

Benchmarking a Tree Tensor Network Algorithm for the HOPS-Method to Simulate Open non-Markovian Quantum Systems

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I hereby declare that this thesis is entirely the result of my own work except where otherwise indicated. I have only used the resources given in the list of references.

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Zusammenfassung

Eine kurze Zusammenfassung der Arbeit auf Deutsch.

Abstract

A brief abstract of this thesis in English.

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1 Introduction

2 Theory

2.1 Non-Markovian Quantum State Diffusion (NMQSD)

We will consider a system S linearly coupled to a bath B of harmonic oscillators. We can split the Hamiltonian of such a model into a system, bath and interaction part

$$\hat{H} = \hat{H}_S \otimes \mathbb{1}_B + \mathbb{1}_S \otimes \hat{H}_B + \hat{H}_{\text{int}}.$$

We assume that the system lives on N sites, and each site couples independently to M harmonic oscillators. The bath Hamiltonian is then given by

$$\hat{H}_B = \sum_{i=1}^N \sum_{\lambda=1}^M v_{i,\lambda} \hat{a}_{i,\lambda}^\dagger \hat{a}_{i,\lambda},$$

where $\hat{a}_{n,\lambda}^\dagger, \hat{a}_{n,\lambda}$ are the bosonic creation and annihilation operators of the λ th harmonic oscillator coupling to site n , and $v_{n,\lambda}$ are constants. The interaction Hamiltonian can be written as

$$\hat{H}_{\text{int}} = \sum_{i=1}^N \sum_{\lambda=1}^M \left(\gamma_{i,\lambda}^* L_i \otimes \hat{a}_{i,\lambda}^\dagger + \text{h.c.} \right)$$

with constants $\gamma_{n,\lambda}$. The system operators \hat{L}_n describe the coupling of the system to the bath modes. In the context of open systems it is useful to define the *bath correlation function*

$$\alpha(\tau) = \frac{1}{\pi} \int_0^\infty d\omega S(\omega) \left[\coth\left(\frac{\omega}{2T}\right) \cos(\omega\tau) - i \sin(\tau) \right]$$

with the *spectral density* $S(\omega)$. The bath correlation function fully characterizes the influence of the environment at temperature T [1].

We are interested in the dynamics of the system S, which can be described in terms of the reduced density matrix

$$\rho(t) = \text{tr}_B \{ \rho_{\text{tot}}(t) \},$$

where $\rho_{\text{tot}}(t)$ is the density matrix of the total system at time t . $\text{tr}_B \{ \dots \}$ denotes the trace over all bath degrees of freedom. We assume that the total system is initially in the state

$$\rho_{\text{tot}}(0) = \rho_S(0) \otimes \rho_{B, \text{therm}},$$

where the bath is in the thermal state

$$\rho_{\text{therm}}^B = \frac{e^{-\hat{H}_B/T}}{Z_B}$$

with the partition function $Z_B = \text{tr}_B \{ e^{-\hat{H}_B/T} \}$

In terms of Non-Markovian Quantum State Diffusion (NMQSD), one obtains the reduced density matrix $\rho(t)$ from an average over pure states

$$\rho(t) = \mathbb{E} [|\Psi_t(z^*)\rangle \langle \Psi_t(z^*)|]. \quad (2.1)$$

The pure states $|\Psi_t(z^*)\rangle \in \mathcal{H}_S$ are vectors in the system Hilbert space, that depend on a family of stochastic processes $z^* := \{z_n^*(t)\}$. The expectation value $\mathbb{E}[\dots]$ can then be computed by taking the average over

different realizations of z^* . For NMQSD, all stochastic processes $z_n^*(t)$ must have the following properties:

$$\mathbb{E}[z_{i,t}] = \mathbb{E}[z_{i,t}^*] = 0, \quad (2.2a)$$

$$\mathbb{E}[z_{i,t} z_{i,t}^*] = 0, \quad (2.2b)$$

$$\mathbb{E}[z_{i,t} z_{i,s}^*] = \alpha(t-s). \quad (2.2c)$$

Each pure state $|\Psi_t(z^*)\rangle$ starts off in the same initial state $|\Psi_{t=0}(z^*)\rangle = |\Psi_0\rangle$ and then evolves according to the Non-Markovian Quantum State Diffusion (NMQSD) equation [2, 3]

