Single-ancilla ground state preparation via Lindbladians

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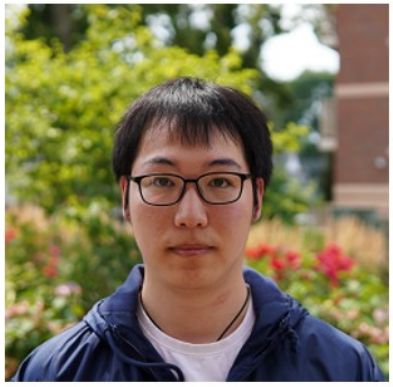
Joint work with

Anthony Chen
(Caltech)



Zhiyan Ding
(Morrey Assistant Prof.)

(Ding, Chen, **Lin**, arXiv:2308.15676)

How to prepare ground state

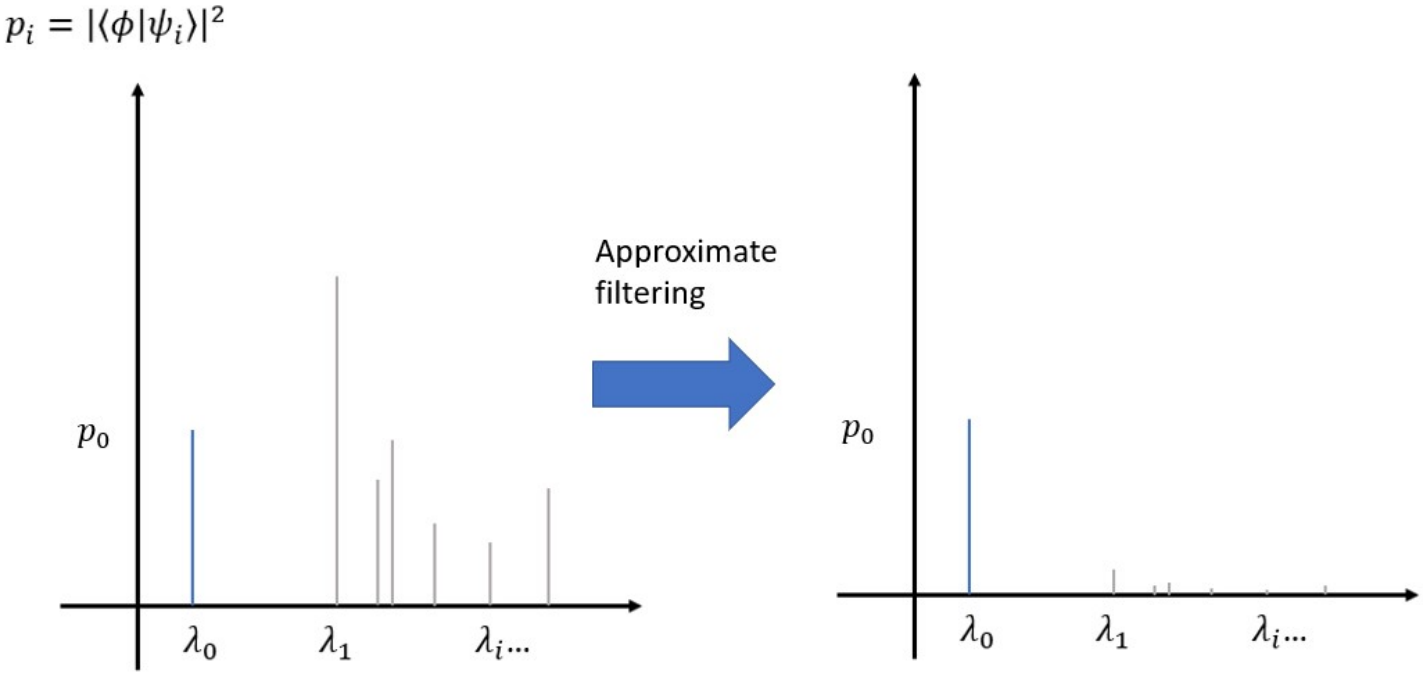
with zero initial overlap?

Ground state problem

$$H|\psi_0\rangle = \lambda_0 |\psi_0\rangle$$

- The problem is QMA-hard in the worst case.
- Common additional assumption: good initial state $|\phi\rangle = U_I|0^n\rangle$: $p_0 = \gamma^2 = |\langle\phi|\psi_0\rangle|^2 = \Omega(1/\mathrm{poly}(n))$.
- Most works (QPE, many post-QPE methods) adopt this assumption (see Yu Tong's tutorial talk, Tuesday's talk in this workshop)

The difficulty of QPE and post-QPE methods



They are essentially filtering methods.

Do not work if $p_0 = |\langle\phi|\psi_0\rangle|^2$ is small (# repetition p_0^{-1})

