Krylov spaces and algebras for efficient simulation of quantum dynamics

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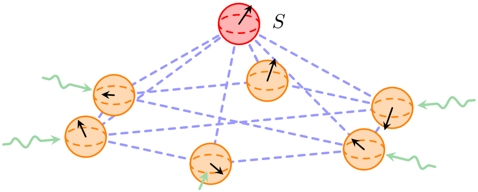


Illustrative application: Dissipative central spin model

$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B \qquad \mathcal{H}_S \simeq \mathbb{C}^2, \quad \mathcal{H}_B \simeq \mathbb{C}^{2^{N_B}}$

$$H_{SB} = H_S \otimes \mathbb{1}_B + H_B + \frac{1}{2}\left(A_x \sigma_x^{(1)} J_x + A_y \sigma_y^{(1)} J_y + A_z \sigma_z^{(1)} J_z\right)$$

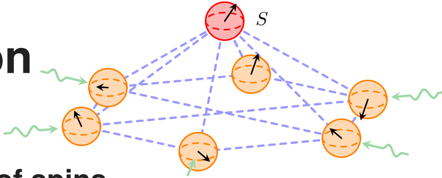
With $H_B = \frac{\lambda}{4} \sum_{2 \le i < k} \sigma_x^{(i)} \sigma_x^{(k)}$.

Collective (Markovian) dissipation $L_B^c = \Lambda J_+$.

We are only interested in reproducing $\rho_S(t) = \mathrm{tr}_B[\rho(t)]$.

Relevant for NV centers.

Goal: Efficient quantum simulation



Task: simulate the evolution of $\rho_S(t)$ for **large numbers of spins.**

Avoid simulating **redundant degrees of freedom** (while retaining a Markovian model)**.**

We would like to find a **smaller** dynamical model that is a **valid quantum model** (a generator in Lindblad form) for a few reasons:

- simulation on quantum computers;
- retain interpretability;
- probe the model's "quantumness".

General setting:

$\mathcal{B}(\mathcal{H}) = \mathbb{C}^{n\times n}$

ρ are density operators:
$\rho \in \mathbb{C}^{n\times n}$, $\rho = \rho^\dagger \geq 0$, $\mathrm{tr}[\rho] = 1$.

$\mathcal{L}$ is a GKLS generator.

ρ_0 is the initial condition.

$$\begin{cases} \dot{\rho}(t) = \mathcal{L}[\rho(t)] \\ y(t) = \mathcal{C}[\rho(t)] \end{cases}, \qquad \rho_0 \in \mathfrak{D}(\mathcal{H})$$

$y(t) \in \mathbb{C}^{m\times m}$ is the **output of interest**, the one we want to reproduce, e.g. $\langle X(t)\rangle, \rho_S(t)$.

$\mathcal{C}$ is a linear output map, e.g. $\mathrm{tr}[X\rho(t)]$ or $\mathrm{tr}_B[\rho(t)]$.

$$\mathcal{L}(\rho) = -i[H,\rho] + \sum_k L_k \rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho\}, \qquad \mathcal{C}(\cdot) = \sum_i E_i \mathrm{tr}(X_i^\dagger \cdot).$$

The problem: quantum model reduction

Given a model $(\mathcal{L}, \mathcal{C})$, we want to find **another, smaller** model $(\check{\mathcal{L}}, \check{\mathcal{C}})$, and a linear initialization map $\Phi : \mathbb{C}^{n\times n} \to \mathbb{C}^{r\times r}$ such that for all $t \geq 0$ and all $\rho_0 \in \mathfrak{D}(\mathcal{H})$, $\check{\rho}_0 = \Phi(\rho_0)$:

- **exact model reduction**

$$\mathcal{C}e^{\mathcal{L}t}(\rho_0) = \check{\mathcal{C}}e^{\check{\mathcal{L}}t}(\check{\rho}_0);$$

- approximate model reduction (in progress)

$$\mathcal{C}e^{\mathcal{L}t}(\rho_0) \approx \check{\mathcal{C}}e^{\check{\mathcal{L}}t}(\check{\rho}_0).$$

Proposed model reduction algorithm (1/4)

Step 1: Compute the **Krylov "observable" operator space** $\mathscr{N}^\perp$, from $\{X_i\}$ as

$$\mathscr{N}^\perp = \text{span}\{\mathcal{L}^{\dagger j}(X_i),\ \forall i, \forall j = 0, \ldots, n^2 - 1\}.$$

We assume $\mathscr{N}^\perp$ has full support: if not reduce the model to the supporting subspace.

