\sigma}_2^z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\hat{\sigma}_1^z \otimes \hat{\sigma}_2^z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

多体

$$\Rightarrow \hat{H} = \underbrace{-\sum_{i=1}^N \hbar \omega_i \hat{\sigma}_i^z}_{\text{イジング模型}} - \underbrace{\sum_{\langle ij \rangle} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z}_{\text{横磁場}} - \mu \sum_{i=1}^N \hat{\sigma}_i^x$$

(1) $\sum_{\langle ij \rangle}$ は 結合した所のみ

Landau-Zener 遷移 (J. Phys. B: At. Mol. Opt. Phys. 56 (2023) 104001).

$$\hat{H} = \underbrace{-\hbar \alpha t \hat{\sigma}_z}_{\text{磁場 } t \text{ 依存}} - \underbrace{\hbar g \hat{\sigma}_x}_{\text{横磁場}} = \hbar \begin{pmatrix} -\alpha t & -g \\ -g & \alpha t \end{pmatrix}$$

from $t \rightarrow -\infty$

$$\hat{H} \sim \hbar \begin{pmatrix} +\alpha |t| & 0 \\ 0 & -\alpha |t| \end{pmatrix} \rightarrow \begin{matrix} \uparrow \\ \text{100\%} \end{matrix} \begin{matrix} |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{matrix}$$

t_0
 $t \rightarrow \infty$

$$\hat{H} \sim \hbar \begin{pmatrix} -\alpha t & 0 \\ 0 & \alpha t \end{pmatrix} \rightarrow \begin{matrix} \uparrow \\ ? \end{matrix} \begin{matrix} |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{matrix}$$

(2) 途中は? $\begin{pmatrix} t=0 \\ 0 & -g \\ -g & 0 \end{pmatrix}$
 $(|0\rangle + |1\rangle) / \sqrt{2}$

★ $g = 0$

$a(-\infty) \rightarrow 0 \quad b(-\infty) \rightarrow 1$

$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$

$$\begin{cases} \frac{\partial}{\partial t} a(t) = i\alpha t a(t) & \therefore a(t) = \exp(i\frac{\alpha t^2}{2}) a(-\infty) \\ \frac{\partial}{\partial t} b(t) = -i\alpha t b(t) & \therefore b(t) = \exp(-i\frac{\alpha t^2}{2}) b(-\infty) \end{cases}$$

↑ 位相が
源から変化する

↑ 基底が変化する

↑ $\nabla^2 \propto \frac{1}{L^2}$ 考慮

★ $g \neq 0$

$\frac{\partial}{\partial t} a(t) = \underline{i\alpha t a(t)} + \underline{i g b(t)}$ $a(t) = \underline{\exp(i\frac{\alpha t^2}{2})} \underline{c(t)}$ 定数変化法 Σ する

$\Rightarrow \exp(i\frac{\alpha t^2}{2}) \frac{\partial}{\partial t} c(t) = i g b(t) \Rightarrow \frac{\partial c}{\partial t} = i g \exp(-i\alpha t^2) d(t)$

$\frac{\partial}{\partial t} b(t) = \underline{i g a(t)} - \underline{i\alpha t b(t)}$ $b(t) = \underline{\exp(-i\frac{\alpha t^2}{2})} \underline{d(t)}$ Σ する

$\Rightarrow \exp(-i\frac{\alpha t^2}{2}) \frac{\partial}{\partial t} d(t) = i g a(t) \Rightarrow \frac{\partial d}{\partial t} = i g \exp(i\alpha t^2) c(t)$

$\therefore \frac{\partial}{\partial t} c(t) = -g^2 \exp(-i\alpha t^2) \int_{-\infty}^t \underline{\exp(i\alpha t'^2)} \underline{c(t')} dt'$ 源から ゆき

Step up Σ する近似的

$\int \underline{a(t)} \underline{b(t)} dt \rightarrow \int \underline{a(t)} \underline{b(t)} dt$ 全 今

$\approx -g^2 \exp(-i\alpha t^2) \int_{-\infty}^t \underline{\exp(i\alpha t'^2)} dt' \underline{c(t)}$ 今 今 今

$\therefore c(t) = \exp(-g^2 \int_{-\infty}^t \exp(-i\alpha t'^2) f_+(t') dt') \underline{c(-\infty)} \rightarrow 0$

同様 $d(t) = \exp(-g^2 \int_{-\infty}^t \exp(+i\alpha t'^2) f_-(t') dt') \underline{d(-\infty)} \rightarrow 1$

★ $d(t \rightarrow \infty)$ 求め

$$d(t \rightarrow \infty) = \exp(-g^2 \int_{-\infty}^{\infty} \exp(i\alpha t_1^2) \int_{-\infty}^{t_1} \exp(-i\alpha t_2^2) dt_1 dt_2)$$

I

$\int_0^{t_1} \textcircled{I_1} + \int_{-\infty}^0 \textcircled{I_2}$
定数

$$\int_{-\infty}^{\infty} \exp(\pm i\alpha t^2) dt = \sqrt{\frac{\pi}{\mp i\alpha}} = \sqrt{\frac{\pm i\pi}{\alpha}} \quad (\text{Fresnel 積分})$$

$$\int_{-\infty}^{\infty} \exp(-\frac{1}{2}\alpha x^2) dx = \sqrt{\frac{2\pi}{\alpha}}$$

ガウス積分

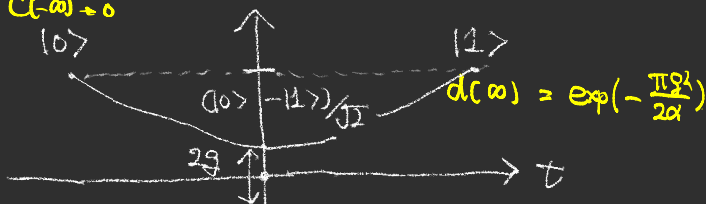
$$I_2 = \sqrt{\frac{i\pi}{\alpha}} \frac{1}{2} \sqrt{\frac{-i\pi}{\alpha}} = \frac{\pi}{2\alpha}$$

$$I_1 = \int_{-\infty}^{\infty} \exp(i\alpha t_1^2) \int_0^{t_1} \exp(-i\alpha t_2^2) dt_1 dt_2$$

$$\int_{\substack{t_1 \rightarrow -t_1 \\ t_2 \rightarrow -t_2}} \exp(i\alpha t_1^2) \int_0^{t_1} \exp(-i\alpha t_2^2) dt_1 dt_2 = -I_1 = 0$$

$$\therefore d(t \rightarrow \infty) = \exp(-\frac{\pi g^2}{2\alpha})$$

$C(-\infty) \rightarrow 0$



$d(-\infty) \rightarrow 1$

$$C(\omega) = \sqrt{1 - \exp(-\frac{\pi g^2}{\alpha})}$$

$\frac{1}{T} \int g(t) dt$ の値

但し T と ω の関係

Step up Landau-Zener $\frac{\hbar^2 \omega^2}{4\alpha}$

$|1\rangle \sim \exp(-\frac{\pi g^2}{\alpha})$ ~~遷移~~
 $|1\rangle \rightarrow |0\rangle$
 $|0\rangle \sim 1 - \exp(-\frac{\pi g^2}{\alpha})$ ~~遷移~~

