CS 59300 – Algorithms for Data Science

Classical and Quantum approaches

Lecture 21 (11/25)

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

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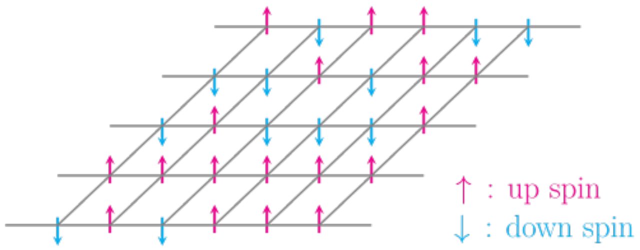
Classical Gibbs sampling: revisited

- Consider a classical spin system (e.g., the Ising model):

$$H_{\text{Ising}} = -\sum_{i \sim j} Z_i Z_j$$



- Eigenstates $\{0,1\}^n$ and eigenvalues $\{E_x\}_{x \in \{0,1\}^n}$
- The goal is to (approximately) sample from the Gibbs distribution:

$$\pi_\beta(x) = \frac{e^{-\beta E_x}}{Z_\beta}, \qquad Z_\beta = \sum_x e^{-\beta E_x}$$

The Metropolis-Hastings algorithm

Set of jump operators $\{A^a\}$ such that A^a is selected with probability $p(a)$

- Example: flip a randomly chosen spin

Let x be the current state

- Pick A^a with probability $p(a)$
- $y \leftarrow A^a$ applied to x
- Accept move with probability $\gamma_\beta(x, y) \coloneqq \min\left\{1, \exp\left(-\beta\left(E_y - E_x\right)\right)\right\}$
- If reject, stay at x

Fact. Under certain conditions, the Gibbs distribution π_β is the unique fixed point.

- Detailed balance (DBC): $e^{-\beta E_x}\gamma_\beta(x, y) = e^{-\beta E_y}\gamma_\beta(y, x)$

Quantum Gibbs sampling

- Let H be a quantum Hamiltonian with eigenstates $\{|\psi_j\rangle\}$ and eigenvalues $\{E_j\}$
- The goal is to (approximately) sample from the "quantum Gibbs distribution":

$$\pi_\beta(|\psi_j\rangle) = \frac{e^{-\beta E_j}}{Z_\beta}$$

- Mixed state:

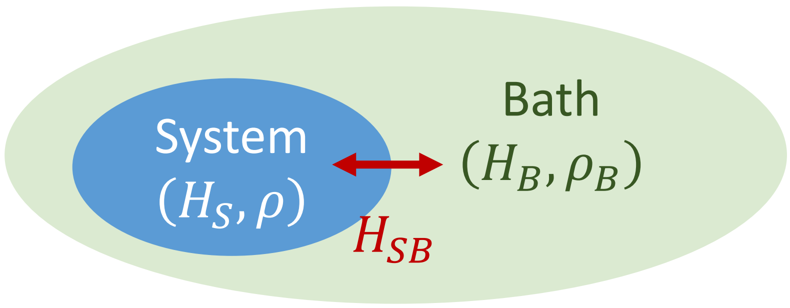
$$\rho_\beta = \sum \frac{e^{-\beta E_j}}{Z_\beta} |\psi_j\rangle\langle\psi_j| = \frac{\exp(-\beta H)}{\mathrm{tr}[\exp(-\beta H)]}$$

Gibbs state

Challenges:

1. Given $|\psi_j\rangle$ cannot calculate the energy E_j exactly
2. Rejection requires backing up after a quantum measurement

Open quantum system



System dimension: d $\ll$ Bath dimension: D

- Total Hamiltonian $H = H_S + H_B + H_{SB}$
- The whole system evolution follows the Liouville-von Neumann equation:

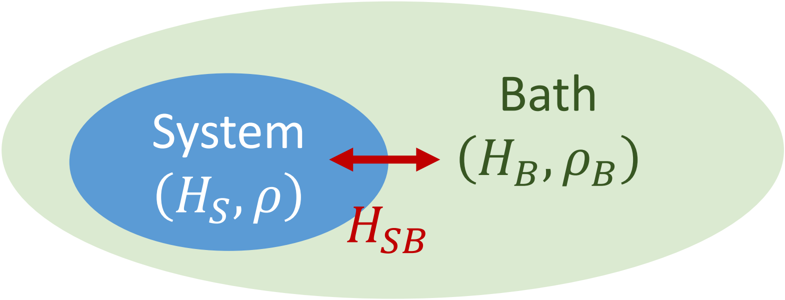
$$\frac{\mathrm{d}\rho_{SB}}{\mathrm{d}t} = -\mathbf{i}[H, \rho_{SB}]$$

- We only care the system part, i.e., $\rho = \mathrm{tr}_B[\rho_{SB}]$

Is it possible to describe the dynamics of ρ **without** simulating the bath?