Fact: $\mathscr{N}^\perp$ **contains all the necessary degrees of freedom** to reproduce the output (e.g. $\rho_S(t)$). Projecting the dynamics on $\mathscr{N}^\perp$ we find a (provably) minimal linear solution:

$$\begin{cases} \dot{x}(t) = Lx(t) \\ y(t) = Cx(t) \end{cases}, \qquad x \in \mathbb{C}^n, \qquad \rho_S(t) \equiv Ce^{Lt}x_0$$

Problem: **Not a quantum model.** How do we obtain one?

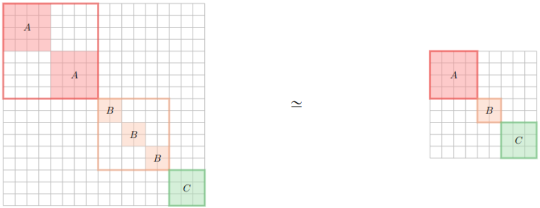
Proposed model reduction algorithm (2/4)

Step 2: Compute the **output algebra** $\mathscr{O} \equiv \mathrm{alg}(\mathscr{N}^\perp)$.

It is the fundamental structure that supports a **quantum probability space**.
Related to DFS and the structure of fixed points of CP maps.

Find U that brings $\mathscr{O}$ to their canonical Wedderburn decomposition $\mathcal{H} = \bigoplus_k \mathcal{H}_{F,k} \otimes \mathcal{H}_{G,k}$

$$\mathscr{O} = U\left(\bigoplus_k \mathfrak{B}(\mathcal{H}_{F,k}) \otimes \mathbb{1}_{G,k}\right)U^\dagger \qquad \simeq \qquad \check{\mathscr{O}} = \bigoplus_k \mathfrak{B}(\mathcal{H}_{F,k}).$$



Proposed model reduction algorithm (3/4)

Step 3: Compute the **CPTP orthogonal projection** $\mathbb{E}|_{\mathscr{O}}^{\dagger} = \mathbb{E}|_{\mathscr{O}}$

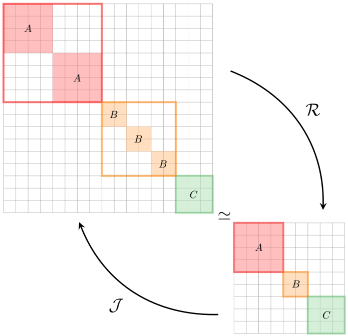
$$\mathbb{E}|_{\mathscr{O}}(X) = U\left(\bigoplus_{k=0}^{K-1} \operatorname{tr}_{\mathcal{H}_{G,k}}\left[W_k X W_k^{\dagger}\right] \otimes \frac{\mathbb{1}_{G,k}}{\dim \mathcal{H}_{G,k}}\right)U^{\dagger}, \qquad \forall X \in \mathcal{B}(\mathcal{H}).$$

$\mathbb{E}|_{\mathscr{O}}[\cdot]$ can be **factorized into CPTP maps**

$$\mathbb{E}|_{\mathscr{O}}[\cdot] = \mathcal{J}\mathcal{R}.$$

$$\check{X} = \mathcal{R}[X] = \bigoplus_k \operatorname{tr}_{\mathcal{H}_{F,k}}[V_k X V_k^{\dagger}] = \bigoplus_k \check{X}_k$$

$$\mathcal{J}[\check{X}] = U\left(\bigoplus_k \check{X}_k \otimes \frac{\mathbb{1}_{F,k}}{\dim \mathcal{H}_{G,k}}\right)U^{\dagger}$$