- ① 横磁場を
I 制御 - 量子機械
- ② α = スピンの
③ スピン遷移 制御

量子制御 時間発展

■ 断熱時間発展 [$\hat{H}(t)$ がゆっくり変化] $\frac{d\hat{H}}{dt} \ll 1$

★ 準備

$$\hat{H}|u_n\rangle = E_n|u_n\rangle$$



固有エネルギーが可数に展開する

step up 固有状態による展開

$$\hat{H}|u_n\rangle = E_n|u_n\rangle$$

直交 $\langle u_m | u_n \rangle = \delta_{mn}$

$$\Rightarrow |\psi\rangle = \sum_n C_n |u_n\rangle$$

完全系 $\sum_n |u_n\rangle \langle u_n| = I$

背景

$$f(x) = \sum_k a_k e^{ikx} \quad (2\pi\hbar)$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dk \hat{f}(k) e^{ikx} \quad (\text{自由})$$

$$\underline{\psi(x)} = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp \underbrace{e^{i\frac{p}{\hbar}x}}_{\text{波数}} \underline{\psi(p)} \quad (\hbar k = p)$$

$$\Leftrightarrow |\psi\rangle$$

$$\Leftrightarrow |p\rangle \langle p| \psi\rangle$$

これ

$$|\psi\rangle = \int_{-\infty}^{\infty} dp \underbrace{I}_{I: \text{恒等演算}} |p\rangle \underbrace{\langle p| \psi\rangle}_{C_p \text{ 係数}}$$

⑦ 未知 $|p\rangle$ の展開

$$\text{逆変換} = \sum_n \underbrace{|u_n\rangle \langle u_n|}_{C_n \text{ 係数}} \psi$$

$|u_n\rangle$ の展開

$$\Rightarrow |\psi\rangle = \sum_n C_n |U_n\rangle \quad \textcircled{II} \quad i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle \quad \text{エネルギー}$$

$$|\psi(t)\rangle = \sum_n C_n(t) |U_n\rangle$$

$$\textcircled{I} \quad i\hbar \sum_n \frac{\partial}{\partial t} C_n(t) |U_n\rangle$$

$$\textcircled{II} \quad \sum_n C_n(t) E_n |U_n\rangle$$

$$\therefore \frac{\partial C_n}{\partial t} = -i \frac{1}{\hbar} E_n C_n(t)$$

$$\text{よ} \quad C_n(t) = \underbrace{C_n(0)}_{\text{初期条件}} \exp(-i \frac{1}{\hbar} E_n t)$$

★ $\hat{H} \rightarrow \hat{H}(t)$ に注意

$$\hat{H}(t) |U_n(t)\rangle = E_n(t) |U_n(t)\rangle \quad \textcircled{II} \quad \boxed{\text{固有状態も変化する}}$$

$$|\psi(t)\rangle = \sum_n \underbrace{C_n(t)}_{\text{定数法}} \exp(-i \frac{1}{\hbar} \int_0^t E_n(t') dt') |U_n(t)\rangle \quad \textcircled{II} \quad \begin{cases} i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle \\ = \hat{H}(t) |\psi(t)\rangle \\ \rightarrow \text{代入} \end{cases}$$

$$\textcircled{I} \quad i\hbar \sum_n \left[\frac{\partial C_n}{\partial t} \exp(\dots) \underbrace{|U_n(t)\rangle}_{\text{再び変化する}} + C_n(t) \exp(\dots) \frac{\partial}{\partial t} |U_n(t)\rangle \right] + \sum_n C_n(t) E_n(t) \exp(\dots) |U_n(t)\rangle$$

$$\textcircled{II} \quad \cancel{\sum_n C_n(t) E_n(t) \exp(\dots) |U_n(t)\rangle}$$

$$\therefore \frac{\partial C_n}{\partial t} = - \sum_m C_m(t) \exp(i \frac{1}{\hbar} \int_0^t dt' (E_m(t') - E_n(t'))) \langle U_m(t) | \frac{\partial}{\partial t} |U_n(t)\rangle$$

$$\textcircled{II} \quad \boxed{\langle U_m(t) | \frac{\partial}{\partial t} |U_n(t)\rangle \rightarrow \text{何?}}$$

$$\textcircled{I} \quad \boxed{\hat{H}(t) \text{ が } \psi < 0 \text{ も考慮する}}$$

$$\frac{dA}{dt} \ll 1$$

$$\textcircled{1} \hat{H}(t) |U_n(t)\rangle = E_n(t) |U_n(t)\rangle$$

(*)

$$\frac{d\hat{H}}{dt} |U_n(t)\rangle + \hat{H}(t) \frac{d}{dt} |U_n(t)\rangle = \frac{dE_n}{dt} |U_n(t)\rangle + E_n(t) \frac{d}{dt} |U_n(t)\rangle$$

左に $\langle U_m(t) |$ ($m \neq n$)

$$\begin{aligned} & \langle U_m(t) | \frac{d\hat{H}}{dt} |U_n(t)\rangle + \overbrace{\langle U_m(t) | \hat{H}(t) }^{\langle U_m(t) | E_n(t) \rangle} \frac{d}{dt} |U_n(t)\rangle \\ &= \frac{dE_n}{dt} \underbrace{\langle U_m(t) | U_n(t) \rangle}_{\substack{\delta_{m,n} \\ \rightarrow 0}} + E_n(t) \langle U_m(t) | \frac{d}{dt} |U_n(t)\rangle \end{aligned}$$

$$\therefore \langle U_m(t) | \frac{d\hat{H}}{dt} |U_n(t)\rangle = - (E_m(t) - E_n(t)) \langle U_m(t) | \frac{d}{dt} |U_n(t)\rangle$$

$$\text{よ} \frac{d\hat{H}}{dt} \Rightarrow 0 \quad \langle U_m(t) | \frac{d}{dt} |U_n(t)\rangle \Rightarrow 0 \quad \textcircled{!!} \boxed{m \neq n \text{ には } 0 \text{ になる}}$$

$$\frac{\partial}{\partial t} C_m(t) = - C_m(t) \langle U_m(t) | \frac{d}{dt} |U_m(t)\rangle$$

$$\text{よ} C_m(t) = C_m(0) \exp\left(- \underbrace{\int_0^t dt \langle U_m(t) | \frac{d}{dt} |U_m(t)\rangle}_{\substack{\textcircled{!!} \\ \text{虚数}}}\right)$$

$$\textcircled{2} \langle U_m(t) | U_m(t) \rangle = 1$$

$$\underbrace{\left(\frac{d}{dt} \langle U_m(t) | \right) |U_m(t)\rangle}_{\left(\langle U_m(t) | \frac{d}{dt} |U_m(t)\rangle \right)^*} + \langle U_m(t) | \frac{d}{dt} |U_m(t)\rangle = 0$$

$$\left(\langle U_m(t) | \frac{d}{dt} |U_m(t)\rangle \right)^*$$

$$\textcircled{!!} \boxed{z + z^* = 0 \text{ なら } z \text{ は純虚数}}$$

$$\textcircled{\nearrow} \boxed{|C_m(t)| = |C_m(0)| \text{ 不変}}$$

step up 断熱時間発展

$$\frac{d\hat{H}}{dt} \rightarrow 0 \quad |C_m(t)| = |C_m(0)|$$

① 基底状態が定常!

$$\Rightarrow \text{step up 量} \rightarrow p_2 - p_1 \rightarrow f(t) = 0 \rightarrow 1$$

$$\hat{H}(t) = f(t) \hat{H}_0 + (1-f(t)) \hat{H}_1$$

$$- \sum_j J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z - \sum_i h_i \hat{\sigma}_i^z$$

