Quantum Gibbs Sampling through Randomized Method

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Quantum Gibbs sampling

- Quantum Gibbs sampling: Given a Hamiltonian H, prepare the thermal state $\sigma = e^{-\beta H}$.
- Designing quantum Gibbs samplers based on Lindblad equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho := \mathcal{L}\rho = \sum_{a\in\mathcal{A}} \underbrace{V_a \rho V_a^\dagger - \frac{1}{2}\{V_a^\dagger V_a, \rho\}}_{\mathcal{L}_a \rho}$$

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- We aim to design a Lindbladian $\mathcal{L}$ such that
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- The first two conditions have been perfectly addressed by [Che+23; CKG23; DLL24; Gil+24].
- The mixing time is much more challenging.
  - Commuting cases
  - Non-commuting local, high temperature [RFA24]

Motivation

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- In general, there are exponential many possible choices of global jump operators.
- The 2D-Toric code case: using symmetries of the system to design global jumps
- How to pick from the exponential many choices without sufficient prior information?
- Just randomly pick from them!

Roadmap

- Construction of a Lindblad dynamic: random unitary design.
- The algorithmic implementation: randomized method.
- The mixing time analysis and implications

The random coupling operators

We choose an ensemble of random coupling operators such that the two-point correlation vanishes:

$$\mathbb{E}\,\langle\psi_i|\,A\,|\psi_j\rangle\,\langle\psi_l|\,A\,|\psi_k\rangle^* = \Theta(1/N)\delta_{i,l}\delta_{j,k}.$$

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This ensemble can be constructed through $A = U_2 D U_2^\dagger$, where

- U_2 is sampled from a unitary 2-design, i.e.,

$$\mathbb{E}[U_2^{\otimes 2} O U_2^{\dagger\otimes 2}] = \mathbb{E}_{U\sim\mathrm{Haar}}[U^{\otimes 2} O U^{\dagger\otimes 2}]\,.$$

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- D is a diagonal random operator with random ± 1 entries without correlation, given by $D = \sigma_z^{p_1} \otimes \sigma_z^{p_2} \otimes \cdots \otimes \sigma_z^{p_n}$, where $p_1, \cdots, p_n$ are independent binary random variable.

The Davies Generator

We consider the Davies generator using the random Hermitian coupling operators:

$$\mathcal{L}_D(\rho) = \mathbb{E}_a \sum_{\omega \in B_H} \gamma(\omega) \left((A_a(\omega))^\dagger \rho A_a(\omega) - \frac{1}{2} \left\{ (A_a(\omega))^\dagger A_a(\omega), \rho \right\} \right),$$

- Let $(|\psi_i\rangle, \lambda_i)$ be the eigenstates and eigenvalues of the Hamiltonian.
- $\omega \in B_H := \text{spec}(H) - \text{spec}(H)$ are the Bohr frequencies
- The operators $A_a(\omega) = \sum_{\lambda_i - \lambda_j = \omega} |\psi_i\rangle \langle\psi_i| A_a |\psi_j\rangle \langle\psi_j|$ are the Fourier components of the Heisenberg evolution of A_a:

$$e^{iHt} A_a e^{-iHt} = \sum_\omega A_a(\omega) e^{i\omega t}.$$

- The weight function $\gamma(\omega) = \min(1, e^{-\beta\omega})$ is chosen to ensure the detailed balance condition.

The integral form reformulation

For the random coupling operator case, the Davies generator is equivalent to the integral form construction in [CKG23; DCL24; DLL24].

Theorem

The random Davies generator can be reformulated as

$$\mathcal{L}_D[\rho] := \mathbb{E}_a\left(K_a \rho K_a^\dagger - \frac{1}{2}\{K_a^\dagger K_a, \rho\}\right),$$

where K_a is expressed as the following integral form:

$$K_a := \int_{-\infty}^{\infty} f(s) e^{iHs} A_a e^{-iHs} \mathrm{d}s = \sum_{i,j\in[N]} \hat{f}(\lambda_i - \lambda_j) \left|\psi_i\right\rangle \left\langle\psi_i\right| A_a \left|\psi_j\right\rangle \left\langle\psi_j\right|.$$

with a weight function f defined such that

$$\hat{f}(\omega) = \sqrt{\gamma(\omega)} \quad \text{for any} \quad \omega \in B_H \subset [-\|H\|, \|H\|].$$