i.e. a kind of **dimension reduction**

Open quantum system



System dimension: d $\ll$ Bath dimension: D

Thermalization

- If you leave a quantum system in contact with a heat bath at temperature $T = 1/\beta$, then the state $\rho(t) = \mathrm{tr}_B[\rho_{SB}(t)]$ forgets its initial condition and converges to the Gibbs state:

$$\rho_\beta = \frac{\exp(-\beta H_S)}{\mathrm{tr}[\exp(-\beta H_S)]}$$

- A physical approach to quantum Gibbs sampling:

Put the quantum spin system into a refrigerator and wait for thermalization

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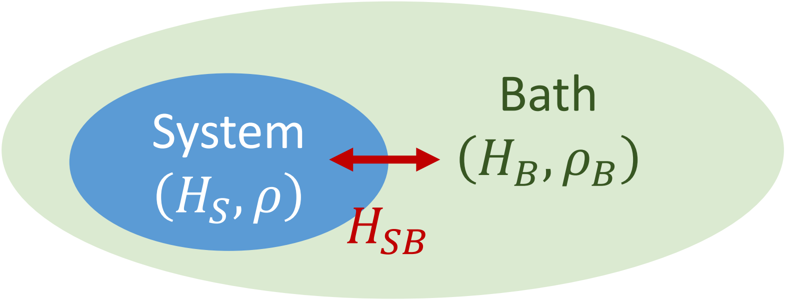
Open quantum system



System dimension: d $\ll$ Bath dimension: D

Is it possible to describe the dynamics of ρ without simulating the bath?

Gorini-Kossakowski-Sudarshan-Lindblad master equation:

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

Lindbladian / Lindblad generator

- $H \in \mathbb{C}^{d \times d}$ is the system Hamiltonian (but is not equal to H_S)
- $L_j \in \mathbb{C}^{d \times d}$ are called the jump operators

Mathematical derivation of the master equation

We want to find a linear map $\mathcal{L}$ such that $V_t = e^{\mathcal{L}t}$ is completely-positive and trace-preserving (CPTP)

Quantum Markov semigroup

- V is CP if and only if $V(\rho) = \sum_i L_i \rho L_i^\dagger$
- V is TP if and only if $\sum_i L_i L_i^\dagger = I$

First consider the CP condition:

- $\mathcal{L} = \lim\limits_{\Delta t \to 0} \frac{V_{\Delta t} - I}{\Delta t}$
- Expand $\mathcal{L}$ under a generic basis $K_1, K_2, \ldots, K_{d^2}$ such that $\mathrm{tr}\left[K_i^\dagger K_j\right] = \delta_{ij}$
  - Set $K_1 = \frac{1}{\sqrt{d}} I$ so that $\mathrm{tr}[K_i] = 0 \;\; \forall i \geq 2$
- $V_{\Delta t}(\rho) = \sum_i L_i \rho L_i^\dagger = \sum_{i,j} c_{i,j}(\Delta t) K_i \rho K_j^\dagger$

Mathematical derivation of the master equation

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Quantum Markov semi-group

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First consider the CP condition:

$$\mathcal{L}\rho = \sum_{i,j=2}^{d^2} g_{ij} K_i \rho K_j^\dagger + \underbrace{\sum_{i=2}^{d^2} \left(g_{i1} K_i \rho + g_{1i} \rho K_i^\dagger \right) + g_{11}\rho}_{\rho G + G^\dagger \rho}$$

$$= \sum_{i,j=2}^{d^2} g_{ij} K_i \rho K_j^\dagger + \rho F + F\rho - \mathbf{i}[H, \rho]$$

$G = F + \mathbf{i}H$

Hermitian

anti-Hermitian

Mathematical derivation of the master equation

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Quantum Markov semi-group

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Then consider the TP condition:

$$\mathcal{L}\rho = \sum_{i,j=2}^{d^2} g_{ij} K_i \rho K_j^\dagger + F\rho + \rho F - \mathbf{i}[H, \rho]$$

- $\mathrm{tr}\left[\frac{\mathrm{d}\rho}{\mathrm{d}t}\right] = \mathrm{tr}[\mathcal{L}\rho] = 0 \quad \Longrightarrow \quad \mathrm{tr}\left[\left(\sum_{i,j=2}^{d^2} g_{ij} K_j^\dagger K_i + 2F\right)\rho\right] = 0 \quad \forall \rho$
- $F = -\frac{1}{2}\sum_{i,j=2}^{d^2} g_{ij} K_j^\dagger K_i$

Mathematical derivation of the master equation

We want to find a linear map $\mathcal{L}$ such that $V_t = e^{\mathcal{L}t}$ is completely-positive and trace-preserving (CPTP)

