Overview of Influence Functionals for Open Quantum Systems

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1 Introduction

The influence functional was first introduced by Feynman and Vernon [1] using the Lagrangian or path integral formulation of quantum mechanics. In classical mechanics, a system with the coordinate x can be defined by the Lagrangian $\mathcal{L}(x, \dot{x}, t)$. The action of the Lagrangian is defined as the time integral of the Lagrangian along some path $x(t)$,

$$S[x(t)] = \int_{t_0}^{t_1} \mathcal{L}(x(t), \dot{x}(t))\, dt \tag{1}$$

According to Hamilton's principle, the path along which the action is stationary, meaning that the action remains constant (to first order) as one deviates from $x(t)$, is the classical path from which we derive the equations of motion of our system (i.e., the Euler-Lagrange equations).

Feynman postulated that the time evolution of the probability amplitude $\psi(x_N, t + N\Delta t)$ from initial state $\psi(x_0, t_0)$ can be written as

$$\psi(x_N, t_0 + N\Delta t) = \lim_{\substack{\Delta t \to 0 \\ N \to \infty}} \int \exp\left[\frac{i}{\hbar} S(x_{k+1}, x_k)\right] \psi(x_k, t_0) \frac{dx_{N-1}}{A} \dots \frac{dx_0}{A}. \tag{2}$$

Note: to simplify notation, the integrals over each coordinate in time were often represented as a functional integral:

$$\mathcal{D}x = \lim_{N \to \infty} \frac{1}{A^N} \int dx_1 \dots dx_N \tag{3}$$

The dominant contributions to Eq. (2) are from the paths whose actions are close to stationary, meaning that the phase only deviates slightly when the path is perturbed. This is the same as the classical path of the system (as stated by Hamilton), defined as when the action $S(x)$ is stationary, or $\delta S / \delta x(t) = 0$.

But for quantum systems whose Hamiltonian is H, Eq. (2) is equivalent to

$$\psi(x, t_0 + N\Delta t) = e^{-iH(N\Delta t)} \psi(x, t_0) \tag{4}$$

and the time evolution of the density matrix $\rho = |\psi\rangle \langle\psi|$ (with Liouvillian $L = [H, \cdot]$) is

$$\rho(x, t_0 + N\Delta t) = e^{-iH(N\Delta t)} \rho(x, t) e^{iH(N\Delta t)} = e^{-iL(N\Delta t)} \rho(x, t) \tag{5}$$

It is arguably easier to consider path integrals in this operator-based representation. The functional derivative (the integration over the coordinates at each time step) now looks like the insertion of the resolution at identity at each time step (see below). Therefore, the key idea that one should keep in mind is the "space-time" aspect of the formalism–that we have our problem coordinates at every step in time.

2 Definition of Influence Functionals

Consider a quantum system composed of a subsystem of interest S (with coordinates or states s) and a bath B (with coordinates b), whose Hamiltonian is of the form $H = H_s + H_{bs}$, where H_s is the Hamiltonian of the subsystem and H_{bs} defines the dynamics of the bath and the coupling of the bath to the subsystem.

We denote the subsystem density matrix by $\rho_s(s_T)$, where s_T is a basis for the density matrix at time T, and the bath density matrix is analogously written as $\rho_b(b_T)$. The basis of the full system is spanned by the product space $\{s\} \otimes \{b\}$. The evolution of the density matrix is given by a linear operator, the Liouville operator L, which we partition as $L = L_s + L_{bs}$ where L_s contains the component operating only on the subsystem and L_{bs} contains the component on the bath and interactions between the subsystem and bath. If we further assume the system dynamics obeys Hamiltonian evolution, then the Liouville action can be written as $L\rho = [H, \rho]$.

Formally, $\rho_s(s_T)$ is obtained by time evolving the entire system and tracing out the bath degrees of freedom. The path integral expression, assuming a second-order Trotter decomposition of the time evolution operator into N timesteps of length Δt, is

$$\begin{aligned}\rho_s(s_T) = \mathrm{Tr}_{b_T}\Bigg[\sum_{s_{t_{N-1}}} \sum_{s_{t'_{N-1}}} \sum_{b_{t_{N-1}}} \sum_{b_{t'_{N-1}}} \cdots \sum_{s_{t_0}} \sum_{s'_{t_0}} \sum_{b_{t_0}} \sum_{b'_{t_0}} \\ \langle\langle s_T, b_T |\, e^{-\frac{i}{2}L_s\Delta t}\, |s_{t_N}, b_{t_N}\rangle\rangle \, \langle\langle s_{t_N}, b_{t_N} |\, e^{-iL_{bs}\Delta t}\, |s_{t'_N}, b_{t'_N}\rangle\rangle \\ \times \langle\langle s_{t'_N}, b_{t'_N} |\, e^{-iL_s\Delta t}\, |s_{t_{N-1}}, b_{t_{N-1}}\rangle\rangle \, \langle\langle s_{t_{N-1}}, b_{t_{N-1}} |\, e^{-iL_{bs}\Delta t}\, |s_{t'_{N-2}}, b_{t'_{N-2}}\rangle\rangle \\ \times \langle\langle s_{t'_{N-2}}, b_{t'_{N-2}} |\, e^{-iL_s\Delta t}\, |s_{t_{N-2}}, b_{t_{N-2}}\rangle\rangle \times \dots \\ \times \langle\langle s_{t_1}, b_{t_1} |\, e^{-iL_{bs}\Delta t}\, |s_{t'_1}, b_{t'_1}\rangle\rangle \, \langle\langle s_{t'_1}, b_{t'_1} |\, e^{-\frac{i}{2}L_s\Delta t}\, |s_{t_0}, b_{t_0}\rangle\rangle \\ \times \langle\langle s_{t_0}, b_{t_0} | \rho(s_{t_0}, b_{t_0})\rangle\rangle \Bigg] \end{aligned} \tag{6}$$