9/12/14/15/16/17/18/19/20/21/22/23/24/25/26/27/28/29/30/31/32/33/34/35/36/37/38/39/40/41/42/43/44/45/46/47/48/49/50/51/52/53/54/55/56/57/58/59/60/61/62/63/64/65/66/67/68/69/70/71/72/73/74/75/76/77/78/79/80/81/82/83/84/85/86/87/88/89/90/91/92/93/94/95/96/97/98/99/100

$$- \Gamma \sum_i \hat{\sigma}_i^x$$

1/3/11/12/13/14/15/16/17/18/19/20/21/22/23/24/25/26/27/28/29/30/31/32/33/34/35/36/37/38/39/40/41/42/43/44/45/46/47/48/49/50/51/52/53/54/55/56/57/58/59/60/61/62/63/64/65/66/67/68/69/70/71/72/73/74/75/76/77/78/79/80/81/82/83/84/85/86/87/88/89/90/91/92/93/94/95/96/97/98/99/100

$$\frac{d\hat{H}}{dt} \rightarrow 0 \quad \hat{H}_0 \text{ a G.S.}$$

Easy

$$\hat{H}_1 \text{ a G.S.}$$

Hard

$$[\hat{H}_0, \hat{H}_1] \neq 0$$

① $\sum_i \hat{\sigma}_i^z$ 保存?

$$\star C_m(t) = 1 \quad C_{n \neq m}(t) = 0 \text{ a 持たず条件は? } - \langle U_m(t) | \frac{d}{dt} | U_m(t) \rangle$$

$$C_m(t) = 1 \quad C_{n \neq m}(t) = 0$$

$$E_m(t) = E_n(t)$$

$$\frac{dC_m}{dt} = \sum_n C_n(t) \exp(i \frac{1}{\hbar} \int_0^t dt' \Delta_{mn}(t')) \frac{\langle U_m(t) | \frac{d\hat{H}}{dt} | U_m(t) \rangle}{\Delta_{mn}(t)}$$

① $C_m(t)$ 定常?

$$\Rightarrow \frac{dC_{n \neq m}}{dt} = \exp(i \frac{1}{\hbar} \int_0^t dt' \Delta_{nm}(t')) \frac{\langle U_n(t) | \frac{d\hat{H}}{dt} | U_n(t) \rangle}{\Delta_{nm}(t)}$$

① 一般に Δ_{nm} は $\Delta_{nm} \approx \Delta_{nm}^{\text{max}} - \Delta_{nm}^{\text{min}}$ と考へ

① $\int dt$ 十分大?

面倒!

$$C_{n \neq m}(t) \approx \int_0^t dt_1 \exp(i \frac{1}{\hbar} \int_0^{t_1} dt_2 \Delta_{nm}(t_2)) \frac{\langle U_n(t_1) | \frac{d\hat{H}}{dt} | U_n(t_1) \rangle}{\Delta_{nm}(t_1)}$$

$$= \frac{-i\hbar}{\Delta_{nm}} \frac{\langle u_m | \frac{dH}{dt} | u_n \rangle}{\Delta_{nm}} \left[\exp\left(\frac{i}{\hbar} \Delta_{nm} t\right) - 1 \right]$$

$$\begin{aligned} & \textcircled{11} |e^{i\theta} - 1|^2 \\ &= (e^{i\theta} - 1)(e^{-i\theta} - 1) \\ &= 2 - e^{i\theta} - e^{-i\theta} \\ &= \frac{2(1 - \cos\theta)}{1} \end{aligned}$$

$$|C_{n \leftarrow m}(t)| = \frac{\hbar}{|\Delta_{nm}|^2} \left| \langle u_m | \frac{dH}{dt} | u_n \rangle \right| \left| 2 \sin\left(\frac{\Delta_{nm} t}{2\hbar}\right) \right|$$

これは大切!
(1) $\hbar < \hbar \omega$...
(2) $\Delta_{nm} \rightarrow 0$...

Step up QA 成功の条件

$\Delta_{nm}(t) = E_n(t) - E_m(t)$ 为

$\frac{1}{T} \frac{1}{\Delta_{nm}^2} \ll 1 \text{ 或 } T \gg \frac{1}{\Delta_{nm}^2}$

$$\begin{aligned} & \textcircled{11} \frac{dH}{dt} \sim \frac{1}{T} \text{ 数} \\ & f(t) = \frac{1}{T} \text{ 最短時刻} \end{aligned}$$

四 1次元-フロップ

★ 1次元-探索問題 [J. Roland and N. Cerf = Phys. Rev. A 65 042308 (2002)]

$N \times a$ 内 1点 指定した状態 $|n\rangle$ を出す $\rightarrow O(N)$ 時間 $\xrightarrow{\text{量子加速}} O(\sqrt{N})$ 時間

$$\hat{H}_0 = \hat{I} - |n\rangle\langle n| \quad \begin{cases} \hat{H}_0 |n\rangle = |n\rangle - |n\rangle = \textcircled{0} |n\rangle \\ \hat{H}_0 |k\rangle = \textcircled{1} |k\rangle \end{cases} \quad \text{G.S.}$$

$$\hat{H}_1 = \hat{I} - |\psi\rangle\langle\psi| = \begin{cases} \hat{H}_1 |\psi\rangle = |\psi\rangle - |\psi\rangle = \textcircled{0} |\psi\rangle \\ \hat{H}_1 |\phi\rangle = \textcircled{1} |\phi\rangle \end{cases} \quad \text{G.S.}$$

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_k |k\rangle \quad (\phi=0) \quad \text{さらに } \langle\psi|\phi\rangle = \frac{1}{N} \sum_k \sum_l \exp(i \frac{2\pi}{N} k l \phi) \langle k|l\rangle = \frac{1}{N} \sum_k \underbrace{\exp(i \frac{2\pi}{N} k \phi)}_{\omega^{k\phi}} \underbrace{\langle k|k\rangle}_{\delta_{kk}} = \textcircled{0} (\phi \neq 0)$$

$$|\phi\rangle = \frac{1}{\sqrt{N}} \sum_k \exp(i \frac{2\pi}{N} k \phi) |k\rangle = \frac{1}{N} \sum_k \underbrace{\exp(i \frac{2\pi}{N} k \phi)}_{\omega^{k\phi}} = \textcircled{0} (\phi \neq 0)$$

$$1\phi + \omega\phi + \omega^2\phi + \dots + \omega^{N-1}\phi = \frac{1-\omega^N\phi}{1-\omega}$$

行列表示 $\langle k|\hat{H}_0|l\rangle \rightarrow A_{kl}$

$$\Rightarrow \begin{pmatrix} 1 & & & 0 \\ & 1 & & \\ & & \ddots & \\ 0 & & & 1 \end{pmatrix}$$

$\langle k|\hat{H}_1|l\rangle \rightarrow B_{kl}$

$$\begin{pmatrix} 1-\frac{1}{N} & & -\frac{1}{N} \\ & \ddots & \\ -\frac{1}{N} & & 1-\frac{1}{N} \end{pmatrix}$$

