CS 59300 – Algorithms for Data Science

Classical and Quantum approaches

Lecture 22 (12/02)

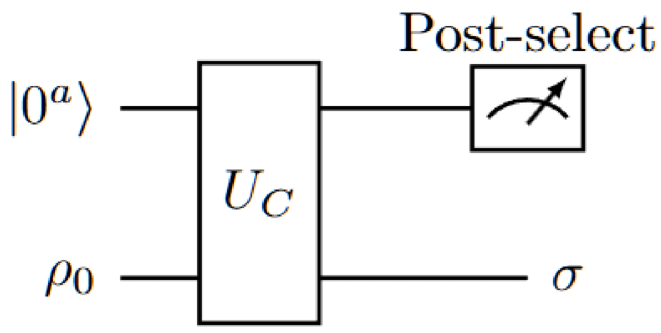
Quantum Gibbs Sampling and Open Quantum Systems

https://ruizhezhang.com/course_fall_2025.html

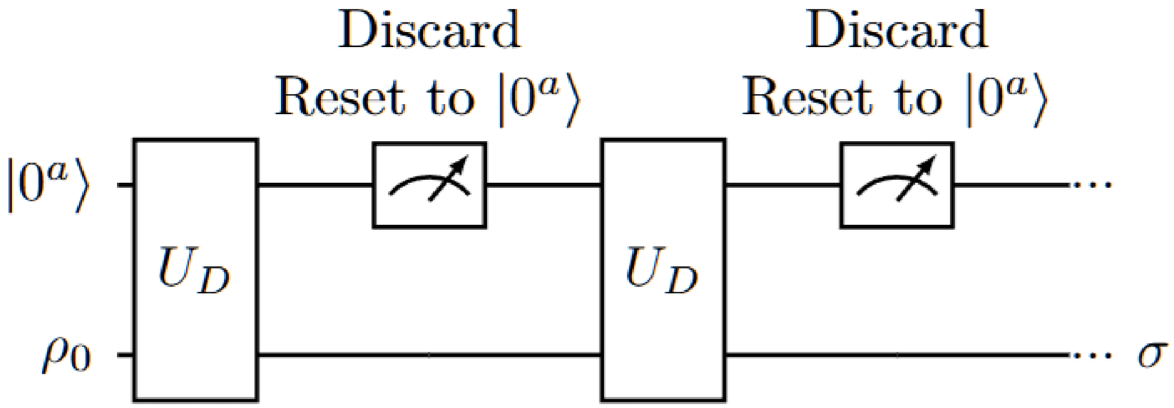
Outline

- Motivation
- Description of open quantum system dynamics
- Quantum simulation algorithms
- Applications
    - State preparation (ground state and Gibbs state)
    - Approximate the non-equilibrium system bath coupled dynamics
    - Simulate quantum field theories
    - Classical and quantum optimizations
    - Model the noise in quantum circuits, quantum error correction, and quantum memory
    - Quantum biology

Coherent vs. dissipative state preparation



(a) Coherent state preparation.



(b) Dissipative state preparation.

Coherent state preparation: LCU, QSVT

- Success probability issue and the initial state preparation cost
- Complexity analysis is rigorous and easy

Dissipative state preparation: Lindblad dynamics

- No post-selection, i.e. success probability $= 1$
- No need a good initial state
- Proving the complexity is hard

Dissipative state preparation workflow

- Suppose the target state is σ
- Design a Lindbladian $\mathcal{L}$ such that σ is its fixed point,

$$\frac{\mathrm{d}\sigma}{\mathrm{d}t} = \mathcal{L}(\sigma) = 0$$

- Apply a Lindblad simulation algorithm that approximately preserves the fixed point:

$$\Phi(\sigma) = \mathrm{tr}_a\left[U_D(|0\rangle\langle 0| \otimes \sigma)U_D^\dagger\right] \approx \sigma$$

- Analyzing the convergence rate (mixing time) of the Lindblad dynamics

$$\tau_{\mathrm{mix}}(\eta) = \min\left\{t : \left\|e^{t\mathcal{L}}\rho - \sigma\right\|_1 \leq \eta, \qquad \forall\rho\right\}$$

  For an n-qubit system, fast mixing if $\tau_{\mathrm{mix}} = \mathrm{poly}(n)$, and rapid mixing if $\tau_{\mathrm{mix}} = \mathrm{polylog}(n)$

- Total complexity $\approx \mathrm{cost}(U_D) \times \tau_{\mathrm{mix}}$

Ground state preparation: toy example

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \mathcal{L}\rho = -\mathbf{i}[H,\rho] + K\rho K^\dagger - \frac{1}{2}\{K^\dagger K, \rho\}$$

- $H = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$, the ground state is $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$
- Jump operator $K = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$
- Initial state $\rho(0) = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$
- Solution: $\rho(t) = \begin{bmatrix} 1 - e^{-t} & 0 \\ 0 & e^{-t} \end{bmatrix}$
- Converge to the ground state exponentially fast

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{bmatrix} = \begin{bmatrix} \rho_{11} & \left(2\mathbf{i} - \frac{1}{2}\right)\rho_{01} \\ \left(-2\mathbf{i} - \frac{1}{2}\right)\rho_{10} & -\rho_{11} \end{bmatrix}$$

$$\rho_{11} = \rho(0)_{11} \cdot e^{-t} = e^{-t}$$

$$\rho_{00} = 1 - \rho_{11} = 1 - e^{-t}$$

$$\rho_{01} = \rho(0)_{01} \cdot e^{\left(2\mathbf{i} - \frac{1}{2}\right)t} = 0$$

Ground state preparation: toy example

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \mathcal{L}\rho = -\mathbf{i}[H,\rho] + \underbrace{K\rho K^\dagger - \frac{1}{2}\{K^\dagger K,\rho\}}_{\mathcal{L}_K(\rho)}$$

- $H = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$, the ground state is $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$
- Jump operator $K = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$
- Initial state $\rho(0) = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$
- $\mathcal{L}_K(|1\rangle\langle 1|) = |0\rangle\langle 0| - |1\rangle\langle 1|$ steer excited state towards the ground state
- $\mathcal{L}_K(|0\rangle\langle 0|) = 0$ preserve the ground state

Ground state preparation

Given a Hamiltonian $H = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$, the jump operator is designed to be:

$$K = \sum_{i,j} \hat{f}(\lambda_i - \lambda_j) |\psi_i\rangle\langle\psi_i|A|\psi_j\rangle\langle\psi_j|$$

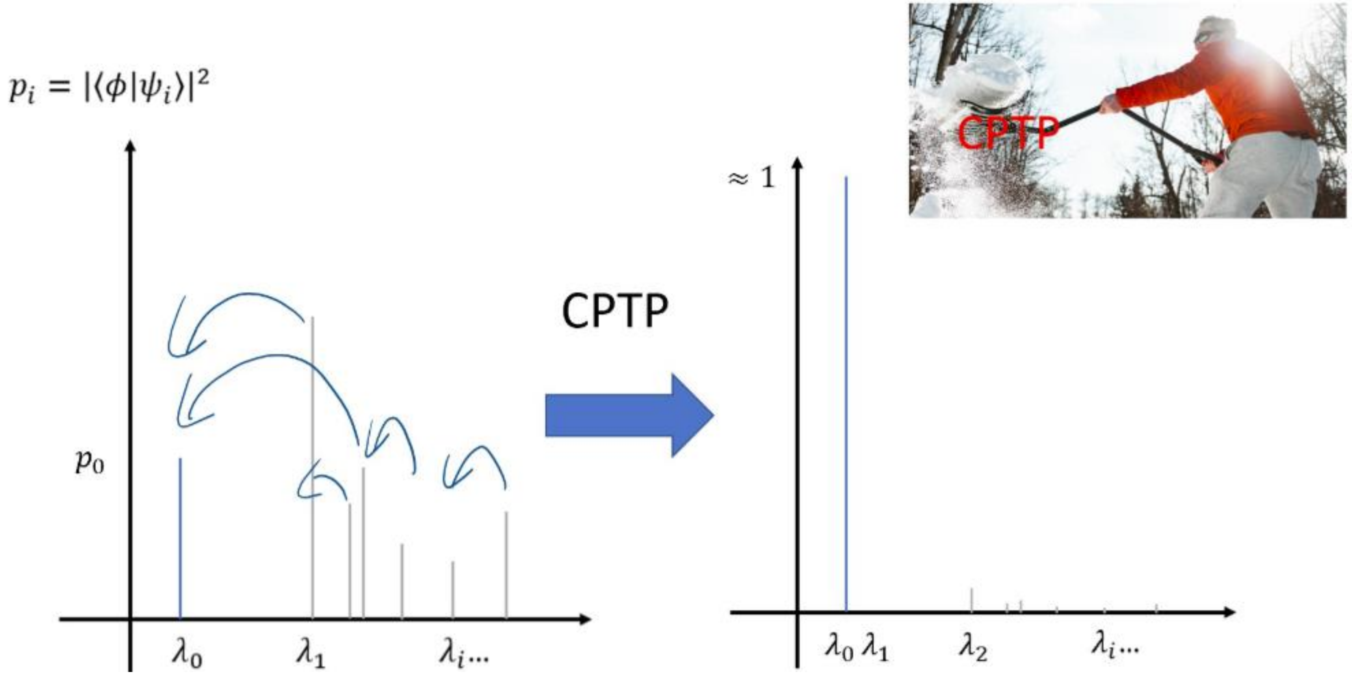
- A is the coupling operator that can be Hermitian and local (e.g. a single Pauli operator)
- $\hat{f}(\omega)$ is a filter function such that $\hat{f}(\omega) = 0$ for any $\omega \geq 0$

$$\mathcal{L}_K(\rho) = K\rho K^\dagger - \frac{1}{2}\{K^\dagger K, \rho\}$$

- $\mathcal{L}_K(|\psi_0\rangle\langle\psi_0|) = 0$ fix the ground state
- $\langle\psi_i|\mathcal{L}_K\left(|\psi_j\rangle\langle\psi_j|\right)|\psi_i\rangle > 0$ if $i < j$ push high energy states towards low energy states
- $\langle\psi_i|\mathcal{L}_K\left(|\psi_j\rangle\langle\psi_j|\right)|\psi_i\rangle = 0$ if $i \geq j$ low energy state $\not\Rightarrow$ high energy state

Ground state preparation

From filtering to shoveling



Ground state preparation

$$K = \sum_{i,j} \hat{f}(\lambda_i - \lambda_j)|\psi_i\rangle\langle\psi_i|A|\psi_j\rangle\langle\psi_j|$$
$$= \int_{-\infty}^{\infty} f(s) e^{\mathbf{i}Hs} A e^{-\mathbf{i}Hs} \mathrm{d}s$$

- The filter function f can be designed to have support of size $\mathcal{O}(\Delta^{-1})$, where Δ is the spectral gap of H
- We can discretize the integral and use LCU to block-encode the jump operator

Ding, Zhiyan, Chi-Fang Chen, and Lin Lin. "Single-ancilla ground state preparation via Lindbladians."