where $\rho(s_{t_0}, b_{t_0})$ is the initial state of the system, and the double bra/ket notation indicates we are working in Liouville space, with the density matrix being a vector in this space. In the above, we have inserted the resolution of identity between each operator.

For simplicity in notation, assume there are no correlations between the subsystem and bath initially such that $|\rho(s_{t_0}, b_{t_0})\rangle\rangle = |\rho_s(s_{t_0})\rangle\rangle\, |\rho_b(b_{t_0})\rangle\rangle$. Also, note that $\langle\langle s_{t'_n}, b_{t'_n} |\, e^{-iL_s\Delta t}\, |s_{t_{n-1}}, b_{t_{n-1}}\rangle\rangle = \langle\langle s_{t'_n} |\, e^{-iL_s\Delta t}\, |s_{t_{n-1}}\rangle\rangle\, \delta_{b_{t'_n}, b_{t_{n-1}}}$. Then, we define the **influence functional** (IF) as

$$\begin{aligned} I(s_{t_1}, s_{t'_1}, ..., s_{t_N}, s_{t'_N}) = \mathrm{Tr}_{b_T}\Bigg[\sum_{b_{t_{N-1}}} \sum_{b_{t_0}} \langle\langle s_{t_N}, b_T |\, e^{-iL_{bs}\Delta t}\, |s_{t'_{N-1}}, b_{t_{N-1}}\rangle\rangle \times \dots \\ \times \langle\langle s_{t_1}, b_{t_1} |\, e^{-iL_{bs}\Delta t}\, |s_{t'_1}, b_{t_0}\rangle\rangle \, \langle\langle s_{t'_1}, b_{t_0} | \rho_b(b_{t_0})\rangle\rangle \Bigg] \end{aligned} \tag{7}$$

This high-dimenional object describes how the path of a subsystem (defined by $s_1, \dots, s_N$) is reweighted due to its interactions with an external bath. The equation of motion for ρ_s (Eq. (6)) becomes

$$\begin{aligned} \rho_s(s_T) = \sum_{s_{t_{N-1}}} \cdots \sum_{s_{t_0}} \Bigg(\langle\langle s_T |\, e^{-\frac{i}{2}L_s\Delta t}\, |s_{t_N}\rangle\rangle \times \langle\langle s_{t'_N} |\, e^{-iL_s\Delta t}\, |s_{t_{N-1}}\rangle\rangle \times \dots \\ \times \langle\langle s_{t'_1} |\, e^{-\frac{i}{2}L_s\Delta t}\, |s_{t_0}\rangle\rangle \, \langle\langle s_{t_0} | \rho_s(s_{t_0})\rangle\rangle \Bigg) \times I(s_{t_1}, s_{t'_1}, s_{t_2}, s_{t'_2}, ..., s_{t_N}, s_{t'_N}) \end{aligned} \tag{8}$$

For a visual explanation, see Fig. 1(a), where we express Eq. (6) as a tensor network diagram and denote the influence functional with a blue box.

Typically, L_{bs} is typically assumed to be diagonal in the basis $\{s\}$. Then Eq. (6) becomes

$$\begin{aligned} \rho_s(s_T) = \sum_{s_{t_{N-1}}} \cdots \sum_{s_{t_0}} \Bigg(\langle\langle s_T |\, e^{-\frac{i}{2}L_s\Delta t}\, |s_{t_N}\rangle\rangle \times \langle\langle s_{t_N} |\, e^{-iL_s\Delta t}\, |s_{t_{N-1}}\rangle\rangle \times \dots \\ \times \langle\langle s_{t_1} |\, e^{-\frac{i}{2}L_s\Delta t}\, |s_{t_0}\rangle\rangle \, \langle\langle s_{t_0} | \rho_s(s_{t_0})\rangle\rangle \Bigg) \times I(s_{t_1}, s_{t_2}, ..., s_{t_N}) \end{aligned} \tag{9}$$

where $I(s_{t_1}, s_{t_2}, ..., s_{t_N})$ is the IF with $s_{t'_n} \to s_{t_n}$. This is depicted in Fig. 1(b).

