Heat Current in Non-Markovian Open Systems

Ruofan Chen
College of Physics and Electronic Engineering, and Center for Computational Sciences, Sichuan Normal University,
Chengdu 610068, China

Abstract. We generalize time-evolving matrix product operators method to nonequilibrium quantum transport problems. The nonequilibrium current is obtained via numerical differentiation of the generating functional which is represented as a tensor network. The approach is numerically exact and the non-Markovian effects are fully taken into account. In the transport process, a part of the heat that flows out from a bath flows into the system and other baths, and the rest is stored in the system-bath coupling part. We take the spin-boson model as a demonstration to show the details of this heat flowing and the establishment of a steady current between two baths.
1. Introduction

Quantum transport at nanoscale has attracted both theoretical and experimental interests for a long time due to the need in device application [1–7]. The quantum effects in low dimensional systems often result in interesting behaviors. For instance, the rectification of heat transfer in nanodevices can be realized by system structural asymmetry [8], the negative differential thermal conductance can show up with certain conditions [9, 10], the Wiedemann-Franz law may be violated at low temperature [11] and the current direction can be reversed by strong interparticle interaction [12].

Beyond the standard linear response approach, exact analytical results are rare for nonequilibrium quantum transport problems, thus there is clearly a considerable need for numerically exact methods. Rigorous non-Markovian and non-perturbative methods for open quantum system include quasi-adiabatic propagator path integral (QUAPI) [13–15], mapping Hamiltonian approach with the density matrix renormalization group [16, 17], multi-configuration time-dependent Hartree method [18, 19] and hierarchical equation of motion [20–24].

The path integral formalism is one of the most suitable approaches to study the open systems. For a system linearly coupled to bosonic baths, the dynamics of the system can be described by the Feynman-Vernon path integral formalism [25–27]. In order to be numerically evaluated, the path integral can be discretized via the QUAPI method. Based on QUAPI, an iterative tensor multiplication scheme for open system dynamics is proposed [14, 28]. The QUAPI method is numerically exact and fully takes non-Markovian effects into account, therefore it has been widely used to investigate reduced dynamics of dissipative systems [29–34]. Such iterative tensor multiplication scheme is also generalized to fermionic environments [35–38] and the corresponding quantum transport problem [39–42].

The major disadvantage of the QUAPI iterative tensor multiplication scheme is that its computational cost scales exponentially with the correlation length and the size of system Hilbert space. Therefore in practical calculation one often encounters memory problem. Recently, it is shown that the QUAPI tensor multiplication scheme can be represented in terms of matrix product state (MPS) and matrix product operator (MPO) [43, 44]. Then the iterative process is amenable to the standard MPS compression algorithm and the computational cost scaling becomes polynomially. This algorithm is called time-evolving matrix product operators (TEMPO) method, which greatly extends the applicability of QUAPI method. The QUAPI and TEMPO method can be generalized to evaluate the system correlation function [31, 45] and heat statistics [46], and to the situation where multiple baths are in the presence [44]. In addition, using generating functional technique the bath dynamics can be related to the system correlation function [47].

In this article, we generalize TEMPO method to the nonequilibrium quantum transport problem. The nonequilibrium current can be obtained via differentiation of the generating functional. Unlike what is done in Ref. [47], where the differentiation of generating functional is handled analytically and then the bath dynamics is formulated as an integral over system correlation function, we directly evaluate the differentiation numerically as in Refs. [39–42]. The generating functional is represented as a real-time path integral in Keldysh formalism and numerically evaluated as a tensor network via QUAPI and TEMPO method. It should be noted that in such evaluation process, we find that although the auxiliary variable in generating functional is a single variable, it needs to be handled consistently with the system variable in QUAPI scheme, i.e., be treated as a path segment. The corresponding details refer to Sec. 3.2.

When the system and bath are coupled, there is an amount of energy stored in the coupling part. Therefore the heat that flows out from a bath not only flows into the system and other baths but is also stored in the system-bath coupling part. This part of energy may be referred to as interaction energy, which is shown to be important to energy transport in nonequilibrium open systems [48–51]. We use the spin-boson model to demonstrate the details of such heat flowing and the establishment of a steady current between two baths.