Gibbs state preparation

$$\rho_\beta = \frac{e^{-\beta H}}{Z_\beta}, \qquad Z_\beta = \mathrm{tr}\left[e^{-\beta H}\right]$$

For coherent state preparation methods (e.g., LCU, QSVT, LCHS), the complexity scales as

$$\sqrt{2^n/Z_\beta}\,\mathrm{poly}(\beta, 1/\epsilon)$$

- At very high temperature ($\beta \to 0$, $\sqrt{2^n/Z_\beta} \sim \mathcal{O}(1)$), the algorithm is efficient
- At low temperature (β large, $\sqrt{2^n/Z_\beta} \sim \sqrt{2^n}$), exponential cost

For dissipative approaches, the complexity varies significantly across different systems

Gibbs state preparation

Complexity

- At low-temperature (very large β), the Gibbs state has large overlap with the ground state, and hence quantum Gibbs sampling is **QMA**-hard in the worst case
- **Bergamaschi-Chen-Liu ’24, Rajakumar-Watson ’24:** there exists a family of local Hamiltonian such that the Gibbs state (with $\beta = \mathcal{O}(1)$) can be prepared in polynomial time by the Davies generator, but classically intractable unless **PH** collapses
- **Rouzé-Franca-Alhambra ’24:** simulating some specific Lindbladian at $\beta = \Omega(\log n)$ to $T = \mathrm{poly}(n)$ for a k-local Hamiltonian is **BQP**-complete
- **Bakshi-Liu-Moitra-Tang ’24:** at high-temperature ($\beta < \beta_c$), the Gibbs state is not entangled (i.e., a linear combination of product states), and can be efficiently prepared classically

Gibbs state preparation: mathematics

Markov semigroup

- For a drift-diffusion process $\{\mathbf{x}_t\}_{t\geq 0}$, we define the Markov semigroup $\{P_t\}_{t\geq 0}$:

$$(P_t f)(\mathbf{x}) \coloneqq \mathbb{E}[f(\mathbf{x}_t) \mid \mathbf{x}_0 = \mathbf{x}] \qquad \text{for} \quad f : \mathbb{R}^d \to \mathbb{R}$$

If $f = \mathbf{1}_S$ for a subset S, then $(P_t f)(\mathbf{x}) = \Pr[\mathbf{x}_t \in S \mid \mathbf{x}_0 = \mathbf{x}]$

- Markov property:

$$P_{t+s} f = P_t P_s f = P_s P_t f \qquad \forall\, f : \mathbb{R}^d \to \mathbb{R}, \forall\, s, t \geq 0$$

- Generator:

$$\mathcal{L} f \coloneqq \lim_{\eta \to 0} \frac{P_\eta f - f}{\eta}$$

Quantum Markov semigroup:

$$(\mathcal{P}_t)_{t\geq 0} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$$

- CPTP maps
- Generator (Lindbladian):

$$\mathcal{L}\rho = \lim_{t \to 0^+} \frac{\mathcal{P}_t(\rho) - \rho}{t}$$

- Ergodicity (unique fixed point)
- Detailed balanced condition
- Spectral gap
- Poincaré and log-Sobolev inequalities

Highly non-trivial!

Interlude: Schrödinger and Heisenberg pictures

The evolution of a quantum system can be viewed from two perspectives:

- Schrödinger picture
  - The state $\rho \mapsto \Phi(\rho)$ is evolving
  - We observe the system by some fixed observable X: $\mathrm{tr}[\Phi(\rho)X]$

$$\mathcal{L}\rho = -\mathbf{i}[H,\rho] + L_j\rho L_j^\dagger - \frac{1}{2}\{L_j^\dagger L_j, \rho\}$$

- Heisenberg picture
  - The state is fixed but the observable $X \mapsto \Phi^\dagger(X)$ is evolving
  - We observe the system by $\mathrm{tr}\left[\rho\Phi^\dagger(X)\right] = \mathrm{tr}[\Phi(\rho)X]$

adjoint w.r.t. $\langle X, Y\rangle = \mathrm{tr}\left[X^\dagger Y\right]$

$$\mathcal{L}^\dagger(X) = \mathbf{i}[H,X] + L_j^\dagger X L_j - \frac{1}{2}\{L_j^\dagger L_j, X\}$$

Mathematicians like this form

Unique fixed point

$$\mathcal{L}\rho = -\mathbf{i}[H,\rho] + \sum_{j=1}^{m}\left(L_j\rho L_j^\dagger - \frac{1}{2}\{L_j^\dagger L_j,\rho\}\right)$$

We want to guarantee that there exists a unique full-rank invariant state σ such that

$$\lim_{\mathrm{t}\to\infty} e^{\mathcal{L}t}\rho = \sigma \quad \forall \rho \in \mathcal{B}(\mathcal{H})$$

Criterion (Old result. See e.g., Ding-Li-Lin ’24, Lemmas 2 and 3):

$$\{H, L_j, L_j^\dagger\}' = \mathrm{span}(\{I\})$$

There is no non-trivial matrix that simultaneously commute with all $H, L_j, L_j^\dagger$

Detailed balanced condition (DBC)

For classical Markov semigroup, the DBC is defined as:

$$\langle f, \mathcal{L}g \rangle_\pi = \langle \mathcal{L}f, g \rangle_\pi$$

$\mathcal{L}$ is self-adjoint w.r.t. the π-weighted inner product

$$\langle f, g \rangle_\pi = \int f(x)g(x)\pi(x)\mathrm{d}x$$

For QMC, due to the non-commutativity, there is no unique way to re-weigh the inner product using the invariant state

- Define the modular operator $\Delta_\sigma(X) \coloneqq \sigma X \sigma^{-1}$
- Define the left and right multiplication operator $L_\sigma(X) \coloneqq \sigma X$ and $R_\sigma(X) \coloneqq X\sigma$
- For any $f: \mathbb{R}_+ \to \mathbb{R}_+$ with $f(1) = 1$, define the operator

$$J_\sigma^f(X) \coloneqq R_\sigma \circ f(\Delta_\sigma)(X) = f(\sigma)Xf(\sigma^{-1})\sigma$$

Detailed balanced condition (DBC)

- For $f = x^{1-s}$,

$$J_\sigma^f(X) = \sigma^{1-s} X \sigma^s$$

The associated inner product is defined as:

$$\langle X, Y \rangle_{\sigma,s} \coloneqq \left\langle X, J_\sigma^f(Y) \right\rangle = \mathrm{tr}\left[\sigma^s X^\dagger \sigma^{1-s} Y\right] = \left\langle J_\sigma^f(X), Y \right\rangle$$

- The QMS $\mathcal{P}_t^\dagger = e^{t\mathcal{L}^\dagger}$ satisfies the J_σ^f-DBC if $\mathcal{L}^\dagger$ is self-adjoint w.r.t. $\langle \cdot, \cdot \rangle_{\sigma,f}$:

$$\left\langle X, \mathcal{L}^\dagger Y \right\rangle_{\sigma,f} = \left\langle J_\sigma^f(X), \mathcal{L}^\dagger Y \right\rangle = \left\langle \mathcal{L} J_\sigma^f(X), Y \right\rangle = \left\langle J_\sigma^f\left(\mathcal{L}^\dagger X\right), Y \right\rangle = \left\langle \mathcal{L}^\dagger X, Y \right\rangle_{\sigma,f}$$

$$\Longleftrightarrow \qquad J_\sigma^f \mathcal{L}^\dagger = \mathcal{L} J_\sigma^f$$

- $s = 1$ is called Gelfand-Naimark-Segal (GNS) DBC

- $s = \frac{1}{2}$ is called Kubo-Martin-Schwinger (KMS) DBC

Detailed balanced condition (DBC)

Let $\mathcal{L}^\dagger$ be a J_σ^f-detailed-balanced Lindbladian:

$$\mathcal{L}^\dagger(X) = \mathbf{i}[H, X] + L_j^\dagger X L_j - \frac{1}{2}\{L_j^\dagger L_j, X\}$$

- $\mathcal{L}^\dagger(I) = 0$ by direct calculation
- J_σ^f-DBC implies that $\mathcal{L}(\sigma) = 0$:

$$0 = \left\langle X, \mathcal{L}^\dagger(I)\right\rangle_{\sigma,f} = \left\langle \mathcal{L}^\dagger(X), I\right\rangle_{\sigma,f} = \left\langle \mathcal{L}^\dagger X, J_\sigma^f(I)\right\rangle = \left\langle \mathcal{L}^\dagger X, \sigma\right\rangle = \langle X, \mathcal{L}(\sigma)\rangle$$

