Quantum algorithmic tools for simulating open quantum systems

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joint work with
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CAUTION
HEAVY PHYSICS JARGON
PLEASE ASK QUESTIONS!

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- After time t the induced channel is the superoperator

$$\exp(t\mathcal{L}[\cdot])$$

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New generic input model

Block-encoding of a Lindbladian

Given a purely dissipative Lindbladian

$$\mathcal{L}[\rho] := \sum_{j\in J}\Big(\boldsymbol{L}_j\rho\boldsymbol{L}_j^\dagger - \frac{1}{2}\boldsymbol{L}_j^\dagger\boldsymbol{L}_j\rho - \frac{1}{2}\rho\boldsymbol{L}_j^\dagger\boldsymbol{L}_j\Big),$$

we say that a unitary matrix is a block-encoding of the Lindblad operators $\{\boldsymbol{L}_j\}_{j\in J}$ if

$$(\left\langle 0^b\right| \otimes \boldsymbol{I}) \cdot \cdot(\left|0^c\right\rangle \otimes \boldsymbol{I}) = \sum_{j\in J} |j\rangle \otimes \boldsymbol{L}_j \quad \text{for} \quad b, c \in \mathbb{N}.$$

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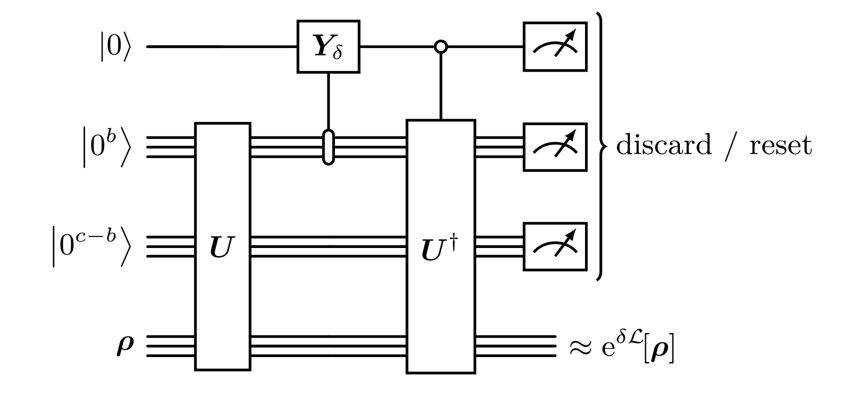
- In principle a block-encoding exists if $\left\|\sum_{j=0}^{m} \boldsymbol{L}_j^\dagger \boldsymbol{L}_j\right\| \leq 1$
- Prior methods depended on $\sum_{j=0}^{m}\left\|\boldsymbol{L}_j^\dagger \boldsymbol{L}_j\right\| \leq 1$

Weak measurement scheme for Lindbladians

Block-encoding of Lindblad generators

We say that the unitary U is a block encoding of the purely irreversible generator $\mathcal{L}$ consisting of Lindblad operators $\boldsymbol{L}_j$ if $(\langle 0^b| \otimes I)U(|0^a\rangle \otimes I) = \sum_{j=0}^{m} |j\rangle \otimes \boldsymbol{L}_j$.



Here $Y_\delta = e^{-i \arcsin \sqrt{\delta} Y}$ for the Pauli-Y gate.

1. Apply $\boldsymbol{U}$.

2. Append an ancilla qubit in state $|0\rangle$ and rotate it with angle $\arcsin\sqrt{\delta}$ controlled on the $\left|0^b\right\rangle$ state (indicating the successful application of a jump).

3. Apply $\boldsymbol{U}^\dagger$ controlled on the ancilla qubit being 0.

4. Measure and discard all but the system register.

Assuming the system register is in the pure state $|\psi\rangle$, this circuit $\boldsymbol{C}$ acts as follows:

$$
\begin{aligned}
|0\rangle\cdot|0^c\rangle|\psi\rangle &\overset{(1)}{\to} |0\rangle\cdot\boldsymbol{U}|0^c\rangle|\psi\rangle\\
&\overset{(2)}{\to} \left(\sqrt{1-\delta}|0\rangle+\sqrt{\delta}|1\rangle\right)\cdot\left(|0^b\rangle\langle 0^b|\otimes\boldsymbol{I}\right)\boldsymbol{U}|0^c\rangle|\psi\rangle \quad + \quad |0\rangle\cdot\left(\boldsymbol{I}-|0^b\rangle\langle 0^b|\otimes\boldsymbol{I}\right)\boldsymbol{U}|0^c\rangle|\psi\rangle\\
&= |0\rangle\cdot\boldsymbol{U}|0^c\rangle|\psi\rangle \quad + \quad \sqrt{\delta}|1\rangle\cdot\left|0^b\right\rangle\underbrace{\left(\left\langle 0^b\right|\otimes\boldsymbol{I}\right)\boldsymbol{U}|0^c\rangle|\psi\rangle}_{|\psi_0'\rangle:=} \quad - \quad (1-\sqrt{1-\delta})|0\rangle\cdot\left(|0^b\rangle\langle 0^b|\otimes\boldsymbol{I}\right)\boldsymbol{U}|0^c\rangle|\psi\rangle\\
&\overset{(3)}{\to} |0\rangle\cdot|0^c\rangle|\psi\rangle \quad + \quad \sqrt{\delta}|1\rangle\cdot\left|0^b\right\rangle|\psi_0'\rangle \quad - \quad (1-\sqrt{1-\delta})|0\rangle\cdot\boldsymbol{U}^\dagger\left(|0^b\rangle\langle 0^b|\otimes\boldsymbol{I}\right)\boldsymbol{U}|0^c\rangle|\psi\rangle\\
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&= |0\rangle\cdot|0^c\rangle\left(\boldsymbol{I}-\underbrace{(1-\sqrt{1-\delta})}_{\frac{\delta}{2}+\mathcal{O}(\delta^2)}\sum_{j\in J}\boldsymbol{L}_j^\dagger\boldsymbol{L}_j\right)|\psi\rangle+\sqrt{\delta}|1\rangle\cdot\left|0^b\right\rangle\sum_{j\in J}|j\rangle\boldsymbol{L}_j|\psi\rangle-\underbrace{(1-\sqrt{1-\delta})}_{\frac{\delta}{2}+\mathcal{O}(\delta^2)}|0\rangle\cdot|0^c\perp\rangle, \quad (3.2)
\end{aligned}
$$

Simulation uses quantum Zeno-like effect

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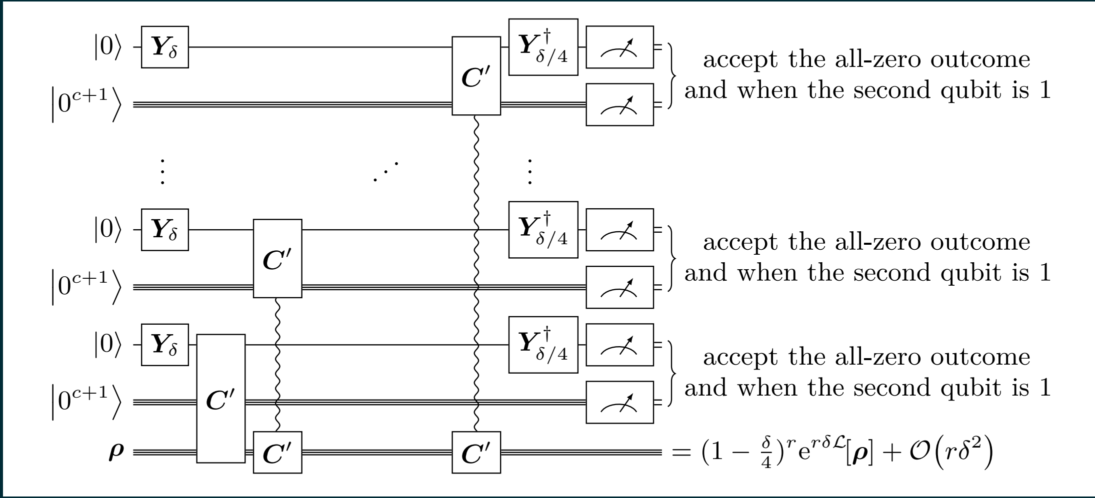
Combine with "compression" cf. "Efficient quantum algorithms for simulating Lindblad evolution" by Richard Cleve, Chunhao Wang (2017)



Davies generator – simulating thermalization?

- $$\mathcal{L}_{Davies}(\rho) = \sum_{a\in A}\sum_{\nu\in B}\gamma(\nu)\left(\underbrace{\boldsymbol{A}_\nu^a\rho(\boldsymbol{A}_\nu^a)^\dagger}_{\text{transition rates}} - \underbrace{\frac{1}{2}((\boldsymbol{A}_\nu^a)^\dagger\boldsymbol{A}_\nu^a\rho + \rho(\boldsymbol{A}_\nu^a)^\dagger\boldsymbol{A}_\nu^a)}_{\text{decay rates}}\right),$$

  where the quantum mechanical transition rates $\boldsymbol{A}_\nu^a$ are defined as

  $$\boldsymbol{A}_\nu^a := \sum_{E_i - E_j = \nu} \boldsymbol{P}_{E_i}\boldsymbol{A}^a\boldsymbol{P}_{E_j} \quad \text{for Bohr frequency} \quad \nu \in spec(\boldsymbol{H}) - spec(\boldsymbol{H}) =: B(\boldsymbol{H}),$$

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- Folklore knowledge: "unphysical exponential relaxation", etc.

