Open Quantum Systems: A Mathematical Introduction, Simulations and Algorithmic Applications

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Outline

1. Introduction
2. Quantum Algorithms for Lindblad Simulation
3. Algorithmic Applications in State-Preparation Problems

Why open quantum system?

- Quantum systems in reality are often interacting with an environment (bath)
- These interaction have a deep impact on the system dynamics (for closed system, we have *unitary* dynamics governed by the Schrödinger equation $\partial_t |\psi(t)\rangle = -\mathrm{i}H|\psi(t)\rangle$)
- The combined system:

$$H = H_{\mathrm{S}} \otimes I_{\mathrm{B}} + I_{\mathrm{S}} \otimes H_{\mathrm{B}} + \lambda H_{\mathrm{SB}} \in L(\mathcal{H}_{\mathrm{S}} \otimes \mathcal{H}_{\mathrm{B}}) \tag{1}$$

  which usually as large dimension and is impossible to simulate directly
- The theory of open quantum system is attempting to identify models that implicity incorporate the effect of the bath.

Feller Semigroups

- V Banach space, a family of operators $T = (T_t)_{t\in\mathbb{R}_+} \subset \mathcal{B}(V)$ is a one-parameter semigroup on V, if (i) $T_0 = I$ the identity operator, (ii) $T_s T_t = T_{s+t}$ for all $s, t \in \mathbb{R}_+$
- A semigroup $\{T_t\}$ on $C_0(E)$ is Feller, if
  - $\{T_t\}$ is Markovian, i.e. $T_t f \geq 0$ for $f \geq 0$
  - $T_t(C_0(E)) \subset C_0(E)$ for all $t \in \mathbb{R}_+$ and $\lim_{t\to 0+} \|T_t f - f\| = 0$ for all $f \in C_0(E)$ (strong continuity)
- The Hille-Yosida-Ray Theorem: The generator of a Feller semigroup has a simple characterization.
  A is the generator of a Feller semigroup on $C_0(E)$, if and only if
  - A is real and satisfies the *positive maximum principle* (i.e. whenever $x_0 \in E$, $f \in \mathscr{D}(A) \cap C_0(E;\mathbb{R})$ are such that $f(x_0) = \|f\|$, we have $(Af)(x_0) \leq 0$.)
  - $\exists \lambda > 0$, s.t. $\lambda I - A$ is surjective.

Completely Positive Maps

- In a (unital) C^* algebra $\mathcal{A}$ we write $a \geq 0$, if and only if $\exists b \in \mathcal{A}$ s.t. $a = b^* b$. We say $\Phi : \mathcal{A} \to \mathcal{B}$ is positive, if $\Phi(x^* x) \geq 0$ for any $x \in \mathcal{A}$.
- We say Φ is k-positive, if

$$I_k \otimes \Phi : M_k(\mathbb{C}) \otimes \mathcal{A} \to M_k(\mathbb{C}) \otimes \mathcal{B} \tag{2}$$

is positive. Φ is completely positive (CP), if it is k-positive for all $k = 1, 2, \cdots$. We say Φ is conservative if $\Phi(I_{\mathcal{A}}) = I_{\mathcal{B}}$.
- **Stinespring Dilation Theorem**: A linear map $\Phi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$ is CP, if and only if $\exists$ a Hilbert space $\mathcal{K}$ and an isometry $V \in \mathcal{B}(\mathcal{H}, \mathcal{H} \otimes \mathcal{K})$, s.t. $\Phi(x) = \mathrm{Tr}_{\mathcal{K}} V x V^*$
- **Kraus Theorem**: Any CP map $\Phi : \mathcal{B}(\mathcal{H}_1) \to \mathcal{B}(\mathcal{H}_2)$ is of the following form:

$$\Phi(X) = \sum_i K_i X K_i^* \tag{3}$$

where $K_i \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)$ and $\sum_i K_i K_i^* = I_{\mathcal{H}_2}$.

Semigroup Generators

Quantum Feller semigroup: $\{T_t\}_{t\in\mathbb{R}_+}$ on a C^* algebra $\mathcal{A}$ is a strongly continuous semigroup such that each T_t is completely positive.

Lindblad, Christensen

Let $\mathcal{L}$ be a bounded linear operator on $\mathcal{A}$, then $\mathcal{L}$ is a generator of a quantum Feller semigroup, if and only if $\exists$ a CP and normal map Φ and an operator $G\in\mathcal{A}$ such that

$$\mathcal{L}(a)=\Phi(a)+G^*a+aG,\quad \forall a\in\mathcal{A}. \tag{4}$$

Proof.