- Relations between DBCs:

$$\boxed{\text{GNS}} \Longleftrightarrow \boxed{\begin{array}{c} f = x^{1-s} \\ s \in [0,1]\backslash\{1/2\} \end{array}} \Longrightarrow \boxed{\begin{array}{c} \text{All other } J_\sigma^f\text{-DBC} \\ \text{(including KMS)} \end{array}}$$

GNS detailed balanced Lindbladian

Davies generator:

$$\mathcal{L}\rho = -i[H_S + H_{LS}, \rho] + g^2 \sum_{\omega} \sum_{a} \left(L_{a,\omega} \rho L_{a,\omega}^{\dagger} - \frac{1}{2} \{ L_{a,\omega}^{\dagger} L_{a,\omega}, \rho \} \right)$$

Engineered Davies generator:

- Choose a set of coupling operator $\{A^a\}_{a \in \mathcal{A}}$
- Let H be the Hamiltonian with eigen-decomposition: $H = \sum_i \lambda_i P_i$, where $P_i = |\psi_i\rangle\langle\psi_i|$
- The jump operator $\{A_\nu^a\}$ are defined as:

$$A^a = \sum_{i,j} P_i A^a P_j = \sum_{\nu \in B_H} A_\nu^a , \qquad B_H := \{\lambda_i - \lambda_j : \lambda_i, \lambda_j \in \mathrm{spec}(H)\}$$

where

$$A_\nu^a = \sum_{\lambda_i - \lambda_j = \nu} P_i A^a P_j , \qquad (A_\nu^a)^\dagger = A_{-\nu}^a, \qquad \Delta_{\rho_\beta} A_\nu^a = e^{-\beta\nu} A_\nu^a$$

GNS detailed balanced Lindbladian

Canonical form:

$$\mathcal{L}\rho = \sum_{a\in\mathcal{A}} c_a \sum_{\nu\in B_H} \gamma_a(\nu)\left(A_\nu^a \rho (A_\nu^a)^\dagger - \frac{1}{2}\{(A_\nu^a)^\dagger A_\nu^a, \rho\}\right)$$

- $\gamma_a(-\nu) = e^{\beta\nu}\gamma_a(\nu)$
  - Examples: $\gamma_a(\nu) = \frac{1}{1+e^{\beta\nu}}$ (Glauber dynamics) or $\gamma_a(\nu) = \min\{1, e^{-\beta\nu}\}$ (Metropolis)
- $c_a \geq 0$
- $A_\nu^a = \sum_{\lambda_i-\lambda_j=\nu} P_i A^a P_j$

To implement a GNS-DB Lindbladian, we need to exactly resolve the Bohr frequencies, which is extremely difficult for a non-commuting Hamiltonian

KMS detailed balanced Lindbladian

Canonical form:

$$\mathcal{L}\rho = -\mathbf{i}[G,\rho] + \sum_{j=1}^{m}\left(L_j\rho L_j^\dagger - \frac{1}{2}\{L_j^\dagger L_j,\rho\}\right)$$

where

$$\Delta_{\rho_\beta}^{-1/2} L_j = L_j^\dagger, \qquad G := -\mathbf{i}\,\tanh\circ\log\left(\Delta_{\rho_\beta}^{1/4}\right)\left(\frac{1}{2}\sum_{j=1}^{m} L_j^\dagger L_j\right)$$

$$\sum_\nu e^{\beta\nu/2}\left(L_j\right)_\nu = L_j^\dagger \qquad G = -\frac{\mathbf{i}}{2}\sum_j\sum_\nu \tanh(-\beta\nu/4)\left(L_j^\dagger L_j\right)_\nu$$

- After choosing a set of jump operators, the coherent term is automatically determined

KMS detailed balanced Lindbladian

- Let $\{A^a\}$ be a set of self-adjoint coupling operators
- $\Delta_{\rho_\beta}^{-1/2} L_j = L_j^\dagger$ implies that $L_j = \Delta_{\rho_\beta}^{1/4} A$ for some self-adjoint operator A

$$L_j = \rho_\beta^{1/4} A \rho_\beta^{-1/4} = \sum_{i,j} e^{-\beta(\lambda_i - \lambda_j)/4} P_i A P_j = \sum_{\nu \in B_H} e^{-\beta\nu/4} A_\nu$$

- For algorithmic purpose, let $q^a(\nu) : \mathbb{R} \to \mathbb{C}$ be a weighing function and define

$$L_a = \sum_{\nu \in B_H} q^a(\nu) e^{-\beta\nu/4} A_\nu = \int_{-\infty}^{\infty} f^a(t) A^a(t) \mathrm{d}t$$

  - $q^a(-\nu) = \overline{q^a(\nu)}$
  - $f^a(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} q^a(\nu) e^{-\beta\nu/4} e^{-\mathbf{i}t\nu} \mathrm{d}\nu$ is the (inverse) Fourier transform
  - $A^a(t) = e^{\mathbf{i}Ht} A^a e^{-\mathbf{i}Ht}$ is the time evolution in the Heisenberg picture

KMS detailed balanced Lindbladian

- Let $\{A^a\}$ be a set of self-adjoint coupling operators
- For algorithmic purpose, let $q^a(\nu) : \mathbb{R} \to \mathbb{C}$ be a weighing function and define

$$L_a = \sum_{\nu \in B_H} q^a(\nu) e^{-\beta\nu/4} A_\nu = \int_{-\infty}^{\infty} f^a(t) A^a(t) \mathrm{d}t$$

- The coherent term G can also be expanded in the eigen-basis of H:

$$G = -\frac{\mathbf{i}}{2} \sum_{a \in \mathcal{A}} \sum_{\nu \in B_H} \tanh\left(-\frac{\beta\nu}{4}\right) \left(L_a^\dagger L_a\right)_\nu$$

- Let $\hat{g}(\nu) \coloneqq \kappa(\nu) \cdot \left(-\frac{\mathbf{i}}{2} \tanh\left(-\frac{\beta\nu}{4}\right)\right)$ be an L^1-integrable function, and $g(t)$ be its Fourier transform

$$G = \int_{-\infty}^{\infty} g(t) H_L(t) \mathrm{d}t = \int_{-\infty}^{\infty} g(t) \sum_{a \in \mathcal{A}} e^{\mathbf{i}Ht} \left(L_a^\dagger L_a\right) e^{-\mathbf{i}Ht} \, \mathrm{d}t$$

KMS detailed balanced Lindbladian

- Let $\{A^a\}$ be a set of self-adjoint coupling operators

$$L_a = \int_{-\infty}^{\infty} f^a(t) A^a(t) \mathrm{d}t$$

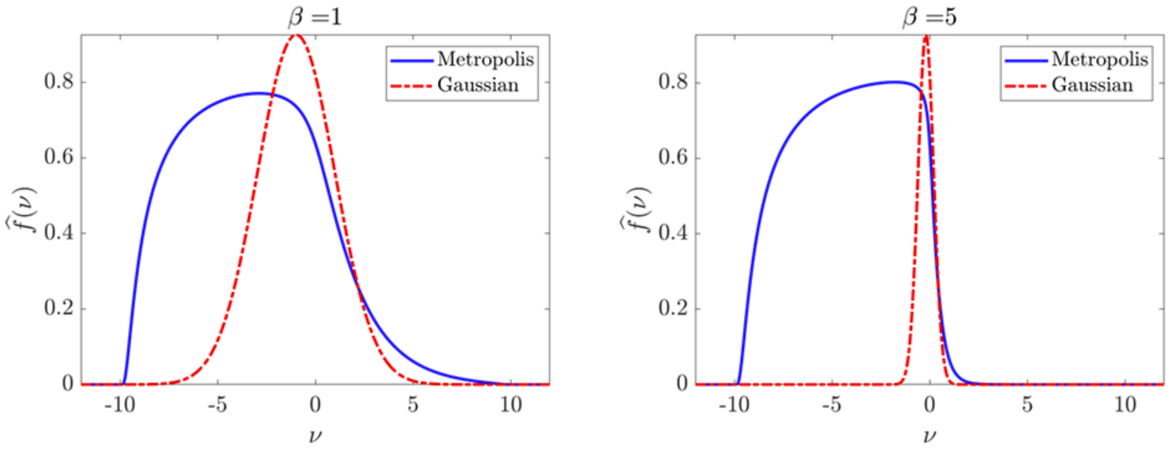
$$G = \int_{-\infty}^{\infty} g(t) H_L(t) \mathrm{d}t$$

- By properly choosing $q(\nu)$ and $\kappa(\nu)$, we can use quadrature to discretize the integrals and use LCU to block-encode $\{L_a\}$ and G
  - Metropolis-type:

    $$\hat{f}(\nu) \propto \min\left\{1, e^{-\beta\nu/2}\right\}$$

  - Gaussian-type:

    $$\hat{f}(\nu) \propto e^{-(\beta\nu+1)^2/8}$$



Spectral gap

- Let $\mathcal{L}$ be a Lindbladian satisfying GNS or KMS DBC
- Recall that for a classical Markov semi-group, the spectral gap is defined as

$$\inf_{f \perp \mathbf{1}} \frac{\mathcal{E}(f,f)}{\langle f,f \rangle_\pi} = \inf_{f \perp \mathbf{1}} \frac{\langle f, -\mathcal{L} f \rangle_\pi}{\langle f,f \rangle_\pi}$$