$$\frac{\partial}{\partial t} |\Psi_t\rangle = -iH_S |\Psi_t\rangle + \sum_{i=1}^N \left(L_i z_{i,t}^* |\Psi_t\rangle - L_i^\dagger \int_0^t ds \alpha(t-s) \frac{\delta |\Psi_t\rangle}{\delta z_{n,s}^*} \right), \quad (2.3)$$

where we omitted the explicit dependency of $|\Psi_t\rangle$ on z^* due to brevity.

2.2 Hierarchy Of Pure States (HOPS)

The NMQSD equation (2.3) cannot easily be solved numerically due to the functional derivative. However, one can bring the equation into a hierarchically structured set of differential equations, the Hierarchy of Pure States (HOPS) [4], which can then be integrated numerically. In this section, we will derive the linear HOPS equation, mainly following the derivation in [5], but the same result is also obtained in [4, 6].

We will start by approximating the bath correlation function (BCF) by a finite sum of exponentials

$$\alpha(\tau) \approx \sum_{\mu=1}^{N_{\text{BCF}}} \alpha_\mu(\tau) := \sum_{\mu=1}^{N_{\text{bath}}} g_\mu e^{-\omega_\mu \tau},$$

with constants g_μ and ω_μ . The total number of terms N_{BCF} corresponds to the number of harmonic oscillators coupling to each site of the system. Such an approximation of the bath correlation function is possible for many systems of interest, and a specific example is given in section ??, where we approximate the BCF of the spin-boson model.

In the following, we will assume that the system lives only on a single site, $N = 1$. The derivation of the HOPS can trivially be expanded to $N > 1$ sites.

We will work with the discrete version of the NMQSD equation (2.3) [5]

$$\Psi_{n+1} = \Psi_n + \Delta \cdot \left\{ -iH_S + \left[L z_n^* - L^\dagger \sum_{m=0}^{n-1} \alpha(n\Delta - m\Delta) \frac{\partial}{\partial z_m^*} \right] \right\} \Psi_n, \quad (2.4)$$

where we introduced the time step Δ , with $t \equiv n \cdot \Delta$, and $z^* = \{z_1^*, z_2^*, \dots, z_n^*\}$ now is a discrete stochastic process. One can easily see that the NMQSD equation is recovered if the limit $\Delta \rightarrow 0$ is taken. The reason for using the discrete version of the NMQSD equation is that we can replace the functional derivative with an ordinary derivative and the derivation becomes much more intuitive.

We define the operator

$$D_\mu^n := \sum_{m=0}^{n-1} \alpha(n\Delta - m\Delta) \frac{\partial}{\partial z_m^*} = g_\mu \sum_{m=0}^{n-1} e^{-\omega_\mu(n-m)\Delta} \frac{\partial}{\partial z_m^*}$$

and the auxillary states

$$\Psi_n^{(\vec{k})} := \prod_{\mu=1}^{N_{\text{BCF}}} (D_\mu^n)^{k_\mu} \Psi_n, \quad (2.5)$$

using an index vector $\vec{k} \in \mathbb{N}_0^{N_{\text{BCF}}}$. The physical pure state is recovered when setting the index vector to zero, $\Psi_n = \Psi_n^{(\vec{0})}$. Using these definitions, we can rewrite the discrete NMQSD equation (2.4):

$$\Psi_{n+1}^{(\vec{0})} = \Psi_n^{(\vec{0})} + \Delta \cdot \left(-iH_S + Lz_n^* - L^\dagger \sum_{\mu=1}^{N_{\text{BCF}}} D_\mu^n \right) \Psi_n^{(\vec{0})} = \Psi_n^{(\vec{0})} + \Delta \cdot (-iH_S + Lz_n^*) \Psi_n^{(\vec{0})} - L^\dagger \sum_{\mu=1}^{N_{\text{BCF}}} \Psi_n^{(\vec{0}+\hat{e}_\mu)},$$

where \hat{e}_μ is the μ -th unit vector.