This article is organized as follows. The detail of the model is given in Sec. 2. The method is presented in Sec. 3. The simulations of the spin-boson model with single and two baths are given in Sec. 4 and 5, respectively. Finally Sec. 6 gives conclusions.
2. Model

Here we consider a system plus multiple baths model. The Hamiltonian is

\[ \hat{H} = \hat{H}_d + \sum_{\alpha} (\hat{H}_\alpha + \hat{H}_{d\alpha}), \]  

where \( \hat{H}_d \) is the system Hamiltonian and \( \hat{H}_\alpha \) is the Hamiltonian of \( \alpha \)th bath. We consider the Caldeira-Leggett type environment [27, 52] for which the bath is described by a collection of harmonic oscillators as

\[ \hat{H}_\alpha = \sum_k \omega_{\alpha k} \hat{b}_\alpha^\dagger \hat{b}_\alpha. \]  

Here \( \hat{b}_\alpha^\dagger (\hat{b}_\alpha) \) creates (annihilates) a boson of state \( k \) in \( \alpha \)th bath with frequency \( \omega_{\alpha k} \). The coupling between the system and \( \alpha \)th bath is given by

\[ \hat{H}_{d\alpha} = \hat{s}_\alpha \sum_k V_{\alpha k} (\hat{b}_\alpha + \hat{b}_\alpha^\dagger), \]  

where \( \hat{s}_\alpha \) is a system operator which couples to boson of state \( k \) in \( \alpha \)th bath with strength \( V_{\alpha k} \). Here \( \hat{s}_\alpha \) of different \( \alpha \) are supposed to commute with each other. The \( \alpha \)th bath is characterized by a spectral function

\[ J_\alpha(\omega) = \sum_k V_{\alpha k}^2 \delta(\omega - \omega_{\alpha k}). \]  

We consider Ohmic spectral functions for which

\[ J_\alpha(\omega) = \lambda_\alpha \omega e^{-\omega/\omega_c}, \]

where \( \lambda_\alpha \) is the coupling strength parameter and \( \omega_c \) is the cutoff frequency of the bath. For simplicity, the cutoff frequency is set to \( \omega_c = 3.5 \) for all baths throughout this article.

We assume that at initial time \( t = 0 \) the total density matrix is separable into system and baths for which

\[ \hat{\rho}(0) = \hat{\rho}_d(0) \prod_\alpha \hat{\rho}_\alpha, \]

where \( \hat{\rho}_d(0) \) is the initial system density matrix and the \( \alpha \)th bath is in thermal equilibrium for which \( \hat{\rho}_\alpha = e^{-\hat{H}_\alpha/T_\alpha} \). Here \( T_\alpha \) is the temperature of \( \alpha \)th bath. Throughout this article we set \( \hbar = k_B = 1 \) and use dimensionless quantities.

The heat current flows out from the \( \alpha \)th bath at time \( t \) is defined as the opposite of the energy change rate for which

\[ I_\alpha(t) = -\langle \dot{\hat{H}}_\alpha(t) \rangle = -i \langle [\hat{H}, \hat{H}_\alpha(t)] \rangle = i \sum_k V_{\alpha k} \omega_{\alpha k} \langle \hat{s}_\alpha(t) \hat{b}_\alpha(t) - \hat{b}_\alpha^\dagger(t) \hat{b}_\alpha(t) \rangle. \]

The system quantum operator \( \hat{s}_\alpha \) commutes with the bath operators \( \hat{b}_\alpha \) and \( \hat{b}_\alpha^\dagger \), therefore the above expression can be written as

\[ I_\alpha(t) = -2 \Im \sum_k V_{\alpha k} \omega_{\alpha k} \langle \hat{s}_\alpha(t) \hat{b}_\alpha(t) \rangle. \]
expectation value of any system operator \( \hat{f}(t) \) via \( \langle \hat{f}(t) \rangle = Z_d^{-1} \text{Tr}_d[\hat{\rho}_d(t)\hat{f}] \), where \( Z_d = \text{Tr}_d[\hat{\rho}_d(t)] \) and \( \text{Tr}_d \) is the trace over the system. However, to evaluate the current formula (8) we need to calculate the quantity \( \langle \hat{s}_\alpha(t)\hat{b}_{\alpha k}(t) \rangle \) which involves bath operator \( \hat{b}_{\alpha k}(t) \). In order to handle such an operator, we define a reduced density matrix with a source term as

\[
\hat{\rho}_d^s(t) = \text{Tr}_E[\hat{\rho}(t)e^{\xi_\alpha \sum_k V_{\alpha k}\omega_{\alpha k}\hat{b}_{\alpha k}}].
\]