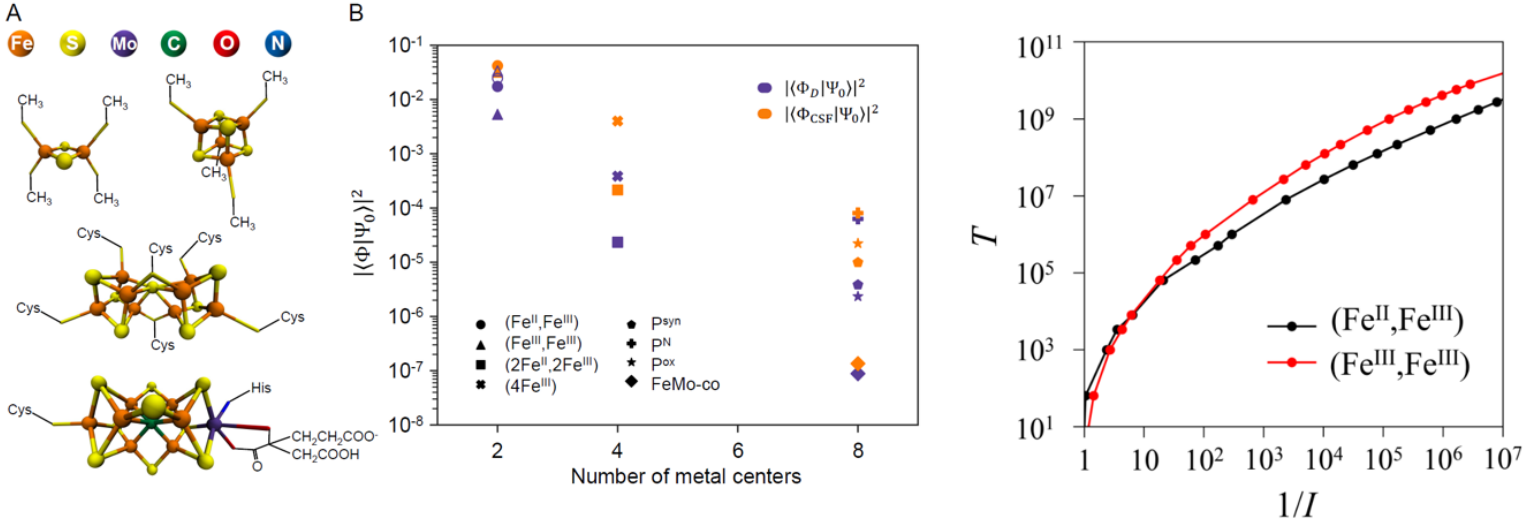
Good initial overlap for strongly correlated systems?

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

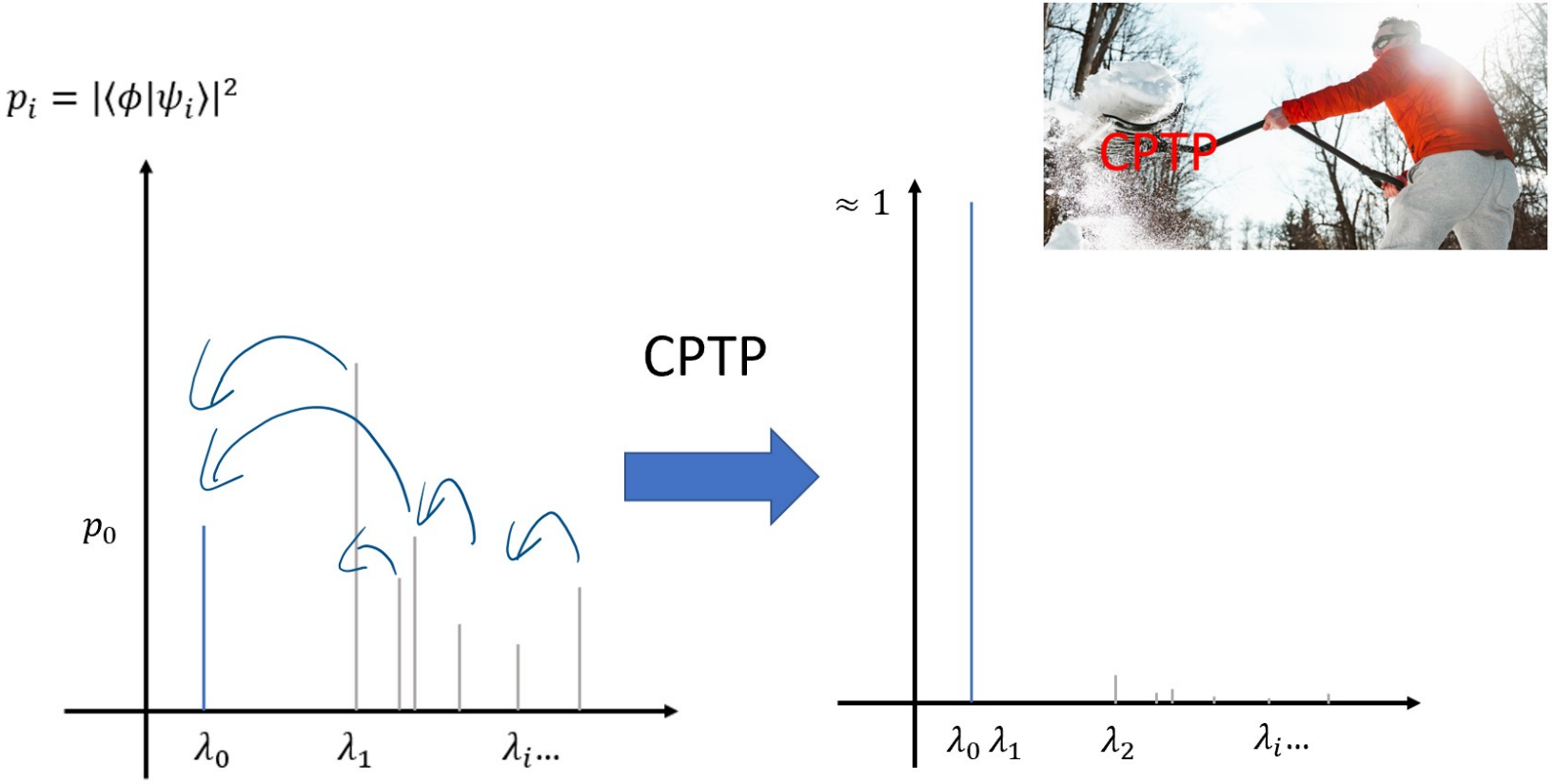


Possible to eliminate p_0 dependence?

- QMA-hardness: cannot prepare ground state just by knowing H.
- $p_0 = \Omega(1/\mathrm{poly}(n))$ is sufficient but not necessary for efficient preparation. Some other assumptions?
- Parameterized circuit (VQE; MPS); Adiabatic; Lindblad
- Open quantum system ideas for preparing thermal states
- Key theoretical assumption: $\mathrm{poly}(n)$ mixing time.

