A New Proposal for Large-Scale First-Principle Calculations of Decoherence in the Caldeira–Leggett Model and Analogous Models

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1. Introduction

Motivation

Decoherence is a key ingredient in the emergence of classical behavior from quantum dynamics. However, direct real-time calculations for a system coupled to a large environment become prohibitively expensive as the number of environmental degrees of freedom increases.

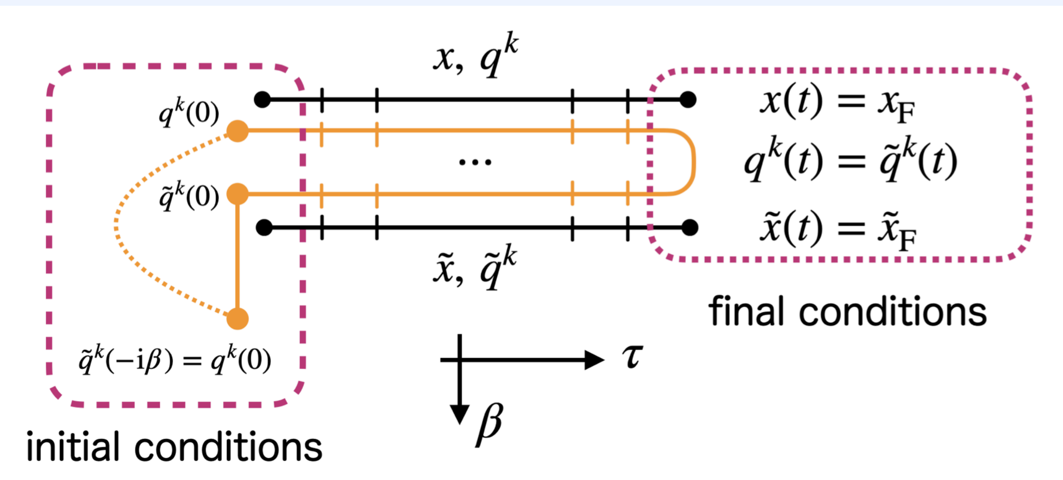
Here we show that, for quadratic Hamiltonians with Gaussian initial states, the reduced dynamics can be reconstructed exactly from a small set of covariance data, leading to a drastic reduction in computational cost.

Caldeira–Leggett model

System X + Environment q_k + Coupling

$$\hat{H} = \frac{\hat{P}^2}{2} + \frac{1}{2}\Omega^2\hat{X}^2 + \sum_{k=1}^{N}\left(\frac{\hat{p}_k^2}{2} + \frac{1}{2}\omega_k^2\hat{q}_k^2\right) - c\,\hat{X}\sum_{k=1}^{N}\hat{q}_k$$

2. Real-time path integral JN-Watanabe arxiv:2503.20699



$$\rho_S(x_F, \tilde{x}_F; t) = \int DxD\tilde{x}\left(\prod_{k=1}^{N_E} Dq^k D\tilde{q}_k\right)\rho_S(x_0, \tilde{x}_0; t)\left(\prod_{k=1}^{N_E}\rho_E^{(k)}(q_0^k, \tilde{q}_0^k, \beta)\right)e^{i(S(x,q)-S(\tilde{x},\tilde{q}))}$$

$$|\rho_S(x_F, \tilde{x}_F; t)| \simeq \exp\left\{-\frac{1}{2}\Gamma_{\rm diag}(t)\left(\frac{x_F+\tilde{x}_F}{2}\right)^2 - \frac{1}{2}\Gamma_{\rm off-diag}(t)\left(\frac{x_F-\tilde{x}_F}{2}\right)^2\right\}$$

3. Our method

Gaussian initial state → Only mean and variance are needed

Quadratic Hamiltonian → Only mean and variance are needed

Assume to be zero

Heisenberg equation

$$\frac{d\hat{z}(t)}{dt} = i[H, \hat{z}(t)] = A\hat{z}(t)$$

$$\hat{z} = \left(\hat{X}, \hat{P}, \hat{q}_1, \hat{p}_1, \ldots, \hat{q}_N, \hat{p}_N\right)^{\top}$$

$$\hat{z}(t) = S(t)\hat{z}(0) \qquad S(t) = e^{At}$$

$$u(t) = e_X^{\top}S(t) \qquad v(t) = e_P^{\top}S(t)$$

Characteristic function

$$\chi(\lambda; t) = \mathrm{Tr}\left[\hat{\rho}\, e^{i\lambda^{\top}\hat{z}(t)}\right] = \exp\left[-\frac{1}{2}\lambda^{\top}\Sigma(t)\,\lambda\right]$$

$$\frac{du(t)}{dt} = u(t)A \qquad \frac{dv(t)}{dt} = v(t)A$$

Covariance matrix

$$\Sigma_{ij}(t) = \frac{1}{2}\langle\,\hat{z}_i(t)\,\hat{z}_j(t) + \hat{z}_j(t)\,\hat{z}_i(t)\,\rangle$$
$$\Sigma_{XX}(t) = u(t)\,\Sigma_0\,u(t)^{\top},$$
$$\Sigma_{XP}(t) = u(t)\,\Sigma_0\,v(t)^{\top},$$
$$\Sigma_{PP}(t) = v(t)\,\Sigma_0\,v(t)^{\top}.$$

$$\Sigma_{XX}(0) = \frac{1}{2\tilde{\Omega}}, \quad \Sigma_{PP}(0) = \frac{\tilde{\Omega}}{2}, \quad \Sigma_{XP}(0) = 0.$$
$$\Sigma_{q_kq_k}(0) = \frac{1}{2\omega_k}\coth\left(\frac{\beta\omega_k}{2}\right),$$
$$\Sigma_{p_kp_k}(0) = \frac{\omega_k}{2}\coth\left(\frac{\beta\omega_k}{2}\right),$$

