

QUPIT: QUasiadiabatic propagator Path Integral Toolkit

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Chapter 1

A Review on QUAPI

In this chapter we give a review of the formalism of the QUAPI [1, 2, 3]. Let us consider a generic many-body system which can be modeled by a finite system of interest coupled to a bath. Let $H(t)$ denote the total Hamiltonian which can split into three parts:

$$H(t) = H_S(t) + H_B + H_{SB}, \quad (1.1)$$

where $H_S(t)$ is the Hamiltonian of the system of interest, H_B is the Hamiltonian of the bath and H_{SB} represents the coupling between the system and the bath. Here we consider the case where only the system Hamiltonian $H_S(t)$ is time-dependent. Let $\rho(t)$ be the total density matrix, then the time evolution of $\rho(t)$ is given by

$$\rho(t) = U(t)\rho(0)U^\dagger(t), \quad (1.2)$$

where

$$U(t) = \text{T exp} \left[-i \int_0^t H(\tau) d\tau \right] = \lim_{\delta t \rightarrow 0} \prod_{t_i=0}^t e^{-iH(t_i)\delta t}. \quad (1.3)$$

Here T is the chronological ordering symbol, and the product is understood in that we take the limit over all the infinitesimal intervals δt . Therefore we can write the density matrix $\rho(t)$ as

$$\rho(t) = \lim_{N \rightarrow \infty} e^{-iH(t_N)\delta t} \dots e^{-iH(t_0)\delta t} \rho(0) e^{iH(t_0)\delta t} \dots e^{iH(t_N)\delta t} \quad (1.4)$$

for $t_0 = 0$ and $\delta t = t/N$.

Now we introduce the reduced density matrix of the system $\rho_B(t) = \text{Tr}_B[\rho(t)]$, which is obtained by tracing the total density matrix over the bath degrees of freedom, then the time evolution of $\rho_B(t)$ is given by

$$\rho_S(s'', s'; t) = \text{Tr}_B \langle s'' | \lim_{N \rightarrow \infty} e^{-iH(t_N)\delta t} \dots e^{-iH(t_1)\delta t} \rho(0) e^{iH(t_1)\delta t} \dots e^{iH(t_N)\delta t} | s' \rangle. \quad (1.5)$$

For numerical evaluation we can employ finite δt in the above expression which approximates the evolution operator $U(t)$ into a product of finite N exponentials. Inserting the identity operator $\int |s\rangle \langle s| ds$ between every two exponentials and relabeling s'', s' as s_N^+, s_N^- gives

$$\begin{aligned} \rho(s_N^+, s_N^-; t) = & \int ds_0^+ \dots ds_{N-1}^+ \int ds_0^- \dots ds_{N-1}^- \\ & \text{Tr}_B [\langle s_N^+ | e^{-iH(t_N)\delta t} | s_{N-1}^+ \rangle \dots \langle s_1^+ | e^{-iH(t_1)\delta t} | s_0^+ \rangle \\ & \times \langle s_0^+ | \rho(0) | s_0^- \rangle \langle s_0^- | e^{iH(t_1)\delta t} | s_1^- \rangle \dots \langle s_{N-1}^- | e^{iH(t_N)\delta t} | s_N^- \rangle]. \end{aligned} \quad (1.6)$$

The integrand in the above expression can be referred as the “influence functional” and we denote it by $I(s_0^\pm, \dots, s_N^\pm)$. The influence functional has an important property which greatly simplify the calculation: nonlocal correlations in the influence functional decay exponentially under certain conditions. For spin-boson model, finite temperature is needed, and for spin-fermion model, finite chemical potential difference or temperature is needed. This property enables practical numerical calculation for the influence functional.

In the discretized form, $\rho(0)$ need to “go” through N steps to arrive at $\rho(t)$. Then nonlocal correlations with all length need to be taken into consideration, which means the influence functional can be written as a product of terms corresponding to different correlation length Δk ,

$$I(s_0^\pm, \dots, s_N^\pm) = \prod_{k=0}^N I_0(s_k^\pm) \prod_{k=0}^{N-1} I_1(s_k^\pm, s_{k+1}^\pm) \cdots \prod_{k=0}^{N-\Delta k} I_{\Delta k}(s_k^\pm, s_{k+\Delta k}^\pm) \cdots I_N(s_0^\pm, s_N^\pm). \quad (1.7)$$

Now suppose the influence functional can be truncated beyond a memory time $\tau_c = N_s \delta t$ for N_s a positive integer, then we have

$$I(s_0^\pm, \dots, s_N^\pm) = \prod_{k=0}^N I_0(s_k^\pm) \prod_{k=0}^{N-1} I_1(s_k^\pm, s_{k+1}^\pm) \cdots \prod_{k=0}^{N-\Delta k} I_{\Delta k}(s_k^\pm, s_{k+\Delta k}^\pm) \cdots \prod_{k=0}^{N-N_s} I_{N_s}(s_0^\pm, s_{N_s}^\pm). \quad (1.8)$$