(Chen-Brandao, 2112.07646), (Chen, Kastoryano, Brandao, Gilyen, 2303.18224)
(Shtanko, Movassagh, 2112.14688), (Rall, Wang, Wocjan, 2210.01670)
(Cubitt, 2303.11962)

Lindblad idea for ground state preparation



From filtering to shoveling.

If works ($\mathrm{poly}(n)$ mixing time), succeeds w.p. 1, independent of p_0 (and initial guess in general)!

Main results (algorithm)

$$H|\psi_i\rangle = \lambda_i |\psi_i\rangle, \quad \lambda_1 - \lambda_0 \geq \Delta.$$

Query $e^{\pm iHt}$. Cost measured by total simulation time.
Error measured by trace norm of ρ w.r.t. some dynamics.
Hopefully, this dynamics converges to ground state.

- Prepare ground state from zero overlap.
- One jump operator. One ancilla qubit.
- Continuous-time simulation:
  $T_{H,\text{total}} = \widetilde{\Theta}\left((1+\|H\|)\Delta^{-1} T^{2+o(1)} \epsilon^{-1-o(1)}\right)$
- Discrete-time simulation (just Lindblad with a large step size)
  $T_{H,\text{total}} = \widetilde{\Theta}(\Delta^{-1} T^{1+o(1)} \epsilon^{-o(1)})$
  Quadratic improvement in T, arbitrary polynomial improvement in ϵ, exponential improvement in $\|H\|$ ($\Rightarrow$ quadratic improvement in gate cost).

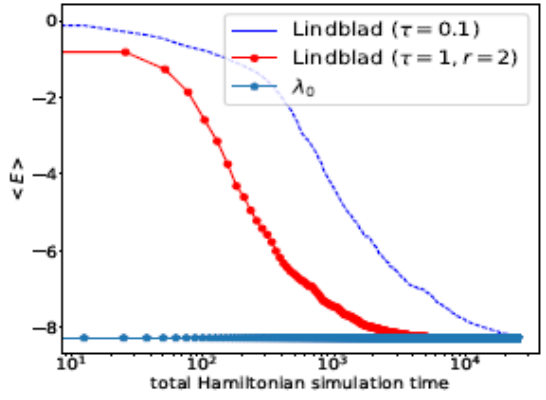
(Ding, Chen, **Lin**, arXiv:2308.15676)

Other results (mixing time)

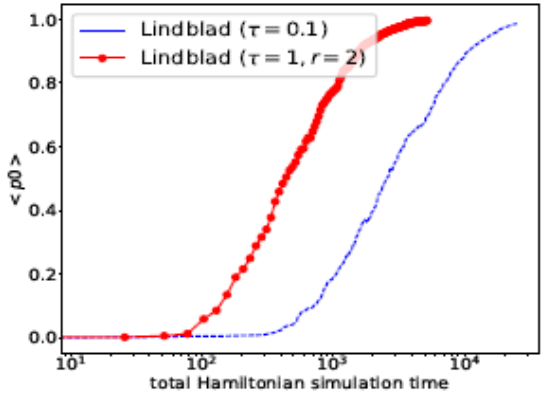
- With random coupling matrix (motivated from eigenstate thermalization hypothesis, ETH), ground state $\rho = |\psi_0\rangle\langle\psi_0|$ is the unique fixed point starting from diagonal $\rho(0)$ (e.g. $\propto I$).
- With random coupling matrix, additional structures on eigenvalue distribution gives $\mathrm{poly}(n)$ mixing time.

(Ding, Chen, **Lin**, arXiv:2308.15676)

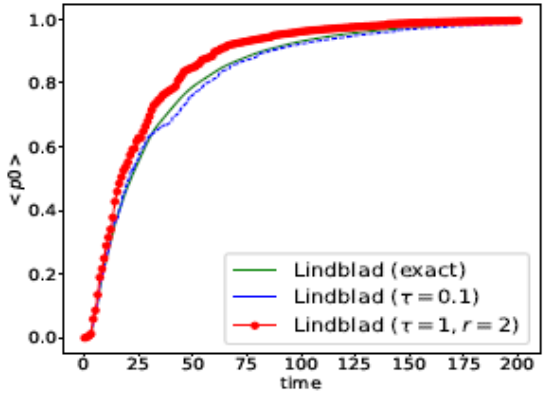
Numerical results (TFIM-6)