Our next goal is to derive an equation of motion for an arbitrary auxiliary state $\Psi_n^{(\vec{k})}$. Using equation (2.5) we can write

$$\Psi_{n+1}^{(\vec{k})} = \prod_{\mu=1}^{N_{\text{BCF}}} \left(D_\mu^{n+1} \right)^{k_\mu} \Psi_{n+1}. \quad (2.6)$$

We can expand

$$D_\mu^{n+1} = (1 - \omega_\mu \cdot \Delta) \left(g_\mu \frac{\partial}{\partial z_n^*} + D_\mu^n \right) + O(\Delta^2)$$

and hence

$$\left(D_\mu^{n+1} \right)^{k_\mu} = (1 - k_\mu \omega_\mu \Delta) \left(g_\mu \frac{\partial}{\partial z_n^*} + D_\mu^n \right)^{k_\mu} + O(\Delta^2).$$

To further simplify eq (2.6), we can use the fact that the physical pure state at time t , Ψ_n , depends only on the stochastic variables $z_1^*, z_2^*, \dots, z_{n-1}^*$, but not on z_n^* , which we can write as $\Psi_n = \Psi_n(z^*|_0^{n-1})$. It follows that $\frac{\partial}{\partial z_n^*} \Psi_n = 0$. Using equation (2.4) we can see $\frac{\partial^2}{\partial z_n^{*2}} \Psi_{n+1} = 0$ and therefore

$$\left(D_\mu^{n+1} \right)^{k_\mu} \Psi_{n+1} = (1 - k_\mu \omega_\mu \Delta) \left(k_\mu g_\mu \left(D_\mu^n \right)^{k_\mu-1} \frac{\partial}{\partial z_n^*} + \left(D_\mu^n \right)^{k_\mu} \right) + O(\Delta^2). \quad (2.7)$$

Inserting equations (2.4) and (2.7) into equation (2.6) and performing some additional algebra, one arrives at

$$\Psi_{n+1}^{(\vec{k})} = \Psi_n^{(\vec{k})} + \Delta \cdot \left(-iH_S - \vec{k} \cdot \vec{\omega} + z_t^* L \right) \Psi_n^{(\vec{k})} + \Delta \cdot L \sum_{\mu=1}^{N_{\text{BCF}}} g_\mu \Psi_n^{(\vec{k}-\hat{e}_\mu)} - \Delta \cdot L^\dagger \sum_{\mu=1}^{N_{\text{BCF}}} \Psi_n^{(\vec{k}+\hat{e}_\mu)}.$$

Performing the limit $\Delta \rightarrow 0$, we obtain the linear HOPS equation for a single site coupled to multiple heat baths:

$$\frac{\partial}{\partial t} \Psi_t^{(\vec{k})} = \left(-iH_S - \vec{k} \cdot \vec{\omega} + z_t^* L \right) \Psi_t^{(\vec{k})} + L \sum_{\mu=1}^{N_{\text{BCF}}} g_\mu \Psi_t^{(\vec{k}-\hat{e}_\mu)} - L^\dagger \sum_{\mu=1}^{N_{\text{BCF}}} \Psi_t^{(\vec{k}+\hat{e}_\mu)}. \quad (2.8)$$

Repeating the derivation for $N > 1$ sites yields

$$\frac{\partial}{\partial t} \Psi_t^{(\vec{k})} = \left(-iH_S - \vec{k} \cdot \vec{\omega} + \sum_{i=1}^N z_{i,t}^* L_i \right) \Psi_t^{(\vec{k})} + \sum_{i=1}^N \left[L_i \sum_{\mu=1}^{N_{\text{BCF}}} g_\mu \Psi_t^{(\vec{k}-\hat{e}_\mu)} - L_i^\dagger \sum_{\mu=1}^{N_{\text{BCF}}} \Psi_t^{(\vec{k}+\hat{e}_\mu)} \right]. \quad (2.9)$$

Note that the HOPS equations do not contain functional derivatives and therefore can be integrated numerically.

