Exact Model Reduction for Continuous-Time Open Quantum Dynamics

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Quantum

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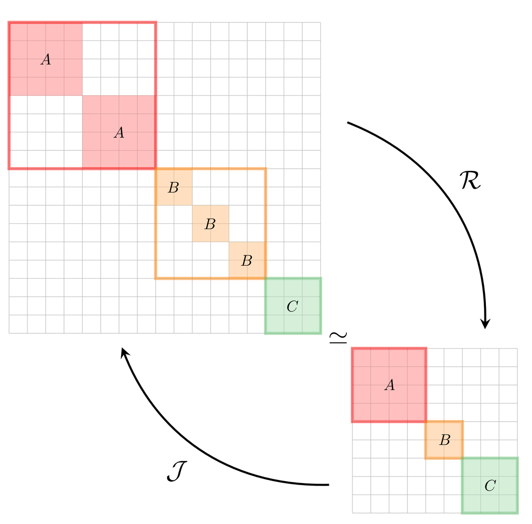
Abstract

We consider finite-dimensional many-body quantum systems described by time-independent Hamiltonians and Markovian master equations, and present a systematic method for constructing *smaller-dimensional*, reduced models that *exactly* reproduce the time evolution of a set of initial conditions or observables of interest. Our approach exploits Krylov operator spaces and their extension to operator algebras, and may be used to obtain reduced *linear* models of minimal dimension, well-suited for simulation on classical computers, or reduced *quantum* models that preserve the structural constraints of admissible quantum dynamics, as required for simulation on quantum computers. Notably, **we prove that the reduced quantum-dynamical generator is still in Lindblad form**. By introducing a new type of *observable-dependent symmetries*, we show that our method provides a non-trivial generalization of techniques that leverage symmetries, unlocking new reduction opportunities. We quantitatively benchmark our method on paradigmatic open many-body systems of relevance to condensed-matter and quantum-information physics. In particular, we demonstrate how our reduced models can quantitatively describe decoherence dynamics in central-spin systems coupled to structured environments, magnetization transport in boundary-driven dissipative spin chains, and unwanted error dynamics on information encoded in a noiseless quantum code.

Theory



In many situations of fundamental and practical relevance, interest may be *a priori* restricted to a subset of initial input states, and a subset of output quantities that depend upon the final, time-evolved state $\rho(t)$ and may be directly associated to or required for computing experimentally accessible properties.

We thus focus on finite dimensional systems $\mathcal{H} \simeq \mathbb{C}^n$ of the type

$$\begin{cases} \dot\rho(t) = \mathcal{L}[\rho(t)] \\ Y(t) = \mathcal{O}[\rho(t)] \end{cases} \quad (1)$$

where

$$\mathcal{L}(\rho) = -i[H,\rho] + \sum_u \left(L_u \rho L_u^\dagger - \frac{1}{2}\{L_u^\dagger L_u, \rho\} \right) \quad (2)$$

and $\mathcal{O}(\cdot) = \sum_i E_i \mathrm{tr}(O_i^\dagger \cdot)$ is a linear output functional (e.g. $\mathcal{O} = \mathrm{tr}_B$) and O_i are observables of interest.

Proposed model-reduction algorithm:

1. Compute the orthogonal to the non-observable subspace, $\mathscr{N}^\perp$, from $\{O_i\}$ as
$$\mathscr{N}^\perp = \mathrm{span}\{\mathcal{L}^{\dagger j}(O_i),\ \forall i, \forall j = 0, \dots, n^2-1\}. \quad (3)$$
We assume $\mathscr{N}^\perp$ has full support: if this is not the case, we can immediately reduce the model to the supporting subspace.
2. Compute the output algebra $\mathscr{O} \equiv \mathrm{alg}(\mathscr{N}^\perp)$. Given $\mathscr{O}$, find the unitary change of base U that brings $\mathscr{O}$ to their canonical Wedderburn decomposition
$$\mathscr{O} = U\left(\bigoplus_k \mathfrak{B}(\mathcal{H}_{F,k}) \otimes \mathbb{1}_{G,k} \right) U^\dagger \quad \simeq \quad \check{\mathscr{O}} = \bigoplus_k \mathfrak{B}(\mathcal{H}_{F,k}). \quad (4)$$
3. Consider the CPTP orthogonal projection $\mathbb{E}|_{\mathscr{O}}^\dagger = \mathbb{E}|_{\mathscr{O}}$ or **conditional expectation**
$$\mathbb{E}|_{\mathscr{O}}(X) = U\left(\bigoplus_{k=0}^{K-1} \mathrm{tr}_{\mathcal{H}_{G,k}}\left[(W_k X W_k^\dagger)(\mathbb{1}_{d_k} \otimes \tau_k) \right] \otimes \mathbb{1}_{G,k} \right) U^\dagger, \qquad \forall X \in \mathcal{B}(\mathcal{H}), \quad (5)$$
with $\tau_k = \frac{\mathbb{1}_{G,k}}{\dim \mathcal{H}_{G,k}}$ and compute its two CPTP factors $\mathcal{J}, \mathcal{R}$ s.t. $\mathbb{E}|_{\mathscr{O}} = \mathcal{J}\mathcal{R}$
$$\mathcal{R}(X) = \bigoplus_k \mathrm{tr}_{\mathcal{H}_{G,k}}(W_k X W_k^\dagger) = \bigoplus_k X_{F,k} = \check{X}, \quad (6)$$
$$\mathcal{J}(\check{X}) = U\left(\bigoplus_k X_{F,k} \otimes \tau_k \right) U^\dagger. \quad (7)$$
4. Define the reduced generator $\check{\mathcal{L}} \equiv \mathcal{J}\mathcal{L}\mathcal{R}$ on $\check{\mathscr{A}}$ and the output function for the reduced model $\check{\mathcal{O}} \equiv \mathcal{O}\mathcal{J}$. Then, for any initial condition $\rho_0 \in \mathfrak{S}$, we have
$$\mathcal{O} e^{\mathcal{L}t}(\rho_0) = \check{\mathcal{O}} e^{\check{\mathcal{L}}t} \mathcal{R}(\rho_0), \quad \forall t \geq 0.$$

Reduced Lindblad dynamics

Theorem: Let $\mathscr{A}$ be a unital $*$-subalgebra of $\mathcal{B}(\mathcal{H})$, and let $\mathcal{R}$ and $\mathcal{J}$ denote the CPTP factorization of $\mathbb{J}|_{\mathscr{A}} = \mathcal{J}\mathcal{R}$, 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 quantum dynamical semigroup.

Observable-dependent symmetries

A *weak symmetry* is a unitary operator S that leaves the dynamics invariant,

$$\mathcal{T}_t(S\rho S^\dagger) = S\mathcal{T}_t(\rho)S^\dagger, \quad \forall t, \forall \rho \in \mathfrak{D}(\mathcal{H}), \quad (8)$$

or, equivalently, $[\mathcal{S}, \mathcal{L}] = 0$, in terms of the super-operator $\mathcal{S}(\cdot) \equiv S \cdot S^\dagger$.
A *strong symmetry* is a unitary operator S that commutes with the Hamiltonian and all the noise operators in $\mathcal{L}$,

$$[H, S] = 0, \quad [L_u, S] = 0, \quad \forall u, \quad (9)$$

where $\mathcal{L} \sim (H, \{L_u\})$ is an arbitrary representation of the semigroup generator. Equivalently, $\mathcal{S}(H) = H$ and $\mathcal{S}(L_u) = L_u, \forall u$.

For any *weak* symmetry operator S, the eigendecomposition of the superoperator $\mathcal{S}$ provides a decomposition of the operator space, $\mathfrak{B}(\mathcal{H}) = \bigoplus_\nu \mathscr{B}_\nu$, where $\mathscr{B}_\nu$ are operator-eigenspaces associated to distinct eigenvalues ν, i.e., $\mathcal{S}(X) = \nu X$ for all $X \in \mathscr{B}_\nu$. Since $\mathcal{S}$ and $\mathcal{L}$ commute, it follows that each subspace $\mathscr{B}_\nu$ is $\mathcal{L}$-invariant. In particular $\mathscr{B}_1$ is an $\mathcal{L}$-invariant $*$-algebra.

