QFlux: From Closed to Open Quantum Dynamics

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Part IV: Open Systems & Dilation

- *Real systems are never isolated*
- *Environment causes:*
  - *Relaxation*
  - *Decoherence*
  - *Energy exchange*
- *Need density matrices, not wavefunctions*
- *Goal: simulate non-unitary dynamics on unitary hardware*

https://qflux.batistalab.com

JCTC_IV.ipynb

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Part IV: Open Systems & Dilation

This tutorial is based on the manuscript

QFlux: Quantum Circuit Implementations for Molecular Dynamics

Part IV - Dilation method for Open Systems

Authors:

Xiaohan Dan, Saurabh Shivpuje, Yuchen Wang, Brandon C. Allen, Delmar G. A. Cabral, Pouya Khazaei, Alexander V. Soudackov, Zixuan Hu, Ningyi Lyu, Eitan Geva, Sabre Kais, and Victor S. Batista

Roadmap for Part IV

- Physics: open systems & **Lindblad dynamics**
- Encoding:
  - Vectorized **density matrices**
  - **Kraus operator** representation
- Core idea: **dilation** = embed non-unitary in a bigger unitary
- Demonstrations:
  - Spin-½
  - Spin chain
  - Double-well proton transfer

PART A — OPEN SYSTEM FOUNDATIONS

What Is an Open Quantum System?

- System + environment → entangled
- Reduced state described by density matrix
- Evolution:

$$\rho(t) = \mathcal{G}(t)\,\rho(0)$$

- Propagator $\mathcal{G}(t)$ is non-unitary

The Lindblad Master Equation

Most general completely positive, trace-preserving Markovian evolution

$$\frac{\partial \rho(t)}{\partial t} = -\frac{\mathrm{i}}{\hbar}[H, \rho(t)] + \frac{1}{2}\sum_n \gamma_n \left(2L_n \rho(t) L_n^\dagger - \rho(t) L_n^\dagger L_n - L_n^\dagger L_n \rho(t)\right)$$

- General Markovian open-system equation
- **Coherent term:** commutator with H
- **Dissipative terms:** jump operators L_n (encode relaxation and dephasing)
- Assumes:
  - Weak coupling
  - Fast bath (Markov)
  - No memory

Where dissipative chemical processes meet quantum information

Why Lindblad Is a Good Starting Point

- Widely used in:
  - Spectroscopy
  - Transport
  - Quantum devices
- Efficient numerically

Warning: Breaks down for:

  - Strong (bath-system) coupling
  - Structured baths
  - Memory effects (Part VI)

QFlux: An Open-Source Python Package for Quantum Dynamics Simulations

PART B — ENCODING OPEN SYSTEMS ON QUBITS

Two Ways to Encode Density Matrices

1. **Vectorization: Superoperator Picture**

- $\rho \rightarrow |\nu_\rho\rangle$ **reshaped in N^2 space:**

$$|\nu_\rho\rangle = [\rho_{11}, \ldots, \rho_{1N}, \rho_{21}, \ldots, \rho_{2N}, \ldots, \rho_{N1}, \ldots, \rho_{NN}]^\top$$

- **Direct propagator:** $\frac{\partial |\nu_\rho(t)\rangle}{\partial t} = -\mathrm{i} H_{\text{eff}} |\nu_\rho(t)\rangle$

$$H_{\text{eff}} = H_C + \mathrm{i} H_D$$

$$H_C = H \otimes \mathbb{I} - \mathbb{I} \otimes H^T \quad ,$$

$$H_D = \frac{1}{2} \sum_n \gamma_n \left[2 L_n \otimes L_n^* - \mathbb{I} \otimes L_n^T L_n^* - L_n^\dagger L_n \otimes \mathbb{I} \right]$$