Let $\mathcal{A}=\mathcal{B}(\mathcal{H})$, define G s.t. $G^*v=\mathcal{L}(|v\rangle\langle u|)u-\frac{1}{2}\langle u,\mathcal{L}(|u\rangle\langle u|)u\rangle v$
Then by $\mathcal{L}$ is conditionally CP (Lindblad-Evans), we can verify that for any $a_i\in\mathcal{A}$ and $\psi_i\in\mathcal{H}$, $\sum_{i,j=1}^n\langle\psi_i,\Phi(a_i^*a_j)\psi_j\rangle\geq 0$ (here the mapping Φ is $a\mapsto\mathcal{L}(a)-G^*a-aG$), which implies that Φ is CP. □

GKSL Theorem

Theorem (Gorini-Kossakowski-Sudarshan, Lindblad)

A bounded linear map $\mathcal{L} \in \mathcal{B}(\mathcal{A})$ is the generator of a uniformly continuous quantum Feller semigroup, if and only if

$$\mathcal{L}(a) = -i[h, a] - \frac{1}{2} \sum_i (L_i^* L_i a - 2L_i^* a L_i + a L_i^* L_i), \quad \forall a \in \mathcal{A}. \tag{5}$$

Here $h = h^* \in \mathcal{A}$, $L_i \in \mathcal{B}(\mathcal{H})$

Proof.

Suppose $\mathcal{L}$ is the generator of such semigroup, then by the preceding theorem, we have $\mathcal{L}(a) = \Phi(a) + G^* a + aG$ for any $a \in \mathcal{A}$. Taking $a = 1$ shows that $G^* + G = -\Phi(1)$ so $G = -\frac{1}{2}\Phi(1) + ih$ for some self-adjoint element $h \in \mathcal{A}$. Then the result follows by Kraus representation. □

Classical Algorithms for Lindblad Simulation

- Non-Hermitian time evolution, $\partial_t \mathrm{vec}(\rho) = \mathbf{L}\mathrm{vec}(\rho)$

$$\begin{aligned}\mathbf{L} &= -i\mathrm{I} \otimes H + iH^T \otimes \mathrm{I} + \sum_k \overline{L}_k \otimes L_k - \frac{1}{2}\mathrm{I} \otimes (L_k^* L_k) - \frac{1}{2} L_k^T L_k^* \otimes \mathrm{I} \\ &= -i\mathrm{I} \otimes H_{\mathrm{eff}} + iH_{\mathrm{eff}}^T \otimes \mathrm{I} + \sum_k \overline{L}_k \otimes L_k\end{aligned} \tag{6}$$

- Unraveling Lindblad dynamics using quantum jump method
  - $\psi(t+\Delta t) = e^{-i\Delta t H_{\mathrm{eff}}}\psi(t)$, $p = 1 - |\psi(t+\Delta t)|^2$ $(\sum_j L_j^* L_j \succeq 0)$
  - With the probability p, the system jumps to $\frac{L_j\psi(t)}{|L_j\psi(t)|}$
  - Equivalent to solving $\mathrm{d}\psi_t = -i(H_{\mathrm{eff}} + \frac{i}{2}\sum_j |L_j\psi_t|^2)\psi_t \mathrm{d}t + \sum_j \left(\frac{L_j\psi_t}{|L_j\psi_t|} - \psi_t\right)\mathrm{d}N_t^j$
- More natural interpretation: wavefunction-trajectories driven by non-Hermitian dynamics and Brownian motion
  - $\mathrm{d}\psi_t = -i\left(H - \frac{i}{2}\sum_{j=1}^M L_j^* L_j\right)\psi_t \mathrm{d}t + \sum_{j=1}^M L_j\psi_t \mathrm{d}W_t^j$
  - Then it can be treated using classical SDE solvers (such as Euler-Maruyama)

Quantum Algorithms for Lindblad Simulation

- Kliesch-Barthel-Gogolin-Kastoryano-Eisert, PRL 2011, $\mathcal{O}(t^2/\varepsilon)$
- Childs-Li, QIC 2017, $\mathcal{O}(t^{3/2}/\sqrt{\varepsilon})$
- Cleve-Wang, ICALP 2017, $\mathcal{O}(t\,\mathrm{polylog}(t/\varepsilon))$
  - Kraus operator: $\mathcal{E}[\rho] = A_0\rho A_0^* + \sum_{j=1}^m A_j\rho A_j^*$, where $A_0 = I - i\Delta t H - \frac{\Delta t}{2}\sum_{j=1}^m L_j L_j^*$ and $A_j = \sqrt{\Delta t} L_j$
  - Block-encoding of A_i + “standard LCU” for quantum channels + oblivious amplitude amplification
  - Require a certain “compression scheme”
- Li-Wang, ICALP 2023, $\mathcal{O}(t\,\mathrm{polylog}(t/\varepsilon))$ without compressed encoding
- **Ding-Li-Lin, PRR 2024**

Higher-Order Series Expansion

- Duhamel's expansion

$$\rho(t) = \exp(t\mathcal{L}_{\mathrm{D}})\rho(0) + \int_0^t e^{(t-t_1)\mathcal{L}_{\mathrm{D}}}\mathcal{L}_{\mathrm{J}}\rho(t_1)\mathrm{d}t_1 \tag{7}$$

$$\rho(t) = \exp(t\mathcal{L}_{\mathrm{D}})\rho(0) + \int_0^t e^{(t-t_1)\mathcal{L}_{\mathrm{D}}}\mathcal{L}_{\mathrm{J}}e^{t_1\mathcal{L}_{\mathrm{D}}}\rho(0)\mathrm{d}t_1 + \int_0^t\int_0^{t_1} * + \cdots \tag{8}$$