Quantum Markov Semigroup

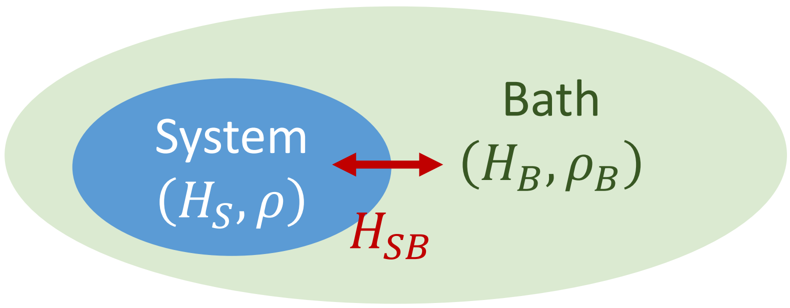
- V is CP if and only if $V(\rho) = \sum_i L_i \rho L_i^\dagger$
- V is TP if and only if $\sum_i L_i L_i^\dagger = I$

By diagonalization, we get that

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

- This derivation gives the most general form of Quantum Markov Semigroup (QMS)
- But H and L_j are decoupled from the physical system

Derivation of the master equation



System dimension: d $\ll$ Bath dimension: D

It remains open to derive the master equation for a given open quantum system from first principles

$$H(t) = H_S \otimes I_B + I_S \otimes H_B + gA_\alpha \otimes B_\alpha$$

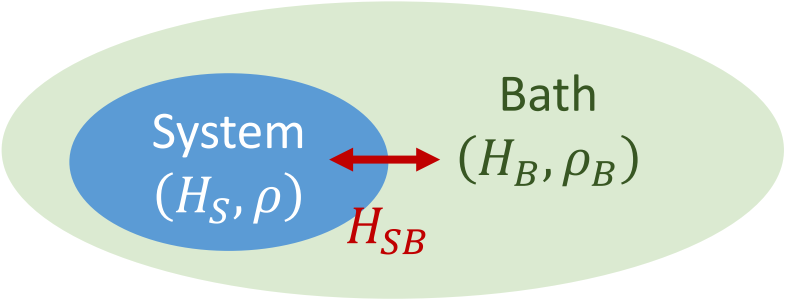
Assumptions:

- **Born approximation:** $\rho_{SB}(t) = \rho(t) \otimes \rho_B$ and ρ_B is stationary
- **Markov approximation:** memoryless
- **Secular approximation (rotating wave approximation)**

Weak coupling assumption

g is very small

Derivation of the master equation



System dimension: d $\ll$ Bath dimension: D

It remains open to derive the master equation for a given open quantum system from first principles

$$H(t) = H_S \otimes I_B + I_S \otimes H_B + g A_\alpha \otimes B_\alpha$$

Davies generator

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

Lamb shift

Bohr frequency $\{\lambda_i - \lambda_j : \lambda_i, \lambda_j \in \mathrm{spec}(H_S)\}$

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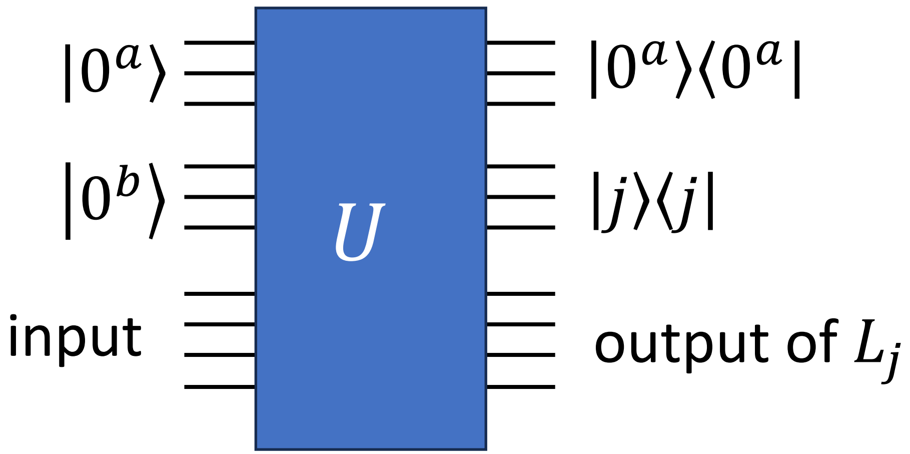
Input model

Block-encoding for the jump operators $\{L_j\}$



$$\sum_j |j\rangle\langle j| \otimes L_j$$

The goal is to simulate $e^{\mathcal{L}t}$ on an initial state $\rho(0)$

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

Quantum simulation algorithms

1. “Quantizing” the classical numerical solvers for ODE/SDE

2. “Quantizing” the Metropolis-Hastings algorithm

A toy example

$$\mathcal{L}\rho = L\rho L^\dagger - \frac{1}{2}\{L^\dagger L, \rho\}$$

- Consider the dilated Hamiltonian: $\widetilde{H} = \begin{bmatrix} & L^\dagger \\ L & \end{bmatrix}$
- We construct a quantum channel:

$$U_D = e^{-\mathbf{i}\widetilde{H}\sqrt{\Delta t}}, \qquad \Phi(\rho) \coloneqq \mathrm{tr}_a\left[U_D(|0\rangle\langle 0|_a \otimes \rho)U_D^\dagger\right]$$