This \( \hat{\rho}_d^s(t) \) may be referred to as generating functional in path integral formalism, which shall be discussed in the following section. Note that \( \hat{\rho}_d^s(t) \) reduces to \( \hat{\rho}_d(t) \) when \( \xi_\alpha = 0 \). Then via differentiation with respect to \( \xi_\alpha \) we have

\[
\sum_k V_{\alpha k}\omega_{\alpha k}\langle \hat{s}_\alpha(t)\hat{b}_{\alpha k}(t) \rangle = Z_d^{-1} \text{Tr}_d \left[ \frac{\delta \hat{\rho}_d^s(t)}{\delta \xi_\alpha} \hat{s}_\alpha \right].
\]

Then the current formula (8) can be evaluated numerically with a finite but small \( \xi_\alpha \) for which

\[
I_{\alpha}(t) = -2\text{Im} Z_d^{-1} \text{Tr}_d \left[ \frac{\hat{\rho}_d^s(t) - \hat{\rho}_d(t)}{\xi_\alpha} \hat{s}_\alpha \right].
\]

The total heat \( Q_\alpha(t) \) that flows out from the \( \alpha \)th bath at time \( t \) is given by a time integral of heat current as

\[
Q_\alpha(t) = \int_0^t I_{\alpha}(t') \text{d}t'.
\]

A part of this heat flows into the system and other baths, and the rest is stored in the coupling part which may be referred to as interaction energy. We denote the system energy change at time \( t \) as

\[
E(t) = \langle \hat{H}_d(t) \rangle - \langle \hat{H}_d(0) \rangle,
\]

and the interaction energy between the system and \( \alpha \)th bath at time \( t \) as

\[
W_\alpha(t) = \langle \hat{H}_{d\alpha}(t) \rangle = 2\text{Re} \sum_k V_{\alpha k}\langle \hat{s}_\alpha(t)\hat{b}_{\alpha k}(t) \rangle.
\]

Since at time \( t = 0 \) the total density matrix (6) is in product state, we have \( \langle \hat{H}_{d\alpha}(0) \rangle = 0 \) and the quantity \( W_\alpha(t) \) defined here is also the interaction energy change \( \langle \hat{H}_{d\alpha}(t) \rangle - \langle \hat{H}_{d\alpha}(0) \rangle \).

Similarly, we can define another reduced density matrix with a source term as

\[
\hat{\rho}_d^{\chi_\alpha}(t) = \text{Tr}_E[\hat{\rho}(t)e^{\chi_\alpha \sum_k V_{\alpha k}\hat{b}_{\alpha k}}],
\]

and a numerical differentiation with a small \( \chi_\alpha \) yields

\[
W_\alpha(t) = 2\text{Re} Z_d^{-1} \text{Tr}_d \left[ \frac{\hat{\rho}_d^{\chi_\alpha}(t) - \hat{\rho}_d(t)}{\chi_\alpha} \hat{s}_\alpha \right].
\]

In this article, we set \( \xi_\alpha = \chi_\alpha = 10^{-3} \), then the error due to numerical differentiation should be at the order of \( O(10^{-3}) \) since \( [(e^x - 1)/x - 1] = O(x) \).

The energy conservation is expressed by \( Q(t) \), \( E(t) \) and \( W(t) \) as

\[
\sum_\alpha Q_\alpha(t) = E(t) + \sum_\alpha W_\alpha(t),
\]

or be expressed by the corresponding time derivates as

\[
\sum_\alpha I_{\alpha}(t) = \dot{E}(t) + \sum_\alpha \dot{W}(t).
\]

The energy conservation is numerically fulfilled for the algorithm described in this article.
3. Method

In this section, we present the basic framework of our method, which includes the path integral formalism, the discretization (QUAPI scheme) and the MPS representation (TEMPO scheme) for path integral formalism.

3.1. Path Integral Formalism

Now we want to express $\hat{\rho}(t)$, $\hat{G}_d^\dagger(t)$ and $\hat{G}_d^\Sigma(t)$ in path integral representation. In this section, we give a basic introduction of the path integral formalism, and a more detailed derivation refers to Appendix A.