- Gaussian quadrature scheme

$$\int *\mathrm{d}t_1\cdots\mathrm{d}t_k \approx \sum_{j_1,\cdots,j_k=1}^{q} w_{j_k}w_{(j_k,j_{k-1})}\cdots w_{(j_k,\cdots,j_1)}\mathcal{F}(s_k,\cdots,s_{(j_k,\cdots,j_1)}) \tag{9}$$

  - We have $\sum_{j_1,\cdots,j_k} w_{(j_k,j_{k-1})}\cdots w_{(j_k,\cdots,j_1)} = \frac{t^k}{(k+1)!}$, $k = 1, 2, \cdots, K$
  - Truncations: $K, q = \mathcal{O}(\log\frac{1}{\varepsilon}/\log\log\frac{1}{\varepsilon})$
  - Overall complexity: $\mathcal{O}(t\,\mathrm{polylog}(t/\varepsilon))$

Li-Wang, ICALP 2023

Lindblad Simulation via Hamiltonian Simulation

- Stinespring dilated evolution:

$$\rho(t+\Delta t) = \mathrm{Tr}_{\mathrm{A}}\left(e^{-i\sqrt{\Delta t}\widetilde{H}}[|\bar{0}\rangle\langle\bar{0}| \otimes \rho(t)]e^{i\sqrt{\Delta t}\widetilde{H}}\right) + \mathcal{O}(\Delta t^2) \tag{10}$$

Dilated Hamiltonian $\widetilde{H} = \begin{pmatrix} \sqrt{\Delta t}H & L_1^* & \cdots & L_m^* \\ L_1 & & & \\ \vdots & & & \\ L_m & & & \end{pmatrix}$

- Recall: unraveling the Lindblad equation using Itô-SDE

$$\mathrm{d}\psi_t = -i\left(H - \frac{i}{2}\sum_{j=1}^{M} L_j^* L_j\right)\psi_t \mathrm{d}t + \sum_{j=1}^{M} L_j \psi_t \mathrm{d}W_t^j \tag{11}$$

Euler-Maruyama scheme $\psi_{n+1} = \left(I - i\Delta t H_{\mathrm{eff}} + \sum_{j=1}^{M}\sqrt{\Delta t}W^j L_j\right)\psi_n =: \mathscr{L}_{1,\Delta t}\psi_n$.

Ding-Li-Lin, PRR 2024

Lindblad Simulation via Hamiltonian Simulation

- k-th order SDE scheme using Itô-Taylor expansion $\mathscr{L}_{k,\Delta t}\psi = \sum_{j=0}^{k} \frac{(\Delta t)^j}{j!} H_{\mathrm{eff}}^j \psi + \sum_\alpha R_\alpha \mathbf{L}_\alpha \psi$
- $R_\alpha = \int_0^{\Delta t} \int_0^{s_{|\alpha|}} \int_0^{s_{|\alpha|-1}} \cdots \int_0^{s_2} \mathrm{d}W_{s_1}^{j_1} \cdots \mathrm{d}W_{s_{|\alpha|}}^{j_{|\alpha|}}$, $\mathbf{L}_\alpha = \prod_{i=1}^{|\alpha|} L_{j_i}$
- $\mathbb{E}[R_\alpha R_\beta] = C_{\alpha,\beta} \Delta t^{|\alpha|+|\beta|-|\alpha^+|} \mathbf{1}_{\alpha^+=\beta^+}$, $\widetilde{R}_\alpha := R_\alpha \Delta t^{-(|\alpha|+|\alpha^0|)/2}$
- We cannot naively define $K_\alpha = \sqrt{\mathbb{E}(\widetilde{R}_\alpha^2)} \Delta t^{(|\alpha|+|\alpha^0|)/2} \mathbf{L}_\alpha$ since $\mathbb{E}(\widetilde{R}_\alpha \widetilde{R}_\beta) \neq 0$
- Kloeden-Platen: orthogonal random variables $\widetilde{R}_\alpha = \sum_{\alpha' \neq 0} c_{\alpha\alpha'} Q_{\alpha'}$ and $\{Q_\alpha\}$ are uncorrelated and normalized, then we have $\mathbb{E}(\mathscr{L} |\psi\rangle\langle\psi| \mathscr{L}^\dagger) = F_0 |\psi\rangle\langle\psi| F_0^* + \sum_\alpha F_\alpha |\psi\rangle\langle\psi| F_\alpha^*$
- Next step: construct the dilated Hamiltonian simulation

Ding-Li-Lin, PRR 2024

Lindblad Simulation via Hamiltonian Simulation

$$\exp^{\mathcal{L}\Delta t}[\rho] = \sum_{j=0}^{S_k} F_j \rho F_j^* + \mathcal{O}(\Delta t^{k+1}) = \mathrm{Tr}_{\mathrm{A}}\left(e^{-i\sqrt{\Delta t}\widetilde{H}}[|\bar{0}\rangle\langle\bar{0}| \otimes \rho(t)]e^{i\sqrt{\Delta t}\widetilde{H}}\right) + \mathcal{O}(\Delta t^{k+1})$$

Matching the terms using asymptotic analysis!