Given a Lindblad generator $\mathcal{L}$, a set of observables $\{O_i\}$ and a unitary operator $S \in \mathfrak{B}(\mathcal{H})$, with associated super-operator $\mathcal{S}(\cdot) = S \cdot S^\dagger$, we say that S is a **$\{O_i\}$-(observable-)dependent symmetry** (ODS) if

$$\mathcal{S}\mathcal{L}^{\dagger n}(O_i) = \mathcal{L}^{\dagger n}(O_i), \quad \forall n \in \mathbb{N}, \forall i. \quad (10)$$

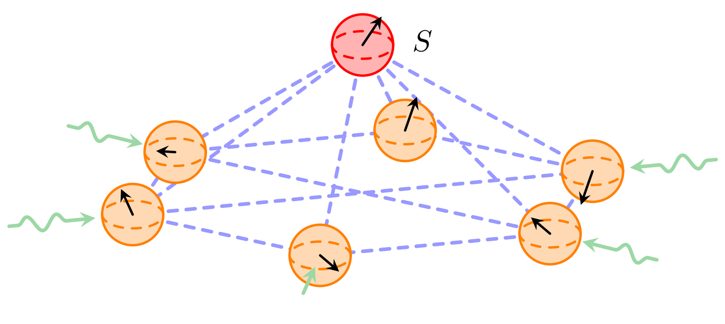
Theorem: Let $\{O_i\} \subset \mathfrak{H}(\mathcal{H})$ be a set of observables, and let $\mathcal{L}$ be a Lindblad generator. Then $\mathscr{O} = \mathrm{alg}\{\mathscr{N}^\perp\} \subsetneq \mathfrak{B}(\mathcal{H})$ if and only if there exists a non-trivial $\{O_i\}$-ODS for $\mathcal{L}$. Furthermore, we have

$$\mathscr{O} = \mathrm{alg}\{\mathscr{N}^\perp\} = \mathbb{C}\mathscr{G}',$$

where $\mathscr{G}$ is the largest group of ODS for the model.

Illustrative application: Dissipative central spin model

We consider a central spin system, S, coupled to a "structured quantum environment," namely, an interacting spin bath, B, responsible for generally non-Markovian dynamics on S, along with a bath inducing Markovian dissipation on B alone. Explicitly, in what follows we label the central spin by 1, while the remaining $N-1 \equiv N_B$ spins correspond to bath spins, whereby $\mathcal{H}_B \simeq \mathbb{C}^{2^{N_B}}$, $\mathcal{H}_S \simeq \mathbb{C}^2$, $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$.

