QFlux: Beyond Lindblad: Non-Markovian Open Quantum Systems

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Part VI: Generalized Quantum Master Equation (GQME)

Non-Markovian dynamics, where the environment has memory

Memory kernels + quantum dilation

https://qflux.batistalab.com

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This tutorial is based on the manuscript

QFlux: Quantum Circuit Implementations for Molecular Dynamics

Part VI - The Generalized Quantum Master Equation

Authors:

Xiaohan Dan, Pouya Khazaei, Ningyi Lyu, Callie Wilson, Ellen Mulvihill, Yuchen Wang, Brandon C. Allen, Delmar G. A. Cabral, Saurabh Shivpuje, Sabre Kais, Victor S. Batista, and Eitan Geva

Why Markovian Dynamics Fails?

- Lindblad assumes memoryless bath
- Real environments have finite correlation times
- Examples:
  - Solvent relaxation
  - Vibronic coupling
  - Long-lived coherences

What Is Non-Markovian Dynamics?

- Future depends on the entire past
- Integro-differential equation
- Environment feeds information back

The GQME: Exact Reduced Dynamics

$$\frac{\partial \hat{\rho}(t)}{\partial t} = -\frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{\rho}(t)] = -\frac{\mathrm{i}}{\hbar}\mathcal{L}\hat{\rho}(t)$$

$$\hat{H} = \sum_{j=1}^{N_e} \hat{H}_j(\hat{\mathbf{R}}, \hat{\mathbf{P}})\,|j\rangle\langle j| + \sum_{j,k=1}^{N_e} \hat{V}_{jk}(\hat{\mathbf{R}})\,|j\rangle\langle k|$$

$$\hat{H}_j(\hat{\mathbf{R}}, \hat{\mathbf{P}}) = \hat{\mathbf{P}}^2/2 + V_j(\hat{\mathbf{R}})$$

$$\mathcal{P}\hat{A} = \hat{\rho}_n(0) \otimes \mathrm{Tr}_n\{\hat{A}\}, \qquad \mathcal{Q} = \mathcal{I} - \mathcal{P}$$

- **GQME:** $$\dot{\sigma}(t) = \underbrace{-\frac{i}{\hbar}\langle L\rangle_n^0 \sigma(t)}_{\text{Instantaneous bath MF}} - \underbrace{\int_0^t K(\tau)\sigma(t-\tau)d\tau}_{\text{memory term bath influence}}$$

$$\langle \mathcal{L}\rangle_n^0(\cdot) = \mathrm{Tr}_n\{\hat{\rho}_n(0)\mathcal{L}\}(\cdot) \qquad \mathcal{K}(\tau) = \frac{1}{\hbar^2}\,\mathrm{Tr}_n\Big\{\mathcal{L}\,\mathrm{e}^{-\mathrm{i}\mathcal{Q}\mathcal{L}\tau/\hbar}\,\mathcal{Q}\mathcal{L}\,\hat{\rho}_n(0)\Big\}$$

Strategy of GQME Simulations

Complete workflow

1. From Hamiltonian of microscopic model (e.g., spin–boson)
2. Compute exact reference (TT-TFD)
3. Build projected Liouvillian
4. Compute memory kernel
5. Solve GQME classically
6. Embed non-unitary propagator into a unitary circuit

Benchmark System: The Spin–Boson Model

$$\hat{H} = \epsilon\,\hat{\sigma}_z + \Gamma\,\hat{\sigma}_x + \sum_{i=1}^{N_n}\left[\frac{\hat{P}_i^2}{2} + \frac{1}{2}\omega_i^2\hat{R}_i^2 - c_i\hat{R}_i\hat{\sigma}_z\right]$$

- Two-level system + harmonic bath.
- **System Parameters:** JCTC_VI.ipynb **Script S.1.1**
  - bias ε
  - coupling Γ
  - temperature β
  - spectral density $J(\omega) = \frac{\pi}{2}\sum_{k=1}^{N_n}\frac{c_k^2}{\omega_k}\,\delta(\omega-\omega_k)$

Initial thermal state:

$$\hat{\rho}(0) = |D\rangle\langle D| \otimes \hat{\rho}_n(0)\,,$$

$$\hat{\rho}_n(0) = \frac{\exp\left[-\beta\sum_{i=1}^{N_n}\left(\frac{\hat{P}_i^2}{2} + \frac{1}{2}\omega_i^2\hat{R}_i^2\right)\right]}{\mathrm{Tr}_n\left\{\exp\left[-\beta\sum_{i=1}^{N_n}\left(\frac{\hat{P}_i^2}{2} + \frac{1}{2}\omega_i^2\hat{R}_i^2\right)\right]\right\}}$$