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The randomized method

Let $\{\mathcal{L}_a\}_{a\in\mathcal{A}}$ be an ensemble of Lindbladians. For $\bar{\mathcal{L}} = \mathbb{E}_{a\sim\mu}\mathcal{L}_a$, we simulate $\bar{\mathcal{L}}$ by the random product approximation

$$e^{T\bar{\mathcal{L}}} \approx e^{\tau\mathcal{L}_M} \cdots e^{\tau\mathcal{L}_1}, \tag{1}$$

- Each $\mathcal{L}_i$ is randomly sampled from μ.
- For fixed T, as $\tau \to 0$, the random product converges to the exact evolution $e^{T\bar{\mathcal{L}}}$.
- Motivated by qDRIFT method in Hamiltonian simulation [Cam19]

The Randomzied Method

- Now we discuss the simulation of $e^{\tau \mathcal{L}_a}$ at each time step.
- Each $\mathcal{L}_a(\rho) = V_a \rho V_a^\dagger - \frac{1}{2}\{\rho, V_a V_a^\dagger\}$ only includes a single jump operator, allowing a simple short-time implementation.

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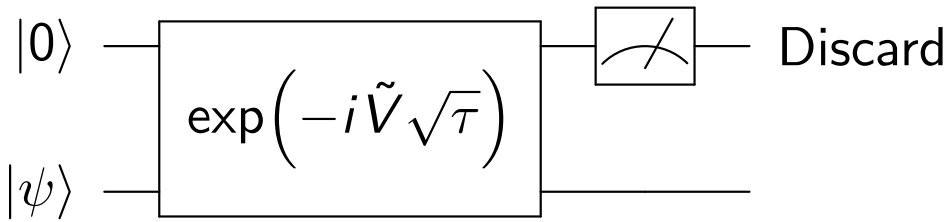
- Dilation-based method.
- Let $\widetilde{V}_a := \begin{pmatrix} 0 & V_a^\dagger \\ V_a & 0 \end{pmatrix}$ be the dilated Hamiltonian on the system coupled with an acilla.

$$e^{\tau \mathcal{L}_a} = \mathrm{Tr}_1[e^{-i\widetilde{V}_a\sqrt{t}}(|0\rangle\langle 0| \otimes \rho)e^{i\widetilde{V}_a\sqrt{t}}] + O(\tau^2)$$



Analysis of the randomized method

Question: How many steps are required for the simulation algorithm to achieve an ϵ error?

- Let $\mathcal{F}_\tau(\mathcal{L}_a) = e^{\tau \mathcal{L}_a} + O(\tau^2)$ be a one-step implementation of a single jump operator.
- The Average channel: $\bar{\mathcal{E}}_{\tau,M} := \left(\mathbb{E}_a \mathcal{F}_\tau(\mathcal{L}_a)\right)^M$.

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Theorem

Suppose $\|V_a\|^2 \leq \lambda$, *(or,* $\|\mathcal{L}_a\|_\diamond \leq \lambda$*), recall* $\bar{\mathcal{L}} = \mathcal{E}_{a\sim\mu}\mathcal{L}_a$, *we have*

$$\left\| \bar{\mathcal{E}}_{\tau,M} - e^{\tau \bar{\mathcal{L}}} \right\|_\diamond = O(\epsilon), \quad \text{if} \quad M \geq \lambda^2 t^2/\epsilon$$

- 1-order Trotter $O\left(|\mathcal{A}|\lambda^2 t^2/\epsilon\right)$.
- sub-optimal dependency on $t, 1/\epsilon$ [CW19; Che+23].
- Avoiding complex oracles of control-circuits.

The algorithmic implementation

- Recall that the integral form of our construction is given by

$$\mathcal{L}_D[\rho] := \mathbb{E}_a\left(K_a \rho K_a^\dagger - \frac{1}{2}\{K_a^\dagger K_a, \rho\}\right),$$

where K_a is expressed as the following integral form:

$$K_a := \int_{-\infty}^{\infty} f(s) e^{iHs} A_a e^{-iHs} \mathrm{d}s$$

- Using the randomized method, we reduce the problem to simulating a jump operator K_a sampled from the ensemble in each time step.
- Each $e^{\tau \mathcal{L}_{K_a}}$ can be implemented by dilation, similar to [DCL24].