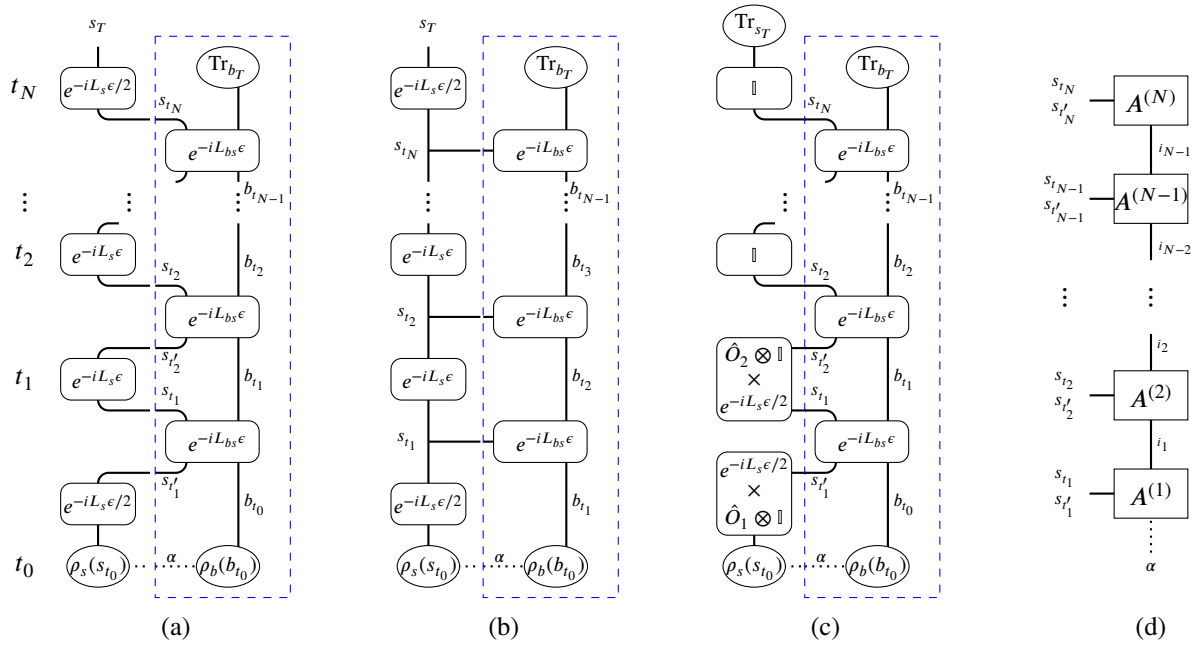


Figure 1: (a, b) Time evolution of $\rho(s_{t_0}) = \sum_\alpha \rho_{s,\alpha}(s_{t_0}) \otimes \rho_{b,\alpha}(s_{t_0})$ in Liouville space with second order Trotter decomposition between system and interaction dynamics. The boxed regions are the traditional and generalized definitions of the influence functional, respectively. (c) Measurement of the time-correlation $\langle \hat{O}_2(t_1)\, \hat{O}_1(t_0) \rangle_\rho$. (d) Matrix product state representation of influence functional. The labels $\{s_{t_m}\}$ and $\{b_{t_m}\}$ index the system and bath states at time step m, respectively. The labels $\{i_m\}$ index the virtual bonds. Lines that connect two tensors (blocks) represent tensor contraction over the labeled indices.

Given that the IF provides the full dynamics of the subsystem, it is straightforward to measure time-correlation functions of the subsystem, $\langle \hat{O}_2(t_1)\, \hat{O}_1(t_0) \rangle_{\rho_s}$ using the influence functional. This is depicted in Fig. 1(c).

However, the IF is a very high-dimensional object; the number of dimensions scales linearly with the total number of time steps N, and the storage requirements of the IF grows exponentially with respect to N. However, if one expects that there is some concept of time locality, meaning that the dynamics of a system depends more heavily on its most recent history instead its state from a long time ago, then one might expect the IF to be low-rank. A natural choice would be to represent the IF as a matrix product state (MPS), with one tensor for each time step, as depicted in Fig. 1(d).

2.1 Simulation of subsystem dynamics with tensor networks

As you may have guessed, one can solve for the IF in a brute-force fashion using tensor networks. One starts in the traditional fashion, representing the initial state $|\rho(t_0)\rangle\rangle$ as a tensor network as an MPS, with one tensor representing each particle. The time evolution operators, $\exp(iL_s\Delta t)$ and $\exp(iL_{bs}\Delta t)$ can be written as MPOs. (A naive SVD-based decomposition (with minimal truncation) typically suffices, but a more informed method would probably yield better results. If the exponential is not known, one can approximate the operator using any variety of time integration schemes, e.g., RK4. Then one would only need to retain singular values with up to $\mathcal{O}(\Delta t^5)$ accuracy.)