★ $|n\rangle$ を 2次元外に 2次元

$$|\bar{n}\rangle = \frac{1}{\sqrt{N-1}} \sum_{k \neq n} |k\rangle$$

行列表示 $\begin{pmatrix} \langle n|\hat{A}|n\rangle & \langle n|\hat{A}|\bar{n}\rangle \\ \langle \bar{n}|\hat{A}|n\rangle & \langle \bar{n}|\hat{A}|\bar{n}\rangle \end{pmatrix}$

$$\hat{I} \rightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad |n\rangle\langle n| \rightarrow \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\hat{H}_0 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$| \psi \rangle \langle \psi | = \begin{pmatrix} \frac{1}{N} & \frac{\sqrt{N-1}}{N} \\ \frac{\sqrt{N-1}}{N} & 1 - \frac{1}{N} \end{pmatrix}$$

$$\textcircled{?} \langle n | \psi \rangle = \frac{1}{\sqrt{N}}$$

$$\begin{aligned} \langle \bar{n} | \psi \rangle &= \frac{1}{\sqrt{N}} \frac{1}{\sqrt{N-1}} \sum_l \sum_{k \neq n} \langle k | l \rangle \\ &= \frac{1}{\sqrt{N(N-1)}} \left\{ \sum_k \left(\sum_l \overset{\delta_{kl}}{\langle k | l \rangle} \right) - \sum_l \overset{\delta_{nl}}{\langle n | l \rangle} \right\} \\ &= \frac{1}{\sqrt{N(N-1)}} \{ N - 1 \} = \sqrt{\frac{N-1}{N}} \end{aligned}$$

$$\hat{H}_1 = \begin{pmatrix} 1 - \frac{1}{N} & -\frac{\sqrt{N-1}}{N} \\ -\frac{\sqrt{N-1}}{N} & \frac{1}{N} \end{pmatrix}$$

$$\begin{aligned}
 \hat{H}(t) &= f(t) \hat{H}_0 + (1-f(t)) \hat{H}_1 \\
 &= \begin{pmatrix} 0 & 0 \\ 0 & f \end{pmatrix} + (1-f) \begin{pmatrix} 1-\frac{1}{N} & -\frac{\sqrt{N-1}}{N} \\ -\frac{\sqrt{N-1}}{N} & \frac{1}{N} \end{pmatrix} \quad (f, f(t)) \\
 &= \begin{pmatrix} \underbrace{(1-f)(1-\frac{1}{N})}_{\frac{1}{2}-\frac{1}{2}} & \underbrace{-(1-f)\frac{\sqrt{N-1}}{N}}_{\hat{\sigma}_x} \\ \underbrace{-(1-f)\frac{\sqrt{N-1}}{N}}_{\hat{\sigma}_x} & \boxed{f + (1-f)\frac{1}{N}} \end{pmatrix} \\
 &\quad \frac{1}{N} + f(1-\frac{1}{N}) = 1 - (1-f)(1-\frac{1}{N}) \\
 &\quad \frac{1}{2} + \frac{1}{2}
 \end{aligned}$$

$$= \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \frac{\Delta}{2} \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix}$$

$\cos \theta \hat{\sigma}_z + \sin \theta \hat{\sigma}_x$

$$\begin{cases} \cos \theta = \frac{1}{\Delta} \left\{ 1 - 2(1-f)(1-\frac{1}{N}) \right\} \\ \sin \theta = \frac{1}{\Delta} 2(1-f) \frac{\sqrt{N-1}}{N} \end{cases}$$

$$\Delta = \sqrt{(1-2(1-f)(1-\frac{1}{N}))^2 + 4(1-f)^2 \frac{N-1}{N^2}} = \sqrt{1-4(1-f)f(1-\frac{1}{N})}$$

★ 厄米共轭-†

$$| \cos \theta \hat{\sigma}_z + \sin \theta \hat{\sigma}_x - \lambda \hat{I} | = \begin{vmatrix} \cos \theta - \lambda & \sin \theta \\ \sin \theta & -\cos \theta - \lambda \end{vmatrix} = \lambda^2 - 1 = 0$$

$\therefore \lambda = \pm 1$

$$\begin{cases} \hat{H}(t) |u_0(t)\rangle = \left(\frac{1}{2} - \frac{\Delta}{2} \right) |u_0(t)\rangle \\ \hat{H}(t) |u_1(t)\rangle = \left(\frac{1}{2} + \frac{\Delta}{2} \right) |u_1(t)\rangle \end{cases}$$

$\xrightarrow{E_0(t)} \quad \xrightarrow{E_1(t)}$

$$\therefore \Delta(t) = E_1(t) - E_0(t) = \Delta$$

★ 断绝条件

$$\frac{df}{dt}(\hat{H}_0 - \hat{H}_1)$$

$$\frac{1}{|\Delta|^2} \left| \langle u_1 | \left(\frac{d\hat{H}}{dt} \right) | u_0 \rangle \right| \ll 1 \quad \text{~~~~~} = \varepsilon \textcircled{4}$$

$$\text{故 } \left| \frac{df}{dt} \right| = \varepsilon \frac{|\Delta|^2}{|\langle u_1 | \hat{H}_0 - \hat{H}_1 | u_0 \rangle|} \equiv \alpha \Delta^2 \quad \textcircled{11} \left\{ \begin{array}{l} \frac{df}{dt} \text{ 是} \\ \text{单同磨加磨} \end{array} \right.$$

$$\frac{df}{dt} = \alpha \left(\underset{1 - \frac{1}{N} + \frac{1}{N}}{1 - 4(1-f)f(1-\frac{1}{N})} \right) = \frac{\alpha}{N} \left(1 + \frac{\alpha \tan^2 \phi}{(1-2f)^2 (N-1)} \right)$$

$$\int_0^1 \frac{df}{1 + \frac{(N-1)(2f-1)^2}{\tan^2 \phi}} = \int_0^T \frac{\alpha}{N} dt$$

$$\sqrt{N-1} (2f-1) = \tan \phi$$

$$2\sqrt{N-1} df = \frac{d\phi}{\cos^2 \phi}$$

$$\frac{1}{2\sqrt{N-1}} \int_{\phi_0}^{\phi_1} \frac{\cancel{\cos^2 \phi}}{\cos^2 \phi} d\phi = \frac{\alpha}{N} T$$

$$\begin{cases} \tan \phi_0 = \sqrt{N-1} (-1) \\ \tan \phi_1 = \sqrt{N-1} (+1) \end{cases}$$

$$\text{故 } T = \frac{N}{2\alpha\sqrt{N-1}} (\phi_1 - \phi_0) \xrightarrow{(N \rightarrow \infty)} \sqrt{N}$$

$$\textcircled{11} \left\{ \begin{array}{l} O(N) \rightarrow \underline{O(\sqrt{N})} \text{ 是?} \end{array} \right.$$

$$\gamma_0 - \gamma_1 = \alpha \sqrt{N} \gamma_2 \gamma_3 \gamma_4 \gamma_5 \gamma_6 \gamma_7 \gamma_8 \gamma_9$$

QA の収束定理 (Morita and Nishimori (2006))

$$|C_{nm}(t)| = \frac{\hbar}{|\Delta_{nm}|} \left| \langle u_m | \frac{d\hat{H}}{dt} | u_n \rangle \right| \left| 2 \sin\left(\frac{\Delta_{nm} t}{2\hbar}\right) \right| \ll 1$$

(★) → (★)

★ QA の一般論

$$\Delta_{nm}(t) = E_m(t) - E_n(t)$$

① 各時刻の固有エネルギーを列挙

$$\hat{H}(t) = \hat{H}_0 + \Gamma(t) \hat{H}_1 \quad \Gamma(t) = \Gamma_0 \rightarrow 0 \quad \text{(★) 定理は nonadiabatic?}$$