The algorithmic implementation

- First, we approximate $e^{\tau \mathcal{L}_{K_a}}$ by the evolution of the dilated Hamiltonian $\tilde{K}_a = |0\rangle\langle 1| \otimes K_a^\dagger + |1\rangle\langle 0| K_a$.
- Next, we evaluate the integral by quadrature: $\tilde{K}_a \approx \sum f(s_l) e^{iHs_l} A_a e^{-iHs_l} \Delta_s := \sum \tilde{K}_l$.
- Applying Trotterization, we only need to implement $e^{-i\tau_l \tilde{K}_l}$
- Note $\tilde{K}_l = \sigma_l \otimes e^{is_l H} A e^{-is_l H}$ with $\sigma_l = w_l \left(\sigma_x \operatorname{Re} f(s_l) + \sigma_y \operatorname{Im} f(s_l)\right)$
- Recall $A = U_2 D U_2^\dagger$, we express the evolution of $\tilde{K}_l$ as

$$e^{-i\tau_l \tilde{H}_l} = (I \otimes e^{is_l H} U_2) e^{-i\tau_l (\sigma_l \otimes D)} (I \otimes U_2^\dagger e^{-is_l H}).$$

- $e^{-i\tau_l(\sigma_l \otimes D)}$ is just a Hamiltonian evolution of Pauli strings [WBA11].

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The mixing time analysis

Theorem

The evolution ρ_t satisfies

- *Let $p_i(t) = \mathbb{E} \langle \psi_i | \rho_t | \psi_i \rangle$ be the diagonal terms. We have*

$$\underbrace{\dot{p}_i = \Theta(1/N) \sum_{k \neq i} \left(\gamma(\lambda_k - \lambda_i) p_k - \gamma(\lambda_i - \lambda_k) p_i\right).}_{\text{Classical Metropolis–Hasting with uniform proposal on the diagonal entries}}$$

- *Let $Q_{ij}(t) = \mathbb{E} \langle \psi_j | \rho_t | \psi_i \rangle$ be the non-diagnonal terms. We have*

$$\underbrace{\dot{Q}_{ij} = -\Theta(1/N) \sum_{k} \frac{1}{2} \left(\gamma(\lambda_k - \lambda_i) + \gamma(\lambda_k - \lambda_j)\right) Q_{ij}.}_{\text{Exponential decaying coherence}}$$

The mixing time analysis

Theorem

Let $r_\beta(H)$ denote the ratio of the states within an energy window above the ground state:

$$r_\beta(H) = \frac{\#\left\{|\psi_i\rangle : \lambda_i \leq \lambda_{\min}(H) + 1/\beta\right\}}{N}.$$

The spectral gap of $\mathcal{L}_D$ is bounded below by $\eta \gtrsim r_\beta(H)$.

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Example

If the spectral density approximately follows the Wigner semi-circle law (with appropriate normalization), we have

$$r_\beta(H) \approx \int_{-2}^{-2+1/\beta} \frac{\sqrt{4-x^2}}{2\pi} \mathrm{d}x = \Omega(\beta^{-3/2}),$$

implying polynomial-time mixing as long β is not exponentially large.

The mixing time analysis

A provable example [Chi+23]:

Lemma

Consider the Hamiltonian given by random sparse Pauli strings:

$$H_{\mathrm{PS}} := \sum_{j=1}^{m} \frac{r_j}{\sqrt{m}} \sigma_j \quad \text{with } \sigma_j \overset{\text{iid}}{\sim} \{I, \sigma_x, \sigma_y, \sigma_z\}^{\otimes n}, r_j \overset{\text{iid}}{\sim} \mathrm{Unif}\{+1, -1\}.$$

If $m \geq Cn^5\beta^4$, *with high probability,* $r_\beta(H) = \Omega(\beta^{-3/2})$.

- Connection with quantum chaos: the level-spacing statistics of a chaotic Hamiltonian is predicted by random matrix theory.

Conclusion

- Preparing the thermal state is quantumly easy if the Hamiltonian satisfies
  - efficient simulability
  - a non-negligible low-energy density.
- Future work
  - Combine random global jump operators and local jump operators
  - Design random jump operators using unitary designs in subspaces.

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