- The spectral gap of $\mathcal{L}$ can be defined in a similar way:

$$\mathrm{gap}(\mathcal{L}) = \inf_{\mathrm{tr}[\sigma X]=0} \frac{\left\langle X, -\mathcal{L}^\dagger X \right\rangle_{\sigma,1/2}}{\langle X, X \rangle_{\sigma,1/2}} = \inf_X \frac{\left\langle X, -\mathcal{L}^\dagger X \right\rangle_{\sigma,1/2}}{\mathrm{Var}[X]},$$

where $\mathrm{Var}[X] \coloneqq \langle X, X \rangle_{\sigma,1/2} - \mathrm{tr}[\sigma X]^2$

Recall that $\langle X, Y \rangle_{\sigma,1/2} = \mathrm{tr}\left[\sigma^{1/2} X^\dagger \sigma^{1/2} Y\right]$

Poincare inequality

$$\chi^2(\rho(t),\sigma) \leq \chi^2(\rho(0),\sigma)e^{-2\mathrm{gap}(\mathcal{L})t}$$

- $\chi^2(\rho,\sigma) \coloneqq \mathrm{tr}\left[\rho\sigma^{-\frac{1}{2}}\rho\sigma^{-\frac{1}{2}}\right] - 1$ is the χ^2-divergence for quantum states
- $\|\rho - \sigma\|_1 \leq \sqrt{\chi^2(\rho,\sigma)}$

$$\left\|\rho(t) - \rho_\beta\right\|_1 \leq \sigma_{\min}\left(\rho_\beta\right)^{-1/2} e^{-\mathrm{gap}(\mathcal{L})t} = Z_\beta e^{\beta\|H\|} e^{-\mathrm{gap}(\mathcal{L})t}$$

- $\tau_{\mathrm{mix}} \sim \mathrm{poly}(n)$ (fast mixing)
- **Applications:** Weakly interacting Fermionic systems (Tong-Zhan ’25), quantum stabilizer code Hamiltonians (2D Toric code, 4D Toric code, Kitaev's quantum double models, etc.) (Alicki-Fannes-Horodeck ’09, Temme-Kastoryano ’15, Ding-Landau-Li-Lin-**Z.** ’24, Hangleiter-Ju-Vazirani ’25)

Modified log-Sobolev inequality

$$D(\rho(t)\|\sigma) \leq D(\rho(0)\|\sigma)e^{-2\alpha t}$$

- $D(\rho\|\sigma) \coloneqq \mathrm{tr}[\rho(\log(\rho) - \log(\sigma))]$ is the quantum relative entropy

- $\|\rho - \sigma\|_1 \leq \sqrt{2 \ln 2\, D(\rho\|\sigma)}$ (quantum Pinsker inequality)

$$\left\|\rho(t) - \rho_\beta\right\|_1 \leq \sqrt{2\log\left(\sigma_{\min}\left(\rho_\beta\right)\right)e^{-\alpha t}} = \sqrt{2\left(\beta\|H\| + \log Z_\beta\right)e^{-\alpha t}}$$

- $\tau_{\mathrm{mix}} \sim \mathrm{polylog}(n)$ (rapid mixing)

- **Applications:** Geometric local Hamiltonian (high temperature) (Rouzé-França-Alhambra ’24), 1D local commuting Hamiltonian (any temperature) (Kochanowski-Alhambra-Capel-Rouzé ’24), weakly interacting quantum systems (Šmíd-Meister-Berta-Bondesan ’25)

Outline

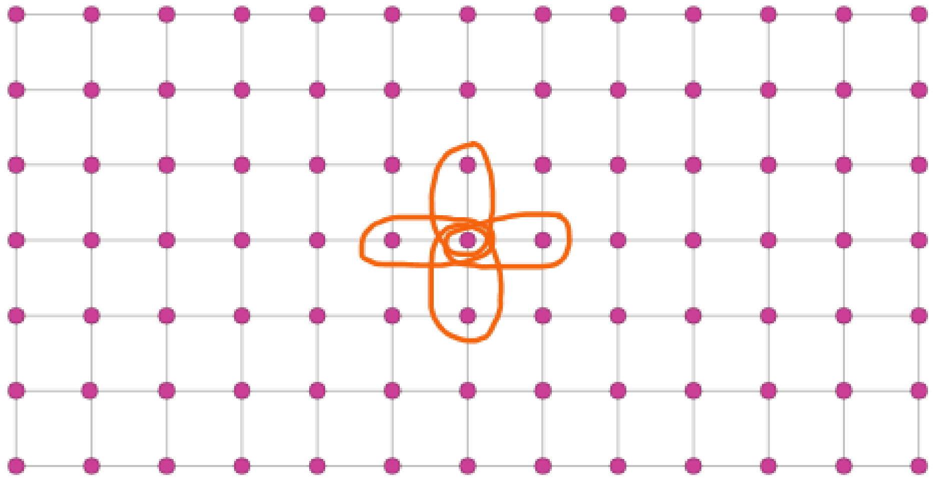
- Motivation
- Description of open quantum system dynamics
- Quantum simulation algorithms
- Applications
- Bonus: Hamiltonian learning from Gibbs states

Hamiltonian learning

- An (unknown) Hamiltonian H acting on n qubits on a D-dimensional lattice

$$H = \sum_{\gamma \in \Gamma} h_\gamma P_\gamma \,, \qquad h_\gamma \in [-1,1], \qquad P_\gamma \in \mathcal{P}_n(q)$$ n-qubit Pauli of degree $\leq q$

- We assume that $\leq d$ terms acting on any qubit i, and Γ contains all admissible terms
- Given d, q, β, and access to the Gibbs state $\rho_\beta \propto e^{-\beta H}$ (without access to $e^{-\mathbf{i}Ht}$)
- The goal is to recover the coefficient vector $\left(h_\gamma\right)_{\gamma \in \Gamma}$
- Example: $D = 2, q = 2, d = 4, |\Gamma| = \mathcal{O}(n)$



Lower bounds

Consider a 2-qubit system with two Hamiltonians:

$$H_0 = -Z \otimes I - \frac{1}{2} I \otimes Z - \frac{1}{2} Z \otimes Z = \begin{bmatrix} -2 & & & \\ & 0 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$$

$$H_1 = -Z \otimes I - \left(\frac{1}{2} - \epsilon\right) I \otimes Z - \left(\frac{1}{2} + \epsilon\right) Z \otimes Z = \begin{bmatrix} -2 & & & \\ & 0 & & \\ & & 1 + 2\epsilon & \\ & & & 1 - 2\epsilon \end{bmatrix}$$

The corresponding Gibbs states (Gibbs distribution) are:

$$\rho_0 = \frac{1}{Z_0} \mathrm{diag}\left(e^{2\beta}, 1, e^{-\beta}, e^{-\beta}\right), \qquad \rho_1 = \frac{1}{Z_1} \mathrm{diag}\left(e^{2\beta}, 1, e^{-\beta+2\beta\epsilon}, e^{-\beta-2\beta\epsilon}\right)$$

An algorithm that can learn the Hamiltonian with ℓ_∞-error ϵ should be able to distinguish ρ_0 and ρ_1

Classical hypothesis testing

Lower bounds

$$\rho_0 = \frac{1}{Z_0}\mathrm{diag}\left(e^{2\beta}, 1, e^{-\beta}, e^{-\beta}\right), \qquad \rho_1 = \frac{1}{Z_1}\mathrm{diag}\left(e^{2\beta}, 1, e^{-\beta+2\beta\epsilon}, e^{-\beta-2\beta\epsilon}\right)$$

- The KL divergence $D_{\mathrm{KL}}\left(\rho_0 \| \rho_1\right) = \mathcal{O}\left(\beta^2\epsilon^2 e^{-2\beta}\right)$ by direct calculation
- Therefore, the sample complexity of 2-qubit Hamiltonian learning is $\Omega\left(e^{2\beta}/(\beta^2\epsilon^2)\right)$

- **Haah-Kothari-Tang '23:** for n-qubit Hamiltonian learning, achieving ℓ_∞-error ϵ with success probability $1-\delta$ requires

$$\Omega\left(\frac{e^{2\beta}}{\beta^2\epsilon^2}\log\left(\frac{n}{\delta}\right)\right)$$

copies of the Gibbs state ρ_β in the worst case

Upper bounds

Step 1: Choose a set of observables $\{O_a\}_a$

Step 2: Measure the expectation value $\{\mathrm{tr}[\rho_\beta O_a]\}_a$

Step 3: Classical parameter learning from the data

	Sample Complexity	Time Complexity	Qubits entangled
Theorem I.2 (Lattices)	$\mathcal{O}\left(\log n \cdot \frac{e^{\mathrm{Poly}(\beta)}}{\beta^2\epsilon^2}\mathrm{Poly}(\log\frac{1}{\epsilon})\right)$	$\mathcal{O}\left(n\log n \cdot \frac{e^{\mathrm{Poly}(\beta)}}{\beta^2\epsilon^2}\mathrm{Poly}(\log\frac{1}{\epsilon})\right)$	$\mathrm{Poly}(\beta, \log\frac{1}{\epsilon})$
Theorem I.1 (Graphs)	$\mathcal{O}\left(\log n \cdot 2^{2^{\mathcal{O}(\beta^4)}\mathrm{Poly}(1/\beta\epsilon)}\right)$	$\mathcal{O}\left(n\log n \cdot 2^{2^{\mathcal{O}(\beta^4)}\mathrm{Poly}(1/\beta\epsilon)}\right)$	$\mathrm{Poly}(\beta, \log\frac{1}{\epsilon})$
[BLMT24, Nar24] (Graphs)	$\mathrm{Poly}\left(n, \frac{1}{\epsilon^{\mathcal{O}(\beta^2)}}\right)$	$\mathrm{Poly}\left(n, \frac{1}{\epsilon^{\mathcal{O}(\beta^2)}}\right)$	$\mathcal{O}(\beta^2\log\frac{1}{\epsilon})$
[HKT22] (High temp, Graphs)	$\mathcal{O}\left(\log(n)\frac{1}{\beta^2\epsilon^2}\right)$	$\mathcal{O}\left(n\log(n)\frac{1}{\beta^2\epsilon^2}\right)$	$\mathcal{O}(\log\frac{1}{\epsilon})$
[AAKS20] (Lattices)	$\mathrm{Poly}(n)\frac{e^{\mathrm{Poly}(\beta)}}{\mathrm{Poly}(\beta)\epsilon^2}$	$2^{\mathcal{O}(n)} \cdot \frac{e^{\mathrm{Poly}(\beta)}}{\mathrm{Poly}(\beta)\epsilon^2}$	$\mathcal{O}(1)$