$\frac{d\Gamma}{dt} < 0$ (単調減少)

$$\begin{cases} \hat{H}_0 = - \sum_j J_j \hat{\sigma}_j^z \text{ etc} \\ \hat{H}_1 = - \sum_{i=1}^N \hat{\sigma}_i^x \text{ (横磁場)} \end{cases}$$

$$\textcircled{\star} \left| \langle u_m | \frac{d\hat{H}}{dt} | u_0 \rangle \right| = - \frac{d\Gamma}{dt} \left| \langle u_m | \sum_{i=1}^N \hat{\sigma}_i^x | u_0 \rangle \right|$$

$$\begin{cases} |u_m(t)\rangle = \sum_k C_{mk}(t) |k\rangle \Rightarrow \boxed{\hat{\sigma}_i^x} \text{ 1 spin flip. } |0\rangle \leftrightarrow |1\rangle \\ \quad \begin{matrix} |100\dots 00\rangle, |100\dots 01\rangle, \\ |100\dots 11\rangle, \dots \end{matrix} \\ \quad \begin{matrix} |100\dots 01\rangle, |100\dots 00\rangle \\ |100\dots 10\rangle \end{matrix} \end{cases}$$

$$\underbrace{\langle u_m(t) | \hat{\sigma}_i^x | u_0(t) \rangle}_{\text{大文字で記述}} = \cos \theta$$

$$\leq - N \frac{d\Gamma}{dt}$$

★ Hopf 定理 (★) 1.

$$\hat{M} = \text{非負値行列} \Rightarrow |\varepsilon_0| \leq \frac{k-1}{k+1} \varepsilon_0 \quad (\varepsilon_0: \text{固有値}) \quad \text{①} \quad \boxed{\hat{M} \text{ 作用!}}$$

$\varepsilon_0 > \varepsilon_1 > \dots$

$$k = \max_{i,j,k} \left\{ \frac{M_{ijk}}{M_{ik}} \right\} \leq \frac{\max_{ij} \{M_{ij}\}}{\min_{ij} \{M_{ij}\}} \quad \text{②} \quad \boxed{M_{ij} \text{ 最小} \geq \max}$$

(行列)
(難?)
(實際使(易)?)

$$\hat{M} = (E_+ \hat{I} - \hat{H}(t))^N \text{ とおす } E_+ \geq E_0^{\max} + P_0 N$$

$$E_+ \hat{I} - \hat{H}(t) = \underbrace{E_+ \hat{I} - \hat{H}_0}_{\text{③ 対角} > 0} + P(t) \sum_{i=1}^N \hat{\sigma}_i^x$$

(大)
(小)

④ M_{ij} が大きい $\Rightarrow$ 対角 $\geq M_{ij}$ が小さい $\Rightarrow$ 非対角 $\geq$

$$\max_{ij} \{M_{ij}\} \leq \left(\underbrace{E_+ - E_0^{\min}}_{\text{差は大き?}} + \underbrace{P_0 N}_{\text{ここは大き?}} \right)^N$$

$$\min_{ij} \{M_{ij}\} = \underbrace{\langle \phi' |}_{\text{↑}} \underbrace{\left((E_+ \hat{I} - \hat{H}_0)^k \left(P(t) \sum_{i=1}^N \hat{\sigma}_i^x \right)^{N-k} \right)}_{\text{↑ } N \text{ 回反転}} \underbrace{|\phi \rangle}_{\text{↓}}$$

⑤ $\boxed{k=0 \text{ が最小!}}$

$$= P(t)^N \langle \phi' | \underbrace{\left(\sum_{i=1}^N \hat{\sigma}_i^x \right) \dots \left(\sum_{i=1}^N \hat{\sigma}_i^x \right)}_{\text{1, 2, } \dots, N \text{ の順番に分ける}} | \phi \rangle$$

$$= P(t)^N N!$$

$$N! \sim e^{-N} N^N$$

$$\therefore k \leq \frac{(E_+ - E_0^{\min} + P_0 N)^N}{N! (P(t))^N} \sim \frac{1}{\sqrt{2\pi N}} \left(\frac{E_+ - E_0^{\min} + P_0 N}{N P(t)} \right)^N e^N$$

[Step up] Stirling 公式

$$N! \sim \sqrt{2\pi N} N^N e^{-N}$$

[Hopf]

$$|E_0| \leq \frac{k-1}{k+1} E_0 \quad (E_0 \text{ は } M \text{ の固有値})$$

$$(E_+ - \lambda_i)^N \leq \frac{k-1}{k+1} (E_+ - \lambda_0)^N \quad \text{① ② ③ ④ ⑤ ⑥ ⑦ ⑧ ⑨ ⑩ ⑪ ⑫ ⑬ ⑭ ⑮ ⑯ ⑰ ⑱ ⑲ ⑳ ㉑ ㉒ ㉓ ㉔ ㉕ ㉖ ㉗ ㉘ ㉙ ㉚ ㉛ ㉜ ㉝ ㉞ ㉟ ㊱ ㊲ ㊳ ㊴ ㊵ ㊶ ㊷ ㊸ ㊹ ㊺ ㊻ ㊼ ㊽ ㊾ ㊿}$$

$$E_+ - \lambda_i \leq \left(\frac{k-1}{k+1} \right)^{1/N} (E_+ - \lambda_0)$$

$$\left[\left(\frac{k-1}{k+1} \right)^{1/N} \right]^N = \left(1 - \frac{2}{k+1} \right)^{\frac{1}{N}} = 1 - \frac{2}{N(k+1)} + \dots \leq 1 - \frac{2}{N(k+1)}$$

$$\leq (E_+ - \lambda_0) - \frac{2}{N(k+1)} (E_+ - \lambda_0)$$

$$\text{よ} \lambda_i - \lambda_0 \geq \frac{2}{N(k+1)} (E_+ - \lambda_0) \sim \frac{2}{Nk} (E_+ - \lambda_0)$$

$$\geq \frac{2\sqrt{2\pi N}}{Nek} (E_+ - \lambda_0) \left(\frac{N}{E_+ - E_0^{\min} + P_0 N} \right)^N P(t)^N = A$$

$$\text{よ} |C_{nm}(t)| \ll 1 \text{ とおける}$$

$$P^{-2N} \frac{dP}{dt}$$

$$-N \frac{dP}{dt} \frac{1}{A^2 P(t)^{2N}} = \delta \ll 1$$

$$-\frac{N}{A^2} \frac{1}{-2N+1} \left(P(t)^{-2N+1} \right) = \delta t + C$$

$$P(t) = \left(\frac{2N-1}{N} A^2 \right)^{\frac{1}{1-2N}} (\delta t + c)^{\frac{1}{1-2N}}$$

Step up QAE 収束定理

$$P(t) \sim t^{-\frac{1}{2N}} z$$

確率基底状態の対称性

古典統計力学

★ 平衡状態

~~量子~~

~~系~~

$$P(\vec{x}) = \frac{1}{Z} \exp(-\beta E(\vec{x})) \quad \left(\beta = \frac{1}{T} \right)$$

温度

$$E(\vec{x}) = - \sum_{\langle ij \rangle} J_{ij} x_i x_j - \sum_{i=1}^N h_i x_i$$

(6)

例 $\rightarrow x_i = \pm 1$ に
2つ!

$$Z = \sum_{\vec{x}} \exp(-\beta E(\vec{x}))$$

★ マルコフ連鎖モンテカルロ法

初期分布

$$P_0(\vec{x}) \xrightarrow{M(\vec{x}|\vec{x}')} P_1(\vec{x}') \rightarrow P_2(\vec{x}'') \rightarrow \dots \rightarrow P_\infty(\vec{x}) = P(\vec{x}) = \frac{1}{Z} \exp(-\beta E(\vec{x}))$$

$$P_{t+1}(\vec{x}) = \sum_{\vec{x}'} \overset{\text{行和}}{M(\vec{x}|\vec{x}')} \overset{\text{カラム}}{P_t(\vec{x}')} \quad (\text{離散マスタ方程式})$$

$$\circ \sum_{\vec{x}} M(\vec{x}|\vec{x}') = 1 \quad (\text{確率保存})$$

$$\circ \sum_{\vec{x}} M(\vec{x}|\vec{x}') P(\vec{x}') = P(\vec{x}) \quad (\text{ついで条件}) \quad \left(\prod_{i=1}^N \text{Zcal (例)} \right)$$

$$t \rightarrow \infty \text{ として } P_\infty(\vec{x}) = \sum_{\vec{x}'} M(\vec{x}|\vec{x}') P_\infty(\vec{x}') \quad P_\infty(\vec{x}) \rightarrow P(\vec{x})$$