$$\begin{bmatrix} F_0 & \cdot & \cdots & \cdot \\ F_1 & \cdot & \cdots & \cdot \\ \vdots & \vdots & \ddots & \vdots \\ F_{M_t} & \cdot & \cdots & \cdot \end{bmatrix} = \begin{bmatrix} I + \Delta t Y_{0,0} + \Delta t^2 Y_{0,1} + \cdots & \cdot & \cdots & \cdot \\ \Delta t^{1/2}(-iY_{1,0}) + \Delta t^{3/2}(-iY_{1,1}) + \cdots & \cdot & \cdots & \cdot \\ \vdots & \vdots & \ddots & \vdots \\ \Delta t(-iY_{M_t,0}) + \Delta t^2(-iY_{M_t,1}) + \cdots & \cdot & \cdots & \cdot \end{bmatrix}$$

Match $(\Delta t)^p$ terms

$$\begin{bmatrix} I + \Delta t(-iX_{0,0} + \mathrm{poly}(X_{j>0,0})) + \Delta t^2(-iX_{0,1} + \mathrm{poly}(X_{j\geq 0,0}, X_{j>0,1})) + \cdots & \cdot & \cdots & \cdot \\ \Delta t^{1/2}(-iX_{1,0}) + \Delta t^{3/2}(-iX_{1,1} + \mathrm{poly}(X_{j\geq 0,0})) + \cdots & \cdot & \cdots & \cdot \\ \vdots & \vdots & \ddots & \vdots \\ \Delta t(-iX_{M_t,0}) + \Delta t^2(-iX_{M_t,1} + \mathrm{poly}(X_{j\geq 0,0})) + \cdots & \cdot & \cdots & \cdot \end{bmatrix}$$

$$\| $$

$$\exp\left(-i\widetilde{H}\sqrt{\Delta t}\right)$$

Ding-Li-Lin, PRR 2024

Thermal State/Ground State Problems

Given H, can we efficiently prepare the ground state $H|\psi_0\rangle = \lambda_0 |\psi_0\rangle$ and the Gibbs state $\rho = \exp(-\beta H)$?

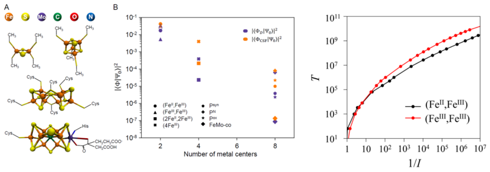
- The problem is QMA-hard in the worst case
- For ground state problems:
  - Common additional assumption: good initial state $|\phi\rangle = U_I |\bar{0}\rangle$ with $p_0 = |\langle\phi|\psi_0\rangle| = \Omega(\frac{1}{\mathrm{poly}(n)})$
  - Most works (QPE, many post-QPE methods, like quantum singular value transformation) adopt this assumption
  - Good initial overlap for strongly correlated system?

nature communications

Evaluating the evidence for exponential quantum advantage in ground-state quantum chemistry

Seunghoon Lee, Joonho Lee, Huanchen Zhai, Yu Tong, Alexander M. Dalzell, Ashutosh Kumar, Phillip Helms, Johnnie Gray, Zhi-Hao Cui, Wenyuan Liu, Michael Kastoryano, Ryan Babbush, John Preskill, David R. Reichman, Earl T. Campbell, Edward F. Valeev, Lin Lin & Garnet Kin-Lic Chan

Nature Communications **14**, Article number: 1952 (2023) | Cite this article



Lee-Lee-Zhai-Tong-EtAl, Nat. Commun. 2023

Lindblad for Thermal State Preparation

- Lindblad dynamics as an algorithmic tool can drive the system to the thermal state: $\lim_{t\to\infty} \rho(t) \approx \rho_\beta = \exp(-\beta H)/\operatorname{Tr}(\exp(-\beta H))$
  (Energy basis: $\rho_\beta \propto \sum_{i=1}^{N} e^{-\beta\lambda_i} |\psi_i\rangle\langle\psi_i|$)
- Quantum detailed balance, and fixes the thermal state

$$A = \sum_{i,j} \langle\psi_i|A|\psi_j\rangle\, |\psi_i\rangle\langle\psi_j|\,, \quad A(t) = \sum_{i,j} e^{i(\lambda_i-\lambda_j)t} \langle\psi_i|A|\psi_j\rangle\, |\psi_i\rangle\langle\psi_j| \tag{12}$$

$$L(\omega) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} A(t) e^{-i\omega t} f(t)\mathrm{d}t = \sum_{\nu} \hat{f}(\omega-\nu) A_{ij} |\psi_i\rangle\langle\psi_j| \tag{13}$$

$$\mathcal{L}_{L_j}[\cdot] = -i[B_j, \cdot] + \int_{\mathbb{R}} \gamma(\omega) \left(L_j(\omega) \cdot L_j(\omega)^* - \frac{1}{2}\{L_j(\omega)^* L_j(\omega), \cdot\} \right) \mathrm{d}\omega \tag{14}$$

  - Finely-tuned coherent term, Detailed balanced weights $\gamma(\omega)/\gamma(-\omega) \sim e^{-\beta\omega}$
  - Detailed balanced Lindbladian: $\sum_j \mathcal{L}_{L_j}[\rho_\beta] \approx 0$