(a) Hamiltonian simulation time vs energy

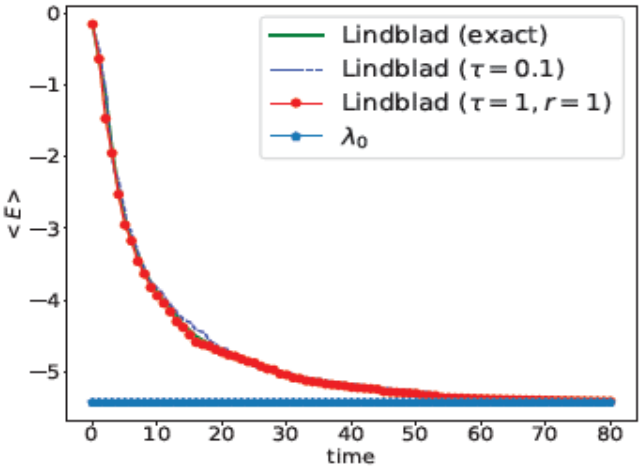


(b) Hamiltonian simulation time vs overlap

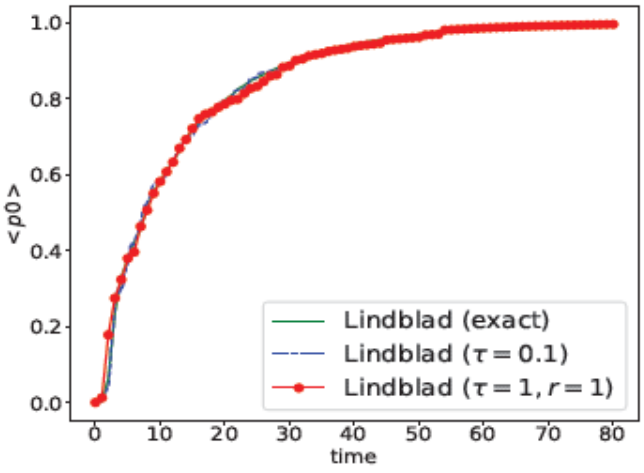


(c) Lindblad simulation time vs overlap

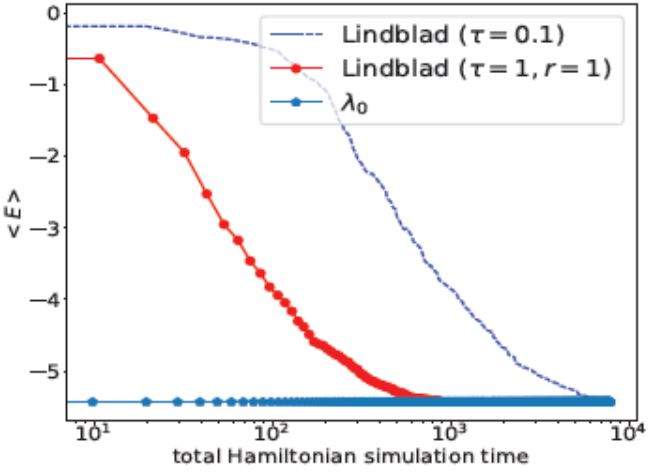
Numerical examples (TFIM-4)



