

9/1

① 量子 $P = -i\hbar \nabla$ (Pauli, Ising, 2 単位系)② 断熱定理・森田 α 定理・CJ 項

9/2

① η - ν 相移② SA/SQA・鈴木 τ - ν 分解③ 量子相転移 (p -spin model)

9/3

① SUSY・7 次元-7 次元方程式

② 抗散モデルの対応

量子 P2-1127 218...

$$\begin{cases} \hat{H}_0 = - \sum_{\langle ij \rangle} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z - \sum_{i=1}^N h_i \hat{\sigma}_i^z \\ \hat{H}_1 = - \prod_i \hat{\sigma}_i^x \end{cases}$$

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

$$f(t) : 0 \rightarrow 1 \text{ (ゆっくり)} \quad \hat{H}_{1 \text{ a.g.}} \rightarrow \hat{H}_{0 \text{ a.g.}} \quad \text{7/29.2.} \quad \text{難in}$$

★ Ising model

元は Heisenberg の 模型

$$\hat{H}_0 = -J \sum_{\langle ij \rangle} (\hat{\sigma}_i^x \hat{\sigma}_j^x + \hat{\sigma}_i^y \hat{\sigma}_j^y + \hat{\sigma}_i^z \hat{\sigma}_j^z) \quad \text{①} \quad \text{互に近接したスピンの相互作用}$$

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad [10] = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, [11] = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

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

$$\hat{\sigma}_z |0\rangle = +1 |0\rangle \quad \text{or} \quad \hat{\sigma}_z |1\rangle = -1 |1\rangle \quad \text{②} \quad \hat{\sigma}_z \rightarrow \sigma = \pm 1 \text{ (古典スピン系)}$$

$$\Rightarrow E(\vec{\sigma}) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \quad (\sigma_i = \pm 1)$$

★ 中置 $\sigma \rightarrow P(\sigma)$ ③ 確率分布

熱中置 $\sigma \rightarrow \sigma'$ (対角項)

量子中置 $\sigma \rightarrow \hat{\sigma}$ (非対角項)

ハミルトン中置 $J \rightarrow J_{ij}$ (スピン)

★ 断熱定理

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle \quad (\text{シュレディンガー方程式})$$

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

$$f(t) = \frac{t}{\tau} \equiv s \quad (\tau: \text{アハラースキ時間})$$

$$i\hbar \frac{d}{ds} |\psi(s)\rangle = \tau \hat{H}(s) |\psi(s)\rangle \quad \textcircled{1} \quad \boxed{\text{ここで } \hat{H}(s) \text{ が定数}}$$

$$\boxed{\text{各時刻}} \quad \hat{H}(s) |j(s)\rangle = E_j(s) |j(s)\rangle \quad \textcircled{2}$$

$$|\psi(s)\rangle = \sum_j C_j(s) |j(s)\rangle \quad \text{展開} \quad \textcircled{3} \quad \boxed{|j(s)\rangle \text{ 基底を固定}} \quad \text{!!}$$

$$[\text{EL } |j(s)\rangle \rightarrow |j\rangle \text{ なら } C_j(s) = C_j(0) \exp(-i \frac{1}{\hbar} \int_0^s dt E_j(t))]$$

$$\textcircled{3} \quad C_j(s) = \hat{C}_j(s) \exp(-i \frac{1}{\hbar} \int_0^s dt E_j(t)) \quad \text{変換} \quad \textcircled{4} \quad \boxed{\tau \phi_j(s) \text{ だけ変換}} \quad \text{!!}$$

$$\textcircled{4} : i\hbar \frac{d}{ds} |\psi(s)\rangle = i\hbar \sum_j \frac{d\hat{C}_j}{ds} \exp(-i \frac{1}{\hbar} \int_0^s dt E_j(t)) |j(s)\rangle + \sum_j \hat{C}_j(s) \tau E_j(s) \exp(-i \frac{1}{\hbar} \int_0^s dt E_j(t)) |j(s)\rangle$$

$$+ i\hbar \sum_j \hat{C}_j(s) \exp(-i \frac{1}{\hbar} \int_0^s dt E_j(t)) \frac{d}{ds} |j(s)\rangle$$

$$\textcircled{5} : \tau \hat{H}(s) |\psi(s)\rangle = \sum_j \hat{C}_j(s) \exp(-i \frac{1}{\hbar} \int_0^s dt E_j(t)) \tau E_j(s) |j(s)\rangle$$

$$\langle k(s) | \tau \hat{H}(s) | \rangle = \sum_j \langle k(s) | \tau E_j(s) | j(s) \rangle \hat{C}_j(s) \quad (\langle k(s) | j(s) \rangle = \delta_{kj} \text{ だけ})$$

$$\therefore \frac{d\hat{C}_k}{ds} = - \sum_j \hat{C}_j(s) \exp(i \frac{1}{\hbar} (\phi_k - \phi_j)) \langle k(s) | \frac{d}{ds} | j(s) \rangle \quad \textcircled{6} \quad \boxed{\hat{C}_k \text{ だけ変換}} \quad \text{!!}$$

$$[\textcircled{6} \text{ だけ } \frac{d\hat{H}}{ds} |j(s)\rangle + \hat{H}(s) \frac{d}{ds} |j(s)\rangle = \frac{dE_j}{ds} |j(s)\rangle + E_j(s) \frac{d}{ds} |j(s)\rangle]$$

$$\left\{ \begin{aligned} \langle k(s) | \frac{d}{ds} | j(s) \rangle &= \frac{1}{E_j(s) - E_k(s)} \langle k(s) | \frac{d\hat{H}}{ds} | j(s) \rangle \quad (j \neq k) \\ \langle k(s) | \frac{d}{ds} | k(s) \rangle &= 0 \quad (\text{by } \langle k(s) | k(s) \rangle = 1) \end{aligned} \right.$$

$$\Rightarrow \frac{d\hat{C}_k}{ds} = \sum_{j \neq k} \frac{e^{i \frac{1}{\hbar} (\phi_k - \phi_j)} \langle k(s) | \frac{d\hat{H}}{ds} | j(s) \rangle}{E_k(s) - E_j(s)} C_j(s) \langle k(s) | \frac{d\hat{H}}{ds} | j(s) \rangle$$