After writing out the time evolution of the full system in space-time as a tensor network, one then performs the tensor contraction. For time evolution in the traditional sense, where $|\rho(t)\rangle\rangle$ is evolved forward in time, one would start from time t_0 and contract the $\exp(i(L_s + L_{bs})\Delta t)$ MPO into the MPS. Then one would compress the resulting MPS, and repeat until one has reached the desired point in time. However, as you all know, the state typically becomes increasingly entangled, so the low-rank approximation/compression step introduces more and more errors.

For IF-based calculations, one would contract the tensor network in the perpendicular direction (see Fig. 2), contracting the "paths" of each of the particles one at a time. Once all of the bath sites have been contracted together, the resulting MPS is simply the IF. Numerical tests show that in many cases, as the bath becomes increasingly continuous, the IF becomes increasingly compressible.

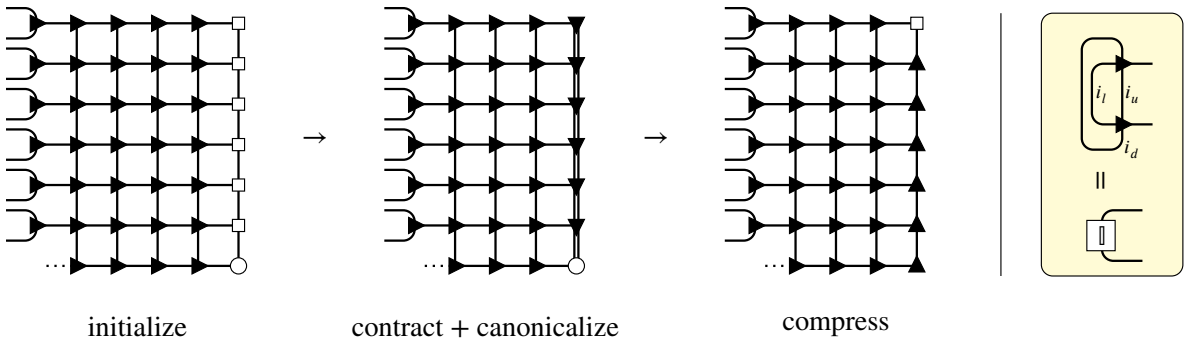


Figure 2: Iteration of transverse contraction scheme to compute IF tensor network. The time evolution operators $e^{-iL_{bs}\epsilon}$ at each time step are the rows of the grid and are each represented as an MPO, and the subsystem of interest is at the left-most site. Before contraction, we first canonicalize each row into left canonical form as indicated by the right pointing triangles along the rows. The rightmost two columns are then contracted and compressed to fixed bond dimension D_I using the standard MPS compression algorithm, where the column is first converted into a canonical form (here, top canonical form) and then compressed by singular value decomposition in the reverse direction (leaving it in bottom canonical form). The canonical form implies that the tensors satisfy an isometric condition (see diagram on the right); e.g. the right pointing arrow implies contraction of a tensor with its complex conjugate over the left, up, and down indices yields the identity matrix. The procedure is repeated until all columns have been contracted.

Quantum dynamics are often described as thermalizing and localizing. In the case of thermalizing dynamics, the results converge "quickly" with respect to IF bond dimension. However, in the case of localizing behavior, traditional TE may exhibit better convergence with respect to bond dimension.

In Fig. 3, we consider the interacting hard-core boson model,

$$H_{HCB} = \sum_j \left[-J(a_j^\dagger a_{j+1} + h.c.) + U n_j n_{j+1} + \frac{K}{2} n_j j^2 \right] \tag{10}$$

and plot the occupancy of a single site (site 21 in a chain of 43 sites) is measured over time for different interaction strengths U. (I believe that we expect an insulating state for $U > J$ (small J/U), and an thermalizing state for $U < J$ (large J/U).) Direct time evolution exhibits better convergence with respect to bond dimension with increased U, whereas IF time evolution exhibits better convergence with decreased U.