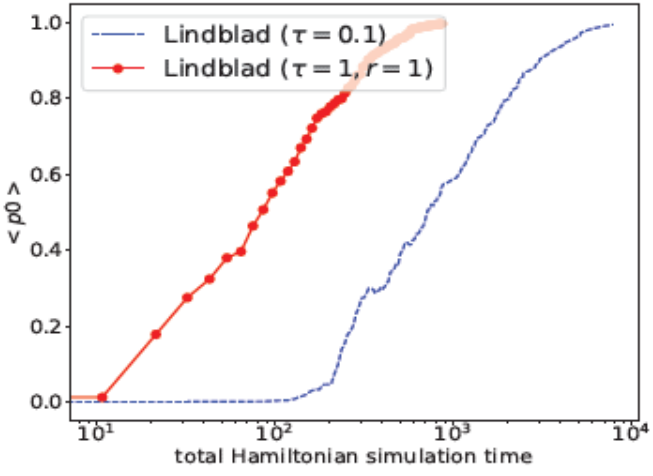
(a) Lindblad simulation time vs energy



(b) Lindblad simulation time vs overlap

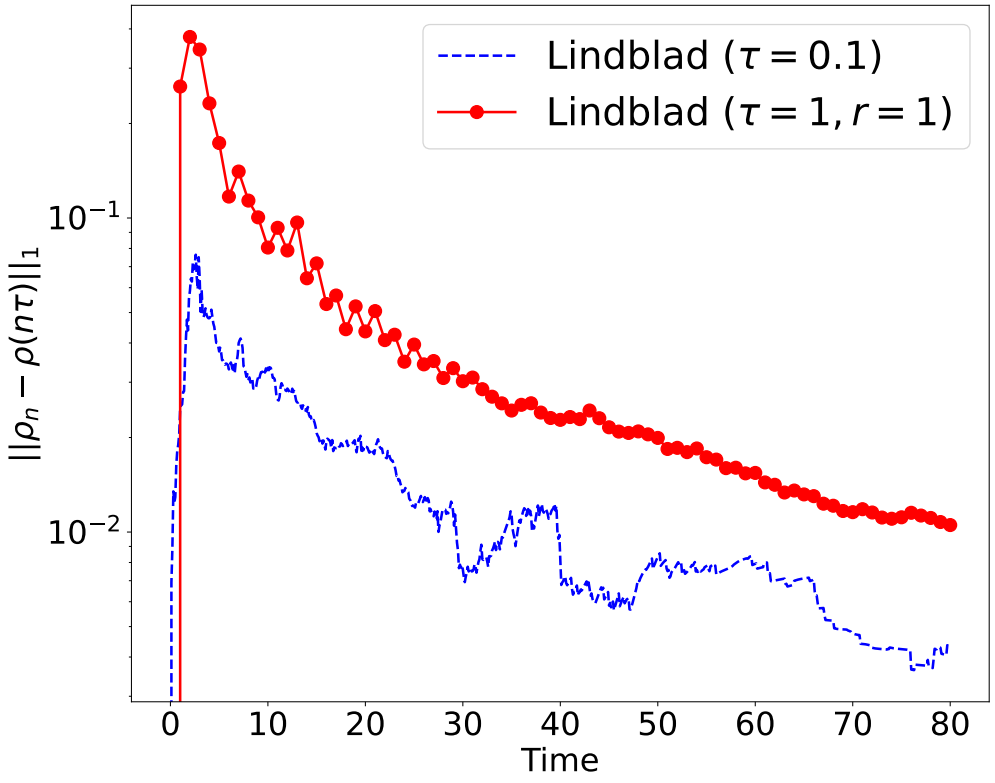


(c) Hamiltonian simulation time vs energy

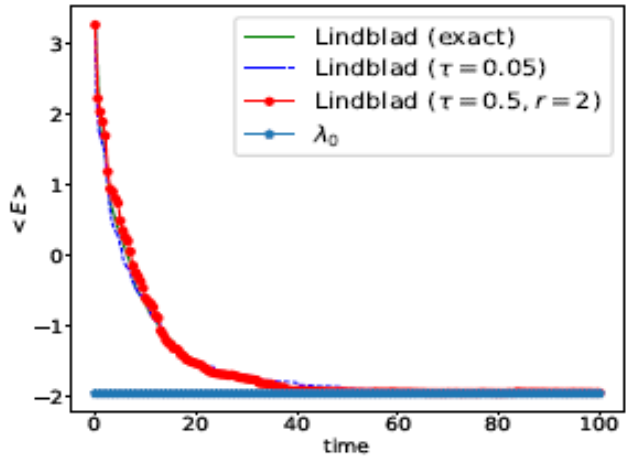


(d) Hamiltonian simulation time vs overlap

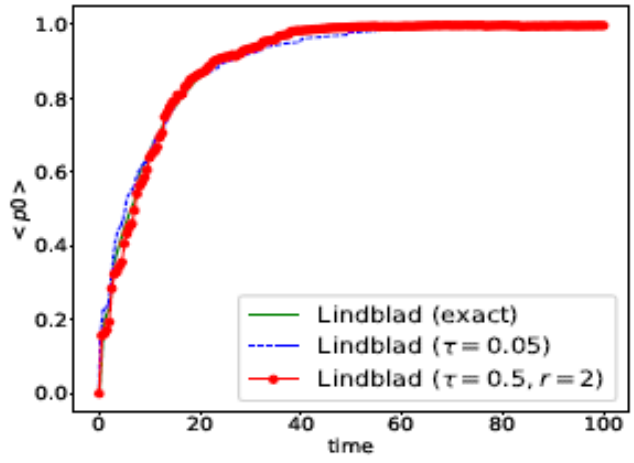
TFIM-4


Lindblad ($\tau = 0.1$)
Lindblad ($\tau = 1, r = 1$)
$||\rho_n - \rho(n\tau)||_1$
10^{-1}
10^{-2}
0
10
20
30
40
50
60
70
80
Time

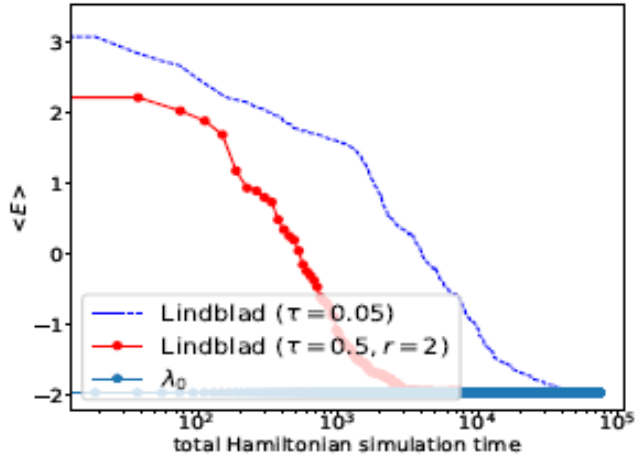
Numerical results (Hubbard-4)



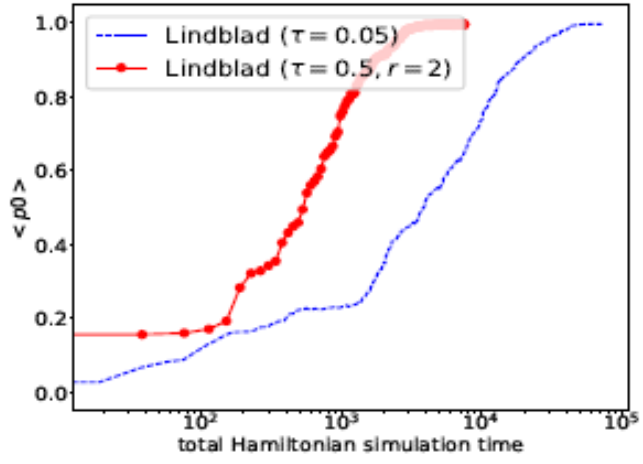
(a) Lindblad simulation time vs energy



(b) Lindblad simulation time vs overlap



(c) Hamiltonian simulation time vs energy

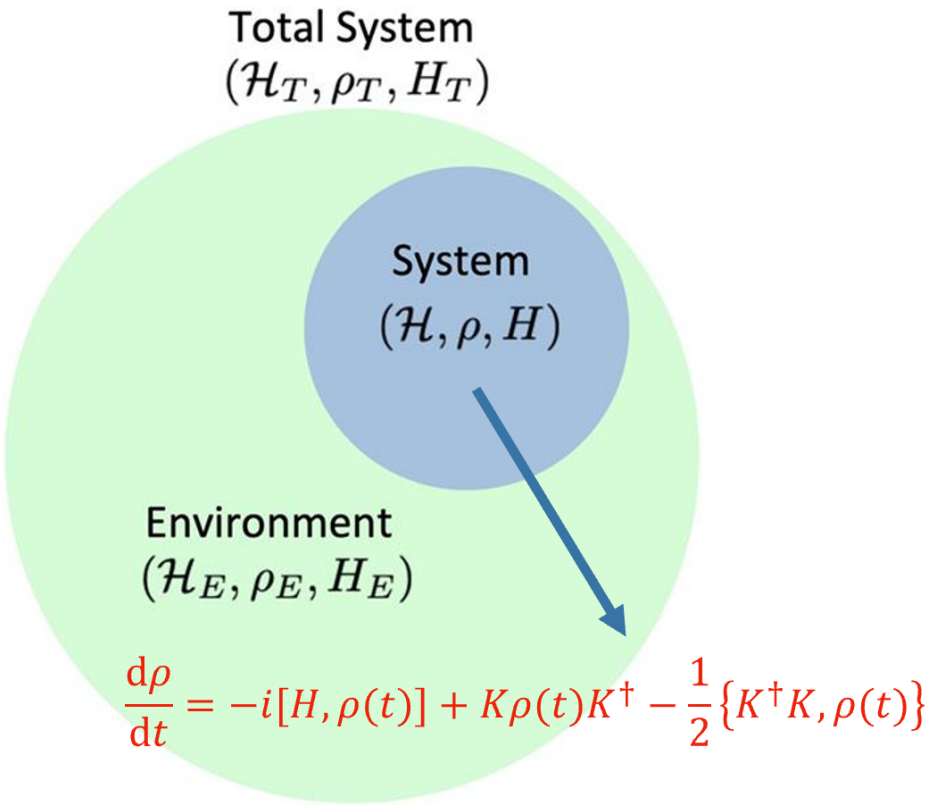


(d) Hamiltonian simulation time vs overlap

Algorithm

Lindblad dynamics for open quantum system

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -i[H, \rho(t)] + \sum_{\alpha} K_\alpha \rho(t) K_\alpha^\dagger - \frac{1}{2}\left\{K_\alpha^\dagger K_\alpha, \rho(t)\right\} .$$