Ohmic spectral density:

$$J(\omega) = \frac{\pi\hbar}{2}\,\xi\,\omega\,e^{-\omega/\omega_c}$$

Reference Dynamics: TT-TFD

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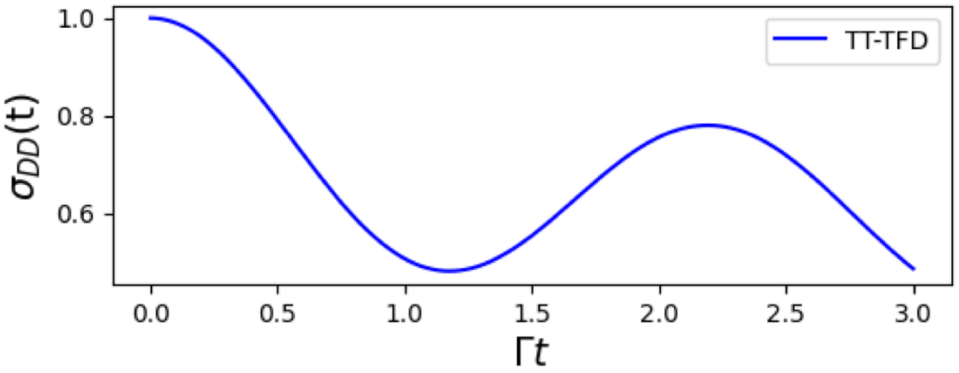
Script S.1.2

- Numerically exact tensor-train method
- Produces σ(t) benchmark
- Shows oscillations + dissipation



Step 1: Projected Liouvillian (No Memory)

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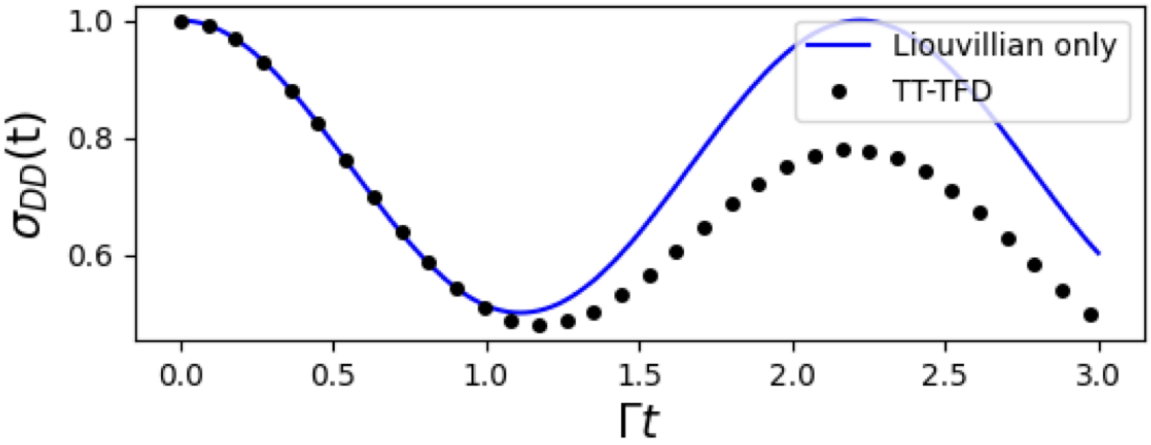
Script S.2.1

Script S.2.1

- Mean-field generator $\langle L \rangle^{0}_{n}$
- Equivalent to closed-system dynamics
- Produces undamped oscillations



Step 2: Building the Memory Kernel

- Solve Volterra equation : JCTC_VI.ipynb **Script S.3.4**

$$\mathcal{K}(t) = \mathrm{i}\dot{\mathcal{F}}(t) - \frac{1}{\hbar}\mathcal{F}(t)\langle\mathcal{L}\rangle_n^0 + \mathrm{i}\int_0^t \mathrm{d}\tau\ \mathcal{F}(t-\tau)\,\mathcal{K}(\tau)$$

- Projection Free Inputs obtained by TT-TFD: **Script S.3.3** JCTC_VI.ipynb

$$\mathcal{F}(t) = \frac{1}{\hbar}\,\mathrm{Tr}_n\left[\mathcal{L}\mathrm{e}^{-\mathrm{i}\mathcal{L}t/\hbar}\hat{\rho}_n(0)\right] \qquad \dot{\mathcal{F}}(t) = -\frac{\mathrm{i}}{\hbar^2}\,\mathrm{Tr}_n\left[\mathcal{L}\mathrm{e}^{-\mathrm{i}\mathcal{L}t/\hbar}\mathcal{L}\hat{\rho}_n(0)\right]$$

$$\hat{\sigma}(t) = \underbrace{\mathcal{G}(t)}\hat{\sigma}(0) = \mathrm{Tr}_n\left[\mathrm{e}^{-\mathrm{i}\mathcal{L}t/\hbar}\,\hat{\rho}_n(0)\right]\hat{\sigma}(0)$$