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- "Local minima in quantum systems" by Chi-Fang Chen, Hsin-Yuan Huang, John Preskill, Leo Zhou Sep 29 2023 arXiv:2309.16596

Back to first principles

- "Coarse graining can beat the rotating-wave approximation in quantum markovian master equations" Christian Majenz, Tameem Albash, Heinz-Peter Breuer, and Daniel A. Lidar. Phys. Rev. A, (2013)

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- $$\mathcal{L}_\beta[\rho] := \sum_{a\in A}\int_{-\infty}^{\infty}\gamma(\omega)\Big(\hat{\boldsymbol{A}}^a(\omega)\rho\hat{\boldsymbol{A}}^a(\omega)^\dagger - \frac{1}{2}\{\hat{\boldsymbol{A}}^a(\omega)^\dagger\hat{\boldsymbol{A}}^a(\omega),\rho\}\Big)d\omega$$

  where $\gamma(\omega) = \min(1, e^{-\beta\omega})$ may be the Metropolis weight or the (smoother) Glauber dynamics weight $\gamma(\omega) = (e^{\beta\omega}+1)^{-1}$, or something similar and

  $$\hat{\boldsymbol{A}}^a(\omega) :\propto \int_{-T/2}^{T/2} e^{-i\omega t} e^{i\boldsymbol{H}t}\boldsymbol{A}^a e^{-i\boldsymbol{H}t}dt \quad \text{for each} \quad a\in A \quad \text{and} \quad \omega\in\mathbb{R}.$$

Discretization + Operator Fourier transform

- We want to turn $\boldsymbol{L}$ to

$$\sum_{\nu} \gamma(\nu) |\nu\rangle \boldsymbol{L}^{(\nu)} \quad \text{where} \quad \boldsymbol{L}^{(\nu)} = \sum_{\psi,\psi' \,:\, \nu = E_{\psi'} - E_{\psi}} |\psi'\rangle\langle\psi'| \boldsymbol{L} |\psi\rangle\langle\psi|$$

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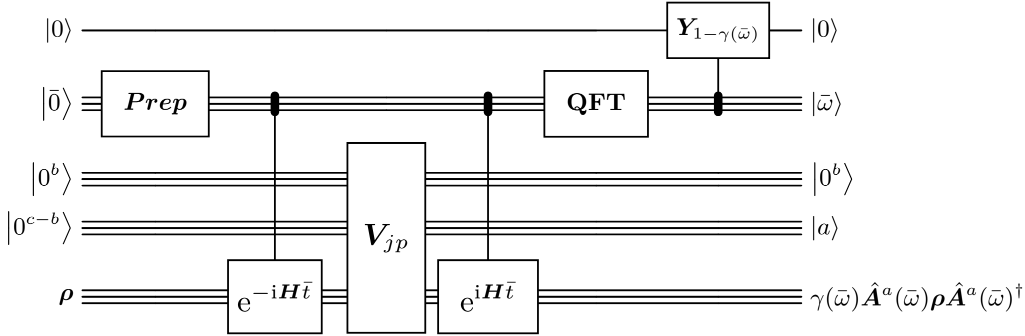
- (Flat) Operator Fourier transform:

$$\underbrace{\sum_{t=-T/2}^{T/2} \frac{1}{T}}_{\text{flat weights}} |t\rangle \boldsymbol{L} \rightarrow \sum_{t} \frac{1}{T} |t\rangle \underbrace{\exp(iHt) \boldsymbol{L} \exp(-iHt)}_{\sum_{\nu} \exp(i\nu t) \boldsymbol{L}^{(\nu)}} \rightarrow \sum_{\nu} \underbrace{\sum_{w} \hat{f}(w-\nu) |w\rangle \boldsymbol{L}^{(\nu)}}_{\text{peak at } \nu}$$

(Show figure from paper block-encoding the jumps.)

Block-encoding the Lindblad operators via quantum operator Fourier transform:



A coherent Szegedy quantum walk type variant

- (Discretized) discriminant proxy

$$\sum_{a\in A}\int\sqrt{\gamma(\omega)\gamma(-\omega)}\hat{\boldsymbol{A}}^{a}(\omega)\otimes\hat{\boldsymbol{A}}^{a*}(\omega)-\frac{\gamma(\omega)}{2}\left(\boldsymbol{A}^{a}(\omega)^{\dagger}\hat{\boldsymbol{A}}^{a}(\omega)\otimes\boldsymbol{I}+\boldsymbol{I}\otimes\hat{\boldsymbol{A}}^{a}(\omega)^{\dagger*}\hat{\boldsymbol{A}}^{a}(\omega)^{*}\right)d\omega$$

- If the mixing time is sufficiently short then provides access to (approximately) the following specific purification of the Gibbs state

$$\left|\sqrt{\boldsymbol{\rho}_\beta}\right\rangle\propto\sum_i e^{-\beta E_i/2}|\psi_i\rangle\otimes\left|\psi_i^*\right\rangle \quad \text{where} \quad \boldsymbol{H}=\sum_i E_i|\psi_i\rangle\langle\psi_i|$$

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- How noise resilient is this algorithm?
- Finally a quadratic improvement for carbon capture?