(Lindblad, CMP 1976) (Gorini-Kossakowski-Sudarshan, JMP 1976)

Lindblad dynamics

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -i[H,\rho(t)] + \sum_{\alpha} K_\alpha \rho(t) K_\alpha^\dagger - \frac{1}{2}\left\{K_\alpha^\dagger K_\alpha, \rho(t)\right\} .$$

Solution map $\mathcal{T}_t : \rho(0) \to \rho(t)$:

- $\mathcal{T}_t$ is not a unitary map.
- $\mathcal{T}_t$ is a completely positive trace-preserving (CPTP) map.
  $\Rightarrow \rho(t)$ is still a density operator.

A simple Lindblad dynamics

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

1-qubit system:

$$H = -Z = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, K = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \rho(0) = |\psi_1\rangle\langle\psi_1| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}.$$

Solution:

$$\rho(t) = \begin{bmatrix} 1 - e^{-t} & 0 \\ 0 & e^{-t} \end{bmatrix} \to |\psi_0\rangle\langle\psi_0| , \quad t \to \infty .$$

Converge to the ground state exponentially fast!

A simple Lindblad dynamics

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

1-qubit system:

$$H = -Z = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, K = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \rho(0) = |\psi_1\rangle\langle\psi_1| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}.$$

- $\mathcal{L}_\mathcal{K}(|\psi_1\rangle\langle\psi_1|) = |\psi_0\rangle\langle\psi_0|$
  Push high energy state to low energy state
- $\mathcal{L}_\mathcal{K}(|\psi_0\rangle\langle\psi_0|) = 0 \Rightarrow \frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = 0$ if $\rho(t) = |\psi_0\rangle\langle\psi_0|$
  Preserve the ground state energy

Ergodic Lindblad dynamics

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -i[H,\rho(t)] + \sum_{\alpha} K_\alpha \rho(t) K_\alpha^\dagger - \frac{1}{2}\left\{K_\alpha^\dagger K_\alpha, \rho(t)\right\} .$$

Ergodic means:

- $\exists \rho_\infty$ (fix point) such that

$$\rho(t) \to \rho_\infty, \quad \forall \rho_0 .$$

- $\exists T$ (mixing time) such that

$$\|\rho(T) - \rho_\infty\| \leq \frac{1}{2}\|\rho(0) - \rho_\infty\|, \quad \forall \rho_0, t \geq T.$$

$\Rightarrow \|\rho(t) - \rho_\infty\| \leq \epsilon$ when $t = \mathcal{O}(T \log(1/\epsilon))$.
Independent of $\rho(0)$!

Lindblad for thermal state (Chen et al, 2303.18224)

- Lindblad dynamics as an algorithmic tool

$$\partial_t \rho(t) = \sum_{\alpha=1}^{N_K} \mathcal{L}_{K_\alpha}[\rho(t)], \quad \mathcal{L}_{K_\alpha}[\rho] = K_\alpha \rho K_\alpha^\dagger - \frac{1}{2}\{K_\alpha^\dagger K_\alpha, \rho\}$$

  can drive the system to the thermal state,

$$\lim_{t\to\infty} \rho(t) \approx \rho_\beta = e^{-\beta H}/Z.$$

- Quantum detailed balance, and fixes the thermal state

$$\sum_{\alpha=1}^{N_K} \mathcal{L}_{K_\alpha}[\rho_\beta] \approx 0.$$

From thermal state to ground state

$$\hat{f}(\omega) = 0 \quad \forall \omega \geq 0, \quad \hat{f}(\omega) = \int_{\mathbb{R}} f(s) e^{i\omega s} \mathrm{d}s. \tag{1}$$

Notice

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

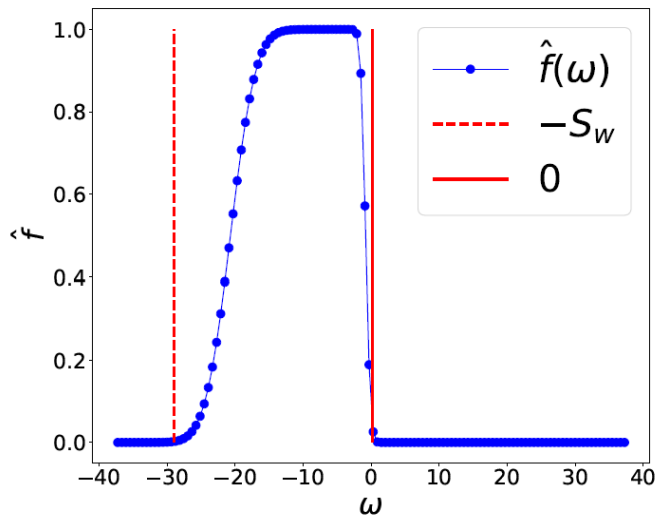
$$= \sum_{i<j} \hat{f}(\lambda_i - \lambda_j) \, |\psi_i\rangle \langle \psi_i | A | \psi_j \rangle \langle \psi_j |$$

Coupling matrix A can be Hermitian and local (and not block diagonal in eigenbasis of H):