Hamiltonian simulation

- Taylor expanding U_D to the second order:

$$U_D = I - i\sqrt{\Delta t}\begin{bmatrix} & L^\dagger \\ L & \end{bmatrix} - \frac{\Delta t}{2}\begin{bmatrix} L^\dagger L & \\ & LL^\dagger \end{bmatrix} + O(\Delta t^{1.5})$$

- We can check that

$$\left\| e^{\mathcal{L}\Delta t}(\rho) - \Phi(\rho) \right\|_1 \sim (\Delta t)^2$$

- For $T = r\Delta t$, we have $\left\| e^{\mathcal{L}T}(\rho) - \Phi^r(\rho) \right\|_1 \sim T\Delta t$

First-order accuracy

High-order Lindblad simulation

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

$$= \underbrace{J\rho + \rho J^\dagger}_{\substack{\mathcal{L}_{\mathrm{D}}\rho \\ \text{“Drifting”}}} + \underbrace{\sum_{j=1}^{m} L_j\rho L_j^\dagger}_{\substack{\mathcal{L}_{\mathrm{J}}\rho \\ \text{“Jump”}}}$$

$$J = -\mathbf{i}H_{\mathrm{eff}}, \qquad H_{\mathrm{eff}} \coloneqq H + \frac{1}{2\mathbf{i}}\sum_{j=1}^{m} L_j^\dagger L_j$$

High-order Lindblad simulation

By Duhamel's principle,

$$\rho(t) = e^{\mathcal{L}t}\rho(0) = e^{\mathcal{L}_{\mathrm{D}}t}\rho(0) + \int_0^t e^{\mathcal{L}_{\mathrm{D}}(t-s)}\mathcal{L}_{\mathrm{J}}\rho(s)\mathrm{d}s$$

Apply Duhamel's principle again to $\rho(s)$:

$$\rho(t) = e^{\mathcal{L}_{\mathrm{D}}t}\rho(0) + \int_0^t e^{\mathcal{L}_{\mathrm{D}}(t-s)}\mathcal{L}_{\mathrm{J}}e^{\mathcal{L}_{\mathrm{D}}s}\rho(0)\mathrm{d}s$$

$$+ \int_{0\le s_1\le s_2\le t} e^{\mathcal{L}_{\mathrm{D}}(t-s_2)}\mathcal{L}_{\mathrm{J}}e^{\mathcal{L}_{\mathrm{D}}(s_2-s_1)}\mathcal{L}_{\mathrm{J}}\rho(s_1)\mathrm{d}s_2\mathrm{d}s_1$$

truncation error

We can iterate this expansion for K-th order

High-order Lindblad simulation

$$\rho(t) = e^{\mathcal{L}_{\mathrm{D}} t}\rho(0) + \sum_{k=1}^{K} \int_{0 \le s_1 \le \cdots \le s_k \le t} e^{\mathcal{L}_{\mathrm{D}}(t-s_k)} \mathcal{L}_{\mathrm{J}} e^{\mathcal{L}_{\mathrm{D}}(s_k - s_{k-1})} \mathcal{L}_{\mathrm{J}} \cdots e^{\mathcal{L}_{\mathrm{D}}(s_2 - s_1)} \mathcal{L}_{\mathrm{J}}\, e^{\mathcal{L}_{\mathrm{D}} s_1} \rho(0) \mathrm{d}s_1 \cdots \mathrm{d}s_k + \text{truncation error}$$

- The integrals can be discretized using Gaussian quadrature
- Need to block-encode $e^{\mathcal{L}_{\mathrm{D}} t}$ and $\mathcal{L}_{\mathrm{J}}$
- For the drifting part,

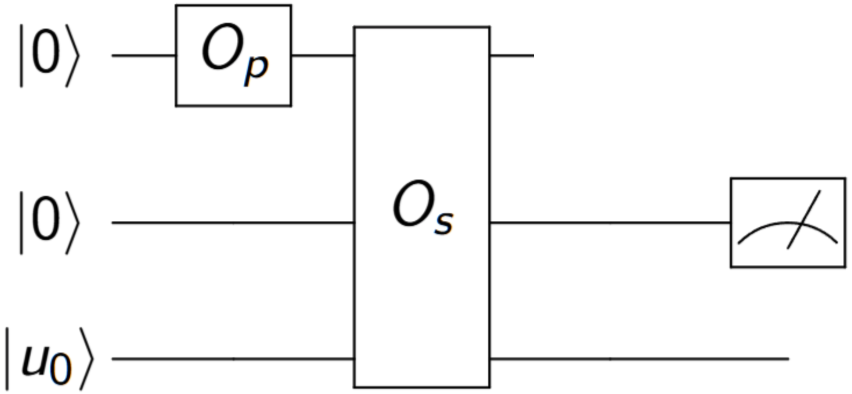
$$e^{\mathcal{L}_{\mathrm{D}} t}\rho = e^{Jt}\rho e^{J^\dagger t} \approx \left(\sum_{\ell=0}^{K'} \frac{J^\ell t^\ell}{\ell!}\right) \rho \left(\sum_{\ell=0}^{K'} \frac{J^\ell t^\ell}{\ell!}\right)^\dagger$$