$\Delta_{kj}(s) = E_k(s) - E_j(s)$

$\hat{H}_0 - \hat{H}_1 = \text{遷移ハミルトン (量子力学的)}$

(151) QA $\begin{cases} C_0(0) = 1 \text{ g.s.s.} \\ C_k(0) = 0 \end{cases} \Rightarrow \begin{cases} C_0(s) = 1 - O(k_c) \\ C_k(s) = O(k_c) \end{cases} \text{ g.s.s.}$

$$\tilde{C}_k(s) = \int_0^s du \frac{e^{i\frac{T}{\hbar}\Delta\phi_{k0}}}{\Delta k_0(u)} \frac{C_0(u)}{1 - O(k_c)} \langle k(s) | \frac{dH}{ds} | 0(u) \rangle = O(k_c)$$

$$= \int_0^s du \frac{e^{i\frac{T}{\hbar}\Delta\phi_{k0}}}{\Delta k_0(u)} \langle k(u) | \frac{dH}{ds} | 0(u) \rangle + O\left(\frac{1}{T^2}\right)$$

$$\uparrow \frac{\hbar}{iT\Delta k_0(u)} \frac{d}{du} e^{i\frac{T}{\hbar}\Delta\phi_{k0}}$$

$$= \int_0^s du \frac{\hbar}{iT} \frac{\langle k(u) | \frac{dH}{ds} | 0(u) \rangle}{\Delta k_0(u)^2} \frac{d}{du} \left(e^{i\frac{T}{\hbar}\Delta\phi_{k0}} \right) \equiv A(u)$$

$$= \frac{i\hbar}{T} \left[A(0) - A(s) e^{i\frac{T}{\hbar}\Delta\phi_{k0}} \right] + \frac{i\hbar}{T} \int_0^s du e^{i\frac{T}{\hbar}\Delta\phi_{k0}} \left(\frac{d}{du} A(u) \right)$$

$$|\tilde{C}_k(s)| < \varepsilon \text{ となる}$$

$$\hat{H}_0 - \hat{H}_1 \sim O(E) \text{ 程度}$$

$$\varepsilon > \frac{2\hbar}{T} \max_s \left(\frac{1}{\Delta k_0(s)^2} \left| \langle k(s) | \frac{dH}{ds} | 0(s) \rangle \right| \right)$$

$\rightarrow 0$ となる条件

Step up 断熱定理

$$T \geq \frac{1}{\varepsilon \Delta k_0(s_{\max})^2} \text{ 程度以上}$$

$$\frac{dH}{ds} = 0 \text{ となる?}$$

$$(151) S^2 H_0 + (1 - S^2) \hat{H}_1$$

$$\rightarrow 2S(\hat{H}_0 - \hat{H}_1)$$

★ 断熱定理の条件

$$\frac{\hbar}{iT\Delta k_0} \frac{d}{du} e^{i\frac{T}{\hbar}\Delta\phi_{k0}}$$

$-B(u)$ 程度

$$\tilde{C}_k(s) = \int_0^s du \frac{e^{i\frac{T}{\hbar}\Delta\phi_{k0}}}{\Delta k_0(u)} \frac{1}{\Delta k_0(u)} \langle k(u) | \frac{dH}{ds} | 0(u) \rangle$$

$$\left[B_{k1}(u) = \frac{1}{i\Delta k_0(u)} \frac{d}{du} B_k(u) \text{ 程度. } (B_1(u) = \frac{B(u)}{i\Delta k_0(u)}) \right]$$

$$= \frac{\hbar}{T} \int_0^s du B_1(u) \frac{d}{du} e^{i\frac{T}{\hbar}\Delta\phi_{k0}} \quad \frac{\hbar}{iT\Delta k_0} \frac{d}{du} e^{i\frac{T}{\hbar}\Delta\phi_{k0}}$$

$$= \frac{\hbar}{T} \left[\underline{B_1(0)} - \underline{B_1(s)} e^{i\frac{T}{\hbar}\Delta\phi_{k0}} \right] + \frac{\hbar}{T} \int_0^s du \frac{e^{i\frac{T}{\hbar}\Delta\phi_{k0}}}{\Delta k_0(u)} \frac{d}{du} B_1(u)$$

$$= + \frac{\hbar^2}{T^2} \int_0^s du B_2(u) \frac{d}{du} e^{i\frac{T}{\hbar}\Delta\phi_{k0}}$$

$$= - \left(\frac{\hbar}{T} \right)^2 \left[B_2(0) - B_2(s) e^{i\frac{T}{\hbar}\Delta\phi_{k0}} \right] - \left(\frac{\hbar}{T} \right)^2 \int_0^s du e^{i\frac{T}{\hbar}\Delta\phi_{k0}} \frac{d}{du} B_2(u)$$

$$(151) S = 0.1 \text{ 程度 } B_k(0) = B_k(1) = 0 \text{ 程度}$$

Step up 李田. 西田 2个 (2007)

$$J = \frac{1}{\kappa} z^{\wedge} \frac{d^m H}{ds^m} \Big|_{s=0.1} = 0.12772$$

$$|\hat{C}_k(1)|_2 \sim \frac{1}{T^{2(m+1)}} \quad (27)$$

★ Counter-diabatic $\hat{H}$

规律 $|n(t)\rangle = e^{i\phi_n(t)} |n(t)\rangle$  $|n(t)\rangle$ 不变

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}'(t) |\psi(t)\rangle \quad \text{where} \quad \hat{H}(t) + H_{\text{int}}(t) \equiv \hat{H}'(t)$$

