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:

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

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

$$\rho(t) = U(t)\rho(0)U^\dagger(t), \tag{1.2}$$

where

$$U(t) = \mathrm{T}\exp\left[-i\int_0^t H(\tau)\,\mathrm{d}\tau\right] = \lim_{\delta t\to 0}\prod_{t_i=0}^{t} e^{-iH(t_i)\delta_t}. \tag{1.3}$$

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

$$\rho(t) = \lim_{N\to\infty} e^{-iH(t_N)\delta t}\cdots e^{-iH(t_0)\delta t}\rho(0)e^{iH(t_0)\delta t}\cdots e^{iH(t_N)\delta t} \tag{1.4}$$

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

Now we introduce the reduced density matrix of the system $\rho_B(t) = \mathrm{Tr}_B[\rho(t)]$, 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

$$\rho_S(s'', s'; t) = \mathrm{Tr}_B\left\langle s''\right| \lim_{N\to\infty} e^{-iH(t_N)\delta t}\cdots e^{-iH(t_1)\delta t}\rho(0)e^{iH(t_1)\delta t}\cdots e^{iH(t_N)\delta t}\left|s'\right\rangle. \tag{1.5}$$

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 $\int |s\rangle\langle s|\,\mathrm{d}s$ between every two exponentials and relabeling s'', s' as s_N^+, s_N^- gives

$$\begin{aligned}\rho(s_N^+, s_N^-; t) = \int \mathrm{d}s_0^+\cdots\mathrm{d}s_{N-1}^+ \int \mathrm{d}s_0^-\cdots\mathrm{d}s_{N-1}^- \\ \mathrm{Tr}_B[\left\langle s_N^+\right|e^{-iH(t_N)\delta t}\left|s_{N-1}^+\right\rangle\cdots\left\langle s_1^+\right|e^{-iH(t_1)\delta t}\left|s_0^+\right\rangle \\ \times\left\langle s_0^+\right|\rho(0)\left|s_0^-\right\rangle\left\langle s_0^-\right|e^{iH(t_1)}\delta t\left|s_1^-\right\rangle\cdots\left\langle s_{N-1}^-\right|e^{iH(t_N)\delta t}\left|s_N^-\right\rangle].\end{aligned} \tag{1.6}$$

The integrand in the above expression can be referred as the "influence functional" and we denote it by $I(s_0^{\pm},\ldots,s_N^{\pm})$. The influence functional has an important property which greatly simply 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,

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

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

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

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

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

and recursively applying this expression yields

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

where

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

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

$$\tilde{\rho}_S(s_1^{\pm},\ldots,s_{N_s}^{\pm}) = \int I(s_0^{\pm},\ldots,s_{N_s}^{\pm})\,\mathrm{d}s_0^{\pm}\,, \tag{1.12}$$

and beyond the first step the evolution step is given by

$$\tilde{\rho}_S(s_{k+1}^{\pm},\ldots,s_{k+N_s}^{\pm}) = \int \tilde{\rho}_S(s_k^{\pm},\ldots,s_{k+N_s-1}^{\pm})I_s(s_k^{\pm},\ldots,s_{k+N_s}^{\pm})\,\mathrm{d}s_k^{\pm}\,. \tag{1.13}$$

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

$$\rho_S(s_k^{+},s_k^{-};t_k) = \int \tilde{\rho}_S(s_{k-N_s+1},\ldots,s_k^{\pm})\,\mathrm{d}s_k^{\pm}\cdots\mathrm{d}s_{k-N_s+1}^{\pm}\,. \tag{1.14}$$

1.1 Spin-Boson Model

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

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

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

$$H_B = \sum_k \omega_k b_k^\dagger b_k, \tag{1.16}$$

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

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

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

$$\boldsymbol{n} \cdot \boldsymbol{\sigma} = \sigma_x \sin\theta\cos\phi + \sigma_y \sin\theta\sin\phi + \sigma_z\cos\theta. \tag{1.18}$$

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

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

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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