(non-unitary)

$$|\nu_\rho(t)\rangle = \mathbf{G}(t) |\nu_\rho(0)\rangle$$

$$|\nu_\rho(t)\rangle = e^{-\mathrm{i} H_{\text{eff}} t} |\nu_\rho(0)\rangle$$

Script S.3.1: JCTC_IV.ipynb
Script S.3.2: JCTC_IV.ipynb

PART B — ENCODING OPEN SYSTEMS ON QUBITS

Two Ways to Encode Density Matrices, cont'd

2. **Kraus representation: Ensemble picture** $\rho(0) = \sum_n p_n(0) \left|\psi_n(0)\right\rangle\!\left\langle\psi_n(0)\right|$

- $\rho \not\rightarrow |\nu_\rho\rangle$
- Evolve ensemble of pure states
- (quantum channels)

$$\rho(t) = \sum_{in} p_n(0) M_i(t) \left|\psi_n(0)\right\rangle\!\left\langle\psi_n(0)\right| M_i^\dagger(t)$$

$$= \sum_{in} p_n(0) \left|\psi_n^i(t)\right\rangle\!\left\langle\psi_n^i(t)\right|$$

$$\rho(t) = \sum_i M_i(t)\rho(0)M_i^\dagger(t) \qquad \left|\psi_n^i(t)\right\rangle = M_i(t)\left|\psi_n(0)\right\rangle \quad \text{(non-unitary)}$$

Fewer qubits than vectorization: Kraus operators $M_i(t)$ are $N \times N$ matrices
Many circuits though

From Propagator to Kraus (Choi Map)

Motivation for UCRs

Script S.1.1: JCTC_IV.ipynb

Choi–Jamiołkowski isomorphism theorem

- Build Choi matrix from propagator : $$C = \sum_{i,j=1}^{N} (E_{ij} \otimes I)\mathbf{G}(t)(I \otimes E_{ij})$$
- Diagonalize → eigenvalues λ_k : $$C = \sum_{k=1}^{N^2} \lambda_k u_k u_k^\dagger$$
- Reshape eigenvectors $\lambda_k u_k$ into N x N matrices → Kraus operators M_k
- Discard small λ_k

PART C — THE CORE IDEA: DILATION

The Fundamental Problem

- Quantum circuits must be unitary
- Lindblad & Kraus are non-unitary
- Solution: embed non-unitary into a larger unitary evolution

Physical Intuition: Irreversibility from Tracing Out

- Enlarge Hilbert space: system + ancilla
- Evolve unitarily in the enlarged space
- Trace out ancilla → non-unitary system dynamics

Sz.-Nagy Dilation Theorem

Core Formula

- For non-unitary M, build the unitary U_M

$$U_M = \begin{pmatrix} M & D_{M^\dagger} \\ D_M & -M^\dagger \end{pmatrix}$$

$$D_M = \sqrt{I - M^\dagger M}$$
$$D_{M^\dagger} = \sqrt{I - M M^\dagger}.$$

$$U_M \begin{pmatrix} \boldsymbol{v} \\ \boldsymbol{0} \end{pmatrix} = \begin{pmatrix} M\boldsymbol{v} \\ \boldsymbol{v}' \end{pmatrix}$$

- One ancilla qubit
- Guarantees unitary embedding

Script S.2.1: JCTC_IV.ipynb

Optimized Dilations

More advanced dilation schemes

Script S.4.5: JCTC_IV.ipynb

- SVD-based dilation
- Walsh diagonal synthesis
- Fewer CNOTs
- Built into QFlux

PART D — CLASSICAL BENCHMARK FIRST

Always Benchmark Classically

Script S.3.3: JCTC_IV.ipynb

- Solve Lindblad with:
  - Matrix exponential
  - ODE Solver (e.g., QuTiP's mesolve)
- Establish reference dynamics
- Only then go quantum