2.3 Computing Expectation Values

Both in linear and non-linear HOPS the density matrix of the system is computed by averaging over multiple realizations of pure states, see equations (2.1) and (2.1). However, mostly one is not interested in the density matrix directly, but in the expectation value of a given operator \hat{A} . In linear HOPS, the average is taken over unnormalized states, and thus the expectation value can be computed as

$$\langle \hat{A} \rangle_t = \frac{\text{tr} \{ \rho(t) \hat{A} \}}{\text{tr} \{ \rho(t) \}} \approx \frac{\text{tr} \{ \frac{1}{N} \sum_{i=1}^N |\Psi_t(z_i^*)\rangle \langle \Psi_t(z_i^*)| \hat{A} \}}{\text{tr} \{ \frac{1}{N} \sum_{i=1}^N |\Psi_t(z_i^*)\rangle \langle \Psi_t(z_i^*)| \}} = \frac{\sum_i \langle \Psi_t(z_i^*) | \hat{A} | \Psi_t(z_i^*) \rangle}{\sum_i \langle \Psi_t(z_i^*) | \Psi_t(z_i^*) \rangle}, \quad (2.10)$$

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where we denote different realizations i of the noise with z_i^* and we used the cyclic property of the trace. In non-linear HOPS the average is taken over normalized states $|\tilde{\Psi}_t(z^*)\rangle$ instead, and thus it holds $\text{tr}\{\rho\} = 1$. The expectation value can then be computed as

$$\langle \hat{A} \rangle_t = \frac{\text{tr}\{\rho(t) \hat{A}\}}{\text{tr}\{\rho(t)\}} \approx \frac{1}{N} \sum_{i=1}^N \langle \tilde{\Psi}_t(z_i^*) | \hat{A} | \tilde{\Psi}_t(z_i^*) \rangle = \frac{1}{N} \sum_{i=1}^N \frac{\langle \Psi_t(z_i^*) | \hat{A} | \Psi_t(z_i^*) \rangle}{\langle \Psi_t(z_i^*) | \Psi_t(z_i^*) \rangle}. \quad (2.11)$$

3 Implementing and testing HOPS

4 Implementing and testing HOMPS

4.1 The BCF of the Spin-Boson model

In this section we want to compute g_j and ω_j such that the bath correlation function

$$\alpha(\tau) = \frac{1}{\pi} \int_0^\infty S(\omega) \left[\coth\left(\frac{\omega}{2T}\right) \cos(\omega\tau) - i \sin(\omega\tau) \right] d\omega = \int_0^\infty I(\omega, \tau) d\omega$$

with the *Debye spectral density*

$$S(\omega) = \eta \frac{\omega\gamma}{\omega^2 + \gamma^2}$$

can be approximated as a sum of exponentials

$$\alpha(\tau) \approx \sum_{j=0}^{N_{BCF}} g_j e^{-\omega_j \tau}.$$

To compute the expansion coefficients g_j and ω_j , we will use a *Matsubara expansion*. First we note that the integrand $I(\omega, \tau)$ is symmetric with respect to ω , $I(-\omega, \tau) = I(\omega, \tau)$. Hence, we can extend the integral over the negative real axis:

$$\alpha(\tau) = \frac{1}{2} \int_{-\infty}^{\infty} I(\omega, \tau) d\omega.$$

We further split the integral into a real and an imaginary part $\alpha(\tau) = a(\tau) + ib(\tau)$, where

$$a(\tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} S(\omega) \coth\left(\frac{\omega}{2T}\right) \cos(\omega\tau) d\omega$$

and

$$b(\tau) = -\frac{1}{2\pi} \int_{-\infty}^{\infty} S(\omega) \sin(\omega\tau) d\omega.$$

Expanding the sine and cosine in terms of exponentials and using the antisymmetry of the hyperbolic cotangent and the Debye spectral density, we can write

$$a(\tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} S(\omega) \coth\left(\frac{\omega}{2T}\right) e^{i\omega\tau} d\omega,$$

$$b(\tau) = -\frac{1}{2\pi i} \int_{-\infty}^{\infty} S(\omega) e^{i\omega\tau} d\omega.$$