Chen-Kastoryano-Brandão-Gilyén, 2023, arXiv:2303.18224

Chen-Kastoryano-Gilyén, 2023, arXiv:2311.09207

One-ancilla Ground State Preparation via Lindbladians

- From thermal state to ground state: $\hat{f}(\omega) = 0 \quad \forall \omega \geq 0$,
- Notice

$$L = \sum_{i<j} \hat{f}(\lambda_i - \lambda_j) A_{ij} |\psi_i\rangle\langle\psi_j| = \int_{\mathbb{R}} f(s) e^{iHs} A e^{-iHs} \mathrm{d}s \tag{15}$$

where $\hat{f}(\omega) = \int_{\mathbb{R}} f(s) e^{i\omega s} \mathrm{d}s$

- One can easily verify that $\mathcal{L}[|\psi_0\rangle\langle\psi_0|] = 0$ (fix ground state)
- $\langle\psi_i|\mathcal{L}[|\psi_j\rangle\langle\psi_j|]|\psi_i\rangle = 0$ for $i \geq j$ (forbid low to high)
- $\langle\psi_i|\mathcal{L}[|\psi_j\rangle\langle\psi_j|]|\psi_i\rangle \neq 0$ for some $i < j$ (push high to low)
- Choice of f

$$\hat{f}(\omega) = \frac{1}{2}\left(\operatorname{erf}\left(\frac{\omega + a}{\delta_a}\right) - \operatorname{erf}\left(\frac{\omega + b}{\delta_b}\right)\right), \quad f(s) = \frac{e^{ias - \frac{\delta_a^2 s^2}{4}} - e^{ibs - \frac{\delta_b^2 s^2}{4}}}{2\pi i s} \tag{16}$$

- Choice of A: local? $A_{ij} \neq 0$ for as much $i < j$ as possible?

Ding-Chen-Lin, PRR 2024

One-ancilla Ground State Preparation via Lindbladians

- First order Trotter

$$\rho(\Delta t) = \underbrace{\exp(\mathcal{L}_H \Delta t)}_{\text{just}\exp(-iH\Delta t)} \exp(\mathcal{L}_L \Delta t)\rho(0) + \mathcal{O}(\Delta t^2) \tag{17}$$

- Dilated Hamiltonian simulation for non-unitary term $\exp(\mathcal{L}_L \Delta t)$ (also 1st order): $\exp(\mathcal{L}_L \Delta t)\rho = \mathrm{Tr}_{\mathrm{A}}(e^{-i\widetilde{L}\sqrt{\Delta t}} |0\rangle\langle 0| \otimes \rho e^{i\widetilde{L}\sqrt{\Delta t}}) + \mathcal{O}(\Delta t^2)$
- Quadrature, second order Trotter, and short-time simulations
  - $L = \sum f(s_l) e^{iHs_l} A e^{-iHs_l} w_l = \sum_l L_l$ (trapezoidal rule)
  - $\exp\left(-i\widetilde{L}\sqrt{\Delta t}\right) = \overleftarrow{\prod_{l=1}} e^{-i\widetilde{L}_l \sqrt{\Delta t}/2} \overrightarrow{\prod_{l=M}} e^{-i\widetilde{L}_l \sqrt{\Delta t}/2} + \mathcal{O}(\Delta t^{3/2})$
  - $\widetilde{L}_l = \sigma_l \otimes A(s_l)$ where $\sigma_l = w_l(X \mathrm{Re}\, f(s_l) + Y \mathrm{Im}\, f(s_l))$, $e^{-i\widetilde{L}_l \sqrt{\Delta t}/2} = (I \otimes e^{iHs_l}) e^{-i\frac{\Delta t}{2}\sigma_l \otimes A(s_l)} (I \otimes e^{iHs_l})$ (Ham.-sim. + ctrl-local)
  - cancellation: $(I \otimes e^{-iHs_{l+1}})(I \otimes e^{iHs_l}) = I \otimes e^{-iH\Delta s}$, avoiding long Hamiltonian simulation

Ab-Initio Eletronic Structure Problem

- Full ab-initio Hamiltonian under 2nd quantization

$$H = \sum_{p,q}^{2L} T_{pq} c_p^\dagger c_q + \frac{1}{2} \sum_{p,q,r,s}^{2L} S_{p,q,r,s} c_p^\dagger c_q^\dagger c_r c_s \tag{18}$$

- Lack geometric locality or sparsity structures, complicating the choice of Lindblad jump operators
- Simplified Hartree-Fock framework (Review Prof. Jin-Peng Liu's first lecture)

$$H_{\mathrm{HF}} = \sum_{p,q=1}^{2L} F_{pq} a_p^\dagger a_q, \quad F_{pq} = h_{pq} + V_{pq}[D] - K_{pq}[D], \quad D_{pq} = \sum_{i=1}^{N_{\mathrm{e}}} \Phi_{pi} \Phi_{qi}^* \tag{19}$$

$$F\Lambda = \Lambda\Phi, \quad \Lambda = \mathrm{diag}(\varepsilon_i) \tag{20}$$

Ground state: $|\mathrm{HF}\rangle = c_1^\dagger \cdots c_{N_{\mathrm{e}}}^\dagger |\mathrm{vac}\rangle$, $(c_1^\dagger, \cdots, c_{2L}^\dagger) = (a_1^\dagger, \cdots, a_{2L}^\dagger)\Phi$

Everything is quasi-free!