Script S.3.2

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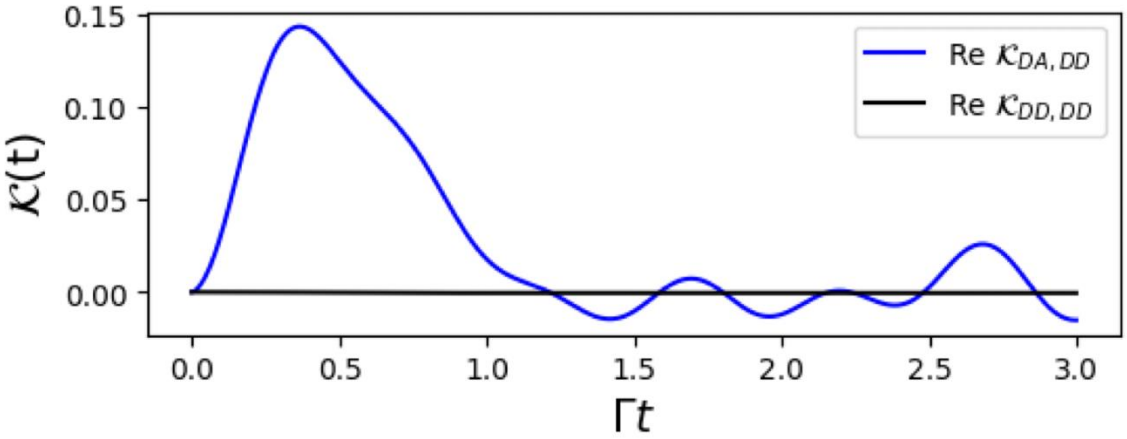
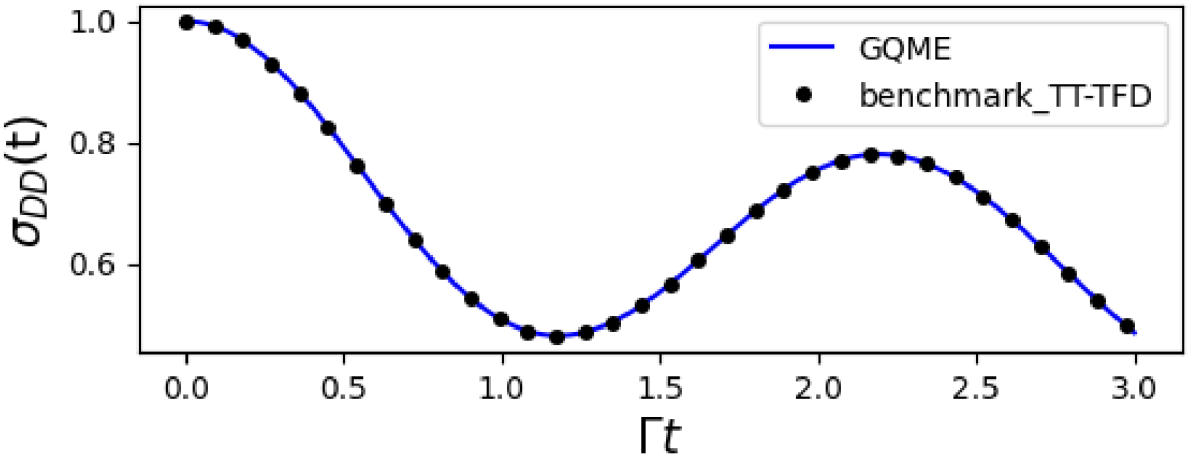
Interpreting the Kernel

- Some elements small → weak direct damping
- Others large → population–coherence transfer
- Kernel decays with bath memory time τ_B



Step 3: Baseline for the GQME

- RK4 time integration: JCTC_VI.ipynb **Script S.4.2**
- Matches TT-TFD exactly



Problem: GQME Is Non-Unitary

- Obtain propagator by TT-TFD:

$$\frac{\partial \mathcal{G}(t)}{\partial t} = -\frac{\mathrm{i}}{\hbar} \langle \mathcal{L} \rangle_n^0 \, \mathcal{G}(t) - \int_0^t \mathrm{d}\tau \, \mathcal{K}(\tau) \, \mathcal{G}(t-\tau)$$