Table 1 in (Chen-Anshu-Nguyen ’25)

KMS condition

For $\rho_\beta \propto e^{-\beta H}$ and $A_H(t) \coloneqq e^{\mathbf{i}Ht} A e^{-\mathbf{i}Ht}$, it holds that

$$\mathrm{tr}\left[O A_H(t) \rho_\beta\right] = \mathrm{tr}\left[A_H(t + \mathbf{i}\beta) O \rho_\beta\right] \quad \forall\, O, A, \text{and } t \in \mathbb{R}$$

Corollary:

$$\mathrm{tr}\left[\rho_\beta\left(O A_{H'}(t + \mathbf{i}\beta/2) - A_{H'}(t - \mathbf{i}\beta/2) O\right)\right] = 0 \quad \forall\, O, A, \text{and } t \in \mathbb{R}$$

if and only if $H' = H + cI$

- Robustness: if the above expectation value is ≈ 0, does it imply that $H' \approx H$?
- Locality: can O and A be restricted to local observables?

Proof of the KMS condition

$$\mathrm{tr}\left[O A_H(t)\rho_\beta\right] = \mathrm{tr}\left[A_H(t+\mathbf{i}\beta)O\rho_\beta\right] = \mathrm{tr}\left[O\rho_\beta A_H(t+\mathbf{i}\beta)\right] \quad \forall O$$

is equivalent to

$$A_H(t)\rho_\beta = \rho_\beta A_H(t+\mathbf{i}\beta) \quad \Leftrightarrow \quad A_H(t) = \rho_\beta A_H(t+\mathbf{i}\beta)\rho_\beta^{-1} = A_H(t)$$

For the Corollary,

$$\mathrm{tr}\left[\rho_\beta\left(O A_{H'}(t+\mathbf{i}\beta/2) - A_{H'}(t-\mathbf{i}\beta/2)O\right)\right] = 0 \quad \forall O$$

is equivalent to

$$(\rho'_\beta)^{1/2} A_{H'}(t)(\rho'_\beta)^{-1/2}\rho_\beta = \rho_\beta(\rho'_\beta)^{-1/2}A_{H'}(t)(\rho'_\beta)^{1/2}$$

$$A_{H'}(t)(\rho'_\beta)^{-1/2}\rho_\beta(\rho'_\beta)^{-1/2} = (\rho'_\beta)^{-1/2}\rho_\beta(\rho'_\beta)^{-1/2}A_{H'}(t) \quad \forall A, t$$

$$(\rho'_\beta)^{-1/2}\rho_\beta(\rho'_\beta)^{-1/2} \propto I \quad \Leftrightarrow \quad H = H' + cI$$

Identifiability equation

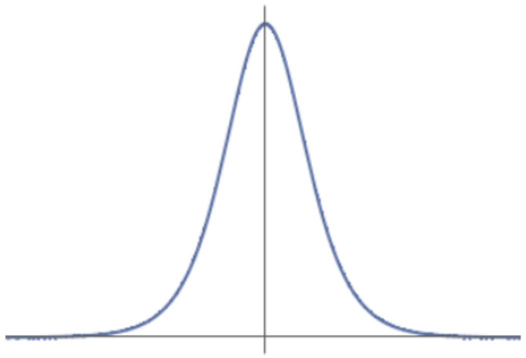
For any observables O and A, KMS inner product: $\langle X, Y\rangle_{\frac{1}{2}} = \mathrm{tr}\left[X^\dagger \sqrt{\rho_\beta} Y \sqrt{\rho_\beta}\right]$

$$\frac{\beta}{2}\langle O, [A, H - H']\rangle_{\frac{1}{2}} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{tr}\left[\rho_\beta\left(O_H^\dagger(t) A_{H'}(t + \mathbf{i}\beta/2) - A_{H'}(t - \mathbf{i}\beta/2) O_H^\dagger(t)\right)\right] g_\beta(t)\mathrm{d}t$$

where $g_\beta(t) = \frac{2}{\beta} g(2t/\beta)$ and

$$g(t) = -\frac{\pi^{3/2}}{2\sqrt{2}(1 + \cosh(\pi t))}$$

Rapidly decaying



Identifiability equation

$$\frac{\beta}{2}\langle O,[A,H-H']\rangle_{\frac{1}{2}} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{tr}\left[\rho_\beta\left(O_H^\dagger(t)A_{H'}(t+\mathbf{i}\beta/2) - A_{H'}(t-\mathbf{i}\beta/2)O_H^\dagger(t)\right)\right]g_\beta(t)\mathrm{d}t$$

- Suppose we take $A \in \{X_i, Y_i, Z_i\}_{i\in[n]}$ a degree-1 Pauli and $O = [A, H - H']$
- Then $\mathrm{LHS} = \|[A,H-H']\|_{\frac{1}{2}} = 0$ only if $[A,H-H'] = 0$

Claim 1: If $\|[A,H-H']\|_{\frac{1}{2}} \approx 0$, by the locality of A and $H-H'$, the Frobenius norm can be bounded by the KMS norm:

$$\|[A,H-H']\|_F \leq f(d,\beta)\cdot\|[A,H-H']\|_{\frac{1}{2}} \approx 0$$

Claim 2: If $\frac{1}{2^n}\|[A,H-H']\|_F^2 \leq \epsilon^2$ for all $A \in \{X_i, Y_i, Z_i\}$, then $\left|h_\gamma - h'_\gamma\right| \leq \epsilon$ for every term P_γ acting on the i-th qubit

Proof of Claim 2

- Using the cyclic property of trace, we have the following identity:

$$\|[A, H - H']\|_F^2 = \mathrm{tr}\left[[A, [A, H - H']](H - H')\right]$$

- Consider a term $(h_\gamma - h'_\gamma)P_\gamma$ in $H - H'$, where P_γ acts on the i-th qubit
- Since $\left[\sigma_i, [\sigma_i, \sigma_j]\right] = 4\sigma_j$, for any $A \in \{X_i, Y_i, Z_i\}$, either $\left[A, [A, P_\gamma]\right] = 0$ or $4P_\gamma$
- Thus, $\sum_{A \in \{X_i, Y_i, Z_i\}} \left[A, [A, P_\gamma]\right] = 8P_\gamma$
- Therefore,

$$3\epsilon^2 \geq \sum_{A \in \{X_i, Y_i, Z_i\}} \|[A, H - H']\|_F^2 \geq 8 \sum_{\gamma \sim i} \mathrm{tr}\left[(h_\gamma - h'_\gamma)P_\gamma(H - H')\right] = 8 \sum_{\gamma \sim i} (h_\gamma - h'_\gamma)^2$$