$$- \hbar \frac{d\phi_n}{dt} e^{i\phi_n} |n(t)\rangle + i\hbar e^{i\phi_n} \frac{d}{dt} |n(t)\rangle$$

$$2. \quad \hat{H}(t) |n(t)\rangle = -\hbar \frac{d}{dt} |n(t)\rangle + i\hbar \frac{d}{dt} |n(t)\rangle$$

$$\boxed{E_n(t) + \hbar \frac{d}{dt}} \quad \hat{H}_{\text{eff}} |n(t)\rangle = \left(-\hbar \frac{d}{dt} - E_n(t) \right) |n(t)\rangle + i\hbar \frac{d}{dt} |n(t)\rangle$$

$$\bullet \langle n(t) | \hat{H}_0 | n(t) \rangle = \left(-\frac{\hbar}{2} \frac{d\phi_n}{dt} - E_n(t) \right) + i\hbar \langle n(t) | \frac{d}{dt} | n(t) \rangle$$

$$\bullet \langle m(t) | \hat{H}(t) | n(t) \rangle = i\hbar \langle m(t) | \frac{d}{dt} | n(t) \rangle$$

$$\therefore \frac{d\phi_n}{dt} = \frac{-1}{\hbar} E_n(t) + i \langle n(t) | \frac{d}{dt} | n(t) \rangle \quad \text{z } \phi \in \mathbb{R} \text{ (2)}$$

$$\text{お } \hat{H}_{\text{eff}}(t) = \sum_{m,n} |m(t)\rangle \langle m(t)| H_{\text{eff}} |n(t)\rangle \langle n(t)|$$

$$= \text{這} \int_{-\infty}^{\infty} |\langle m(t) | \frac{d}{dt} | n(t) \rangle| \langle n(t) |$$

$$\textcircled{2} \text{ 例 } \langle m(t) | \frac{d}{dt} | n(t) \rangle = \frac{1}{E_n(t) - E_m(t)} \langle m(t) | \frac{dH}{dt} | n(t) \rangle$$

Step up HCD IR

$$\hat{H}_{cb}(t) = i\hbar \sum_{m \neq n} \frac{\langle m(t) | \frac{dH}{dt} | n(t) \rangle}{E_n(t) - E_m(t)} |m(t)\rangle \langle n(t)| \quad \text{with } \frac{1}{E_n(t) - E_m(t)} \propto |n(t)\rangle$$

11 $|m(t)\rangle \langle m(t)| \pi \sigma_z$

★ 现实的有CD项

$$\langle m | \hat{H}_{\text{cd}} | n \rangle = i \frac{\langle m | \frac{d\hat{H}}{dt} | n \rangle}{E_n - E_m} \quad \textcircled{11} \quad \begin{array}{|l} E_n - E_m \dots? \\ \hat{H} \text{ 的交换?} \end{array}$$

$$\langle m | [\hat{H}_{\text{cd}}, \hat{H}] | n \rangle = \langle m | \hat{H}_{\text{cd}} E_n - E_m \hat{H}_{\text{cd}} | n \rangle$$

$$\text{故 } i \langle m | \frac{d\hat{H}}{dt} | n \rangle = \langle m | [\hat{H}_{\text{cd}}, \hat{H}] | n \rangle$$

(非对角项)

$$G(t) = \frac{d}{dt} \hat{H}(t) + i [\hat{H}_{\text{cd}}, \hat{H}] \quad \textcircled{11} \quad \begin{array}{|l} \text{因为 } \hat{H}_{\text{cd}} \text{ 为反对称} \end{array}$$

↑ 厄米共轭!

Step up Sel's Polkovnikov α 变分 (2017)

$$\min_A \text{Tr}[G^2] \quad G = \frac{d}{dt} \hat{H}(t) + i [\hat{A}, \hat{H}]$$

$$\delta G = i [\delta A, \hat{H}]$$

$$\text{故 } 2 \text{Tr}[G \delta G] = 2i \text{Tr}[G [\delta A, \hat{H}]] = 0$$

Step up) $\text{Tr} \geq [\dots]$

$$\text{Tr}[AB] = \text{Tr}[BA] \quad (\text{循环性})$$

$$\text{Tr}[A[BC]] = \text{Tr}[[C,A]B]$$

$$[\text{Tr}[ABC] - \text{Tr}[ACB]]$$

$$\text{Tr}[AB]$$

$$\therefore 2i \text{Tr}[[\hat{H}, G] \delta A] = 0 \quad \text{故 } [\hat{H}, G] = 0 \quad \text{合理}$$

$$G_2(t) = \frac{d}{dt} \hat{H}(t) \quad \text{且 } \hat{H} \text{ 为厄米算符, } A \text{ 为厄米算符}$$

$$A = i [\hat{H}, \frac{d}{dt} \hat{H}(t)] \propto \text{但 } \frac{d}{dt} \hat{H}(t) \text{ 为反对称}$$

$$[\frac{d}{dt} \hat{H}(t) = \frac{d}{dt} (\lambda \hat{H}_0 + (1-\lambda) \hat{H}_1) = \hat{H}_0 - \hat{H}_1]$$

$$\propto i [\hat{H}_0, \hat{H}_1] \quad \textcircled{11} \quad \begin{array}{|l} \text{因为 } \hat{H}_0, \hat{H}_1 \text{ 为厄米算符} \end{array}$$

$$\text{实际 } \langle m | [A, \hat{H}] | n \rangle = \langle m | \hat{A} E_n - E_m \hat{A} | n \rangle \quad \text{故}$$

$$\langle m | \hat{A} | n \rangle$$

$$\star \langle n(t) | \frac{d}{dt} | n(t) \rangle = 0 \quad (\text{by } \langle n(t) | n(t) \rangle = 1)$$

$$\left(\frac{d}{dt} \langle n(t) | \right) | n(t) \rangle + \langle n(t) | \frac{d}{dt} | n(t) \rangle = 0 \quad \text{①}$$

$$(\langle n(t) | \frac{d}{dt} | n(t) \rangle)^* = - \langle n(t) | \frac{d}{dt} | n(t) \rangle$$

$$\text{もし } | n(t) \rangle \rightarrow e^{i\theta(t)} | n(t) \rangle$$

$$\langle n(t) | e^{-i\theta} \frac{d}{dt} e^{i\theta} | n(t) \rangle = i \frac{d\theta}{dt} + \langle n(t) | \frac{d}{dt} | n(t) \rangle = 0 \quad \text{②}$$