Kraus form

- For the jump part, $\mathcal{L}_J = \sum_{j=1}^{m} L_j \rho L_j^\dagger$

Block-encoding Kraus operators

- Let $A_1, A_2, \ldots, A_m$ be Kraus operators and let U_i be the corresponding $(\alpha_i, n', 0)$-block-encodings



$$O_p|0\rangle = \frac{1}{\|\alpha\|_2}\sum_{j=1}^{m}\alpha_j|j\rangle$$

$$O_s = \sum_{j=1}^{m}|j\rangle\langle j| \otimes U_j$$

- $|0\rangle|u_0\rangle \mapsto \frac{1}{\|\alpha\|_2}\sum_{j=1}^{m}|j\rangle A_j|u_0\rangle$
- Density matrix: $\rho_0 \mapsto \tilde{\rho} \coloneqq \sum_{j,j'}|j\rangle\langle j'| \otimes A_j\rho_0 A_j^\dagger$
- Trace out the first ancilla register: $\mathrm{tr}_a[\tilde{\rho}] = \sum_j A_j\rho_0 A_j^\dagger$

High-order Lindblad simulation

$$\rho(t) = e^{\mathcal{L}_{\mathrm{D}}t}\rho(0)$$

$$+ \sum_{k=1}^{K} \int_{0\le s_1 \le \cdots \le s_k \le t} e^{\mathcal{L}_{\mathrm{D}}(t-s_k)}\mathcal{L}_{\mathrm{J}} e^{\mathcal{L}_{\mathrm{D}}(s_k - s_{k-1})}\mathcal{L}_{\mathrm{J}} \cdots e^{\mathcal{L}_{\mathrm{D}}(s_2-s_1)}\mathcal{L}_{\mathrm{J}}\, e^{\mathcal{L}_{\mathrm{D}}s_1}\rho(0)\mathrm{d}s_1 \cdots \mathrm{d}s_k$$

$$+ \text{truncation error}$$

- The integrals can be discretized using Gaussian quadrature
- Use truncated Taylor series to approximate $e^{\mathcal{L}_{\mathrm{D}}t}$
- Block-encode the Kraus forms and use a big LCU to combine all the terms
- Total complexity: $\mathcal{O}\left(t\|\mathcal{L}\|_{\mathrm{be}} \log\left(\frac{t\|\mathcal{L}\|_{\mathrm{be}}}{\epsilon}\right)\right)$ where $\|\mathcal{L}\|_{\mathrm{be}} \coloneqq \|H\| + \frac{1}{2}\sum_{j=1}^{m}\left\|L_j\right\|^2$

Li, Xiantao, and Chunhao Wang. "Simulating Markovian open quantum systems using higher-order series expansion."

Lindblad simulation via Hamiltonian simulation

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = J\rho + \rho J^\dagger + \sum_{j=1}^{m} L_j \rho L_j^\dagger , \qquad J = -\mathbf{i}H - \frac{1}{2}\sum_{j=1}^{m} L_j^\dagger L_j$$

Unraveling

- Thinking about $\rho(t) = \mathbb{E}[|\psi_t\rangle\langle\psi_t|]$:

$$\frac{\mathrm{d}\mathbb{E}[|\psi_t\rangle\langle\psi_t|]}{\mathrm{d}t} = J\mathbb{E}[|\psi_t\rangle\langle\psi_t|] + \mathbb{E}[|\psi_t\rangle\langle\psi_t|]J^\dagger + \sum_{j=1}^{m} L_j \mathbb{E}[|\psi_t\rangle\langle\psi_t|]L_j^\dagger$$

- Reverse-engineer an SDE for $|\psi_t\rangle$ using Itô’s lemma:

$$\mathrm{d}|\psi_t\rangle = J|\psi_t\rangle\mathrm{d}t + \sum_{j=1}^{m} L_j|\psi_t\rangle \mathrm{d}W_t^j$$

independent 1d Brownian motion

Lindblad simulation via Hamiltonian simulation

$$\mathrm{d}|\psi_t\rangle = J|\psi_t\rangle \mathrm{d}t + \sum_{j=1}^{m} L_j|\psi_t\rangle \mathrm{d}W_t^j$$