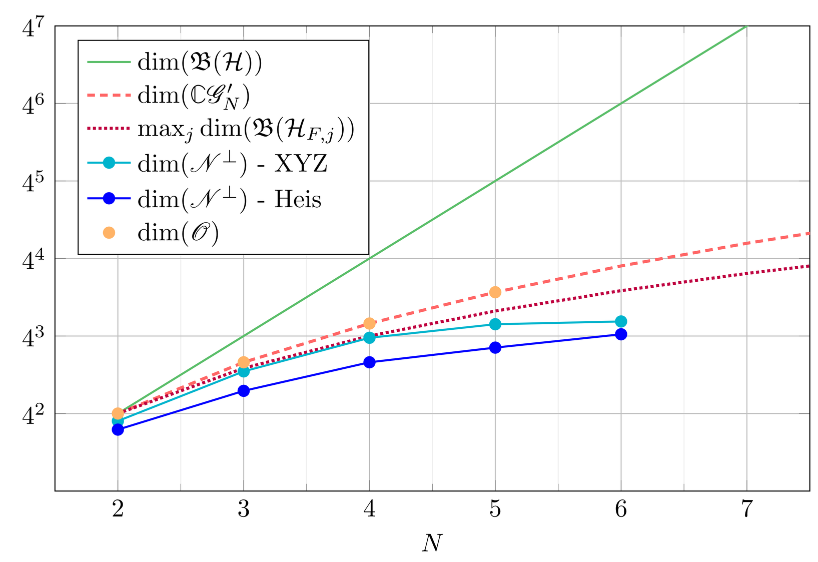


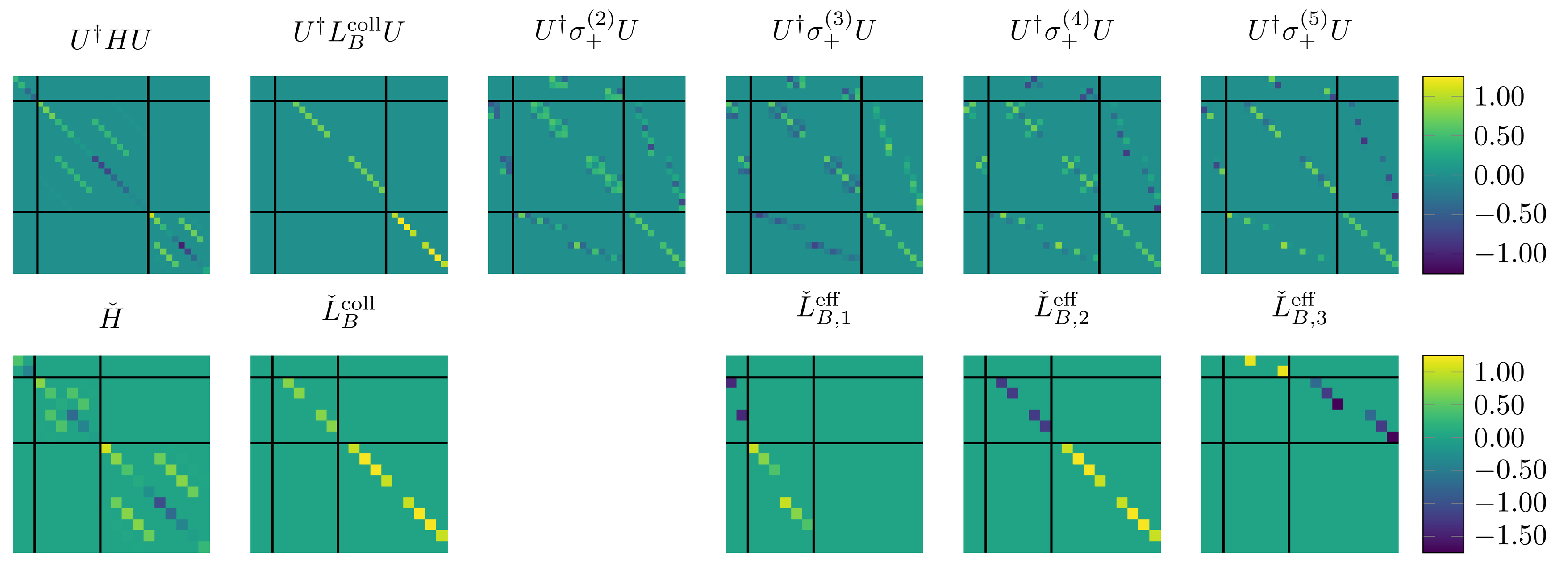
The full dynamics for the joint system-bath state $\rho(t) \in \mathfrak{D}(\mathcal{H}_S \otimes \mathcal{H}_B)$ is determined by the joint system-bath Hamiltonian which reads

$$H_{SB} = \underbrace{\frac{1}{2}\left(\omega_1 \sigma_z^{(1)} + \eta \sigma_x^{(1)}\right)}_{H_S} + \underbrace{\frac{\lambda}{4}\left(2J_x^2 - \frac{N_B}{2}\mathbb{1}_{2^N}\right)}_{H_B^{\mathrm{Ising}}} + \underbrace{\frac{1}{2}\left(A_x\sigma_x^{(1)}J_x + A_y\sigma_y^{(1)}J_y + A_z\sigma_z^{(1)}J_z\right)}_{H_{\mathrm{Int}}}$$