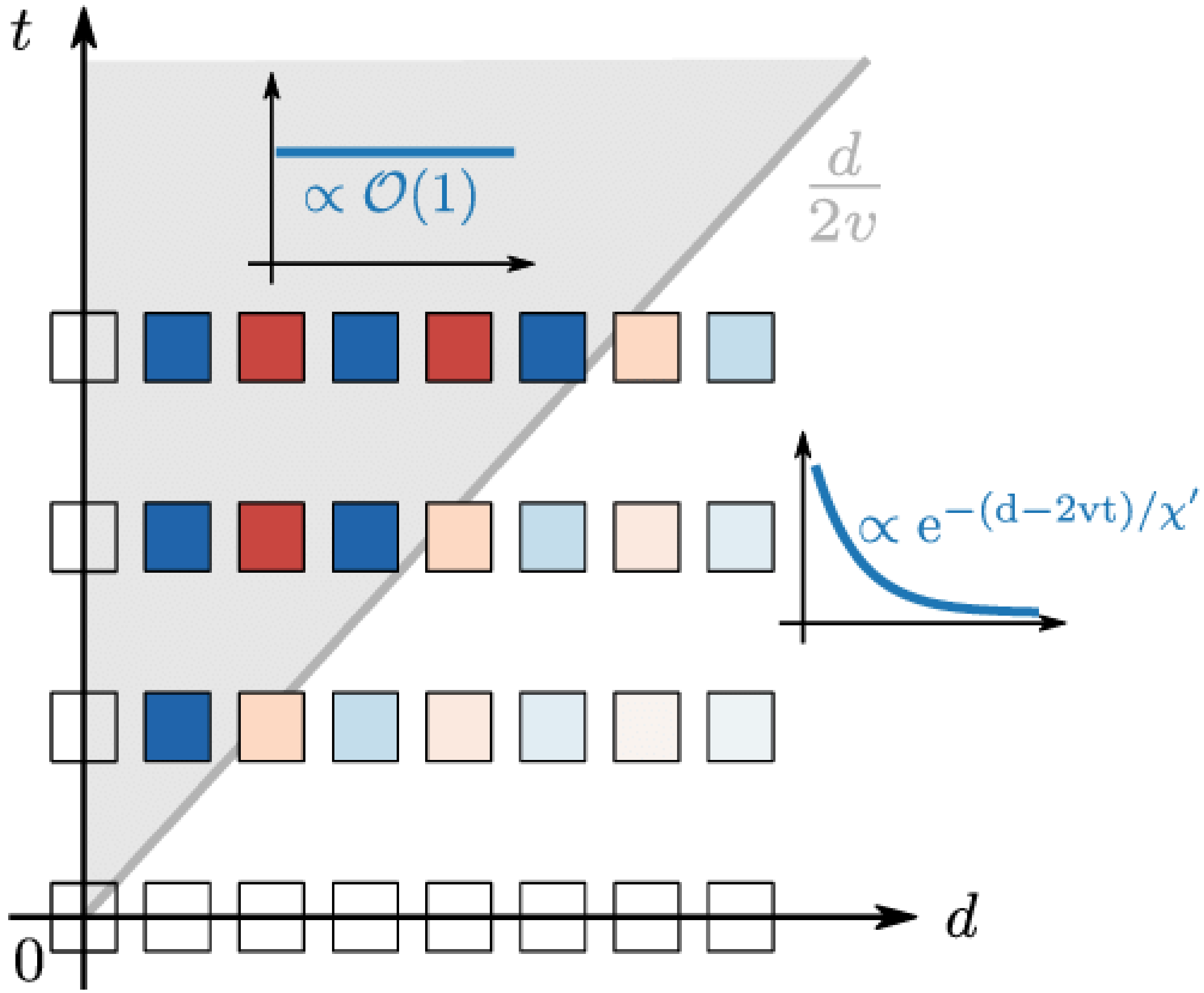
$\blacksquare$

Identifiability equation

$$\frac{\beta}{2}\langle O,[A,H-H']\rangle_{\frac{1}{2}} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{tr}\left[\rho_\beta\left(O_H^\dagger(t)A_{H'}(t+\mathbf{i}\beta/2) - A_{H'}(t-\mathbf{i}\beta/2)O_H^\dagger(t)\right)\right]g_\beta(t)\mathrm{d}t$$

- Since g_β is a rapid decaying function, RHS can be approximated by local measurements
  - Lightcone argument / Lieb-Robinson bound: a local observable evolved by a local Hamiltonian for a short period of time is still a (quasi-)local observable

Lieb-Robinson bound



(Lienhard et al. '18)

Identifiability equation

$$\frac{\beta}{2}\langle O,[A,H-H']\rangle_{\frac{1}{2}} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{tr}\left[\rho_\beta\left(O_H^\dagger(t)A_{H'}(t+\mathbf{i}\beta/2) - A_{H'}(t-\mathbf{i}\beta/2)O_H^\dagger(t)\right)\right] g_\beta(t)\mathrm{d}t$$

- Since g_β is a rapid decaying function, RHS can be approximated by local measurements
    - Lightcone argument / Lieb-Robinson bound: a local observable evolved by a local Hamiltonian for a short period of time is still a (quasi-)local observable

Issues:

1. The imaginary-time evolution $A_{H'}(t+\mathbf{i}\beta/2) = {\rho'_\beta}^{1/2} A_{H'}(t) {\rho'_\beta}^{-1/2}$ is well-known to be a nasty operator
2. The operator $O_H^\dagger(t)$ in RHS depends on the unknown Hamiltonian H

Proof of the identification equation

Recall that in the canonical form of the GNS-DB lindbladian, we decompose an operator w.r.t. the Bohr frequency:

$$A = \sum_{i,j} P_i A P_j = \sum_{\nu \in B_H} A_\nu$$

We will use a double decomposition:

$$A = \sum_{\nu_2 \in B_{H_2}} \sum_{\nu_1 \in B_{H_1}} \left(A_{\nu_1}\right)_{\nu_2}$$

Identities:

- $[A, H_2 - H_1] = \sum_{\nu_1,\nu_2} \left(A_{\nu_1}\right)_{\nu_2} (\nu_1 - \nu_2)$
- $e^{H_2} e^{-H_1} A e^{H_1} e^{-H_2} - e^{-H_2} e^{H_1} A e^{-H_1} e^{H_2} = \sum_{\nu_1,\nu_2} \left(A_{\nu_1}\right)_{\nu_2} \cdot 2\sinh(\nu_2 - \nu_1)$

Proof of the identities

$$[A, H] = AH - HA = \sum_{\nu \in B_H} \sum_{i,j:\lambda_i - \lambda_j = \nu} P_i A P_j H - H P_i A P_j = \sum_{\nu \in B_H} \sum_{i,j:\lambda_i - \lambda_j = \nu} (-\nu) P_i A P_j = \sum_{\nu \in B_H} -\nu A_\nu$$

- For the first identity,

$$[A, H_2 - H_1] = \sum_{\nu_1 \in B_{H_1}} \nu_1 A_{\nu_1} - \sum_{\nu_2 \in B_{H_2}} \nu_2 A_{\nu_2} = \sum_{\nu_1, \nu_2} \left(A_{\nu_1}\right)_{\nu_2} (\nu_1 - \nu_2)$$

$$e^H A e^{-H} = \sum_{\nu \in B_H} \sum_{i,j:\lambda_i - \lambda_j = \nu} e^H P_i A P_j e^{-H} = \sum_{\nu \in B_H} \sum_{i,j:\lambda_i - \lambda_j = \nu} e^\nu P_i A P_j = \sum_{\nu \in B_H} e^\nu A_\nu$$

- For the second identity,

$$e^{H_2} e^{-H_1} A e^{H_1} e^{-H_2} - e^{-H_2} e^{H_1} A e^{-H_1} e^{H_2} = \sum_{\nu_1, \nu_2} \left(A_{\nu_1}\right)_{\nu_2} \cdot \underbrace{\left(e^{\nu_2 - \nu_1} - e^{\nu_1 - \nu_2}\right)}_{2 \sinh(\nu_2 - \nu_1)}$$

■

Commutator difference in time domain

$$[A, H_2 - H_1] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[e^{H_2} e^{-H_1} A_{H_1}(t) e^{H_1} e^{-H_2} - e^{-H_2} e^{H_1} A_{H_1}(t) e^{-H_1} e^{H_2} \right]_{H_2}(-t) \cdot g(t) \mathrm{d}t$$

where $\hat{g}(\omega) \coloneqq -\frac{\omega}{2\sinh(\omega)}$ and

$$g(t) \coloneqq \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{g}(\omega) e^{-\mathbf{i}\omega t} \mathrm{d}\omega = -\frac{\pi^{3/2}}{2\sqrt{2}(1 + \cosh(\pi t))}$$

Proof.

- By the second identity,

$$\begin{aligned} e^{H_2} e^{-H_1} A_{H_1}(t) e^{H_1} e^{-H_2} - e^{-H_2} e^{H_1} A_{H_1}(t) e^{-H_1} e^{H_2} &= \sum_{\nu_1, \nu_2} \left(A_{H_1}(t)_{\nu_1} \right)_{\nu_2} \cdot 2\sinh(\nu_2 - \nu_1) \\ &= \sum_{\nu_1, \nu_2} \left(A_{H_1}(t)_{\nu_1} \right)_{\nu_2} \cdot e^{\mathbf{i}\nu_1 t} \cdot 2\sinh(\nu_2 - \nu_1) \end{aligned}$$

Commutator difference in time domain

$$[A, H_2 - H_1] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[e^{H_2} e^{-H_1} A_{H_1}(t) e^{H_1} e^{-H_2} - e^{-H_2} e^{H_1} A_{H_1}(t) e^{-H_1} e^{H_2}\right]_{H_2}(-t) \cdot g(t) \mathrm{d}t$$

where $\hat{g}(\omega) \coloneqq -\frac{\omega}{2\sinh(\omega)}$ and

$$g(t) \coloneqq \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{g}(\omega) e^{\mathbf{i}\omega t} \mathrm{d}\omega = -\frac{\pi^{3/2}}{2\sqrt{2}(1 + \cosh(\pi t))}$$

Proof.

- By the first identity,

$$[A, H_2 - H_1] = \sum_{\nu_1, \nu_2} \left(A_{\nu_1}\right)_{\nu_2} (\nu_1 - \nu_2) = \sum_{\nu_1, \nu_2} \left(A_{\nu_1}\right)_{\nu_2} \hat{g}(\nu_2 - \nu_1) \cdot 2\sinh(\nu_2 - \nu_1)$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \sum_{\nu_1, \nu_2} \left(A_{\nu_1}\right)_{\nu_2} \cdot 2\sinh(\nu_2 - \nu_1) \cdot e^{-\mathbf{i}(\nu_2 - \nu_1)t} g(t) \mathrm{d}t$$

$\blacksquare$

Proof of the identification equation

$$\frac{\beta}{2}\langle O,[A,H-H']\rangle_{\frac{1}{2}}=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{tr}\left[\rho_\beta\left(O_H^\dagger(t)A_{H'}(t+\mathbf{i}\beta/2)-A_{H'}(t-\mathbf{i}\beta/2)O_H^\dagger(t)\right)\right]g_\beta(t)\mathrm{d}t$$

- We apply the previous identity with $H_1 \coloneqq \frac{\beta}{2}H',\ H_2 \coloneqq \frac{\beta}{2}H,\ \rho \coloneqq \rho_\beta \propto e^{-\beta H},\ \rho' \coloneqq \rho'_\beta \propto e^{-\beta H'}$:

$$\begin{aligned}[A,H_2-H_1]&=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left[e^{H_2}e^{-H_1}A_{H_1}(t)e^{H_1}e^{-H_2}-e^{-H_2}e^{H_1}A_{H_1}(t)e^{-H_1}e^{H_2}\right]_{H_2}(-t)\cdot g(t)\mathrm{d}t\\&=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left[\sqrt{\rho^{-1}}\sqrt{\rho'}A_{H_1}(t)\sqrt{(\rho')^{-1}}\sqrt{\rho}-\sqrt{\rho}\sqrt{(\rho')^{-1}}A_{H_1}(t)\sqrt{\rho'}\sqrt{\rho^{-1}}\right]_{H_2}(-t)\cdot g(t)\mathrm{d}t\end{aligned}$$