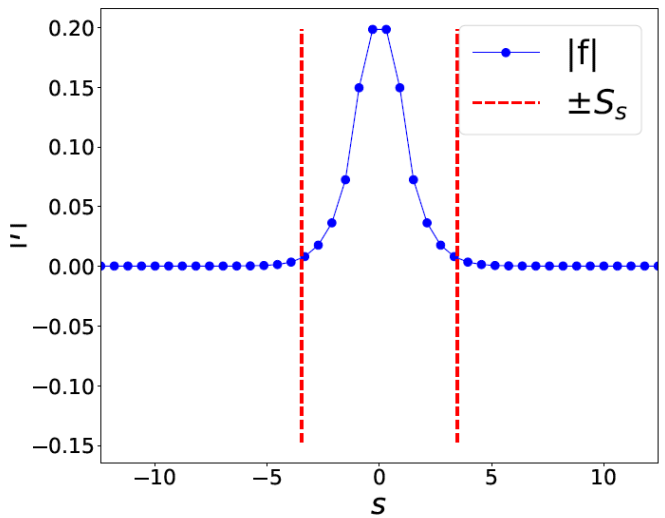
- $\mathcal{L}_K(|\psi_0\rangle \langle \psi_0|) = 0$ fix ground state
- $\langle \psi_i | \mathcal{L}_K(|\psi_j\rangle \langle \psi_j|) |\psi_i\rangle > 0$ for $i < j$ high $\Rightarrow$ low
- $\langle \psi_i | \mathcal{L}_K(|\psi_j\rangle \langle \psi_j|) |\psi_i\rangle = 0$ for $i \geq j$ low $\not\Rightarrow$ high

One possible choice of f

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



(a) $\hat{f}(\omega)$



(b) $f(s)$

$$a, S_w = \Theta(\|H\|), b, \delta_b = \Theta(\Delta) \quad \Rightarrow S_s = \Theta(\Delta^{-1}).$$

New method (Lindblad for ground state)

Lindblad dynamics with one jump operator

$$\partial_t \rho(t) = -i[H, \rho(t)] + K\rho(t)K^\dagger - \frac{1}{2}\left\{K^\dagger K, \rho(t)\right\}$$

- One jump operator $K = \int_{-\infty}^{\infty} f(s) e^{iHs} A e^{-iHs}\, \mathrm{d}s$
- $\mathcal{L}_K(|\psi_0\rangle\langle\psi_0|) = 0$
  fix ground state
- $\langle\psi_i|\,\mathcal{L}_K(|\psi_j\rangle\langle\psi_j|)\,|\psi_i\rangle > 0$ for some $i < j$
  push high energy states towards low energy states

(Ding, Chen, **Lin**, arXiv:2308.15676)

Quantum simulation of Lindblad dynamics

Generic:

- (Kliesch et al, arXiv:1105.3986): $\mathcal{O}(T^2/\epsilon)$.
- (Childs-Li, arXiv:1611.05543): $\mathcal{O}(T^{1.5}/\epsilon^{0.5})$
- (Cleve-Wang, arXiv:1612.09512): $\mathcal{O}(T\mathrm{polylog}(T/\epsilon))$
- (Li-Wang, arXiv:2212.02051): $\mathcal{O}(T\mathrm{polylog}(T/\epsilon))$. Simplified implementation. Reduced gate complexity in # jump operator

New algorithms in the current context:

- Complex form of jump operator $K = \int_{-\infty}^{\infty} f(s) e^{iHs} A e^{-iHs} \, \mathrm{d}s$.
- Need fixed point and not dynamics.

Simulation:

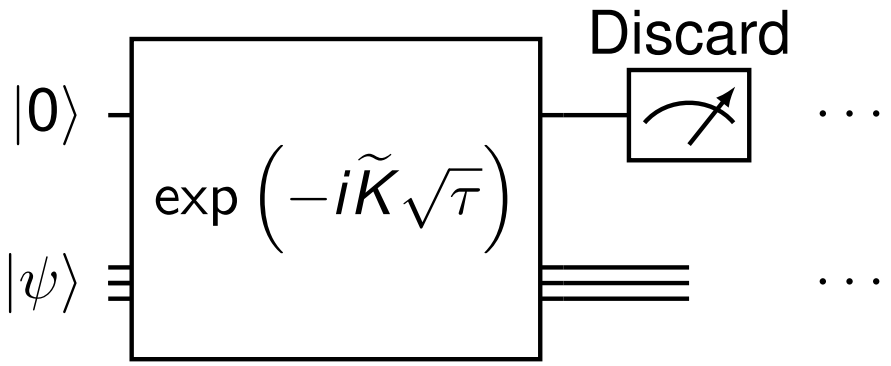
- First order Trotter:

$$\rho(\tau) = \underbrace{\exp(\mathcal{L}_H \tau)}_{\exp(-iH\tau)} \exp(\mathcal{L}_K \tau)\rho(0) + \mathcal{O}(\tau^2)$$

Note $\exp(\mathcal{L}_K \tau)$ is not a unitary operator.

- Use idea[1]: Let $\widetilde{K} = |0\rangle\langle 1| \otimes K^\dagger + |1\rangle\langle 0| \otimes K$

$$\mathrm{Tr}_a\left(\exp\left(-i\widetilde{K}\sqrt{\tau}\right)|0\rangle\langle 0| \otimes \rho \exp\left(i\widetilde{K}\sqrt{\tau}\right)\right) = \exp(\mathcal{L}_K \tau)\rho(0) + \mathcal{O}(\tau^2)$$



[1] (Cleve-Wang,arXiv:1612.09512)

Simulate $\exp\left(-i\widetilde{K}\sqrt{\tau}\right)$

- Quadrature:

$$K \approx \sum \underbrace{f(s_l)e^{iHs_l}Ae^{-iHs_l}\Delta_s}_{K_l}$$

- Second order Trotter:

$$\exp\left(-i\widetilde{K}\sqrt{\tau}\right) \approx \exp\left(-i\sum_l \widetilde{K}_l\sqrt{\tau}\right)$$

$$= \underbrace{\prod_{l=1}^{\leftarrow} \exp\left(-i\widetilde{K}_l\sqrt{\tau}/2\right) \prod_{l=L}^{\rightarrow} \exp\left(-i\widetilde{K}_l\sqrt{\tau}/2\right)}_{W(\tau)} + \mathcal{O}(\tau^{3/2})$$