定常分布 目標分布

Step up 詳細な条件

$$M(\vec{x}|\vec{x}') P(\vec{x}') = M(\vec{x}'|\vec{x}) P(\vec{x}) \Rightarrow \text{詳細条件 ok!}$$

$$\textcircled{1} \sum_{\vec{x}} M(\vec{x}|\vec{x}') P(\vec{x}') = \sum_{\vec{x}} \underbrace{M(\vec{x}'|\vec{x})}_{\text{DBC}} \underbrace{P(\vec{x})}_{\text{確率値 } 0.1} = P(\vec{x}) \text{ ok!}$$

★ 遷移行列 = 提案 × 受理

$$M(\vec{x}|\vec{x}') = \underbrace{C(\vec{x}|\vec{x}')}_{\vec{x}' \text{ から } \vec{x} \text{ へ提案}} \cdot \underbrace{A(\vec{x}|\vec{x}')}_{\text{受け入れ OK/NG}}$$

$$\textcircled{\text{例}} \quad C(\vec{x}|\vec{x}') = \frac{1}{N} \quad (\vec{x}' \text{ へおす})$$

$$\vec{x}' = \{+1, -1, +1\}$$

$$\vec{x} = \{+1, +1, +1\}$$

① $N=3$ なら 1 spin flip

Step up 受け入れ方法

$$A(\vec{x}|\vec{x}') = \min \left\{ 1, \frac{P(\vec{x})}{P(\vec{x}')} \frac{C(\vec{x}'|\vec{x})}{C(\vec{x}|\vec{x}')} \right\}$$

$$M(\vec{x}|\vec{x}') = \cancel{C(\vec{x}|\vec{x}')} \cdot \boxed{\frac{P(\vec{x})}{P(\vec{x}')} \frac{C(\vec{x}'|\vec{x})}{C(\vec{x}|\vec{x}')}} < 1$$

$$M(\vec{x}|\vec{x}') = \cancel{C(\vec{x}|\vec{x}')} \times 1 = \frac{P(\vec{x})}{P(\vec{x}')} \Rightarrow \text{DBC ok!}$$

$$\Rightarrow \text{乱数 } r \in (0, 1] \text{ を生成} \quad \begin{cases} r < \frac{P(\vec{x})}{P(\vec{x}')} (= \exp(-\beta \Delta E)) \text{ なら OK!} \\ \Delta E \leq 0 \text{ の時} \Rightarrow \vec{x}' \rightarrow \vec{x} \quad \text{otherwise なら NG!} \end{cases}$$

★ 量子系 Λ .

$$Z = \sum_{\vec{x}} \exp(-\beta E(\vec{x})) = \text{Tr}[\exp(-\beta \hat{H})]$$

固有値 (= 対角成分)

$$P(\vec{x}) \rightarrow \hat{\rho} = \frac{1}{Z} \exp(-\beta \hat{H}) \quad (\text{密度行列})$$

$$\begin{aligned} \langle A(\vec{x}) \rangle &= \sum_{\vec{x}} A(\vec{x}) P(\vec{x}) \\ &= \text{Tr}[\hat{A} \hat{\rho}] \quad (\text{期待値}) \end{aligned}$$

Step up 量子 + 統計

$$\hat{\rho} = \frac{1}{Z} \exp(-\beta \hat{H}) = \frac{1}{Z} \exp(-\beta E_n) \underbrace{|n\rangle\langle n|}_{\text{統計}} \quad \boxed{\text{量子}}$$

量子モンテカルロ法 ($\hat{H} = \hat{H}_0 + \hat{H}_1$ [$\hat{H}_0, \hat{H}_1 \neq 0$])

★ 行列 α 級 u

$$e^{\hat{A}+\hat{B}} \neq e^{\hat{A}} e^{\hat{B}} \quad [\hat{A}, \hat{B}] \neq 0.$$

Step up Campbell-Baker-Hausdorff の公式

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-[\hat{A}, \hat{B}]/2}$$

$$e^{t(\hat{A}+\hat{B})} = \cancel{I} + \cancel{t(\hat{A}+\hat{B})} + \frac{t^2}{2}(\hat{A}+\hat{B})^2 + \dots$$

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

$$e^{t\hat{A}} = I + t\hat{A} + \frac{1}{2}t^2\hat{A}^2$$

$$\underline{e^{t\hat{A}}e^{t\hat{B}}} = (I + t\hat{A} + \frac{1}{2}t^2\hat{A}^2 + \dots)(I + t\hat{B} + \frac{1}{2}t^2\hat{B}^2 + \dots)$$

$$= \cancel{I} + \cancel{t(\hat{A}+\hat{B})} + \frac{1}{2}t(\cancel{\hat{A}^2} + \cancel{\hat{B}^2} + \underline{2\hat{A}\hat{B}}) + \dots$$

$$- \frac{t^2}{2}(\hat{A}\hat{B} - \hat{B}\hat{A}) \approx e^{-\frac{t^2}{2}[\hat{A}, \hat{B}]}$$

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

★ 鈴木・ロッド-分解

$$e^{-\beta\hat{H}} = (e^{-\frac{\beta}{M}(\hat{H}_0 + \hat{H}_1)})^M \quad (M: \text{トロッコ-数})$$

$$\left[e^{-\frac{\beta}{M}(\hat{H}_0 + \hat{H}_1)} = e^{-\frac{\beta}{M}\hat{H}_0} e^{-\frac{\beta}{M}\hat{H}_1} e^{-\frac{\beta}{2M}[\hat{H}_0, \hat{H}_1]} \right] \quad \xrightarrow{1 \left(\frac{\beta}{M} \ll 1 \right)}$$

$$\approx (e^{-\frac{\beta}{M}\hat{H}_0} e^{-\frac{\beta}{M}\hat{H}_1})^M \quad \textcircled{1} \quad \boxed{\text{具体的な表現がない}}$$

Step up 完全系 $\sum_{\vec{\sigma}} \dots$ (はたわ)

$$\hat{I} = \sum_{\vec{\sigma}} |\vec{\sigma}\rangle \langle \vec{\sigma}|$$

$$\sum_j A_{ij} B_{jk}$$

$$\sum_{[\vec{\sigma}_1, \vec{\sigma}_2, \dots, \vec{\sigma}_M]} |\vec{\sigma}_M\rangle \langle \vec{\sigma}_M| e^{-\frac{\beta}{M}\hat{H}_0} |\vec{\sigma}_{M-1}\rangle \langle \vec{\sigma}_{M-1}| e^{-\frac{\beta}{M}\hat{H}_1} |\vec{\sigma}_{M-2}\rangle \langle \vec{\sigma}_{M-2}| \dots$$

$$\textcircled{1} \quad \left[\langle \vec{\sigma}_{i+1} | e^{-\frac{\beta}{M}\hat{H}} | \vec{\sigma}_i \rangle = \text{遷移行列} \right]$$