Wigner function — Tracing out the environment

$$W(z;t) = \frac{1}{(2\pi)^d}\int d^d\lambda\, e^{-i\lambda^{\top}z}\chi(\lambda;t) = \frac{1}{2\pi\sqrt{\det\Sigma_X(t)}}\exp\left[-\frac{1}{2}(X \quad P)\,\Sigma_X^{-1}(t)\begin{pmatrix}X\\P\end{pmatrix}\right],$$

Reduced density matrix

$$\rho_X(Y, Y'; t) = \int dP\, e^{iP(Y-Y')}W_X\left(\frac{Y+Y'}{2}, P; t\right).$$

$$\Gamma_{\rm diag}(t) = \frac{1}{\Sigma_{XX}(t)}$$

$$\Gamma_{\rm off-diag}(t) = 4\left(\Sigma_{PP}(t) - \frac{\Sigma_{XP}^2(t)}{\Sigma_{XX}(t)}\right)$$

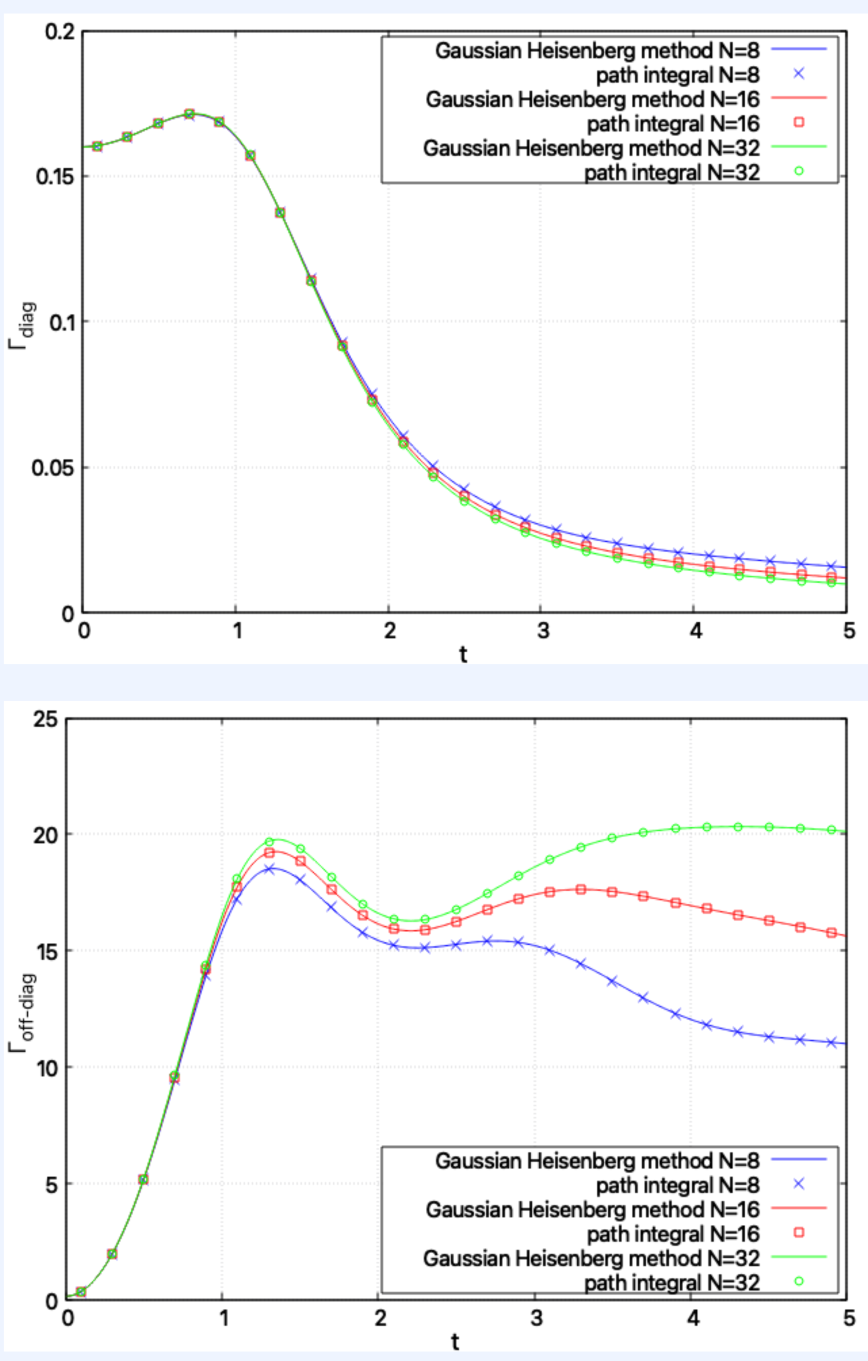
Computational cost:

$$\mathcal{O}(D^3) \gg \mathcal{O}(2nN)$$

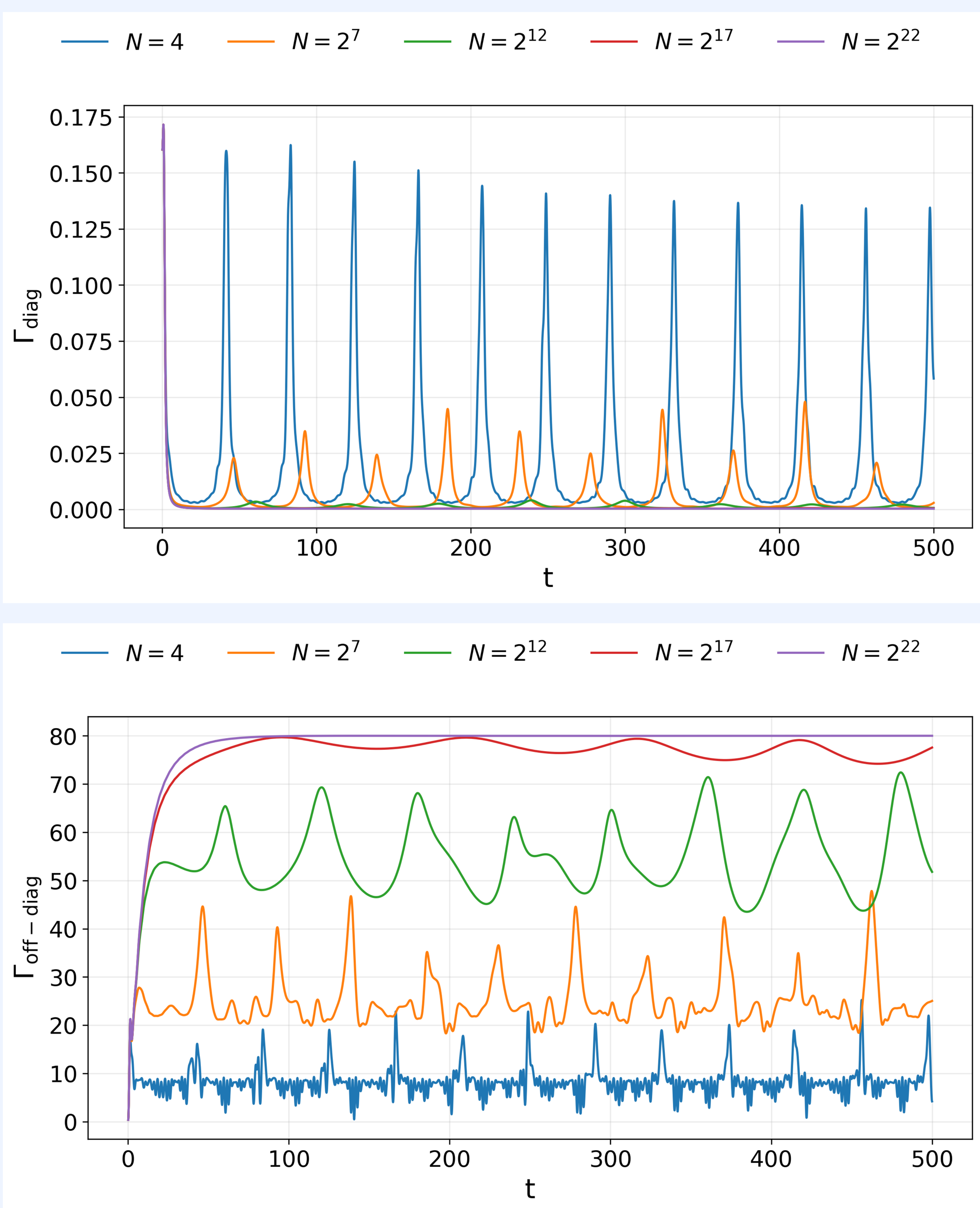
$$N = 32,\ t = 5 \quad \longrightarrow \quad N = 2^{22},\ t = 500$$

$$D = 2N_t(1+N_E) + N_\beta N_E$$

4. Results



Excellent agreement across the whole interval $0 < t < 5$



The approach to the thermal behavior becomes clearer as N is increased.

Summary:

1. We reformulate the open-system problem in terms of a linear propagator and a Gaussian covariance reconstruction, making explicit which part of the dynamics is truly needed for the reduced observables.
2. The method we used here depends on two assumptions: the Hamiltonian is quadratic, and the initial state is Gaussian. Under those conditions, the propagator method is exact.
3. We have applied this method to the von-Neumann measurement problem and obtained some promising results. (Today's talk by Professor Jun Nishimura)