QFlux: An Open-Source Python Package for Quantum Dynamics Simulations

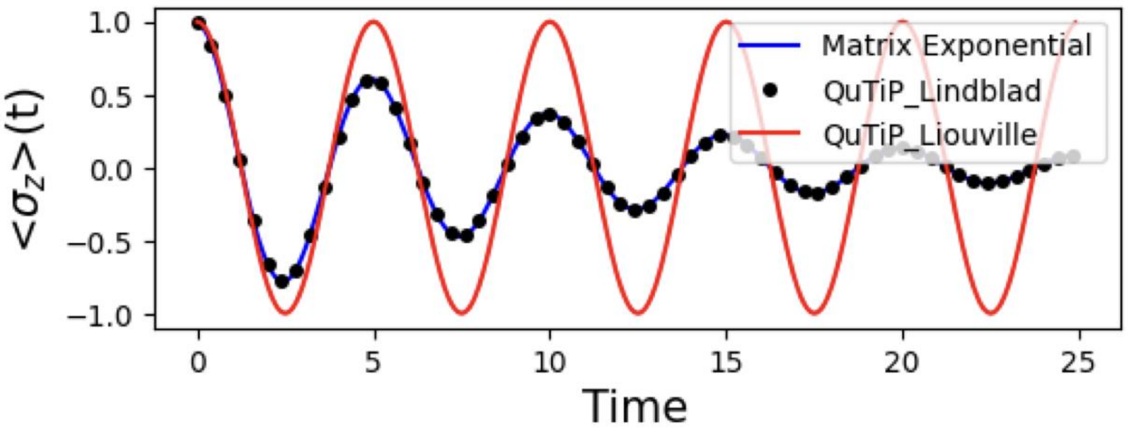
PART E — EXAMPLES

Example 1a — Spin-½ with Dissipation

Script S.4.1-S.4.4: JCTC_IV.ipynb

- Hamiltonian: $H = E_0\,\sigma^z + \Delta\,\sigma^x$ $\qquad E_0 = 0,\ \Delta = 0.1 \times 2\pi.$

$$\frac{\partial \rho(t)}{\partial t} = -\frac{\mathrm{i}}{\hbar}[H, \rho(t)] + \gamma\left[\sigma^+\rho(t)\sigma^- - \frac{1}{2}\{\sigma^-\sigma^+, \rho(t)\}\right]$$



PART E — EXAMPLES

Example 1b — Amplitude Damping

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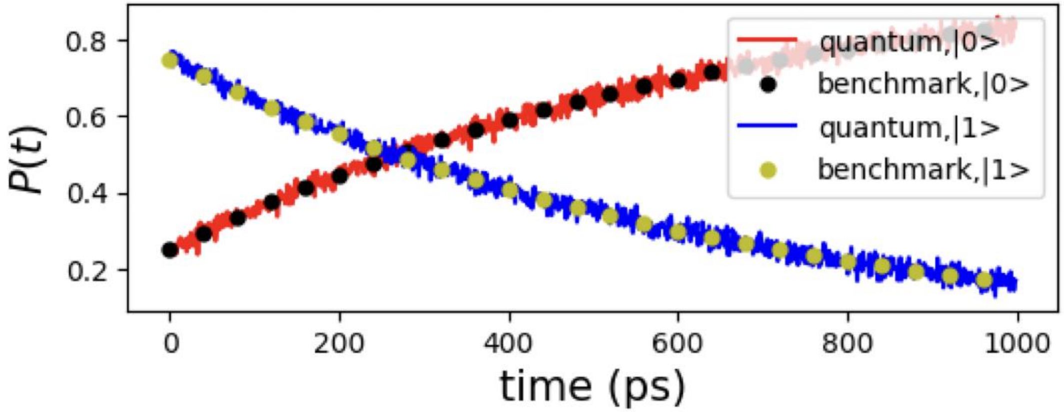
- Hamiltonian: $H = E_0\,\sigma^z + \Delta\,\sigma^x$ $E_0 = 0$ and $\Delta = 0.$

$$\frac{\partial \rho(t)}{\partial t} = \gamma\left[\sigma^+\rho(t)\sigma^- - \frac{1}{2}\{\sigma^-\sigma^+, \rho(t)\}\right]$$