Euler-Maruyama scheme:

$$|\psi_{n+1}\rangle = |\psi_n\rangle + J|\psi_n\rangle\Delta t + \sum_{j=1}^{m} L_j|\psi_n\rangle\sqrt{\Delta t}\,W^j \sim \mathcal{N}(0,1) =: L_{1,\Delta t}(|\psi_n\rangle)$$

$$\mathbb{E}[|\psi_{n+1}\rangle\langle\psi_{n+1}|] = \mathbb{E}\left[L_{1,\Delta t}(|\psi_n\rangle)L_{1,\Delta t}(|\psi_n\rangle)^\dagger\right]$$

$$= \underbrace{(I + J\Delta t)}_{F_0}\mathbb{E}[|\psi_n\rangle\langle\psi_n|](I + J\Delta t)^\dagger + \sum_{j=1}^{m}\underbrace{\left(\sqrt{\Delta t}L_j\right)}_{F_j}\mathbb{E}[|\psi_n\rangle\langle\psi_n|]\left(\sqrt{\Delta t}L_j\right)^\dagger$$

Kraus form: $\rho_{n+1} = \sum_{j=0}^{m} F_j \rho_n F_j^\dagger$

Lindblad simulation via Hamiltonian simulation

$$\rho_{n+1} = \sum_{j=0}^{m} F_j \rho_n F_j^\dagger =: \mathcal{K}[\rho_n]$$

- Since Euler-Maruyama is a first-order scheme,

$$\rho_{n+1} = \rho_n + \mathcal{L}\rho_n \Delta t + \mathcal{O}(\Delta t^2) = e^{\mathcal{L}\Delta t}\rho_n + \mathcal{O}(\Delta t^2)$$

Our goal is to find a dilated Hamiltonian $\widetilde{H}$ such that

$$\mathcal{K}[\rho] \approx \mathrm{tr}_a\left[e^{-\mathbf{i}\widetilde{H}\sqrt{\Delta t}}(|0\rangle\langle 0| \otimes \rho)e^{\mathbf{i}\widetilde{H}\sqrt{\Delta t}}\right]$$

- Stinespring representation of a Kraus form:

Taylor expand and match the terms

$$\mathcal{K}[\rho] = \mathrm{tr}_a\left[\begin{bmatrix} F_0 & * & * & * \\ F_1 & * & * & * \\ \vdots & * & * & * \\ F_m & * & * & * \end{bmatrix}(|0\rangle\langle 0| \otimes \rho)\begin{bmatrix} F_0 & * & * & * \\ F_1 & * & * & * \\ \vdots & * & * & * \\ F_m & * & * & * \end{bmatrix}^\dagger\right]$$

Lindblad simulation via Hamiltonian simulation

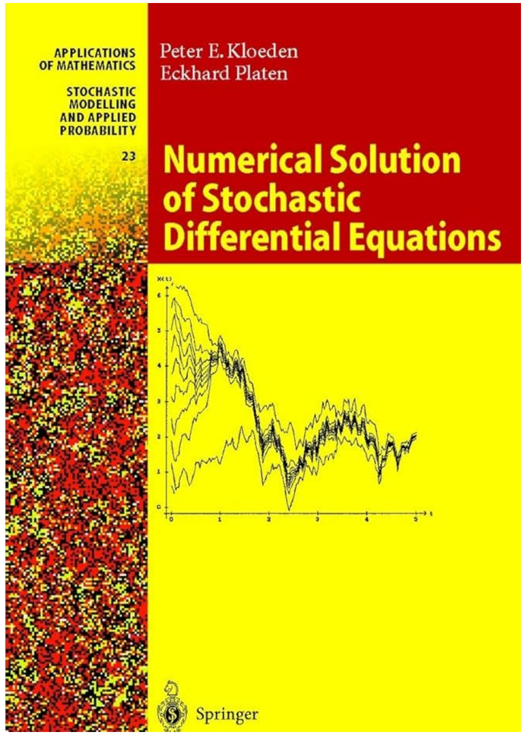
$$\widetilde{H} = \begin{bmatrix} \sqrt{\Delta t} H & L_1^\dagger & \cdots & L_m^\dagger \\ L_1 & 0 & 0 & 0 \\ \vdots & 0 & 0 & 0 \\ L_m & 0 & 0 & 0 \end{bmatrix}, \qquad \mathcal{K}[\rho] = \mathrm{tr}_a \left[e^{-\mathbf{i}\widetilde{H}\sqrt{\Delta t}} (|0\rangle\langle 0| \otimes \rho) e^{\mathbf{i}\widetilde{H}\sqrt{\Delta t}} \right] + \mathcal{O}(\Delta t^2)$$