- Taking the KMS inner product with O, we have

$$\langle O,[A,H-H']\rangle_{\frac{1}{2}}=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\begin{pmatrix}\left\langle O,\left[\sqrt{\rho^{-1}}\sqrt{\rho'}A_{H_1}(t)\sqrt{(\rho')^{-1}}\sqrt{\rho}\right]_{H_2}(-t)\right\rangle_{\frac{1}{2}}\\-\left\langle O,\left[\sqrt{\rho}\sqrt{(\rho')^{-1}}A_{H_1}(t)\sqrt{\rho'}\sqrt{\rho^{-1}}\right]_{H_2}(-t)\right\rangle_{\frac{1}{2}}\end{pmatrix}\cdot g(t)\mathrm{d}t$$

Proof of the identification equation

For the first term in the integral,

$$\left\langle O, \left[\sqrt{\rho^{-1}}\sqrt{\rho'}A_{H_1}(t)\sqrt{(\rho')^{-1}}\,\sqrt{\rho}\right]_{\beta H/2}(-t)\right\rangle_{\frac{1}{2}}$$

$$= \mathrm{tr}\left[\sqrt{\rho}O^{\dagger}\sqrt{\rho}\left[\sqrt{\rho^{-1}}\sqrt{\rho'}A_{H_1}(t)\sqrt{(\rho')^{-1}}\,\sqrt{\rho}\right]_{\beta H/2}(-t)\right]$$

$$= \mathrm{tr}\left[O^{\dagger}\left[\sqrt{\rho'}A_{H_1}(t)\sqrt{(\rho')^{-1}}\,\rho\right]_{\beta H/2}(-t)\right]$$

$$= \mathrm{tr}\left[O^{\dagger}_{\beta H/2}(t)\sqrt{\rho'}A_{\beta H'/2}(t)\sqrt{(\rho')^{-1}}\,\rho\right]$$

$$= \mathrm{tr}\left[O^{\dagger}_{H}\left(\frac{\beta}{2}t\right)\sqrt{\rho'}A_{H'}\left(\frac{\beta}{2}t\right)\sqrt{(\rho')^{-1}}\,\rho\right]$$

$$= \mathrm{tr}\left[O^{\dagger}_{H}\left(\frac{\beta}{2}t\right)A_{H'}\left(\frac{\beta}{2}t+\mathbf{i}\frac{\beta}{2}\right)\rho\right]$$

Proof of the identification equation

For the second term in the integral,

$$
\begin{aligned}
&\left\langle O, \left[\sqrt{\rho}\sqrt{(\rho')^{-1}}A_{H_1}(t)\sqrt{\rho'}\sqrt{\rho^{-1}}\right]_{\beta H/2}(-t)\right\rangle_{\frac{1}{2}} \\
&= \mathrm{tr}\left[\sqrt{\rho}O^\dagger\sqrt{\rho}\left[\sqrt{\rho}\sqrt{(\rho')^{-1}}A_{H_1}(t)\sqrt{\rho'}\sqrt{\rho^{-1}}\right]_{\beta H/2}(-t)\right] \\
&= \mathrm{tr}\left[O^\dagger\left[\rho\sqrt{(\rho')^{-1}}A_{H_1}(t)\sqrt{\rho'}\right]_{\beta H/2}(-t)\right] \\
&= \mathrm{tr}\left[O^\dagger_{\beta H/2}(t)\,\rho\sqrt{(\rho')^{-1}}A_{H_1}(t)\sqrt{\rho'}\right] \\
&= \mathrm{tr}\left[O^\dagger_H\left(\frac{\beta}{2}t\right)\rho A_{H'}\left(\frac{\beta}{2}t - \mathbf{i}\frac{\beta}{2}\right)\right]
\end{aligned}
$$

Proof of the identification equation

Therefore, we have

$$\langle O,[A,H-H']\rangle_{\frac{1}{2}} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{tr}\left[O_H^\dagger\left(\frac{\beta}{2}t\right)A_{H'}\left(\frac{\beta}{2}t+\mathbf{i}\frac{\beta}{2}\right)\rho - O_H^\dagger\left(\frac{\beta}{2}t\right)\rho A_{H'}\left(\frac{\beta}{2}t-\mathbf{i}\frac{\beta}{2}\right)\right]\cdot g(t)\mathrm{d}t$$
$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{tr}\left[\rho\left(O_H^\dagger\left(\frac{\beta}{2}t\right)A_{H'}\left(\frac{\beta}{2}t+\mathbf{i}\frac{\beta}{2}\right) - A_{H'}\left(\frac{\beta}{2}t-\mathbf{i}\frac{\beta}{2}\right)O_H^\dagger\left(\frac{\beta}{2}t\right)\right)\right]\cdot g(t)\mathrm{d}t$$

By changing the variable $t \mapsto \frac{\beta}{2}t$, we obtain the identification equation:

$$\langle O,[A,H-H']\rangle_{\frac{1}{2}} = \frac{2}{\beta}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{tr}\left[\rho\left(O_H^\dagger(t)A_{H'}(t+\mathbf{i}\beta/2) - A_{H'}(t-\mathbf{i}\beta/2)O_H^\dagger(t)\right)\right]\cdot g_\beta(t)\mathrm{d}t$$

$\blacksquare$

Two remaining issues of using the identification equation

1. The imaginary-time evolution $A_{H'}(t+\mathbf{i}\beta/2) = {\rho'_\beta}^{1/2} A_{H'}(t) {\rho'_\beta}^{-1/2}$ is well-known to be a nasty operator

   → Regularization via operator Fourier transform

2. The operator $O_H^\dagger(t)$ in RHS depends on the unknown Hamiltonian H

Operator Fourier transform

Given a Hamiltonian H and an operator A, define the operator Fourier transform $\hat{A}_H$ by:

$$\hat{A}_H[\omega] := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A_H(t) \cdot e^{-\mathbf{i}\omega t} f(t) \mathrm{d}t$$

where $f(t) \propto e^{-\sigma^2 t^2}$ is a Gaussian filter and $\hat{f}(\omega) \propto e^{-\omega^2/4\sigma^2}$ is another Gaussian

Properties:

- $e^{\beta H} \hat{A}_H[\omega] e^{-\beta H} = \left(\widehat{e^{\beta H} A e^{-\beta H}}\right)_H[\omega]$
- $\hat{A}_H[\omega] = \sum_{\nu \in B_H} A_\nu \cdot \hat{f}(\omega - \nu)$
- $A = C_\sigma \cdot \int_{-\infty}^{\infty} A_H[\omega] \mathrm{d}\omega$
- $\hat{A}_H[\omega] = e^{-\beta\omega + \sigma^2\beta^2} \cdot e^{\beta H} \hat{A}_H[\omega - 2\sigma^2\beta] e^{-\beta H}$

"soft" Bohr decomposition

Operator Fourier transform

$$\hat{A}_H[\omega] = e^{-\beta\omega+\sigma^2\beta^2} \cdot e^{\beta H}\hat{A}_H[\omega - 2\sigma^2\beta]e^{-\beta H}$$

- $\hat{A}_H[\omega]$ has a uniformly bounded norm:

$$\left\|\hat{A}_H[\omega]\right\| \leq \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\|A\| \cdot |f(t)|\mathrm{d}t \leq \|A\|$$

- For any ω', it holds that

$$\left\|e^{\beta H}\hat{A}_H(\omega')e^{-\beta H}\right\| \leq e^{\beta\omega'+\sigma^2\beta^2}\|A\|$$

  which is independent of the system size for any bounded operator A

- Without OFT, $\left\|e^{\beta H}Ae^{-\beta H}\right\|$ can be $\exp\big(\mathcal{O}(n)\big)$ in the worst case

OFT has a “regularization” effect

Decomposing the identification equation into high- and low-frequency parts

$$\frac{\beta}{2}\langle O,[A,H-H']\rangle_{\frac{1}{2}} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{tr}\left[\rho\left(O_H^\dagger(t)A_{H'}(t+\mathbf{i}\beta/2)\ -A_{H'}(t-\mathbf{i}\beta/2)O_H^\dagger(t)\right)\right]g_\beta(t)\mathrm{d}t$$

$$\simeq \int_{|\omega'|\le\Omega'}\int_{-\infty}^{\infty}\mathrm{tr}\left[\rho\left(O_H^\dagger(t)\left(\hat{A}_{H'}[\omega']\right)_{H'}(t+\mathbf{i}\beta/2)\ -\left(\hat{A}_{H'}[\omega']\right)_{H'}(t-\mathbf{i}\beta/2)O_H^\dagger(t)\right)\right]g_\beta(t)\mathrm{d}t\,\mathrm{d}\omega'$$

$$+\int_{|\omega'|>\Omega'}\frac{\beta}{2}\left\langle O,\left[\hat{A}_{H'}(\omega'),H-H'\right]\right\rangle_{\frac{1}{2}}d\omega'$$

We have:

$$\int_{|\omega'|\le\Omega'}\left(\hat{A}_{H'}[\omega']\right)_{H'}(t+\mathbf{i}\beta/2)\mathrm{d}\omega' = \int_{|\omega'|\le\Omega'}\left(e^{-\beta H'/2}\hat{A}[\omega']e^{\beta H'/2}\right)_{H'}(t)\mathrm{d}\omega'$$

$$= \int_{|\omega'|\le\Omega'}\left(\hat{A}_{H'}[\omega'-\sigma^2\beta]\right)_{H'}(t)\cdot e^{-\beta\omega'/2+\sigma^2\beta^2/4}\mathrm{d}\omega'$$