仮想的時刻

★ 遷移行列

$$\begin{matrix} \uparrow & \downarrow \\ \uparrow & \downarrow \end{matrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \vec{\sigma}_t$$

$$\langle \vec{\sigma}_{t+1} | e^{-\frac{\beta P}{M} A_0} | \vec{\sigma}_t \rangle = \delta(\vec{\sigma}_{t+1}, \vec{\sigma}_t) \exp\left(\frac{\beta P}{M} \sum_j J_j \sigma_j^x \sigma_j^z\right)$$

$$\langle \hat{\sigma}_{t+1} | e^{-\frac{\beta P}{M} A_1} | \vec{\sigma}_t \rangle = \frac{N}{\pi} \langle \vec{\sigma}_{t+1} | e^{\frac{\beta P}{M} \hat{\sigma}_i^x} | \vec{\sigma}_t \rangle \quad (\star)$$

行列の指数関数

$$e^{\frac{\beta P}{M} \hat{\sigma}_i^x} = \frac{1}{2} \left(1 + \frac{\beta P}{M} \hat{\sigma}_i^x + \frac{1}{2} \left(\frac{\beta P}{M} \right)^2 (\hat{\sigma}_i^x)^2 + \frac{1}{3!} \left(\frac{\beta P}{M} \right)^3 (\hat{\sigma}_i^x)^3 + \dots \right)$$

$$= \cosh\left(\frac{\beta P}{M}\right) \frac{1}{2} + \sinh\left(\frac{\beta P}{M}\right) \hat{\sigma}_i^x$$

$$(\star) = \cosh\left(\frac{\beta P}{M}\right) \begin{pmatrix} 1 & \tanh\left(\frac{\beta P}{M}\right) \\ \tanh\left(\frac{\beta P}{M}\right) & 1 \end{pmatrix}$$

非対角は $\vec{\sigma}_t \rightarrow \vec{\sigma}_{t+1}$ の遷移

仮想的な矢印

$$e^{k \vec{\sigma}_t \vec{\sigma}_{t+1}} = \begin{matrix} \vec{\sigma}_{t+1} \\ \uparrow \\ \downarrow \end{matrix} \begin{pmatrix} e^k & e^{-k} \\ e^{-k} & e^k \end{pmatrix} = e^k \begin{pmatrix} 1 & e^{-2k} \\ e^{-2k} & 1 \end{pmatrix}$$

$\vec{\sigma}_t \vec{\sigma}_{t+1}$ を表せるのか?

$$e^{-2k} = \tanh\left(\frac{\beta P}{M}\right) \quad k = -\frac{1}{2} \log_2 \tanh\left(\frac{\beta P}{M}\right) \quad \text{有効相互作用}$$

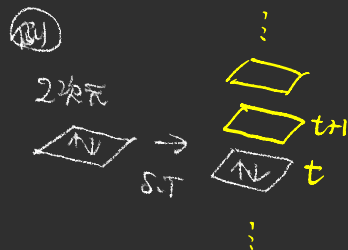
$$\boxed{P \rightarrow \infty \Rightarrow k \rightarrow 0} \quad \boxed{P \rightarrow 0 \Rightarrow k \rightarrow \infty}$$

[Step up] 量子系 $\rightarrow$ 古典系 (ST 分解)

d次元量子系 $\rightarrow$ (d+1)次元古典系
 A_0, A_1 ST

$$\boxed{\vec{\sigma}_t \cdot \vec{\sigma}_{t+1} = \pm 1}$$

MCMC 法



$$\langle \vec{\sigma}_{t+1} | \underbrace{e^{a \vec{\sigma}_t^x}}_{\beta a - \text{部 行标的指数函数}} | \vec{\sigma}_t \rangle \approx \langle \sigma_{it+1} | \underbrace{e^{k \sigma_{it} \sigma_{it+1}}}_{\underbrace{P(\vec{\sigma})}_{a - \text{部 随机分布}}} | \sigma_{it} \rangle \quad \textcircled{+} \underbrace{U_{\text{random}}}_{\text{负熵问题}}$$

Stochastic "随机的"

Stoquastic $\uparrow$

Non-Stochastic $\uparrow$

$$\therefore \dots \langle \vec{\sigma}_{t+2} | \underbrace{e^{-\frac{\beta}{M} H_0}}_{\frac{M}{2} + \vec{\sigma}_0} | \sigma_{t+1} \rangle \langle \sigma_{t+1} | e^{-\frac{\beta}{M} H_1} | \sigma_t \rangle \dots$$

$$\rightarrow \prod_{t=1}^M \exp\left(+ \frac{\beta}{M} \sum_{ij} J_{ij} \sigma_{it} \sigma_{jt} + k \sum_{i=1}^N \sigma_{it} \sigma_{it+1}\right) \quad \textcircled{\text{古典系}}$$

Hopfield モデル = QA.

★ モデル

不変性に満たす

Hebb 則

$$H = - \frac{1}{2N} \sum_{i,j} J_{ij} \sigma_i \sigma_j$$

$$J_{ij} = \frac{1}{p} \sum_{\mu=1}^p \xi_i^{\mu} \xi_j^{\mu} \quad (\xi_i^{\mu} = \pm 1)$$

$$= - \frac{1}{2Np} \sum_{i,j} \sum_{\mu} \xi_i^{\mu} \xi_j^{\mu} \sigma_i \sigma_j = - \frac{N}{2p} \sum_{\mu} \left(\sum_i \xi_i^{\mu} \sigma_i / N \right)^2$$

★ 直交性. $\vec{\xi}^{\mu} = (\xi_1^{\mu}, \xi_2^{\mu}, \dots, \xi_N^{\mu})$

$$\frac{1}{N} \vec{\xi}^{\mu} \cdot \vec{\xi}^{\nu} = \frac{1}{N} \sum_{i=1}^N \xi_i^{\mu} \xi_i^{\nu}$$

大数の法則

$$\left[\begin{array}{l} \mu = \nu \\ \mu \neq \nu \end{array} \right] \rightarrow \left[\begin{array}{l} \langle \xi_i^{\mu} \xi_i^{\nu} \rangle = 1 \\ = 0 \end{array} \right] = \delta_{\mu\nu}$$

★ 統計力学の P 平均

$$Z = \sum_{\{\sigma\}} \exp(-\beta H) \quad \left[\rightarrow -\beta f = \frac{1}{N} \log Z \right]$$

5a 2 次 $\Rightarrow$ 積分の法則?

$$= \sum_{\{\sigma\}} \exp\left(\frac{\beta}{2N} \sum_{i,j} J_{ij} \sigma_i \sigma_j\right)$$

$$= \sum_{\{\sigma\}} \exp\left(\frac{N\beta}{2p} \sum_{\mu} \left(\frac{1}{N} \sum_i \xi_i^{\mu} \sigma_i\right)\right)$$

1 体問題化.