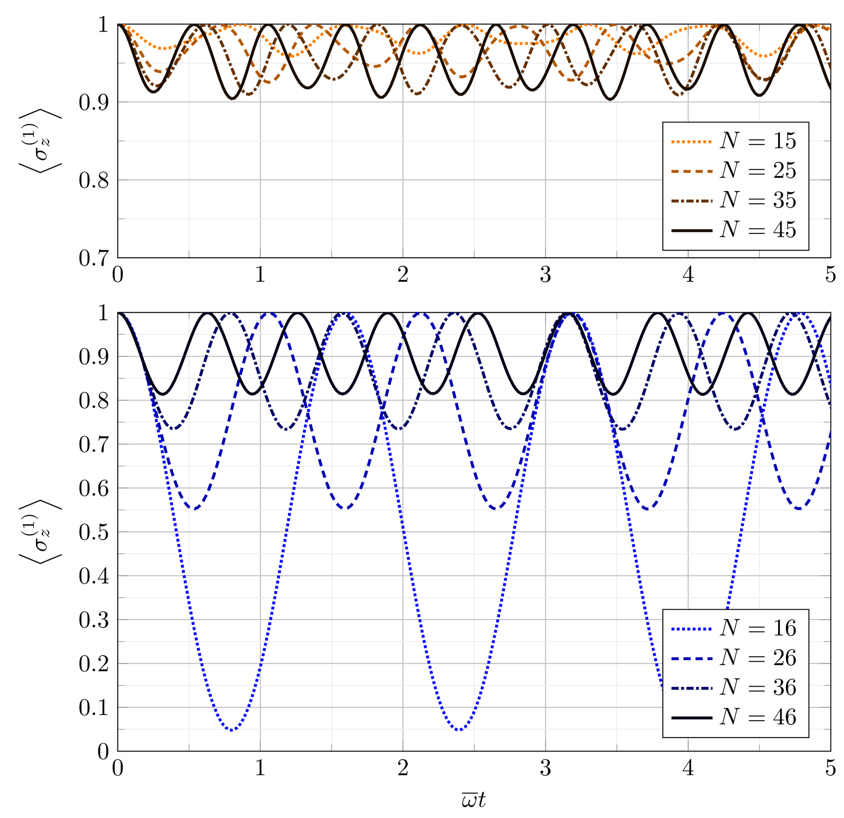
with $J_u \equiv \frac{1}{2}\sum_{k=2}^N \sigma_u^{(k)}$ denoting total bath-spin angular momentum operators, and by two types of dissipations: either *collective* bath dissipation, $L_B^c = \Lambda J_+$, or *local* dissipation on the bath-spins, $L_B^i = \delta\sigma_+^{(i)}$. **We are only interested in reproducing the system's state (⇒ observable reduction):** $\rho_S(t) = \mathrm{tr}_B[\rho(t)]$

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. Furthermore, in the blocks of the reduced Hamiltonian and noise operators, we observe that i) under strong symmetry (case with collective dissipation) each block is invariant; while ii) under weak symmetry (case with local dissipation) there is communication between blocks in the diagonal due to non-zero off-diagonal blocks in the noise operators. The dimension of the largest block grows with N^2, meaning that we can efficiently parallelize the simulation if the symmetry is strong.