To solve the integrals, we will use the residual theorem. Consider the contour ξ in figure ?? . Because of the exponential $e^{i\omega\tau}$, the contribution along ξ_2 vanishes as we take the limit $R \rightarrow \infty$. This leaves us with

$$\begin{aligned} a(\tau) &= \frac{1}{2\pi} \oint_{\xi} S(\omega) \coth\left(\frac{\omega}{2T}\right) e^{i\omega\tau} d\omega = i \sum_{\{\omega_j\}} \text{Res}\left(S(\omega) \coth\left(\frac{\omega}{2T}\right); \omega_j\right) e^{i\omega_j\tau} \\ &= i \sum_{\{\omega'_j\}} \text{Res}\left(S(\omega); \omega'_j\right) \coth\left(\frac{\omega'_j}{2T}\right) e^{i\omega'_j\tau} + i \sum_{\{\omega''_j\}} \text{Res}\left(\coth\left(\frac{\omega}{2T}\right); \omega''_j\right) S(\omega''_j) e^{i\omega''_j\tau}, \\ b(\tau) &= -\frac{1}{2\pi} \oint_{\xi} S(\omega) e^{i\omega\tau} d\omega = - \sum_{\{\omega'_j\}} \text{Res}\left(S(\omega); \omega'_j\right) e^{i\omega'_j\tau}, \end{aligned}$$

where ω_j are the poles of $S(\omega) \coth\left(\frac{\omega}{2T}\right)$, ω'_j the poles of $S(\omega)$, ω''_j the poles of $\coth\left(\frac{\omega}{2T}\right)$, and we used the residue theorem. We also assumed $\omega'_j \neq \omega''_b$ for all a, b , which is the case for almost all γ and T . Next, we need to compute the poles and residues. The Debye spectral density has simple poles at $\omega'_j = \pm i\gamma$, with residuals

$$\text{Res}(S(\omega); \pm i\gamma) = \lim_{\omega \rightarrow i\gamma} (\omega \mp i\gamma) S(\omega) = \frac{\eta\gamma}{2}.$$

The poles of the hyperbolic cotangent $\coth\left(\frac{\omega}{2T}\right)$ lie on the imaginary axis, $\omega''_j = 2\pi iTa$ with $a \in \mathbb{Z}$, and are again simple poles with residuals

$$\text{Res}\left(\coth\left(\frac{\omega}{2T}\right); 2\pi iTj\right) = \lim_{\omega \rightarrow 2\pi iTj} (\omega - 2\pi iTj) \coth\left(\frac{\omega}{2T}\right) = \lim_{\lambda \rightarrow 0} 2T\lambda \coth(\lambda) = 2T,$$

where we used the identities $\coth(x + i\pi n) = \coth(x)$ for $n \in \mathbb{Z}$ and $\lim_{x \rightarrow 0} x \coth(x) = 1$. With this, we are now equipped to solve the integrals:

$$b(\tau) = -\frac{\eta\gamma}{2} e^{-\gamma\tau},$$

$$a(\tau) = i\frac{\eta\gamma}{2} \coth\left(\frac{i\gamma}{2T}\right) e^{-\gamma\tau} + i \sum_{j=1}^{\infty} 2T S(2\pi iTj) e^{-2\pi Tj\tau}.$$

Putting the results together, we can write

$$\alpha(\tau) = a(\tau) + ib(\tau) = \sum_{j=0}^{\infty} g_j e^{-\omega_j \tau}$$

with

$$g_0 = \frac{\eta\gamma}{2} \left(\cot\left(\frac{\gamma}{2T}\right) - i \right); \quad \omega_0 = \gamma,$$

$$g_i = \eta \frac{4\pi T^2 j \gamma}{4\pi^2 T^2 j^2 - \gamma^2}; \quad \omega_j = 2\pi Tj \quad \text{for } j \leq 1. \quad (4.1)$$

The result is similar to the one obtained in [7] (up to a different normalization).

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