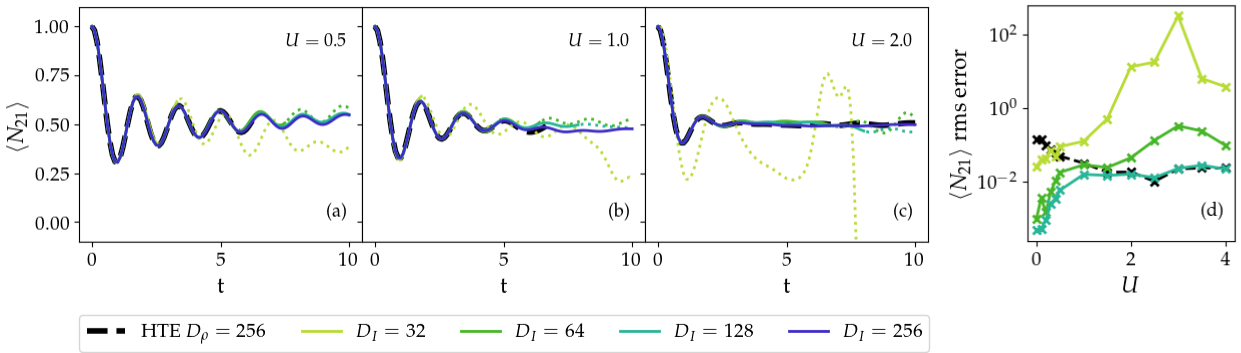


Figure 3: Expectation values of the site-occupancy $\langle N_i(t) \rangle$ for the hard-core boson model of length $L = 43$ at lattice site $i = 21$ for different coupling strengths $U = 0.5$, 1.0, and 2.0 (a-c). Lines become dotted after divergence of >0.03 with respect to the $D_I = 256$ IF results. (d) The r.m.s. errors with respect to the $D_I = 256$ IF results as a function of U. For these calculations, the initial state is a pure product state with alternating spins, $|0, 1, 0, 1, ...\rangle$. Time evolution is performed using Trotter steps with a $N = 100$ time steps of $\Delta t = 0.1$. Compared to the $U = 0$ case, a larger bond dimension is needed, particularly at around $U = 3.0$ where the r.m.s. error peaks. In contrast, the HTE dynamics converge more quickly with increasing U.

2.2 Analytical Solution for the Spin-Boson Model

In the case of a subsystem coupled to a bath of non-interacting harmonic oscillators, one can obtain an analytical solution of the influence functional.

Consider a particle of mass m coupled to a bath of harmonic oscillators with mass m_j and frequencies ω_j. The Hamiltonian is

$$H = \underbrace{\frac{p_s^2}{2m_0} + V_0(q_s)}_{H_s} + \underbrace{\sum_j \frac{P_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2\left(Q_j - \frac{c_j}{m_j\omega_j^2}q_s\right)^2}_{H_{bs}} \tag{11}$$

where q_s, p_s are the position and momentum coordinates for the spin/particle of interest, and Q_j, P_j are the coordinates of the j^{th} oscillator. Coefficient c_j is the coupling strength between the particle and the j^{th} oscillator. The interaction between the particle and bath is captured by the spectral density function,

$$J(\omega) = \frac{\pi}{2}\sum_j \frac{c_j^2}{m_j\omega_j}\delta(\omega - \omega_j) \tag{12}$$

This is perhaps more evident once the bath is represented in second quantized form (in units where $\hbar = 1$ and dropping all constants),

$$H = H_s(q_s, p_s) + \int_0^\infty d\omega\ \left[q_s\left(g(\omega)a_\omega + g^*(\omega)a_\omega^\dagger\right) + \omega a_\omega^\dagger a_\omega\right] \tag{13}$$

where H_s is the Hamiltonian for the particle and $|g(\omega)|^2 = \frac{1}{\pi}J(\omega)$ is the system-bath coupling strength. (To arrive here, one simply expands the square term in H_{bs}, plugs in the definitions for the coordinates X, P in second quantization, and hides the q_s^2 term in the new H_s.)

In the continuous limit (time step $\epsilon \to 0$), the influence functional of the harmonic bath is

$$\begin{aligned} I = \exp\Bigg(&-\frac{1}{\hbar}\int_0^t dt' \int_0^{t'} dt''\ \left(q_s^+(t') - q_s^-(t')\right)\left(\alpha(t-t'')q_s^+(t'') - \alpha^*(t'-t'')q_s^-(t'')\right) \\ &-\frac{i}{\hbar}\int_0^t dt' \int_0^\infty d\omega \frac{J(\omega)}{\pi\omega}\left(q_s^+(t')^2 - q_s^-(t')^2\right)\Bigg) \end{aligned} \tag{14}$$

where α is the bath response function

$$\alpha(t) = \frac{1}{\pi}\int_0^\infty d\omega J(\omega)\left(\coth\left(\frac{\beta\omega\hbar}{2}\right)\cos(\omega t) - i\sin(\omega t)\right) \tag{15}$$

$$\tag{16}$$

assuming that the initial state of the bath is $\rho_b = e^{-\beta H_b}$, with H_b is the Hamiltonian for the uncoupled harmonic oscillator bath. When discretizing in time, and denoting $q_s^\pm(t_k)$ as $s_{t_k}^\pm$ to simplify notation, the influence function takes the form

$$I = \exp\left\{-\frac{1}{\hbar}\sum_{k=1}^N\sum_{k'=1}^k (s_{t_k}^+ - s_{t_k}^-)(\eta_{kk'}s_{t_{k'}}^+ - \eta_{kk'}^* s_{t_{k'}}^-)\right\} \tag{17}$$

where

$$\eta_{k,k'} = \int_{t_{k-1}}^{t_k}\int_{t_{k'-1}}^{t_{k'}} \alpha(t'-t'')dt''dt' \quad \text{for} k \neq k' \tag{18}$$

$$\eta_{k,k} = \int_{t_{k-1}}^{t_k}\int_{t_{k-1}}^{t'} \alpha(t'-t'')dt''dt' \tag{19}$$

The diagonal terms capture the second term in Eq. (14) and the off-diagonal terms capture the first term. Notice that they only depend on $k - k'$, or the difference between the two points in time. See Eq. (12) in Ref. [2] for explicit expressions for $\eta_{kk'}$.