Step up 大数の法則 ① = 1/N-1/N. 2 次 1/N 平均変換

$$\int dx \exp\left(-\frac{a}{2} x^2 + \textcircled{b} x\right) \stackrel{\textcircled{1} \text{ 次}}{\leftarrow} \sqrt{\frac{\pi}{a}} \exp\left(\frac{\textcircled{b}^2}{2a}\right) \quad \textcircled{2} \text{ 次}$$

$$= \sum_{\{\sigma\}} \prod_{\mu} \int dz_{\mu} \exp\left(\sqrt{\frac{N\beta}{p}} \frac{z_{\mu}}{N} \sum_{i=1}^N \xi_i^{\mu} \sigma_i\right) \quad \int dz = \int \frac{dz}{\sqrt{2\pi}} \exp\left(-\frac{1}{2} z^2\right)$$

$z_{\mu} \rightarrow \sqrt{N} z_{\mu}$

$$= \sum_{\{\sigma\}} \prod_{\mu} \int dz_{\mu} \exp\left(-\frac{\textcircled{N}}{2} z_{\mu}^2 + \sqrt{\frac{\beta}{p}} z_{\mu} \sum_{i=1}^N \xi_i^{\mu} \sigma_i\right) \quad \textcircled{O(N)} \quad \textcircled{11} \quad N^2 \text{ 次元!}$$

Step up 比較② 和 1次で

$$\sum_{i=1}^N \prod_{i=1}^N = \prod_{i=1}^N \sum_{i=1}^N$$

$$= \prod_{\mu} \int dz_{\mu} \exp\left(-\frac{N}{2} z_{\mu}^2\right) \prod_{i=1}^N \left[\sum_{\sigma_i} \exp\left(\sqrt{\frac{\beta}{p}} \sum_{\mu} z_{\mu} \sum_{i=1}^M \sigma_i\right) \right] 2 \cosh\left(\sqrt{\frac{\beta}{p}} \sum_{\mu} z_{\mu} \sum_{i=1}^M \sigma_i\right)$$

$$= \prod_{\mu} \int dz_{\mu} \exp\left(-\frac{N}{2} \sum_{\mu} z_{\mu}^2 + N \left(\frac{1}{N} \sum_{i=1}^N \log 2 \cosh\left(\sqrt{\frac{\beta}{p}} \sum_{\mu} z_{\mu} \sum_{i=1}^M \sigma_i\right) \right)\right)$$

$- N \beta f(\{z_{\mu}\})$

Step up 比較③ 鞍点法

$$\int dx \exp(N f(x)) \rightarrow \sum_i \exp(N f(x_i^*))$$

$$x^* = f'(x_i^*) = 0$$

① 鞍点法

Step up 比較④: 大数法則

$$\frac{1}{N} \sum_{i=1}^N f(x_i) \rightarrow \langle f(x) \rangle_x$$



$$-\beta f(\{z_{\mu}\}) = -\frac{1}{2} \sum_{\mu} z_{\mu}^2 + \left\langle \log \left(2 \cosh\left(\sqrt{\frac{\beta}{p}} \sum_{\mu} z_{\mu} \sum_{i=1}^M \sigma_i\right) \right) \right\rangle_{\mathcal{S}}$$

$$\partial z_{\mu} = -z_{\mu} + \left\langle \sqrt{\frac{\beta}{p}} \sum_{i=1}^M \sigma_i \tanh\left(\sqrt{\frac{\beta}{p}} \sum_{\mu} z_{\mu} \sum_{i=1}^M \sigma_i\right) \right\rangle_{\mathcal{S}} = 0$$

$$z_{\mu} = \left\langle \sqrt{\frac{\beta}{p}} \sum_{i=1}^M \sigma_i \tanh\left(\sqrt{\frac{\beta}{p}} \sum_{\mu} z_{\mu} \sum_{i=1}^M \sigma_i\right) \right\rangle_{\mathcal{S}} \quad (\text{鞍点方程式})$$

$\beta \rightarrow \infty$

$$\rightarrow \sum_{i=1}^M \sigma_i \text{sign}\left(\sum_{\mu} z_{\mu} \sigma_i\right) \quad \text{①} \quad z_{\mu} \rightarrow \sqrt{\frac{\beta}{p}} z_{\mu} \text{ 以 } \beta \rightarrow \infty \text{ 変換}$$

★ QA の 表 示

$$\hat{H} = -\frac{1}{2N} \sum_{ij} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z - \Gamma \sum_{i=1}^N \hat{\sigma}_i^x \quad \textcircled{11} \text{ 横磁場の連続近似}$$

$$Z = \text{Tr} \left[\exp \left(\frac{\beta}{2N} \sum_{ij} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z + \beta \Gamma \sum_{i=1}^N \hat{\sigma}_i^x \right) \right]$$

$$\rightarrow \sum_{\text{S.T.}} \sum_{\{\sigma\}} \exp \left(\underbrace{\frac{\beta}{2NM} \sum_{i,j} \sum_{t=1}^M J_{ij} \sigma_{it} \sigma_{jt}}_{M \times N \text{ 間の相互作用}} + \underbrace{k \sum_{it} \sigma_{it} \sigma_{it+1}}_{M \times N \text{ 間の相互作用}} \right)$$

↓

$$\prod_{it} \int d\alpha_{it} \exp \left(-\frac{N}{2} \alpha_{it}^2 + \sqrt{\frac{\beta}{M\Gamma}} \alpha_{it} \sum_{i=1}^N \sum_{t=1}^M \sigma_{it} + k \sum_{it} \sigma_{it} \sigma_{it+1} \right)$$

1次元 Ising 磁場の Ising モデル (★)

Step up 静的近似

$$Z_{it} \rightarrow Z_M$$

⑪ (Lipshitz 条件) 対称性の仮定

破局の外を考慮

$$\star \Rightarrow \exp \left(\underbrace{\left| \frac{\beta}{\Gamma} \right| \frac{1}{M}}_{\text{1次元 Ising 磁場の Ising モデル}} \sum_{it} \underbrace{Z_M \sum_{i=1}^M \sigma_{it}}_{\text{1次元 Ising 磁場の Ising モデル}} + k \sum_{it} \sigma_{it} \sigma_{it+1} \right)$$

$Z_M \rightarrow \int \frac{1}{M} Z_M$ " $\frac{1}{M} h_i$ に依存する?

Step up S.T. の変換

$$\prod_{i=1}^N \exp \left(h_i \hat{\sigma}_i^z + \Gamma \hat{\sigma}_i^x \right) \stackrel{\text{S.T.}}{=} \prod_{it} \exp \left(\frac{h_i}{M} \hat{\sigma}_i^z \right) \exp \left(\frac{\Gamma}{M} \hat{\sigma}_i^x \right) = \prod_{it} \exp \left(\frac{h_i}{M} \sigma_{it} + k \sigma_{it} \sigma_{it+1} \right)$$

⑩ 1次元 Ising 磁場の Ising モデル

$$= \prod_{i=1}^N \exp \left(\left(\sqrt{\frac{\beta}{\Gamma}} \sum_{t=1}^M Z_M \sum_{i=1}^M \sigma_{it} \right) \hat{\sigma}_i^z + \beta \Gamma \hat{\sigma}_i^x \right) \quad \textcircled{11} \text{ 1次元 Ising 磁場の Ising モデル}$$

Step up $h_i \hat{\sigma}_i^z + \Gamma \hat{\sigma}_i^x$ の変換

$$\begin{pmatrix} h_i & \Gamma \\ \Gamma & -h_i \end{pmatrix} \Rightarrow \lambda_{\pm} = \pm \sqrt{h_i^2 + \Gamma^2}$$

$$Z = \pi \int_{\mu} d\vec{z}_{\mu} \exp\left(-\frac{N}{2} \vec{z}_{\mu}^2 + \frac{N}{2} \log \underbrace{\text{Tr} \left[\exp \left(\sqrt{\frac{\beta}{p}} \Sigma \vec{z}_{\mu} S_i^{\mu} \delta_i^z + \beta \uparrow \delta_i^x \right) \right]}_{\exp(\gamma_+) + \exp(\gamma_-)}\right)$$

$$-\beta f(\{\vec{z}_{\mu}\}) = -\frac{1}{2} \Sigma \vec{z}_{\mu}^2 + \frac{1}{N} \sum_{\mu=1}^N \log 2 \cosh \beta \sqrt{\left(\frac{1}{p} \Sigma \vec{z}_{\mu} S_i^{\mu} \right)^2 + p^2}$$

大数法则