量子断絶近似 (QA) (2014)

$$\star \text{ 試行状態 (ansatz) } | s \rangle = \bigotimes_{i=1}^N \left(\frac{1}{\sqrt{2}} (| \uparrow \rangle + | \downarrow \rangle) \right) \quad (\text{重畳})$$

$$| \vec{r}, \vec{p} \rangle = \prod_{k=1}^P e^{-i \vec{p}_k \cdot \hat{H}_1} e^{-i \vec{r}_k \cdot \hat{H}_0} | s \rangle \quad \text{③}$$

$$F_P(\vec{r}, \vec{p}) = \langle \vec{r}, \vec{p} | \hat{H}_0 | \vec{r}, \vec{p} \rangle \quad \text{④}$$

★ QA の関係

$$U(T) = \exp \left(-i \frac{1}{T} \int_0^T dt' \hat{H}(t') \right)$$

$$= \exp \left(-i \frac{\Delta t}{T} \sum_{k=1}^n \hat{H}_k \right) \quad (\text{近似}) \quad \hat{H}_k = H(k \Delta t)$$

Step up | 鈴木-121 分解

$$\Delta t = \frac{T}{n}$$

$$e^{t(\hat{A}+\hat{B})} \approx \left(e^{\frac{t}{n}\hat{A}} e^{\frac{t}{n}\hat{B}} \right)^n \quad (\text{Lie-Trotter})$$

$$\approx \left(e^{\frac{t}{2n}\hat{A}} e^{\frac{t}{n}\hat{B}} e^{\frac{t}{2n}\hat{A}} \right)^n \quad (\text{Suzuki-Trotter})$$

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

$$\rightarrow e^{t\hat{A}} e^{t\hat{B}} = \left(\hat{I} + t\hat{A} + \frac{t^2}{2}\hat{A}^2 \right) \left(\hat{I} + t\hat{B} + \frac{t^2}{2}\hat{B}^2 \right) = \hat{I} + t(\hat{A}+\hat{B}) + t^2\hat{A}\hat{B} + \frac{t^2}{2}(\hat{A}^2+\hat{B}^2)$$

$$(\text{誤差}) = -\frac{t^2}{2} [\hat{A}, \hat{B}]$$

$$\text{②} \rightarrow -\frac{t}{2} \left(\frac{t}{n} \right) [\hat{A}, \hat{B}] \quad \text{③}$$

$$\text{BCH 公式を用いて}$$

$$e^{t(\hat{A}+\hat{B})} = e^{t\hat{A}} e^{t\hat{B}} e^{t^2 [\hat{A}, \hat{B}]} \quad \text{④}$$

$$U(T) \approx \prod_{k=1}^n \exp(-i \frac{\Delta t}{\hbar} \hat{H}_k) \quad \hat{H}_k = f_k \hat{H}_0 + (1-f_k) \hat{H}_1$$

$$\approx \prod_{k=1}^n \exp(-i \frac{\Delta t}{\hbar} f_k \hat{H}_0) \exp(-i \frac{\Delta t}{\hbar} (1-f_k) \hat{H}_1)$$

①

変数分離
QA → QAOA

②

$n \rightarrow \infty$ まで QAOA
有限でいい! (NISQ)

★ 最適化原理 (1956)

Step up $g(t)$: 制御パラメータ

$$\frac{dx}{dt} = f(x, g) \text{ に対して } \min_g \{ F(x(T)) \} \text{ を求む}$$

$$\Rightarrow J = F(x(T)) + \int_0^T \lambda(t) \left(f(x, g) - \frac{dx}{dt} \right) dt \text{ を求む}$$

$$\delta \lambda: \frac{dx}{dt} = \frac{\partial p}{\partial \lambda} \quad \text{① 変数分離}$$

$$\delta x: \frac{d\lambda}{dt} = -\frac{\partial p}{\partial x} \quad \text{② 変数分離}$$

$$\left[\frac{\partial F}{\partial x} \delta x(T) - \int_0^T dt \lambda(t) \left(-\frac{d}{dt} \delta x \right) \right] = \left[\frac{\lambda(t) \delta x(t)}{\lambda(t) \delta x(t)} \right]_0^T - \int_0^T dt \left(\frac{d\lambda}{dt} \delta x \right)$$

$$\delta x(t): \frac{\lambda(t)}{\lambda(t)} = -\nabla F(x(t)) \quad \text{① 変数}$$

$$\Rightarrow g^*(t) = \arg \min_g \{ P(x^*, g) \} \text{ を求む}$$

QAOA

$$F(T) = \langle \hat{\sigma}_x, \hat{\sigma}_y | \hat{H}_0 | \hat{\sigma}_x, \hat{\sigma}_y \rangle \text{ を最小化}$$

$$\text{ith } \frac{d}{dt} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle \quad \text{① 変数分離}$$

$$(-i\hbar \frac{d}{dt} \langle \psi(t) | = \langle \psi(t) | \hat{H}(t)$$

$$\Rightarrow J = F(T) + \int_0^T \left\{ \langle \lambda(t) | \hat{H} - i\hbar \frac{d}{dt} | \psi(t) \rangle + \langle \psi(t) | \hat{H}(t) + i\hbar \frac{d}{dt} | \lambda(t) \rangle \right\} dt$$