Note: see Ref. [3] for extensions to anharmonic baths and Ref. [4] for extensions to fermionic baths.

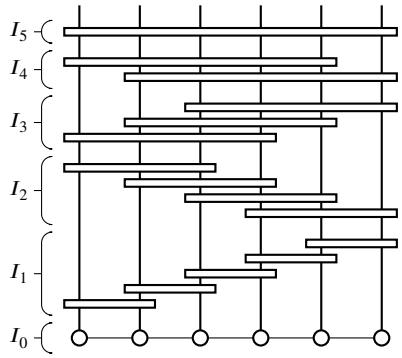
2.2.1 Approximate Numerical Solution

Notice that the influence functional is composed of terms containing two points in time, and that the off-diagonal $\eta_{kk'}$ only depends on $\Delta k = k - k'$. In the quasi-adiabatic propagator path integral (QUAPI) scheme [2, 5], "long-distance" terms with $\Delta k > \Delta k_{\max}$ are discarded, yielding

$$I \approx \prod_{k=0}^{N} I_0(s_k^{\pm}) \prod_{k=0}^{N-1} I_1(s_k^{\pm}, s_{k+1}^{\pm}) \dots \prod_{k=0}^{N-\Delta k} I_{\Delta k}(s_k^{\pm}, s_{k+\Delta k}^{\pm}) \dots \prod_{k=0}^{N-\Delta k_{\max}} I_{\Delta k_{\max}}(s_k^{\pm}, s_{k+\Delta k_{\max}}^{\pm}) \tag{20}$$

There are various numerical implementations of QUAPI [6, 7], including a tensor network implementation [8, 9, 10]. Notably, in Ref. [10], the authors demonstrate sublinear computational cost for systems with time-independent Gaussian baths by using a divide-and-conquer strategy with the tensor network representation. They claim that the divide-and-conquer algorithm reduces computational cost from $\mathcal{O}(N^2)$ singular value decompositions (SVDs) to $\mathcal{O}(N \log N)$ SVDs, where N is the number of time steps. By using only finite memory of N_c time steps, the cost is reduced to $\mathcal{O}(N_c \log N_c)$ SVDs.

While there is no reason to explicitly construct the influence functional (the above methods avoid doing so if all one is interested in is the dynamics of the subsystem), one could:



If only a finite memory (a finite Δk) is considered, the resulting IF is guaranteed by construction to be low-rank because of the finite temporal correlation lengths. (However, if infinite memory is considered, the resulting IF may still be low-rank.)

3 Relation to Nakajima-Zwanzig

This section is a summary of the work by Ivander et al (Ref. [11]). Apologies for the change in notation. Also, for clarification, in the following N will represent the number of time steps, but because we bisect each of the coordinates, there are $2N$ space-time coordinates. Coordinates x_{2n} corresponds to a time of n time steps.

The authors define the reduced dynamics evolution operator U_N, which evolves the initial state $\rho(t_0)$ to time the state at time t_N:

$$\langle\langle x_{2N} | \rho_N \rangle\rangle = \sum_{x_0^{\pm}} U_N(x_{2N}^{\pm}, x_0^{\pm}) \langle\langle x_0^{\pm} | \rho_0 \rangle\rangle \tag{21}$$

The idea is to define U_n using the influence functional formulation and the Nakajima-Zwanzig memory kernel formulation in order to find an relation between the two.

As introduced at the beginning of this document, in the IF formulation, the dynamics of the subsystem (coupled to an external bath) is given by

$$\begin{aligned}\rho(N\Delta t) = \rho_N &= \mathrm{Tr}_B\left[\rho_{tot}(N\Delta t)\right] \\ &= \sum_{x_0^\pm \dots x_{2N-1}^\pm} G_{x_0^\pm, x_1^\pm} G_{x_1^\pm, x_2^\pm} \dots G_{x_{2N-1}^\pm, x_{2N}^\pm} \langle x_0^+|\rho_0|x_0^-\rangle I(x_1^\pm, x_3^\pm, \dots x_{2N-1}^\pm)\end{aligned} \tag{22}$$

where $G_{x_m^\pm, x_{m+1}^\pm}$ is the propagator for just the subsystem over **half** a time step,

$$\begin{aligned}G_{x_m^\pm, x_{m+1}^\pm} &= \langle x_m^+|e^{-i\frac{\Delta t}{2}H_s}|x_{m+1}^+\rangle\langle x_{m+1}^-|e^{i\frac{\Delta t}{2}H_s}|x_m^-\rangle \\ &= \langle\langle x_{m+1}^\pm|\, e^{-i\frac{\Delta t}{2}L_s}\,|x_m^\pm\rangle\rangle\ .\end{aligned} \tag{23}$$

For clarity, here is U_N written out explicitly for a few small $N = 1, 2$, and 3:

$$U_1(i,k) = \sum_j G_{i,j} I_0(j) G_{j,k} \tag{24}$$

$$U_2(i,m) = \sum_{j,k} G_{i,j} I_0(j) F_{j,k} I_0(k) I_1(j,k) G_{k,m} \tag{25}$$

$$U_3(i,n) = \sum_{j,k,m} G_{i,j} I_0(j) F_{j,k} I_1(j,k) I_0(k) F_{k,m} I_2(j,m) I_1(k,m) I_0(m) G_{m,n} \tag{26}$$

$$\dots \tag{27}$$

where $F = GG$ is the propagator for just the subsystem over the full time step.