- After tracing out,

$$\mathrm{Tr}_a\left(\exp\left(-i\widetilde{K}\sqrt{\tau}/2\right)|0\rangle\langle 0| \otimes \rho \exp\left(i\widetilde{K}\sqrt{\tau}/2\right)\right)$$

$$= \mathrm{Tr}_a\left(W(\tau)|0\rangle\langle 0| \otimes \rho W^\dagger(\tau)\right) + \mathcal{O}(\tau^2), \qquad \text{Next: } \exp\left(-i\widetilde{K}_l\sqrt{\tau}/2\right)$$

Simulate $\exp\left(-i\widetilde{K}_l\sqrt{\tau}/2\right)$

- Let $A(s) = e^{iHs}Ae^{-iHs}$,

$$\widetilde{K}_l = \sigma_l \otimes A(s_l) \quad \text{where} \quad \sigma_l := w_l(\sigma_x \operatorname{Re} f(s_l) + \sigma_y \operatorname{Im} f(s_l))$$

$\Rightarrow$

$$\exp\left(-i\frac{\sqrt{\tau}}{2}\sigma_l \otimes A(s_l)\right) = (I \otimes e^{iHs_l})\underbrace{e^{-i\frac{\sqrt{\tau}}{2}\sigma_l \otimes A}}_{=:\widetilde{A}_l(\sqrt{\tau})}(I \otimes e^{-iHs_l}).$$

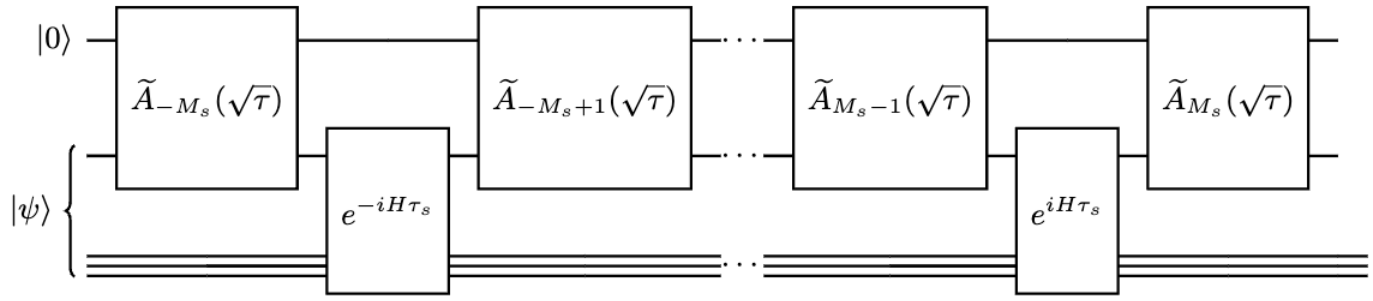
Hamiltonian simulation+controlled local operator $\left(\widetilde{A}_l\right)$

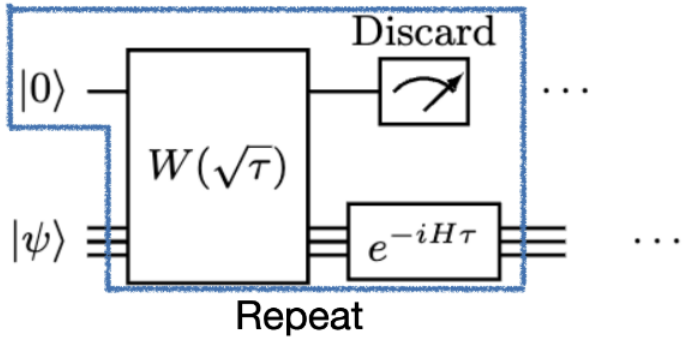
- $s_l \to s_{l+1}$

$$(I \otimes e^{-iHs_{l+1}})(I \otimes e^{iHs_l}) = I \otimes e^{-iH\Delta s}$$

Avoid long Hamiltonian simulation

Continous Lindblad simulation





One ancilla qubit, simple gates

Theorem

For simulation time T and precision ϵ, the total Hamiltonian simulation time is

$$T_{H,\text{total}} = \widetilde{\Theta}\left(T^{2+o(1)}\epsilon^{-1-o(1)}\right), \qquad \textit{First order accuracy}$$

Discrete-time Lindblad simulation

- Why first order? first order Trotter at the beginning

$$\rho(\tau) = \exp(\mathcal{L}_H \tau) \exp(\mathcal{L}_K \tau)\rho(0) + \mathcal{O}(\tau^2)$$

- Notice $\exp(\mathcal{L}_H \tau) \exp(\mathcal{L}_K \tau)(|\psi_0\rangle \langle\psi_0|) \approx |\psi_0\rangle \langle\psi_0|$.
  Always fixes the ground state

- Simulate a discrete Lindblad with $\tau = \mathcal{O}(1)$

$$\rho(n\tau) = (\exp(\mathcal{L}_H \tau)\exp(\mathcal{L}_K \tau))^n \rho(0)$$

$\exp\left(-i\widetilde{K}_l\sqrt{\tau}/2\right) \approx (W(\sqrt{\tau}/r))^r$ choose proper r

Theorem

For simulation time $T = N\tau$ and precision ϵ, the total Hamiltonian simulation time is

$$T_{H,\text{total}} = \widetilde{\Theta}\left(T^{1+o(1)}\epsilon^{-o(1)}\right).$$

Conclusion

- Open quantum system (Lindblad dynamics) is a potential candidate for ground state preparation.
- Early fault-tolerant quantum algorithm:
  Lindblad dynamics can be simulated with one ancilla qubit and simple gates.
- Replace assumption on p_0 by mixing time.
- What can help further: More jumps operators? Coherent contribution? Non-Markovian? Variational?

Acknowledgment

Thank you for your attention!

Lin Lin
https://math.berkeley.edu/~linlin/

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