$$\delta | \psi \rangle: \langle \lambda(t) | \hat{H}(t) + i\hbar \frac{d}{dt} | \lambda(t) \rangle = 0 \quad \therefore +i\hbar \frac{d}{dt} | \lambda(t) \rangle = \hat{H}(t) | \lambda(t) \rangle \quad \text{② 変数}$$

$$\delta \langle \lambda |: (\hat{H} - i\hbar \frac{d}{dt}) | \psi(t) \rangle = 0 \quad \therefore i\hbar \frac{d}{dt} | \psi(t) \rangle = \hat{H}(t) | \psi(t) \rangle \quad \text{① 変数}$$

$$\delta \langle \psi |: (\hat{H} - i\hbar \frac{d}{dt}) | \lambda(t) \rangle = 0 \quad \therefore i\hbar \frac{d}{dt} | \lambda(t) \rangle = \hat{H}(t) | \lambda(t) \rangle$$

$$\therefore | \lambda(t) \rangle = | \psi(t) \rangle$$

$$\delta \langle \psi(t) | : \hat{H}_0 | \vec{r}, \vec{p} \rangle + i\hbar | \chi(t) \rangle = 0 \quad \therefore | \chi(t) \rangle \propto \hat{H}_0 | \vec{r}, \vec{p} \rangle$$

($i\hbar [\langle \psi(t) | \chi(t) \rangle]_0^T$) ② 1 ① 1/2

$$P(\psi, \lambda, f) = \langle \chi(t) | \hat{H}(t) | \psi(t) \rangle + \langle \psi(t) | \hat{H} | \chi(t) \rangle$$

$$= 2 \operatorname{Re} \langle \chi(t) | \hat{H}(t) | \psi(t) \rangle \text{ a min } \exists \lambda \exists f$$

$$\frac{\partial P}{\partial f} = 2 \operatorname{Re} \langle \chi(t) | \hat{H}_0 - \hat{H}_1 | \psi(t) \rangle = \phi(t)$$

$$\phi(t) > 0 \text{ 7h } \frac{f(t)}{H_{\max}} \rightarrow 0 \quad \phi(t) < 0 \text{ 7h } \frac{f(t)}{H_{\max}} \rightarrow 1$$

① 1 bay-bay 制御

★ Quantum Schrödinger Bridge $|i\rangle \rightarrow |f\rangle$ 決めるための Lagrangian

$$J = \int_0^T \operatorname{Tr}[H(t)^2] dt + \int_0^T dt \left\{ \langle \chi(t) | iH(t) + \frac{d}{dt} | \psi(t) \rangle + \langle \psi(t) | -iH(t) + \frac{d}{dt} | \chi(t) \rangle \right\}$$

$\frac{d}{dt} | \psi(t) \rangle = -iH | \psi(t) \rangle$

$$\therefore P(\psi, \lambda, H) = \operatorname{Tr}[H(t)^2] - 2 \operatorname{Im} \langle \chi(t) | H(t) | \psi(t) \rangle$$

$i\bar{z} - i\bar{z}^* = -2y$

$$\delta H = 2 \operatorname{Tr}[H(t) \delta H] - 2 \operatorname{Im} \langle \chi(t) | \delta H | \psi(t) \rangle = 0$$

① 1 $\sum_n |\ln X_n| = I \mathcal{E}$

$$= \operatorname{Tr}[| \psi(t) \rangle \langle \chi(t) | \delta H]$$

$$\hat{H}(t) = i (| \psi(t) \rangle \langle \chi(t) | - | \chi(t) \rangle \langle \psi(t) |)$$

$$\left\{ \begin{array}{l} \delta | \psi(t) \rangle : \langle \chi(t) | i\hat{H} - \frac{d}{dt} \langle \chi(t) | = 0 \quad \therefore \frac{d}{dt} \langle \chi(t) | = -i\hat{H} \langle \chi(t) | \\ \delta \langle \chi(t) | : iH | \psi(t) \rangle + \frac{d}{dt} | \psi(t) \rangle = 0 \quad \therefore \frac{d}{dt} | \psi(t) \rangle = -i\hat{H} | \psi(t) \rangle \end{array} \right.$$

$$\frac{d\hat{H}}{dt} = i \left(\frac{d}{dt} | \psi(t) \rangle \langle \chi(t) | + | \psi(t) \rangle \frac{d}{dt} \langle \chi(t) | - \frac{d}{dt} | \chi(t) \rangle \langle \psi(t) | - | \chi(t) \rangle \frac{d}{dt} \langle \psi(t) | \right) = 0 \text{ (定数)}$$

$-iH | \psi(t) \rangle$ $iH \langle \chi(t) |$ $-iH | \chi(t) \rangle$ $iH \langle \psi(t) |$

量子マテリアル

★ $\beta \rightarrow \infty$ の場合

① Q.A. 12 章 9.5

$$P(\vec{\sigma}) = \frac{1}{Z} \exp(-\beta E(\vec{\sigma})) \rightarrow \hat{P} = \frac{1}{Z} \exp(-\beta \hat{H})$$

$$Z = \int \exp(-\beta E(\vec{\sigma})) \quad Z = \text{Tr}[\exp(-\beta \hat{H})]$$

★ 横磁場の表現

$$\hat{H}_1 = -\Gamma \sum_i \hat{\sigma}_i^x \quad e^{P(A+B)} \approx (e^{PA} e^{PB})^M$$

$$\begin{aligned} Z &= \text{Tr} \left\{ \exp \left[-\beta \left(\hat{H}_0(\vec{\sigma}_k) + \hat{H}_1(\vec{\sigma}_k) \right) \right] \right\} \\ &= \text{Tr} \left\{ \prod_{k=1}^M \exp \left(-\frac{\beta}{M} \hat{H}_0 \right) \exp \left(-\frac{\beta}{M} \hat{H}_1 \right) \right\} \\ &= \text{Tr} \left\{ \prod_{k=1}^M \exp \left(-\frac{\beta}{M} \hat{H}_0(\vec{\sigma}_k) \right) |\delta_k\rangle \langle \delta_k| \exp \left(-\frac{\beta}{M} \hat{H}_1 \right) \right\} \end{aligned}$$

① 対称化

② Suzuki-Trotter!