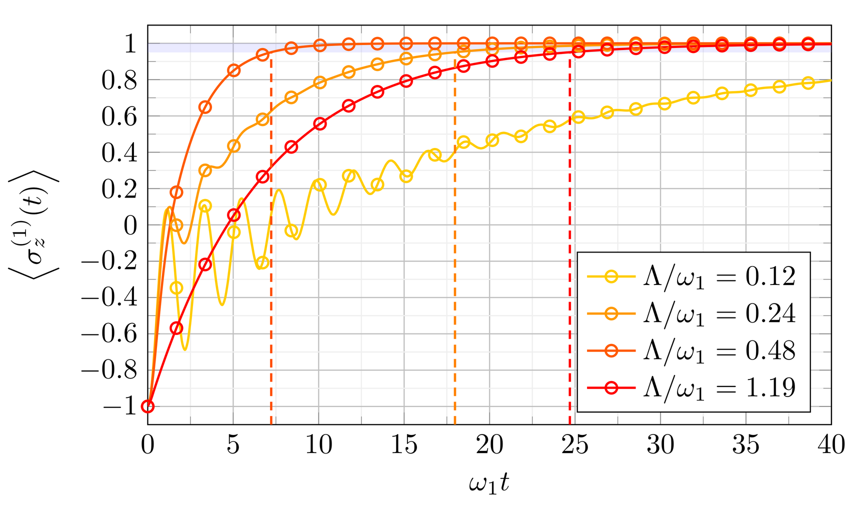


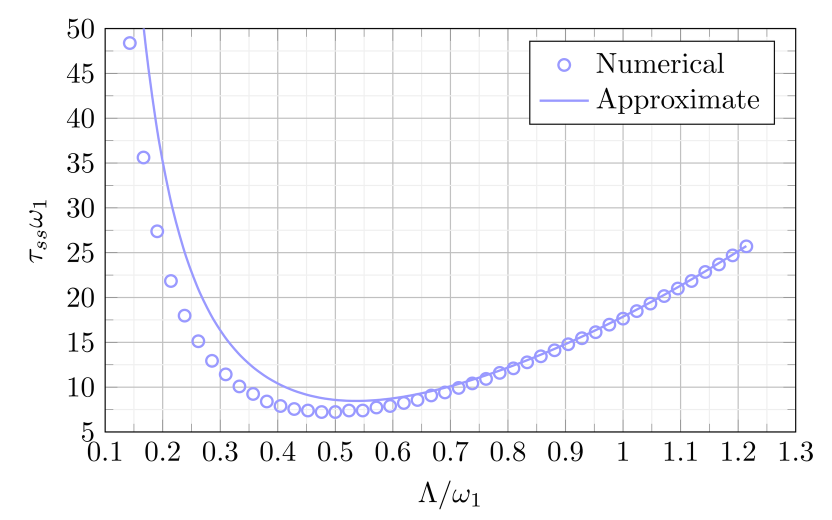


This fact allows us to simulate the reduced model very efficiently and to reach high number of spins. Representative results are shown on the right, where the expectation values $\langle \sigma_z^{(1)} \rangle$ for odd and even N are plotted against time in a setting with no dissipation. Our results suggest that a "self-decoupling" effect still occurs for $\lambda \gg \overline{\omega}$, as manifested by the fact that the spin polarization approximately oscillates periodically or freezes out for even or odd N, respectively. For larger number of spins, however, the difference between odd and even N tends to diminish.



To validate our procedure, we compare the numerical solution of the full vs. reduced models also in the collective dissipative setting. In the bottom left figure we compare the central spin's polarization for the full (dotted line) and reduced model (solid line), resulting in exact agreement, as expected. Interestingly, as the strength Λ of the dissipation increases, we observe a transition from a regime where the trajectory reaches equilibrium slowly, with oscillation, to one where the equilibrium is reached more rapidly, and with no oscillation – showing a *non-monotonic* behavior of the convergence time τ_{ss}, which we quantity in terms of the time taken for $\langle\sigma_z^{(1)}(t)\rangle$ to remain confined within 5% of its asymptotic value. Considering a **single initial condition (⇒ reachable or dual reduction)**, e.g. $\rho_0 = |1\rangle\langle 1| \otimes |0\dots 0\rangle\langle 0 \dots 0|$, we can further reduce the model and obtain an even easier model to study to obtain an approximate curve of the non-monotonic behavior of $\tau_{ss} \approx \ln(0.05)/2\Lambda^2$.





Conclusion

We presented a **general framework for exact model reduction of quantum dynamics, ensuring CPTP**. It has been applied to:

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

Outlook: Approximate model reduction (in progress) and connection with adiabatic elimination techniques (in progress).