$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}A_{H'}(t+t')\underbrace{\left(\int_{|\omega'|\le\Omega'}e^{-\mathbf{i}(\omega'-\sigma^2\beta)t'}e^{-\beta\omega'/2+\sigma^2\beta^2/4}\mathrm{d}\omega'\right)f(t')}_{h_+(t')}\mathrm{d}t'$$

Decomposing the identification equation into high- and low-frequency parts

$$\frac{\beta}{2}\langle O,[A,H-H']\rangle_{\frac{1}{2}} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{tr}\left[\rho\left(O_H^\dagger(t)A_{H'}(t+\mathbf{i}\beta/2)\ -A_{H'}(t-\mathbf{i}\beta/2)O_H^\dagger(t)\right)\right]g_\beta(t)\mathrm{d}t$$

$$\simeq \int_{|\omega'|\le\Omega'}\int_{-\infty}^{\infty}\mathrm{tr}\left[\rho\left(O_H^\dagger(t)\left(\hat{A}_{H'}[\omega']\right)_{H'}(t+\mathbf{i}\beta/2)\ -\left(\hat{A}_{H'}[\omega']\right)_{H'}(t-\mathbf{i}\beta/2)O_H^\dagger(t)\right)\right]g_\beta(t)\mathrm{d}t\,\mathrm{d}\omega'$$

$$+\int_{|\omega'|>\Omega'}\frac{\beta}{2}\langle O,\left[\hat{A}_{H'}(\omega'),H-H'\right]\rangle_{\frac{1}{2}}d\omega'$$

Similarly, we have:

$$\int_{|\omega'|\le\Omega'}\left(\hat{A}_{H'}[\omega']\right)_{H'}(t-\mathbf{i}\beta/2)\mathrm{d}\omega'$$

$$=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}A_{H'}(t+t')\underbrace{\left(\int_{|\omega'|\le\Omega'}e^{-\mathbf{i}(\omega'+\sigma^2\beta)t'}e^{\beta\omega'/2+\sigma^2\beta^2/4}\mathrm{d}\omega'\right)f(t')\mathrm{d}t'}_{h_-(t')}$$

Decomposing the identification equation into high- and low-frequency parts

$$
\begin{aligned}
&\frac{\beta}{2}\langle O,[A,H-H']\rangle_{\frac{1}{2}} \\
&\simeq \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{tr}\left[\rho\left(h_{+}(t')O_H^{\dagger}(t)A_{H'}(t+t')-h_{-}(t')A_{H'}(t+t')O_H^{\dagger}(t')\right)\right]g_\beta(t)\mathrm{d}t\,\mathrm{d}t' \\
&+\int_{|\omega'|>\Omega'}\frac{\beta}{2}\langle O,[\hat{A}_{H'}(\omega'),H-H']\rangle_{\frac{1}{2}}d\omega'
\end{aligned}
$$

- $|h_{+}(t)|,|h_{-}(t)|=\mathcal{O}\left(e^{-\sigma^2t^2}\right)$, i.e. rapidly decaying
- No imaginary time evolution in the observable
- The high-frequency term is negligible when we take a sufficiently large threshold Ω'

Two remaining issues of using the identification equation

1. The imaginary-time evolution $A_{H'}(t+\mathbf{i}\beta/2) = {\rho'_\beta}^{1/2} A_{H'}(t) {\rho'_\beta}^{-1/2}$ is well-known to be a nasty operator

   → Regularization via operator Fourier transform

2. The operator $O_H^\dagger(t)$ in RHS depends on the unknown Hamiltonian H

   → $\|[A, H-H']\|_{\frac{1}{2}}^2 = \langle [A, H-H'], [A, H-H'] \rangle_{\frac{1}{2}} \leq 2d \cdot \sup_\gamma \left| \langle [A, P_\gamma], [A, H-H'] \rangle_{\frac{1}{2}} \right|$

Hamiltonian learning via the identification equation

Define the general truncated observables:

$$\Delta[\![G, H'; O, A]\!] \coloneqq \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(h_+(t') O_G^\dagger(t) A_{H'}(t+t') - h_-(t') A_{H'}(t+t') O_G^\dagger(t') \right) g_\beta(t) \mathrm{d}t \, \mathrm{d}t'$$

Claim 3. When $H' = H$,

$$\mathrm{tr}\left[\rho_\beta \Delta[\![G, H; O, A]\!]\right] = 0 \quad \forall G, O, A$$

Proof.

$$\begin{aligned} &\mathrm{tr}\left[\rho_\beta \Delta[\![G, H; O, A]\!]\right] \\ &\simeq \int_{-\infty}^{\infty} \int_{|\omega'| \le \Omega'} \underbrace{\mathrm{tr}\left[\rho_\beta \left(O_G^\dagger(t) \left(\hat{A}_H[\omega']\right)_H (t + \mathbf{i}\beta/2) - \left(\hat{A}_H[\omega']\right)_H (t - \mathbf{i}\beta/2) O_G^\dagger(t) \right)\right]}_{=\,0 \text{ by the KMS condition}} \mathrm{d}\omega' \, g_\beta(t) \mathrm{d}t \end{aligned}$$

Hamiltonian learning via the identification equation

Define the general truncated observables:

$$\Delta[\![G, H'; O, A]\!] := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(h_+(t') O_G^\dagger(t) A_{H'}(t+t') - h_-(t') A_{H'}(t+t') O_G^\dagger(t') \right) g_\beta(t) \mathrm{d}t \, \mathrm{d}t'$$

Naïve Algorithm

- $\mathcal{E} \leftarrow \epsilon$-net of the local Hamiltonians
- For each $H' \in \mathcal{E}$:
  - Measure the observables

$$\{\Delta[\![G, H'; [A, P_\gamma], A]\!] : \forall G \in \mathcal{E}, i \in [n], A \in \{X_i, Y_i, Z_i\}, \gamma \sim i\}$$

  - If the expectations values are all small, then output H'

Issue:

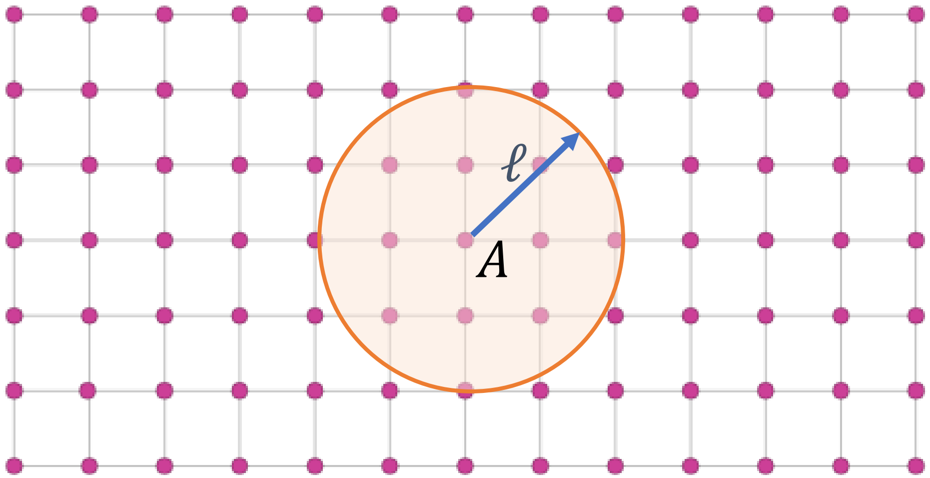
- $\mathcal{E}$ has $\exp(\mathcal{O}(m))$ elements, where m is the number of terms in H
- $m = \mathcal{O}(n)$ for a 2-local H on a 2d lattice

Hamiltonian learning via the identification equation

Define the general truncated observables:

$$\Delta[\![G, H'; O, A]\!] \coloneqq \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(h_+(t') O_G^\dagger(t) A_{H'}(t+t') - h_-(t') A_{H'}(t+t') O_G^\dagger(t') \right) g_\beta(t) \mathrm{d}t \, \mathrm{d}t'$$

- A and $O = [A, P_\gamma]$ are local operators
- Rapid decay of $h_+, h_-, g_\beta \Longrightarrow$ only short-time evolution involved
- Lieb-Robinson bound: G and H' can be truncated to within a neighborhood around i



$$\|A_{H_\ell}(t) - A_H(t)\| \le \mathcal{O}\left(\frac{(2dt)^\ell}{\ell!}\right)$$

Hamiltonian learning via the identification equation

Define the general truncated observables:

$$\Delta[\![G, H'; O, A]\!] := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(h_+(t') O_G^\dagger(t) A_{H'}(t+t') - h_-(t') A_{H'}(t+t') O_G^\dagger(t') \right) g_\beta(t) \mathrm{d}t \, \mathrm{d}t'$$

Efficient Algorithm

- For each $i \in [n]$:
  - $\mathcal{E}_i \leftarrow \epsilon$-net of the local Hamiltonians acting on a neighborhood of i
  - For each $H'_\ell \in \mathcal{E}_i$:
    - Measure the observables using $\mathcal{O}(\log n)$ copies of the Gibbs state ρ_β
    $$\left\{ \Delta[\![G_\ell, H'_\ell; [A, P_\gamma], A]\!] : \forall G_\ell \in \mathcal{E}_i, A \in \{X_i, Y_i, Z_i\}, \gamma \sim i \right\}$$
    - If the expectations values are all small, set the local patch of our estimate to be H'_ℓ