③ 演算子の順序
 $\sum_k |\delta_k\rangle \langle \delta_k| = \hat{I}$ ④ $\hat{I} = \sum_k |\delta_k\rangle \langle \delta_k|$ だが $\delta_k \rightarrow \delta_{k+1}$ とする⑤ $\hat{H}_1$ の横磁場

$$\exp \left(\frac{\beta \Gamma}{M} \hat{\sigma}_i^x \right) = \hat{I} + \frac{\beta \Gamma}{M} \hat{\sigma}_i^x + \frac{1}{2} \left(\frac{\beta \Gamma}{M} \right)^2 (\hat{\sigma}_i^x)^2 + \dots$$

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

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

$$\left[e^{-2k} = \tanh \left(\frac{\beta \Gamma}{M} \right) \right]$$

$$= \cosh \left(\frac{\beta \Gamma}{M} \right) e^k \begin{pmatrix} e^k & e^{-k} \\ e^{-k} & e^k \end{pmatrix} \langle \delta_k | e^{k \delta_k \delta_{k+1}} | \delta_k \rangle$$

$$\therefore \prod_{k=1}^M \exp \left(-\frac{\beta}{M} \hat{H}_0(\vec{\sigma}_k) + k \sum_{i=1}^N \delta_{ik} \delta_{i,k+1} \right) = \text{古典シミュレーション}$$

Step up) 量子古典シミュレーション stochastic.

$$e^{a \delta^x} \rightarrow e^{f(a) \delta_k \delta_{k+1}}$$



d次元量子



d+1次元古典

① δ^x は OK!② 一般化
一般化は OK!
Non-stochastic

解折的p770-7

★ p-spin model

$$\hat{H}_0 = -\frac{J}{N^{p-1}} \sum_{i_1, \dots, i_p} \hat{\sigma}_{i_1}^z \hat{\sigma}_{i_2}^z \dots \hat{\sigma}_{i_p}^z = -NJ \left(\frac{1}{N} \sum_i \hat{\sigma}_i^z \right)^p$$

$$Z = \text{Tr} \exp(-\beta(\hat{H}_0 + \hat{H}_1))$$

$$\stackrel{\text{ST.}}{\downarrow} \text{Tr} \sum_{\vec{\sigma}} \prod_{k=1}^M \exp\left(-\frac{\beta}{M} H_0(\vec{\sigma}_k) + K \sum_{i=1}^N \sigma_{ik} \sigma_{i, k-1}\right) \left[K = -\frac{1}{2} \ln \tanh\left(\frac{\beta J}{M}\right) \right]$$

$$\stackrel{\text{同相模型}}{\downarrow} = \sum_{\vec{\sigma}} \prod_{k=1}^M \exp\left(\frac{N\beta J}{M} \left(\frac{1}{N} \sum_{i=1}^N \sigma_{ik}\right)^p + K \sum_{i=1}^N \sigma_{ik} \sigma_{i, k-1}\right) \quad \text{① 怎么计算?}$$

step up 技巧① $\rightarrow m_k$ with $\int dm \delta(NM - \sum_i \sigma_i)$

$$1 = \int dm \delta(NM - \sum_i \sigma_i)$$

$$\int dm \int dm \exp(-Nm\tilde{m} + \tilde{m} \sum_i \sigma_i)$$

step up 技巧②

$$\delta(NM - \sum_i \sigma_i) = \int d\tilde{m} \exp(-\tilde{m}(NM - \sum_i \sigma_i))$$

$$= \int dm \int d\tilde{m} \exp\left(\frac{N\beta J}{M} \sum_k m_k^p - N \sum_k m_k \tilde{m}_k\right)$$

$$\times \left(\prod_{k=1}^M \sum_{\sigma_k} \exp(\tilde{m}_k \sigma_k + K \sigma_k \sigma_{k-1}) \right)^N \quad \text{① 怎么计算?}$$

3个2个都是 m_k 的
1D Ising model

★ 静态近似 $m_k \rightarrow m$

$\tilde{m}_k \rightarrow \tilde{m}$ δx 由来

$$\text{②} = \prod_{k=1}^M \sum_{\sigma_k} \exp\left(\frac{\beta J m^p}{M} \sigma_k + K \sigma_k \sigma_{k-1}\right)$$

① 怎么计算?

$$= \text{Tr} \left[\prod_{k=1}^M \exp\left(\frac{\beta J m^p}{M} \hat{\sigma}_k^z + \frac{\beta J}{M} \hat{\sigma}_k^x \hat{\sigma}_{k-1}^x\right) \right] \stackrel{\text{②}}{\rightarrow}$$

结果计算麻烦!

$$\left[\hat{A} = \frac{\beta}{M} \begin{pmatrix} \tilde{m} & \Gamma \\ \Gamma & -\tilde{m} \end{pmatrix} \rightarrow \Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \right.$$

$$\det(\hat{A} - \lambda \hat{I}) = (\lambda - \tilde{m})(\lambda + \tilde{m}) - \Gamma^2 = 0$$

$$\therefore \lambda_{\pm} = \pm \sqrt{\tilde{m}^2 + \Gamma^2}$$

$$= \text{Tr}(U \Lambda^N U^{-1}) = 2 \cosh \beta \sqrt{\tilde{m}^2 + \Gamma^2}$$

$$Z = \int dm \int d\tilde{m} \exp(N \left[\beta J(m)^P - \beta m \tilde{m} + \ln 2 \cosh \beta \sqrt{\tilde{m}^2 + P^2} \right])$$

step up) 鞍点法 ($N, \beta \rightarrow \infty$)

$$I = \int dx \exp(-N f(x)) \sim \exp(-N f(x^*))$$

$$x^*: \frac{\partial f}{\partial x} = 0 \text{ 且 } \max_{x^*} f(x^*) \text{ (鞍点)}$$