Proposed model reduction algorithm (4/4)

Step 4: Reduction (main result)

Define the **reduced generator** $\check{\mathcal{L}} \equiv \mathcal{J}\mathcal{L}\mathcal{R}$ on $\check{\mathscr{O}}$ and the output function $\check{\mathcal{C}} \equiv \mathcal{C}\mathcal{J}$.
Then, for any initial condition $\rho_0 \in \mathfrak{D}(\mathcal{H})$, we have

$$\mathcal{C}e^{\mathcal{L}t}(\rho_0) = \check{\mathcal{C}}e^{\check{\mathcal{L}}t}\mathcal{R}(\rho_0), \quad \forall t \geq 0.$$

$\mathscr{O}$ is also the **minimal algebra** that supports such a reduction.

Theorem: Let $\mathscr{A}$ be a unital $*$-subalgebra of $\mathcal{B}(\mathcal{H})$, and let $\mathbb{E}_{\mathscr{A}} = \mathcal{J}\mathcal{R}$ CPTP, as defined above. Then for any Lindblad generator $\mathcal{L}$, its reduction to $\mathscr{A}$,

$$\check{\mathcal{L}} \equiv \mathcal{R}\mathcal{L}\mathcal{J},$$

is also a Lindblad generator, that is, $\check{\mathcal{L}} : \check{\mathscr{A}} \to \check{\mathscr{A}}$ and $\{e^{\check{\mathcal{L}}t}\}_{t\geq 0}$ is a QDS.

An interpretation with symmetries

$U \in \mathfrak{B}(\mathcal{H})$, $U^\dagger U \equiv \mathbb{1}$, $\mathcal{U}(\cdot) = U \cdot U^\dagger$ is a **symmetry** when

$$e^{\mathcal{L}^\dagger t}\mathcal{U} = \mathcal{U} e^{\mathcal{L}^\dagger t}, \quad \forall t \geq 0.$$

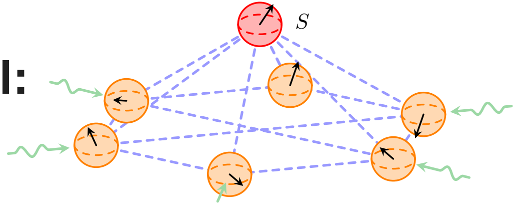
If a generator $\mathcal{L}$ enjoys a group of symmetries $\mathscr{G}$ **and** $\{X_j\} \subseteq \mathscr{G}'$ then $\mathscr{O} \subseteq \mathscr{G}'$. Hence the presence of symmetries may imply model reduction onto $\mathscr{G}'$ (which is an algebra).

Def: We define an **observable-dependent symmetry (ODS)** U for an observable X if $\mathcal{U}(\rho) = U\rho U^\dagger$ satisfies

$$\mathcal{U} e^{\mathcal{L}^\dagger t}(X) = e^{\mathcal{L}^\dagger t}(X) \quad \forall t \geq 0.$$

Thm: Let $\mathscr{G}$ be the group of ALL ODS for $(\mathcal{L}, \mathcal{C})$. Then $\mathscr{G}' = \mathscr{O}$, the output algebra.

Dissipative central spin model: Symmetries



With $H_B = \frac{\lambda}{4}\sum_{2\leq i<k} \sigma_x^{(i)}\sigma_x^{(k)}$, **bath permutations are (strong) symmetries** for this model AND all observables of interest $O_S \otimes \mathbb{1}_B$