Recall the Nakajima-Zwanzig (NZ) equation,

$$\dot\rho_s(t) = \frac{i}{\hbar} L_s \rho(t) + \int_0^t \mathcal{K}(t,\tau)\rho(\tau) + \mathcal{I}(\tau) d\tau \tag{28}$$

where $\mathcal{K}$ is the memory kernel and $I(t)$ is the inhomogeneous term that goes to zero when the total density matrix is factorized, or $\rho(0) = \rho_s(0) \otimes \rho_B$. Discretizing in time, with N time steps of size Δt, we obtain

$$\rho_N = (1 - \frac{i}{\hbar}\Delta t L_s)\rho_{N-1} + \Delta t^2 \sum_{m=1}^N \mathcal{K}_{N,m}\rho_{m-1} \tag{29}$$

where $\mathcal{K}_n$ is the discrete-time memory kernel at time step n. The goal is to relate $\mathcal{K}_N$ to the set of contributions to the influence functional $\{I_k\}$.

The authors define the reduced dynamics evolution operator U_N such that

$$\langle\langle x_{2N}|\rho_N\rangle\rangle = \sum_{x^\pm} U_N(x_{2N}^\pm, x_0^\pm)\,\langle\langle x_0^\pm|\rho_0\rangle\rangle \tag{30}$$

From Eq. (29), we obtain

$$U_N = (1 - \frac{i}{\hbar}\Delta t L_s)U_{N-1} + \Delta t^2 \sum_{m=1}^N \mathbf{K}_{N,m} U_{m-1} \tag{31}$$

$$U_0 = \mathbb{I}. \tag{32}$$

For $N = 1$,

$$\frac{\rho_1 - \rho_0}{\Delta t} = -\frac{i}{\hbar} L_s \rho_0 + \mathcal{K}_{1,1}\rho_0 \Delta t \tag{33}$$

$$U_1 = (1 - \frac{i}{\hbar} L_s \Delta t) + \mathcal{K}_{1,1}\Delta t^2 \tag{34}$$

$$(\mathcal{K}_{1,1})_{ik} = \frac{1}{\Delta t^2}\left[\sum_j G_{ij} I_j^0 G_{jk} + \frac{i}{\hbar}(L_s\Delta t - 1)_{ik}\right] \tag{35}$$

For $N = 2$,

$$\frac{\rho_2 - \rho_1}{\Delta t} = -\frac{i}{\hbar} L_s \rho_1 + \left[\mathcal{K}_{2,2}\rho_1 + \mathcal{K}_{2,1}\rho_0\right] \Delta t \tag{36}$$

$$\tag{37}$$

Note that in the case of a time-independent Hamiltonian, so the kernel $\mathcal{K}_{m,m'}$ only depends on the difference $m - m'$. For example, $\mathcal{K}_{2,1} = \mathcal{K}_{3,2} \equiv \mathcal{K}_1$. Then, since

$$\rho_2 = (1 - \frac{i}{\hbar}\Delta t L_s)\rho_1 + \Delta t^2 \left(\mathcal{K}_0\rho_1 + \mathcal{K}_1\rho_0\right) \tag{38}$$

$$= (1 - \frac{i}{\hbar}\Delta t L_s + \Delta t^2 \mathcal{K}_0)\rho_1 + \Delta t^2 \mathcal{K}_1 \rho_0 \tag{39}$$

$$= U_1\rho_1 + \Delta t^2 \mathcal{K}_1 \rho_0 \tag{40}$$

As one continues, one finds

$$\mathcal{K}_0 = \frac{1}{\Delta t^2}(U_1 - (1 - \frac{i}{\hbar}\Delta t L_s)) \tag{41}$$

$$\mathcal{K}_1 = \frac{1}{\Delta t^2}(U_2 - U_1 U_1) \tag{42}$$

$$\mathcal{K}_2 = \frac{1}{\Delta t^2}(U_3 - U_2 U_1 - U_1 U_2 + U_1 U_1 U_1) \tag{43}$$

$$\dots \tag{44}$$

$\mathcal{K}_0$ can be interpreted as the deviation of the system dynamics from the pure (decoupled) dynamics within a time step. $\mathcal{K}_1$ captures effects that cannot be captured with one time step (within $\mathcal{K}_0$). More generally, $\mathcal{K}_m$ captures the effects that cannot be capture with $m - 1$ time steps. The N-time memoery kernel $\mathcal{K}_N$ is the N^{th} order cumulant in the cumulant expansion of the memory kernel.