★ 鞍点方程

$$\partial m = \tilde{m} = P J m^{P-1}$$

$$\partial \tilde{m}: m = \frac{\tilde{m}}{\sqrt{\tilde{m}^2 + P^2}} \tanh(\beta \sqrt{\tilde{m}^2 + P^2})$$

$$\textcircled{1} \begin{cases} \beta \rightarrow \infty \text{ 且 } P \neq 0 \text{ 时 (QA)} \\ P \rightarrow 0 \text{ 且 } \beta \neq 0 \text{ 时 (SA)} \end{cases}$$

★ QAOA

$$P_{\vec{\alpha}, \vec{\gamma}}(\zeta) = |\langle \zeta | \vec{\alpha}, \vec{\gamma} \rangle|^2$$

$$Z = \frac{1}{\zeta} \int d\vec{r} \int d\vec{\alpha} \exp(-\beta E(\vec{\zeta})) P_{\vec{\alpha}, \vec{\gamma}}(\vec{\zeta})$$

$$P = |\alpha \rangle \langle \alpha|$$

$$|\alpha, \gamma\rangle = \exp(-i\alpha \hat{H}_1) \exp(-i\gamma \hat{H}_0) \left(\frac{1}{\sqrt{2}} \sum_{i=1}^N (|1\rangle + |i\rangle) \right)$$

$$|\alpha, \gamma\rangle = \left(\frac{1}{\sqrt{2}} \right) \sum_{\zeta} \exp(-i\alpha \hat{H}_1) \exp(-i\gamma \hat{H}_0) |\zeta\rangle$$

$$\begin{aligned} &= \left(\frac{1}{\sqrt{2}} \right)^N \int dm \int d\tilde{m} \sum_{\zeta} \exp(-i\alpha \hat{H}_1) \exp(-iN\gamma m^P - Nm\tilde{m} + \tilde{m} \sum_{i=1}^N \zeta_i) \\ &\quad (\cos \alpha \hat{I} + i \sin \alpha \hat{\sigma}^x) \quad (\cosh \tilde{m} + \sinh \tilde{m} \hat{\sigma}^z) \end{aligned}$$

$$= \left(\frac{1}{\sqrt{2}} \right)^N \int dm \int d\tilde{m} \exp(-iN\gamma m^P - Nm\tilde{m})$$

$$\times (\cos \alpha \cosh \tilde{m} \hat{I} + i \sin \alpha \cosh \tilde{m} \hat{\sigma}^x + \sinh \alpha \sinh \tilde{m} \hat{\sigma}^y + \cos \alpha \sinh \tilde{m} \hat{\sigma}^z)$$

于是

$$Z = \int d\alpha \int d\gamma \sum_{\zeta_1 \zeta_2} \sum_{\zeta} \int dm_0 \int dm_1 \int dm_2 \int d\tilde{m}_1 \int d\tilde{m}_2$$

$$\times \exp(+N\beta J m_0^P - iN\gamma J m_1^P + iN\gamma J m_2^P - Nm_0 \tilde{m}_0 - N\tilde{m}_1 m_1 - Nm_2 \tilde{m}_2)$$

$$\times \text{Tr}[\hat{A}^\dagger(\alpha, m_2) e^{\tilde{m}_0 \hat{\sigma}^z} \hat{A}(\alpha, m_1)]$$

虚時間量子P2-127

$$i\hbar \frac{d}{dt} \psi(x,t) = \hat{H}(x,t) \psi(x,t) \quad (\text{実時間}) \quad \left[\hat{H}(x,t) = -\hbar^2 \frac{\partial^2}{\partial x^2} + V(x) \right]$$

$$\Rightarrow -\frac{d}{dt} \psi(x,t) = \hat{H}(x,t) \psi(x,t) \quad (\text{虚時間}) \quad \left[\psi(x,T) = \exp\left(-\int_{t_0}^T dt \hat{H}(x,t)\right) \psi(x,0) \right]$$

① 規格化を気にせず

$$t = -i\tau \quad \left[-\frac{d}{d\tau} \psi(x,\tau) = -\hat{H}(x,\tau) \psi(x,\tau) \quad (\text{随伴}) \right]$$

(backward/adjoint)

$$\Rightarrow P(x,\tau) = \psi(x,\tau) \tilde{\psi}(x,\tau) \quad \text{① 此の方程式が必要?}$$

$$\frac{\partial}{\partial \tau} P(x,\tau) = \left[\frac{\partial \psi}{\partial \tau} \right] \tilde{\psi} + \psi \left[\frac{\partial \tilde{\psi}}{\partial \tau} \right] = -\hbar^2 \left(\frac{\partial^2 \psi}{\partial x^2} \tilde{\psi} + \psi \frac{\partial^2 \tilde{\psi}}{\partial x^2} \right)$$

-Hψ Hψ̃ J(x,t) = 確率流

$$= -\hbar^2 \frac{\partial}{\partial x} \left(-\frac{\partial \psi}{\partial x} \tilde{\psi} + \psi \frac{\partial \tilde{\psi}}{\partial x} \right) \quad \text{① Fokker-Planck?}$$