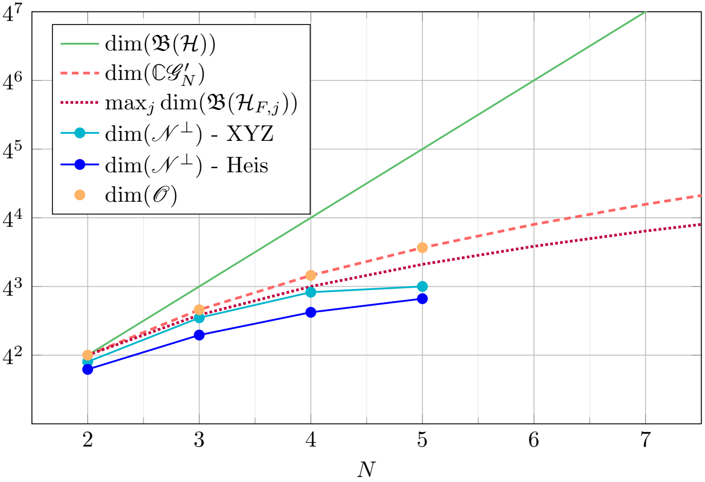
$$[U, O_S \otimes \mathbb{1}_B] = 0, \quad \Rightarrow O_S \otimes \mathbb{1}_B \in \mathscr{G}'.$$

We are able to find a reduced quantum model to reproduce this dynamics.

If we change the bath Hamiltonian to $H_B = \sum_{2\leq i<k} B_{ik}\, \vec{\sigma}^{(i)} \cdot \vec{\sigma}^{(k)}$ then **bath permutations are no longer symmetries for the model BUT are observable dependent symmetries**.

How much are we reducing?

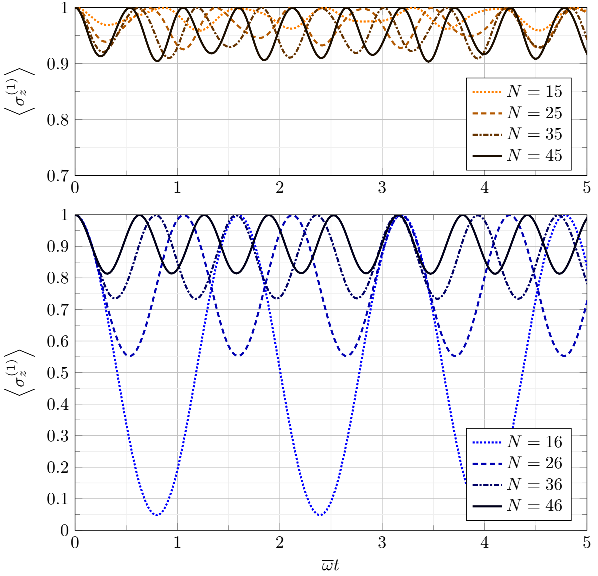
The dimension of $\mathscr{O} = \mathscr{G}'$ scales with N^3 while the dimension of $\mathfrak{B}(\mathcal{H})$ is 4^N.



Large number of spins

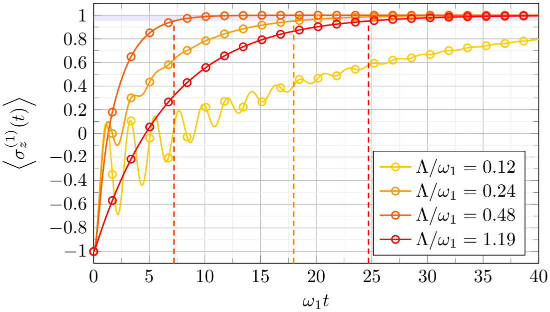
Simulation with no dissipation and strong intra-bath coupling (i.e. $\lambda/\bar{\omega} = 20$).

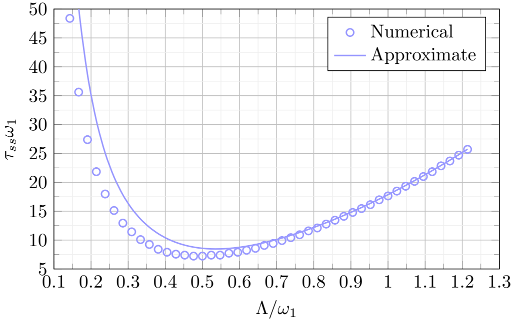
A self-decoupling effect occurs for $\lambda >> \bar{\omega}$ which was previously observed only up to $N_B = 14$.