Solving Quasi-free and Quadratic Lindblad Dynamics

- See the wonderful paper: Barthel-Zhang, J. Stat. Mech. 2022
- Quadratic Hamiltonian $H = \sum_{p,q=1}^{2L} F_{pq} a_p^\dagger a_q$
- Quasi-free: linear jump operators $L_{p,+} = \sum_{r=1}^{M} a_r^\dagger L_{r,p}$, $L_{q,-} = \sum_{r=1}^{M} a_r J_{q,r}$, $L_{r,p}, J_{q,r} \in \mathbb{C}$
- One-particle reduced density matrix (1-RDM) $P_{ij} = \mathrm{Tr}\left(\rho a_j^\dagger a_i\right)$ is a $2L$ by $2L$ matrix
- The Lindblad equation
  $\partial_t \rho = -i[H,\rho] + \sum_p (L_{p,+}\rho L_{p,+}^\dagger - \frac{1}{2}\{L_{p,+}^\dagger L_{p,+}, \rho\}) + \sum_q (L_{q,-}\rho L_{q,-}^\dagger - \frac{1}{2}\{L_{q,-}^\dagger L_{q,-}, \rho\})$
- The equation of motion of P_{ij} is closed!

$$\partial_t P(t) = -i[F, P(t)] + B - \frac{1}{2}[P(t)(B+C) + (B+C)P(t)] \tag{21}$$

  where $B_{ij} = \sum_{p=1}^{M} L_{ip} L_{jp}^*$ and $C_{ij} = \sum_{p=1}^{M} J_{ip} J_{jp}^*$
- For quadratic jump $Q_s = \sum_{i,j} (Q_s)_{i,j} a_i^\dagger a_j$ with Hermitian coefficients, we can also derive a closed EOM for 1-RDM

Linear Bulk Dissipation

- Joint work with Yongtao Zhan (Caltech IQIM) and Lin Lin (UC Berkeley)
- Bulk dissipation: $\mathcal{A}_{\mathrm{I}} = \{a_p^\dagger\}_{p=1}^{2L} \cup \{a_p\}_{p=1}^{2L}$
- Thouless theorem

$$\int_{\mathbb{R}} f(s) e^{iHs} a_p^\dagger e^{-iHs} \mathrm{d}s = \int_{\mathbb{R}} f(s) \sum_{r=1}^{2L} a_r^\dagger (e^{iFs})_{r,p} e^{iHs} e^{-iHs} \mathrm{d}s = \sum_{r=1}^{2L} a_r^\dagger (\hat{f}(F))_{r,p} =: L_{p,+} \tag{22}$$

$$\int_{\mathbb{R}} f(s) e^{iHs} a_q e^{-iHs} \mathrm{d}s = \int_{\mathbb{R}} f(s) \sum_{r=1}^{2L} (e^{-iFs})_{q,r} a_r e^{iHs} e^{-iHs} \mathrm{d}s = \sum_{r=1}^{2L} a_r (\hat{f}(-F))_{q,r} =: L_{q,-} \tag{23}$$

- $\hat{f}(\omega) = 1$ on $[-2\|H\|_2, -\Delta]$ and $\hat{f}(\omega) = 0$ on $[0, +\infty)$, $B + C = \hat{f}^2(F) + \hat{f}^2(-F) = I$
- Then the EOM of 1-RDM takes the following form, with the unique stationary point $P^\star = \hat{f}(F)$

$$\partial_t P(t) = -i[F, P(t)] - P(t) + \hat{f}(F) \tag{24}$$

Li-Zhan-Lin, 2024, arXiv:2411.01470

Linear Bulk Dissipation

- In the energy basis $\widetilde{P} = \Phi^\dagger P \Phi = \left(\mathrm{Tr}\left(\rho c_j^\dagger c_i\right)\right)_{1\le i,j\le 2L}$
- $\Lambda = \mathrm{diag}(\varepsilon_i)$ with $\varepsilon_1 \le \cdots \le \varepsilon_{N_\mathrm{e}} \le 0 < \varepsilon_{N_\mathrm{e}+1} \le \cdots \le \varepsilon_{2L}$
- Stationary state $\widetilde{P}^\star = \hat{f}(\Lambda) = \mathrm{diag}(\underbrace{1,\cdots,1}_{N_\mathrm{e}},\underbrace{0,\cdots,0}_{2L-N_\mathrm{e}})$ (achieved without explicitly diagonalizing the 1-RDM)
- $\|P_1(t) - P_2(t)\|_\mathrm{F} = e^{-t}\|P_1(0) - P_2(0)\|_\mathrm{F}$, mixing time $\equiv \log 2$
- The convergence rate is universal and is independent of any chemical details or starting point!

