

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:

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

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

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

Chapter 2

Reference

Bibliography

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