- Propagation: $\hat{\sigma}(t) = \mathcal{G}(t) \, \hat{\sigma}(0)$
- Propagator $\mathcal{G}(t)$ is not unitary
- Quantum circuits require unitary gates
- Need embedding

Key Idea: Sz.-Nagy Dilation

$$\mathcal{U}_{\mathcal{G}'}(t) = \begin{pmatrix} \mathcal{G}'(t) & \mathcal{D}_{\mathcal{G}'^{\dagger}}(t) \\ \mathcal{D}_{\mathcal{G}'}(t) & -\mathcal{G}'^{\dagger}(t) \end{pmatrix} \qquad \begin{aligned} \mathcal{D}_{\mathcal{G}'}(t) &= \sqrt{I - \mathcal{G}'^{\dagger}(t)\mathcal{G}'(t)} \\ \mathcal{D}_{\mathcal{G}'^{\dagger}}(t) &= \sqrt{I - \mathcal{G}'(t)\mathcal{G}'^{\dagger}(t)} \end{aligned}$$

$$\hat{\sigma}(t) = \mathcal{G}'(t)\hat{\sigma}(0) \xrightarrow{\text{dilation}} \mathcal{U}_{\mathcal{G}'}(t) \begin{pmatrix} \hat{\sigma}(0)^{\top} \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Quantum Workflow

1. Solve GQME → get $\mathcal{G}(t)$
2. Rescale to contraction
3. Build dilated unitary $\mathcal{U}_{\mathcal{G}'}(t)$
4. Compile into quantum gate
5. Measure populations

Circuit Architecture

Compact Circuit

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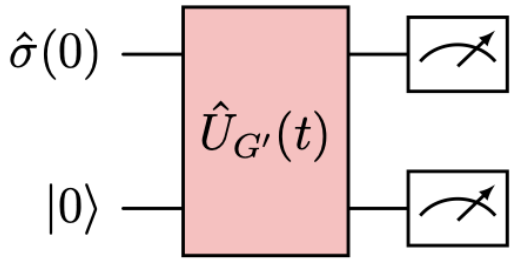
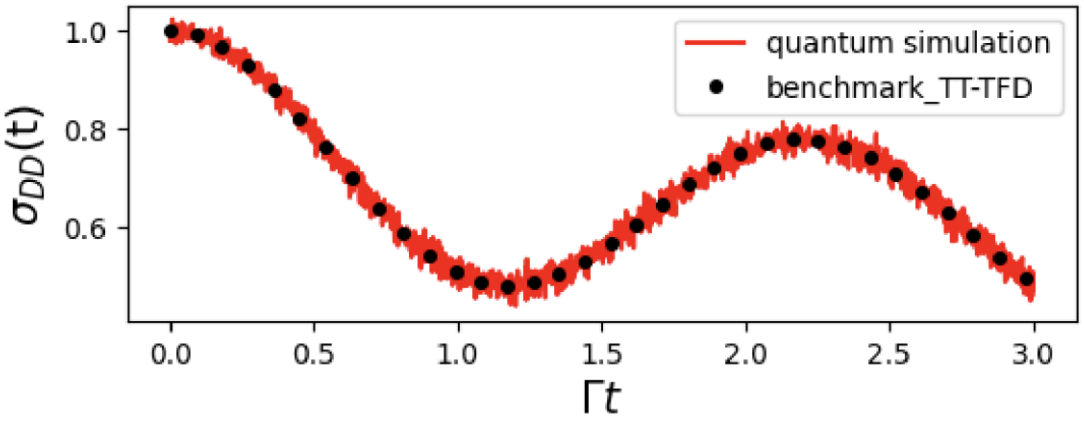
Script S.6.1

Script S.6.2

- 3 qubits total
  - 2 system (vectorized density matrix)
  - 1 dilation ancilla
  - One global unitary gate





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Script S.6.3

Quantum Results vs Exact

Memory Effects: Non-Markovian Quantum Simulations

- QASM simulation
- Excellent agreement with TT-TFD
- Noise only from sampling

Big Picture Take-Home

- GQME gives formally exact reduced dynamics
- Memory kernels capture bath history
- Sz.-Nagy dilation enables quantum simulation
- QFlux provides an end-to-end workflow

Conceptual Unification

All simulation methods unified by Qflux under unitary embeddings

- Closed systems → unitary evolution
- Markov open systems → Lindblad + dilation
- Non-Markov → GQME + memory + dilation

Closing the Series (for now)

- Part I: Classical and Quantum Workflows
- Part II–III: Closed systems
- Part IV–V: Markov open systems
- Part V: Variational methods
- Part VI: non-Markovian memory