Li-Zhan-Lin, 2024, arXiv:2411.01470

Quadratic Bulk Dissipation

- $\mathcal{A}_{\mathrm{II}} = \{a_i^\dagger a_j : 1 \le i, j \le 2L\}$
- Jump operators are upper-triangular under the eigenbasis (cannot be Hermitian)
  $L_{ij} = \int_{\mathbb{R}} e^{iHs} a_i^\dagger a_j e^{-iHs} \mathrm{d}s = \sum_{p,q=1}^{2L} \hat{f}(\varepsilon_p - \varepsilon_q) c_p^\dagger c_q \Phi_{ip}^* \Phi_{jq} = \sum_{p<q} c_p^\dagger c_q \Phi_{ip}^* \Phi_{jq}$
- orthogonal columns:
  - $\sum_{i,j=1}^{2L} L_{ij}^* L_{ij} = \sum_{ij} \sum_{p<q} \sum_{r<s} c_q^\dagger c_p c_r^\dagger c_s \Phi_{ip} \Phi_{jq}^* \Phi_{ir}^* \Phi_{js} = \sum_{p<q} c_q^\dagger c_p c_p^\dagger c_q = \sum_{p<q} (1 - n_p) n_q$
  - Simularly $\mathcal{L}_L^\dagger [c_r^\dagger c_s] = \sum_{ij} L_{ij}^* c_r^\dagger c_s L_{ij} - \frac{1}{2}\{L_{ij}^* L_{ij}, c_r^\dagger c_s\} = -\frac{1}{2}(M_r + M_s + 1) c_r^\dagger c_s$ for $r \neq s$ with $M_k = \sum_{p<k}(1 - n_p) + \sum_{q>k} n_q$
  - $\mathcal{L}_L^\dagger [c_r^\dagger c_r] = \sum_{q>r} (1 - n_r) n_q - \sum_{p<r} (1 - n_p) n_r$
- EOM of 1-RDM: $\partial_t \widetilde{P}_{sr} = \begin{cases} -\mathrm{i}\left(\varepsilon_s - \varepsilon_r\right) \widetilde{P}_{sr} - \frac{1}{2} \left\langle \left(M_r + M_s + 1\right) c_r^\dagger c_s \right\rangle & r < s, \\ -\mathrm{i}\left(\varepsilon_s - \varepsilon_r\right) \widetilde{P}_{sr} - \frac{1}{2} \left\langle c_r^\dagger c_s \left(M_r + M_s + 1\right) \right\rangle & r > s. \end{cases}$
  $\partial_t \widetilde{P}_{rr} = -\langle M_r n_r \rangle + \sum_{q>r} \langle n_q \rangle$

Li-Zhan-Lin, 2024, arXiv:2411.01470

Mean-field and Spectral Gap Analysis

mean-field qualitative analysis

mean-field approximation

- diagonal $\partial_t \widetilde{P}_{rr} \approx -\langle M_r \rangle \widetilde{P}_{rr} + \sum_{q>r} \widetilde{P}_{qq}$ and $M_k \succeq 1$ for $r < N_{\mathrm{e}}$ and $r > N_{\mathrm{e}} + 1$
- off-diagonal $\partial_t \widetilde{P}_{sr} \approx \left[-\frac{1}{2}\left(1 + \langle M_r + M_s \rangle\right) + \mathrm{i}\left(\varepsilon_r - \varepsilon_s\right)\right] \widetilde{P}_{sr}$ and $M_r + M_s \succeq 0$

spectral gap analysis

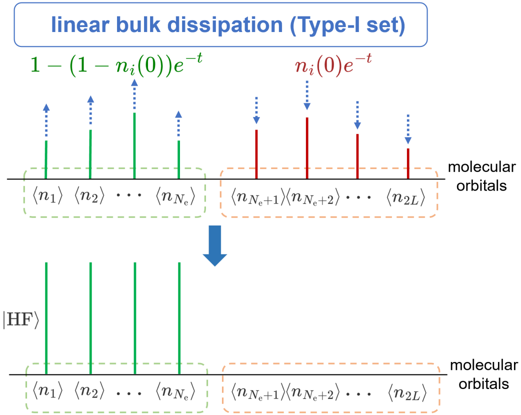
Theorem (**Li**-Zhan-Lin, 2024)

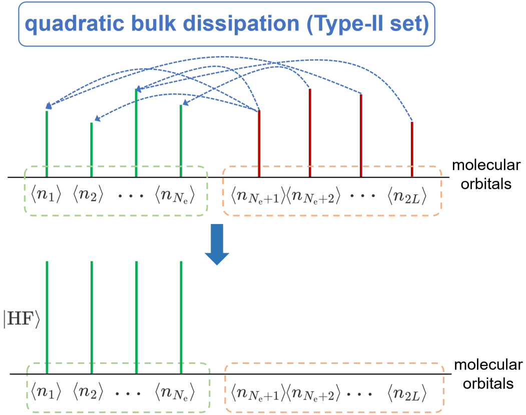
Let $H_{\mathrm{dp}} = \frac{1}{2}\sum_k L_k^* L_k$ *be the frustration-free parent Hamiltonian of the ground state* $|\psi_0\rangle$ *s.t.* $[H, H_{\mathrm{dp}}] = 0$, *then the spectral gap of* $\mathcal{L}$ *is equal to the gap of* H_{dp}.