- This is a generalization of the toy example

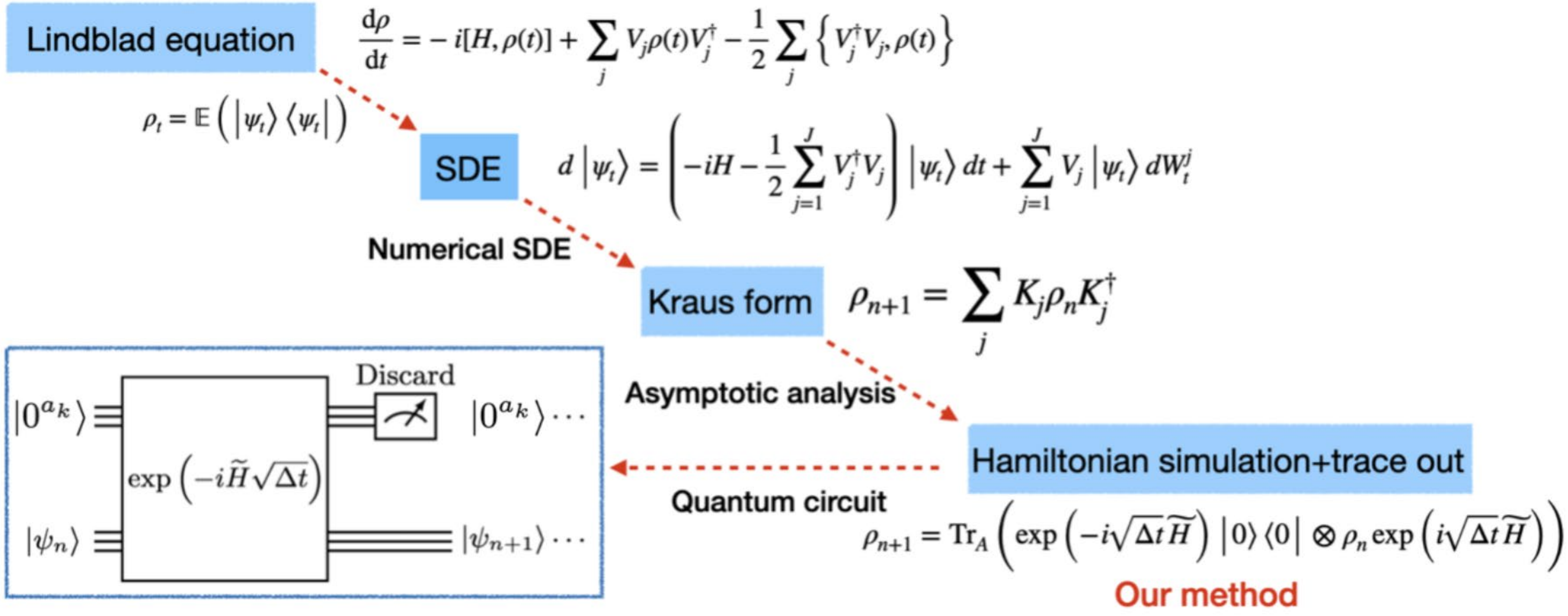
Three-step framework for k-th order Lindblad simulation

- Step 1: find a weak scheme of order k for the SDE
  (e.g., Itô-Taylor-expansion)
- Step 2: formulate the Kraus form
- Step 3: construct the dilated Hamiltonian

$$\widetilde{H} = \begin{bmatrix} H_0 & H_1^\dagger & \cdots & H_S^\dagger \\ H_1 & 0 & 0 & 0 \\ \vdots & 0 & 0 & 0 \\ H_S & 0 & 0 & 0 \end{bmatrix}$$



Lindblad simulation via Hamiltonian simulation



For a k-th order scheme, the simulation error is $\|\rho_T - \rho_N\|_1 = \mathcal{O}\left(T\|\mathcal{L}\|_{\mathrm{be}}\Delta t^k\right)$

Ding, Zhiyan, Xiantao Li, and Lin Lin. "Simulating open quantum systems using Hamiltonian simulations."

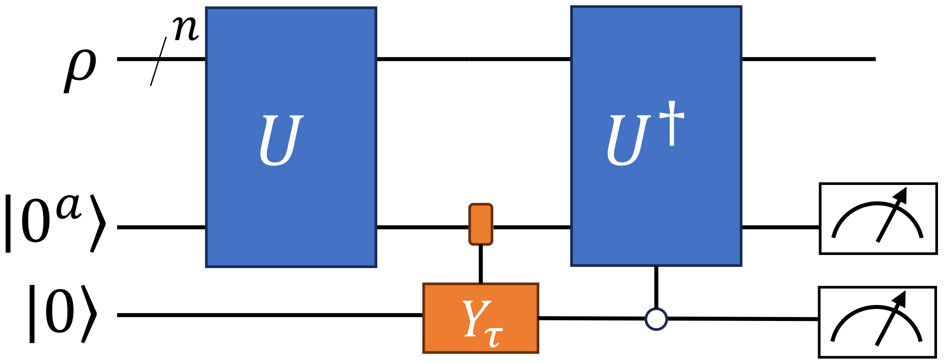
Quantum Metropolis algorithm

Let x be the current state

- Pick A^a with probability $p(a)$
- $y \leftarrow A^a$ applied to x
- Accept move with probability $\gamma_\beta(x, y) \coloneqq \min\left\{1, \exp\left(-\beta\left(E_y - E_x\right)\right)\right\}$
- If reject, stay at x

How to revert in quantum?