Dual procedure: Reachable reduction

Considering a single initial condition, e.g. $\rho_0 = |1\rangle\langle 1| \otimes |0\ldots 0\rangle\langle 0\ldots 0|$ we can further reduce the model with a **dual procedure** (reachable reduction) of what we just described.





$N_B = 5$, collective dissipation $L_B^c = \Lambda J_+$.

Take home ideas

1. **Algebras** and **CPTP projectors** provide CPTP-preserving model reduction.

2. The Krylov based-algorithm are equivalent to finding ODS

3. Observable-dependent symmetries allow us to go beyond simple symmetry-based model reduction.

Conclusion

General framework for model reduction of quantum dynamics, ensuring CPTP.
It has been applied to:

- (classical) Hidden Markov models **[arXiv:2208.05968 – IEEE Trans. Aut. Contr.]**
- (deterministic) Disc.-time case **[arXiv:2307.06319 – IEEE Trans. Inf. Theo.]**
- (deterministic) Cont.-time case **[arXiv:2412.05102 – Quantum]**
- (stochastic) Disc.-time quantum traj. **[arXiv:2403.12575 – IEEE Contr. Sys. Lett.]**
- (stochastic) Cont.-time quantum traj. **[arXiv:2501.13885 – Annales Henri Poincaré]**
- (deterministic) Controlled quantum dynamics **[arXiv:2510.25546]**

Outlook

- Approximate model reduction (in preparation);
- Connection with adiabatic elimination techniques (in preparation).

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Thanks for your attention!

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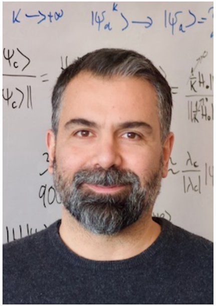
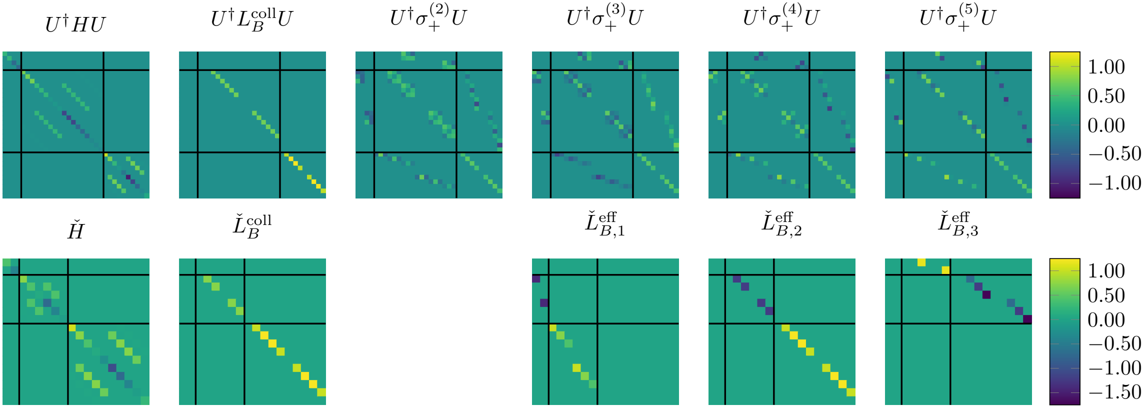


Group's website →

Reduced dynamics operators ($N_B = 4$)



$U \in \mathfrak{B}(\mathcal{H})$, $U^\dagger U = \mathbb{1}$ is a:

- **strong symmetry** for $\mathcal{L}$ if $[H, U] = [L_k, U] = 0 \Rightarrow$ each block is invariant;
- **weak symmetry** for $\mathcal{L}$ if $[\mathcal{L}, U \cdot U^\dagger] = 0 \Rightarrow$ there is comunication between blocks.