$$\rho(0) = \frac{1}{4}\begin{pmatrix} 1 & 1 \\ 1 & 3 \end{pmatrix}$$



$$P_0 = A_0 n_d \sqrt{N_{000}/N}$$

$$P_1 = A_0 n_d \sqrt{N_{011}/N}$$

PART E — EXAMPLES

Example 2 — Spin-½ Chain: Many-Body Dissipation

$$H = \sum_{n=0}^{N-1} \Omega_n \sigma_n^z - \frac{1}{2} \sum_{n=0}^{N-2} \left(J_{n,n+1}^x \hat{\sigma}_n^x \hat{\sigma}_{n+1}^x + J_{n,n+1}^y \hat{\sigma}_n^y \hat{\sigma}_{n+1}^y + J_{n,n+1}^z \hat{\sigma}_n^z \hat{\sigma}_{n+1}^z \right)$$

$$\dot{\rho}(t) = -\mathrm{i}[H, \rho(t)] + \frac{1}{2} \sum_{m=1}^{2} \sum_{n=0}^{N-1} \gamma_{m,n} \left[2L_{m,n}\rho(t)L_{m,n}^\dagger - \rho(t)L_{m,n}^\dagger L_{m,n} - L_{m,n}^\dagger L_{m,n}\rho(t) \right]$$

- Amplitude + dephasing noise:

$$L_{1,n} = \hat{\sigma}_n^- \qquad L_{2,n} = \hat{\sigma}_n^+ \hat{\sigma}_n^-$$

- Observable: survival amplitude

$$A_s(t) = \sqrt{\mathrm{Tr}[\rho(t)\rho(0)]} \qquad A_s(t) = \sqrt{|\langle \tilde{\nu}_\rho(t) | \tilde{\nu}_\rho(0) \rangle|}$$

- Shows relaxation and loss of revivals

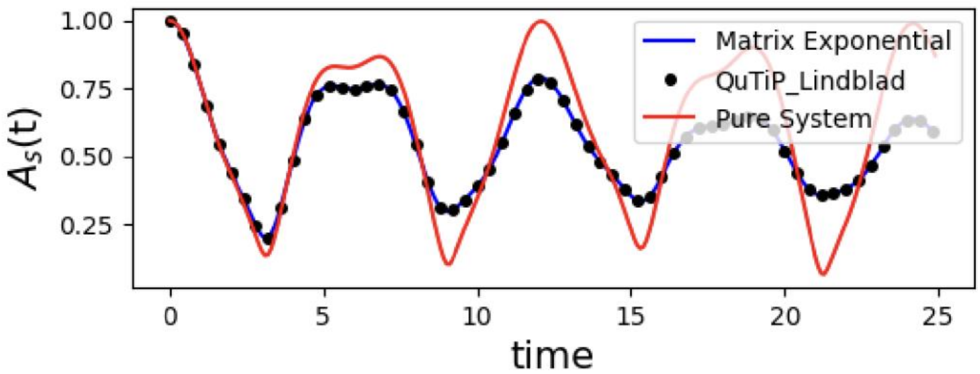
Parameter	$n = 0$	$n \neq 0$
Ω_n	0.65	1.0
$J_{n,n+1}^x$	0.75	1.0
$J_{n,n+1}^y$	0.75	1.0
$J_{n,n+1}^z$	0.0	0.0