It is easy to see that (1.8) becomes (1.7) when $N_s \rightarrow \infty$, i.e., this approach becomes exact when $\tau_c \rightarrow \infty$. In addition, we have

$$\begin{aligned} I(s_0^\pm, \dots, s_N^\pm) &= I(s_0^\pm, \dots, s_{N-1}^\pm) I_0(s_N^\pm) \cdots I_{\Delta k}(s_{N-\Delta k}^\pm, s_N^\pm) \cdots I_{N_s}(s_{N-N_s}^\pm, s_N^\pm) \\ &= I(s_0^\pm, \dots, s_{N-1}^\pm) \frac{I(s_{N-N_s}^\pm, \dots, s_N^\pm)}{I(s_{N-N_s}^\pm, \dots, s_{N-1}^\pm)}, \end{aligned} \quad (1.9)$$

and recursively applying this expression yields

$$I(s_0^\pm, \dots, s_N^\pm) = I(s_0^\pm, \dots, s_{N_s}^\pm) I_s(s_1^\pm, \dots, s_{N_s+1}^\pm) \cdots I_s(s_{N-N_s}^\pm, \dots, s_N^\pm), \quad (1.10)$$

where

$$I_s(s_k^\pm, \dots, s_{k+N_s}^\pm) = \frac{I(s_k^\pm, \dots, s_{k+N_s}^\pm)}{I(s_k^\pm, \dots, s_{k+N_s-1}^\pm)}. \quad (1.11)$$

To integrate (1.10), we define a multiple time system reduced density matrix $\tilde{\rho}_S(s_k^\pm, \dots, s_{k+N_s-1}^\pm)$ with an initial condition $\tilde{\rho}_S(s_0^\pm, \dots, s_{N_s-1}^\pm) = 1$ for which all initial elements are one. Then the first evolution step for (1.10) is given by

$$\tilde{\rho}_S(s_1^\pm, \dots, s_{N_s}^\pm) = \int I(s_0^\pm, \dots, s_{N_s}^\pm) ds_0^\pm, \quad (1.12)$$

and beyond the first step the evolution step is given by

$$\tilde{\rho}_S(s_{k+1}^\pm, \dots, s_{k+N_s}^\pm) = \int \tilde{\rho}_S(s_k^\pm, \dots, s_{k+N_s-1}^\pm) I_s(s_k^\pm, \dots, s_{k+N_s}^\pm) ds_k^\pm. \quad (1.13)$$

Then the time-local ($t_k = k\delta t$) reduced density matrix is obtained by summing over all intermediate states for which

$$\rho_S(s_k^+, s_k^-; t_k) = \int \tilde{\rho}_S(s_{k-N_s+1}^\pm, \dots, s_k^\pm) ds_k^\pm \cdots ds_{k-N_s+1}^\pm. \quad (1.14)$$

1.1 Spin-Boson Model

The system Hamiltonian of the spin-boson model describes a two level system for which

$$H_S(t) = \frac{1}{2} \mathbf{B}(t) \cdot \boldsymbol{\sigma}, \quad (1.15)$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ which is the Pauli matrices vector and $\mathbf{B}(t)$ is the external field. The bath Hamiltonian describes a collection of phonon modes for which

$$H_B = \sum_k \omega_k b_k^\dagger b_k, \quad (1.16)$$

where b_k^\dagger (b_k) creates (annihilates) a phonon with frequency ω_k . The system-bath coupling is taken to be

$$H_{SB} = \frac{1}{2} \sum_k V_k (\mathbf{n} \cdot \boldsymbol{\sigma}) (b_k + b_k^\dagger), \quad (1.17)$$

where \mathbf{n} is a unit vector with spherical angle θ, ϕ for which $\mathbf{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$, and

$$\mathbf{n} \cdot \boldsymbol{\sigma} = \sigma_x \sin \theta \cos \phi + \sigma_y \sin \theta \sin \phi + \sigma_z \cos \theta. \quad (1.18)$$

This unit vector \mathbf{n} describes the system-bath coupling angle θ, ϕ . The bath can be characterized by the spectral density

$$J(\omega) = \sum_k V_k^2 \delta(\omega - \omega_k) = \alpha \omega^s \Theta(\omega - \omega_c), \quad (1.19)$$

where α is the control parameter, Θ is the heavy step function and ω_c is the cutoff frequency of the phonon modes. The exponential factor describes the type of bath: when $0 < s < 1$ we have a sub-Ohmic form, when $s = 1$ we have an Ohmic form, and when $s > 1$ we have a super-Ohmic form.

Chapter 2

Reference

Bibliography

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