Step up 7.4.1-7.3.2 方程式

$$\frac{\partial}{\partial \tau} P(x,\tau) = -\hbar^2 \frac{\partial}{\partial x} J(x,\tau) \quad (\text{連続方程式})$$

$$\left[J(x,\tau) = -\hbar^2 \frac{\partial P}{\partial x} + f(x,\tau) P(x,\tau) \right]$$

$$\left[\text{拡散方程式} f(x,\tau) = -\frac{\partial V}{\partial x} \right]$$

$$dx = -\frac{\partial V}{\partial x} d\tau + \sqrt{2\hbar} dW \quad (\hbar = T)$$

$$t \rightarrow \infty \quad f(x,t) = -\frac{\partial}{\partial x} V(x) \text{ あり}$$

$$J(x,\infty) \rightarrow 0 \quad (\text{平衡状態})$$

$$P(x,\infty) \propto \exp\left(-\frac{1}{\hbar} V(x)\right)$$

$$\star \psi = P/\tilde{\psi} \quad \frac{\partial \psi}{\partial x} = \frac{1}{\tilde{\psi}} \frac{\partial P}{\partial x} - \frac{P}{\tilde{\psi}^2} \frac{\partial \tilde{\psi}}{\partial x} f(x,\tau)$$

$$\frac{\partial}{\partial \tau} P(x,\tau) = \hbar^2 \frac{\partial^2 P}{\partial x^2} - 2\hbar^2 P(x,\tau) \left[\frac{\partial}{\partial x} \left(\ln \tilde{\psi} \right) \right] \quad (\text{forward FP})$$

$$\star \tilde{\psi} = P/\psi \quad \frac{\partial \tilde{\psi}}{\partial x} = \frac{1}{\psi} \frac{\partial P}{\partial x} - \frac{P}{\psi^2} \frac{\partial \psi}{\partial x} f(x,\tau)$$

$$\frac{\partial}{\partial \tau} P(x,\tau) = -\hbar^2 \frac{\partial^2 P}{\partial x^2} - 2\hbar^2 P(x,\tau) \left[\frac{\partial}{\partial x} \left(-\ln \psi \right) \right] \quad (\text{backward FP})$$

拡散方程式

$$dx = f(x,\tau) d\tau + \sqrt{2\hbar} dW$$

$$\text{or } dy = -f(y, T-\tau) d\tau + \sqrt{2\hbar} dW$$

★ T=2 1/4 - 1/11 分解.

$$\left(-\frac{\partial^2}{\partial x^2} + V(x)\right) \psi(x) = E \psi(x) \quad \textcircled{11} \quad \boxed{\text{1階Eがeasy}}$$

Step up T=2 1/4 - 1/11 分解.

$$\hat{A} = \frac{\partial}{\partial x} + \frac{1}{2}V'(x)$$

$$\hat{A}^\dagger = -\frac{\partial}{\partial x} + \frac{1}{2}V'(x)$$

$$\hat{A} \psi(x) = 0 \text{ なら } \psi(x) \propto \exp\left(-\frac{1}{2}V(x)\right)$$

$$\begin{aligned} \hat{A}^\dagger \hat{A} &= \left(-\frac{\partial}{\partial x} + \frac{1}{2}V'(x)\right) \left(\frac{\partial}{\partial x} + \frac{1}{2}V'(x)\right) \\ &= -\frac{\partial^2}{\partial x^2} + \boxed{\frac{1}{4}V'(x)^2 - \frac{1}{2}V''(x)} \equiv \hat{H}_{\text{SUSY}}(x) \end{aligned}$$

位置と力に依存

Step up SUSY 1/11 分解

$$H_{\text{SUSY}} = \hat{A}^\dagger \hat{A} \quad A = \frac{\partial}{\partial x} + \frac{1}{2}V(x)$$

$$\hat{H}_{\text{SUSY}} \psi(x) = 0 \quad \psi(x) \propto \exp\left(-\frac{1}{2}V(x)\right)$$

① $\frac{1}{2}V(x)$ は
T=2 1/4 2階

② $\frac{1}{2}V(x)$ は
T=2 1/4 2階

③ $V(x) = \frac{1}{2}x^2$ ($V'(x) = x$) 調和振動子!

★ 拡散モデル $P_0(x)$: T=2 1/4 分布 $\xrightarrow{\text{生成}} P_T(x)$: 作り出し分布 $\xrightarrow{\text{生成}} P_T(x)$: 作り出し分布

(基底状態) $V(x)$ を学習! (基底状態) $V(x)$ を学習!

途中

$$P(x,t) = \psi_t(x) \tilde{\psi}_t(x)$$

$$\psi_t(x) = \sqrt{P(x,t)} \text{ は g.s. に } \hat{H}_{\text{SUSY}} \text{ を作用}$$

$$V_t(x) = -\log P(x,t) \quad \textcircled{11} \quad \boxed{\text{スコア登場!}}$$

forward $dx = f(x,t)dt + \sqrt{2D}dw$ $\textcircled{11} \quad \boxed{\text{f-g 生成過程}}$

① $P_0(x)$ は x を生成. 2階② $P_t(x)$ を生成 $\rightarrow P_t(x)$ は作り出し分布

$$S(x,t) = \frac{\partial}{\partial x} \log P_t(x) \text{ を学習!}$$

Step up 72P2, 72P1

余計.

$$S(x, t) = \frac{\partial}{\partial x} \log P(x, t) \text{ じゃ!}$$

$$\log \tilde{\pi}_1(x) + \log \pi_1(x)$$

[forward]

$$f_+(x, t) = 2D \frac{\partial}{\partial x} \log \tilde{\pi}_1(x) = f(x, t) \text{ じゃ!}$$

学習した72P2を50

$$f_+ + f_- = 2D \frac{\partial}{\partial x} \log P(x, t)$$

[backward]

$$f_-(x, t) = 2D \frac{\partial}{\partial x} \log \pi_1(x) = -f(x, t) + 2D \frac{\partial}{\partial x} \log P(x, t)$$

逆方向の力

$$\textcircled{3} \Rightarrow dr = (f(x, t) - 2D \frac{\partial}{\partial x} \log P(x, t)) dt + \sqrt{2D} dw \text{ じゃ!}$$

追加項 (P(x, t) じゃ!)

⑪

学習の精度を

★ 追加の項を正体.