Weak measurement



discard/reset

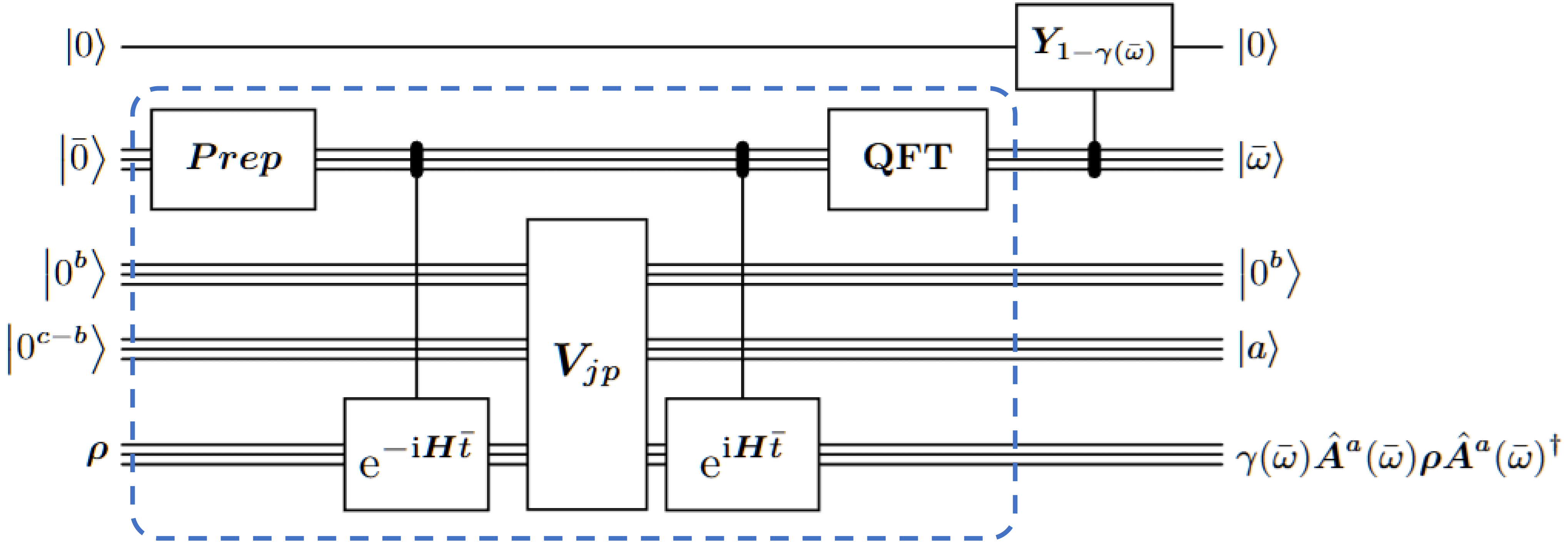
$$\approx \; I + \tau\mathcal{L} + \mathcal{O}(\tau^2) \approx e^{\tau\mathcal{L}}$$

$$Y_\tau = |0^a\rangle\langle 0^a| \otimes \begin{bmatrix} \sqrt{1-\tau} & -\sqrt{\tau} \\ \sqrt{\tau} & \sqrt{1-\tau} \end{bmatrix} + (I - |0^a\rangle\langle 0^a|) \otimes I$$

Block-encoding the Lindbladian

$$\sum_{a,\overline{\omega}} \sqrt{\gamma(\overline{\omega})}|\overline{\omega}\rangle \otimes |a\rangle \otimes \hat{A}^a(\overline{\omega})$$

Calculate the “accept” probability based on the energy difference



a QPE-like circuit

Quantum Metropolis algorithm

Weak measurement implementation costs:

- Suppose the Lindblad simulation time is T
- #steps for weak measurement implementation is T/τ
- Total approximation error $= \frac{T}{\tau} \cdot \tau^2 = T\tau$
- We need to take $\tau \sim \frac{1}{T}$ for small error
- The total #steps $\sim T^2$

➢ It can be improved to $\tilde{O}(T)$ using a complicated "compression" technique (Chen-Kastoryano-Brandão-Gilyén '23)

➢ Simplified quantum Gibbs sampling algorithm using QPE (Irani-Jiang '24)