QUPIT: QUasiadiabatic propagator Path Integral Toolkit

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Chapter 1

General Formulation of QUAPI

In this chapter we give a review of the general 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

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

Chapter 2

Reference

Bibliography

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