The kernel K is expressed in terms of $\{I_k\}$ by matching the multipliers of U_k recursively. By writing $\{U_k\}$ in terms of $\{I_k\}$, the authors obtain

$$\mathcal{K}_{0,ik} = \frac{1}{\Delta t^2}\left[\sum_j G_{ij} I_0(j) G_{jk} - \left(1 - \frac{i}{\hbar}\Delta t L_s\right)_{ik}\right] \tag{45}$$

$$\mathcal{K}_{1,im} = \frac{1}{\Delta t^2}\left[\sum_{jk} G_{ij} I_0(j) F_{jk} \tilde{I}_1(j,k) I_0(k) G_{km}\right] \tag{46}$$

$$\mathcal{K}_{2,ip} = \frac{1}{\Delta t^2}\left[\sum_{jkn} G_{ij} F_{jk} F_{kn} \left[\tilde{I}_2(j,n) I_1(j,k) I_1(k,n) + \tilde{I}_1(j,k)\tilde{I}_1(k,n)\right] I_0(j) I_0(k) I_0(n) G_{np}\right] \tag{47}$$

$$\dots \tag{48}$$

where $\tilde{I}(i,j) = I(i,j) - 1$ and is small in magnitude. The authors show that each term in K_n is represented by each Dyck path of order N, allowing them to obtain expressions for larger N kernels. We refer the reader to the actual paper for more details, but here is a summary of some of their results:

- I_N (multiplicity 1) contributes most to the memory kernel K_N
- Typically $I_k(i,j) \to 1$ as $k \to \infty$. As a result,terms with large multiplicities contribute less to K_N and decay exponentially as multiplicity grows.
- In QUAPI, we only keep I_k terms for $k < k_{\max}$. The approximation first shows up in $\mathcal{K}_2$, with

$$\tilde{I}_2(j,n) I_1(j,k) I_1(k,n) + \tilde{I}_1(j,k)\tilde{I}_1(k,n) \to \tilde{I}_1(j,k)\tilde{I}_1(k,n) \tag{49}$$

- Numerical simulations demonstrate that sub-Ohmic environments have slow decay of I_N and K_N. Ohmic baths see fast decay. (In Ref. [10], they show efficient calculations for super-Ohmic baths, though I believe they focused on long-memory calculations.)

- The authors generalize the formulation to driven systems.

The authors also present a scheme for extracting the bath spectral density from reduced system dynamics. The basic idea is as follows.

1. One extracts U_N by measuring all trajectories from linearly-independent initial states. (This data can be from experiment or numerical simulation.)
2. Memory kernels $\mathcal{K}$ can be obtained from U
3. Influence functional can be obtained from $\mathcal{K}$
4. Take the logarithm of the IF to obtain $\eta_{k,k'}$, and extract the spectral density using the Fourier transform (and additional basic mathematical manipulation.

References

[1] R. P. Feynman and F. L. Vernon. "The theory of a general quantum system interacting with a linear dissipative system". In: *Annals Phys.* 24 (1963), pp. 118–173.

[2] N. Makri and D. E. Makarov. "Tensor propagator for iterative quantum time evolution of reduced density matrices. I. Theory". In: *J. Chem. Phys* 102 (1995), p. 4600.

[3] E. Aurell, R. Kawai, and K. Goyal. "An operator derivation of the Feynman–Vernon theory, with applications to the generating function of bath energy changes and to an-harmonic baths". In: *J. Phys. A: Math. Theor.* 53 (2020), p. 275303.

[4] M. Cirio et al. "The Fermionic influence superoperator: a canonical derivation for the development of methods to simulate the influence of a Fermionic environment on a quantum system with arbitrary parity symmetry". In: *arXiv:2108.09094* (2021).

[5] D. E. Makraov and N. Makri. "Path integrals for dissipative systems by tensor multiplication. Condensed phase quantum dynamics for arbitrarily long time". In: *Chem. Phys. Lett.* 221 (1994), pp. 482–491.

[6] A. Strathearn, B. W. Lovett, and P. Kirton. "Efficient real-time path integrals for non-Markovian spin-boson models". In: *New J. Phys.* 19 (2017), p. 093009.

[7] S. Chatterjee and N. Makri. "Real-time path integral methods, quantum master equations, and classical vs quantum memory". In: *J. Phys. Chem. B* 123 (2019), pp. 10470–10482.

[8] A. Strathearn et al. "Efficient non-Markovian quantum dynamics using time-evolving matrix product operators". In: *Nature Communications* 9 (2018), p. 3322.

[9] M. R. Jorgensen and F. A. Pollock. "Exploiting the causal tensor network structure of quantum processes to efficiently simulate non-Markovian path integrals". In: *Phys. Rev. Lett.* 123 (2019), p. 240602.

[10] M. Cygorek et al. "Sublinear Scaling in Non-Markovian Open Quantum Systems Simulations". In: *Phys. Rev. X* 14 (2024), p. 011010.

[11] F. Ivander, L. P. Lindoy, and J. Lee. "Unified Framework for Open Quantum Dynamics with Memory". In: *arXiv:2312.13233* (2024).