PART E — EXAMPLES

Example 2 — Spin-½ Chain: Many-Body Dissipation

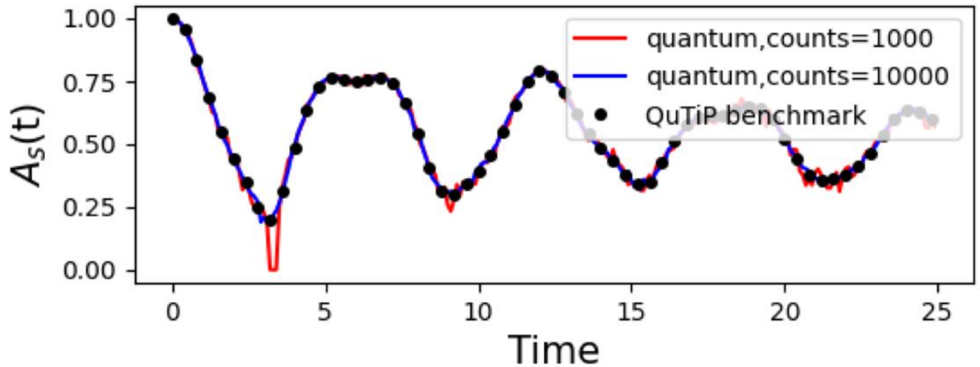
JCTC_IV.ipynb

Script S.5.7



JCTC_IV.ipynb

Script S.5.8



PART E — EXAMPLES

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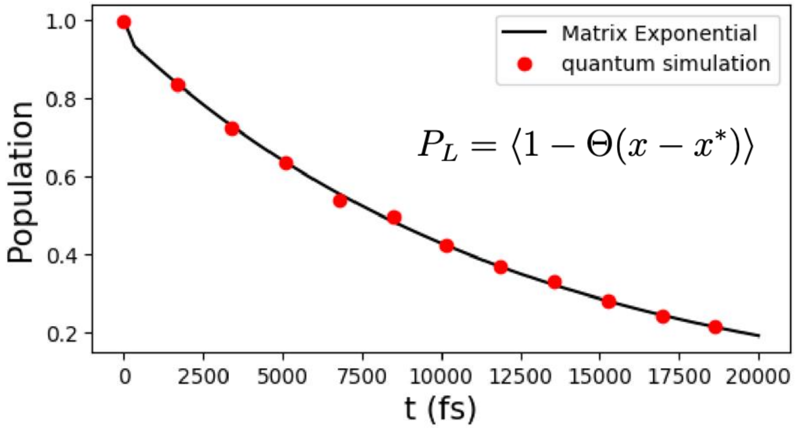
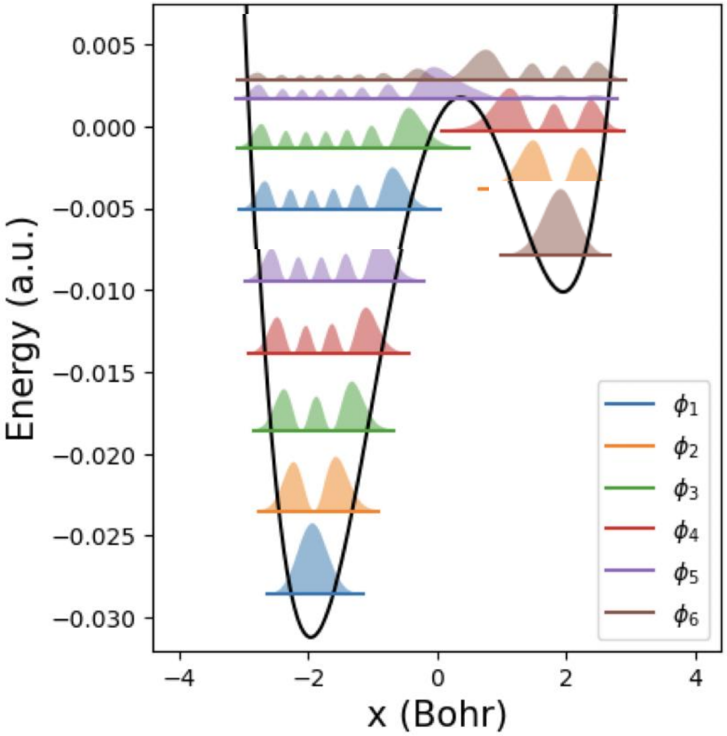
Example 3 — Double-Well Proton Transfer

Script S.6.6-S.6.9

- Proton in DNA base-pair double well
- Initial state localized in right well
- Lindblad bath drives barrier crossing





Take-Home Messages

- We can now simulate:
  dissipation, decoherence, dephasing, relaxation, and chemical kinetics on quantum hardware.
- Open systems require non-unitary evolution implemented by dilation
- Two encodings:
  - Vectorization → fewer circuits, more qubits
  - Kraus → fewer qubits, more circuits
- QFlux unifies:
  - Classical benchmarks
  - Dilation circuits
  - Chemical realism