Type I: $H_{\mathrm{dp}} = \frac{1}{2}\sum_{p \le N_{\mathrm{e}}}(1 - n_p) + \frac{1}{2}\sum_{q > N_{\mathrm{e}}} n_q$, $\Delta_{\mathcal{L}} = \frac{1}{2}$ (number orbitals commute with H!)
Type II: $H_{\mathrm{dp}} = \frac{1}{2}\sum_{p<q}(1 - n_p) n_q$, $\Delta_{\mathcal{L}} = \frac{1}{2}$

Li-Zhan-Lin, 2024, arXiv:2411.01470

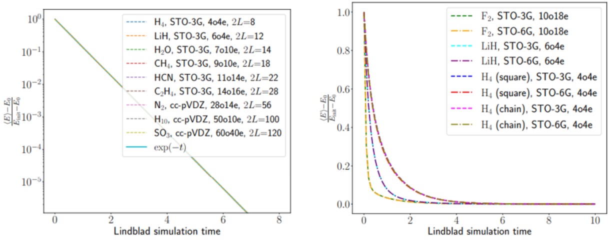
Conceptual Illustration

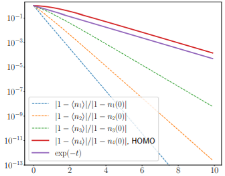




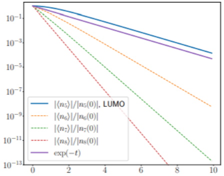
Li-Zhan-Lin, 2024, arXiv:2411.01470

Numerical Validations

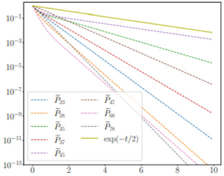




(a) Convergence of the diagonal entries $\widetilde{P}_{rr} = \langle n_r\rangle$ of the 1-RDM for $r \le N_e$



(b) Convergence of the diagonal entries $\widetilde{P}_{rr} = \langle n_r\rangle$ of the 1-RDM for $r \ge N_e + 1$



(c) Convergence of the off-diagonal entries of the 1-RDM. We plot $|\widetilde{P}_{ij}|/|\widetilde{P}_{ij}(0)|$ for each curve.

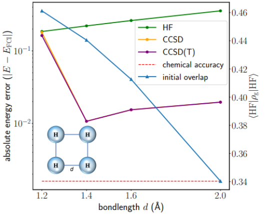
Li-Zhan-Lin, 2024, arXiv:2411.01470

Transferability to Full *Ab Initio* Case

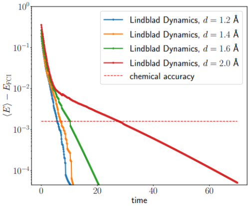
- Full configuration iteraction (FCI) space

$$\mathcal{F}_{N_\mathrm{e}} = \{|\Psi\rangle : \langle\Psi|N|\Psi\rangle = N_\mathrm{e}\} \subset \mathcal{F}, \quad \dim\mathcal{F}_{N_\mathrm{e}} = \binom{2L}{N_\mathrm{e}} \tag{25}$$

- Operator reduction using active space idea (only take r orbitals around the Fermi surface): $\mathcal{S}_\mathrm{I}$, $\mathcal{S}_\mathrm{II}$, $\mathcal{T}_\mathrm{II}$ and starting from Hartree-Fock or low-excited Slater determinants
- Even work for strongly correlated systems with $\mathcal{T}_\mathrm{II}$ set coupling operators



(a) The accuracy of the HF, CCSD and CCSD(T) energy and the initial overlap between the HF state and the true ground state ρ_g under difference bondlengths for square H_4 system in STO-3G



(b) The energy error relative to FCI energy vs. Lindblad simulation time for $d = 1.2, 1.4, 1.6$ and 2.0 Å

Li-Zhan-Lin, 2024, arXiv:2411.01470

Play More with Lindbladians?

- Ding-Li-Lin, 2024, arXiv:2404.05998: Efficient Gibbs samplers with detailed-balance condition
- Ding-Li-Lin-Zhang, 2024, arXiv:2410.01206: Low-Temp. Gibbs states for 2D toric code
- Tamascelli-Smirne-Huelga-Plenio, PRL 2018; Park-Huang-Zhu-Yang-Chan-Lin, PRB 2024
  Simulating non-equilibrium system-bath coupling dynamics via Lindbladians
- Barthel-Zhang, J. Stat. Mech. 2022; Huang-Lin-Park-Zhu, 2024, arXiv:2411.08741
  Understand the Lindblad/general Liouville dyanmics in quasi-free or quadratic systems
- Chen-Lu-Wang-Liu-Li, 2023, arXiv:2311.15587
  Using the Lindblad equation as an algorithmic tool for classical optimization
- Bardet-Capel-Gao-EtAl, PRL 2023; Fang-Lu-Tong, 2024, arXiv:2404.11503
  Understanding the mixing time of Lindblad dynamics for state preparation problems

Thank You!

If you have any questions, feel free to ask!