Splitting the evolution time into $N$ steps that $\delta t = t/N$ with $N \to \infty$ yields the total density matrix as

$$\hat{\rho}(t) = e^{-i\hat{H}\delta t} \cdots e^{-i\hat{H}\delta t} \hat{\rho}(0)e^{i\hat{H}\delta t} \cdots e^{i\hat{H}\delta t}.$$  \hspace{1cm} (19)

We insert the identity operator into every time step and label the time steps starting from $\hat{\rho}(0)$ to the leftmost as $(t_0^+,\ldots,t_N^+)$ and the steps to the rightmost as $(t_0^-,\ldots,t_N^-)$. Due to the cyclic property

$$\langle \hat{f}(t) \rangle = \text{Tr}\left[e^{-i\hat{H}t} \hat{\rho}(0)e^{i\hat{H}t} \hat{f}\right] = \text{Tr}\left[e^{i\hat{H}t} \hat{f}e^{-i\hat{H}t} \hat{\rho}(0)\right],$$  \hspace{1cm} (20)

we can think the evolution starts from time 0 then experiences an evolution $e^{-i\hat{H}t}$, and after a measurement of $\hat{f}$ returns back to time 0 by a backward evolution $e^{i\hat{H}t}$. Therefore the set of time steps $(t_0^+,\ldots,t_N^+,t_N^-,\ldots,t_0^-)$ forms a closed time contour $C$ shown in Fig. 1, which is usually referred to as Keldysh contour [4, 53–55]. The path from $t_0^+$ to $t_N^+$ corresponds the forward evolution operator $e^{-i\hat{H}t}$ and thus we call it forward branch. Correspondingly, we call the path from $t_N^-$ to $t_0^-$ the backward branch.

![Figure 1. The Keldysh contour C. The upper is the forward branch and the lower is the backward branch.](image)

On the contour, we can define free bath Green’s functions, which are useful to describe path integral formalism. If $t'$ succeeds $t''$ on the contour then we denote it by $t' \succ t''$. With this ordering, the free bath Green’s function on the contour $C$ is defined as

$$G_{ak}(t',t'') = \langle T_C \hat{b}_{ak}(t')\hat{b}_{ak}^\dagger(t'') \rangle_0,$$  \hspace{1cm} (21)

where $T_C$ is the contour ordered operator and $\langle \cdots \rangle_0$ means the expectation value in the free bath. To be specific,

$$G_{ak}(t',t'') = \begin{cases} \langle \hat{b}_{ak}(t')\hat{b}_{ak}^\dagger(t'') \rangle_0, & t' \geq t''; \\ \langle \hat{b}_{ak}(t'')\hat{b}_{ak}(t') \rangle_0, & t'' \succ t'. \end{cases}$$  \hspace{1cm} (22)

The contour ordered Green’s function can be split into four nonequilibrium Green’s function blocks as

$$G_{ak}(t',t'') = \begin{bmatrix} G_{ak}^{++}(t',t'') & G_{ak}^{+-}(t',t'') \\ G_{ak}^{-+}(t',t'') & G_{ak}^{--}(t',t'') \end{bmatrix},$$  \hspace{1cm} (23)

where in $G^{++}$ ($G^{--}$) both $t'$, $t''$ are on the forward (backward) branch, and in $G^{+-}$ ($G^{-+}$) $t'$ is on the forward (backward) branch and $t''$ is on the backward (forward) branch.
The matrix element of the reduced density matrix is
\[
\langle s'|\hat{\rho}_d(t)|s''\rangle = \text{Tr}_{\Xi}[\langle s'|e^{-i\hat{H}_t}\hat{\rho}(0)e^{i\hat{H}_t}|s''\rangle].
\] (24)

Relabeling \(s' = s(t_+^N) = s^+_N\) and \(s'' = s(t^-_N) = s^-_N\), then the corresponding set \((s^+_0, \ldots, s^+_N, s^-_N, \ldots, s^-_0)\) forms a path of \(s(t)\) on the contour \(\mathcal{C}\). Following standard procedures \([25, 26, 56, 57]\), the reduced density matrix can be presented as a path integral as
\[
\rho_d(s^+_N) = \langle s^+_N|\hat{\rho}_d(t)|s^-_N\rangle = \left(\prod_\alpha Z_\alpha^{(0)}\right) \int \mathcal{D}[s]K[s]F[s],
\] (25)

where \(Z_\alpha^{(0)}\) is the free partition function of the \(\alpha\)th bath and \(K[s]\) is the propagator of the bare system. Here the integral over \(\mathcal{D}[s]\) indicates the summation over all the possible path on the contour \(\mathcal{C}\) with boundary condition \(s^+_N = s'\) and \(s^-_N = s''\).

The term \(F[s]\) is the total influence functional which is the production of influence functional of each bath \(F_\alpha[s]\) for which \(F[s] = \prod_\alpha F_\alpha[s]\). The quantity \(F_\alpha[s]\) is the Feynman-Vernon influence functional of \(\alpha\)th bath for which
\[
F_\alpha[s] = e^{-\int_0^t dt' f_\alpha dt'' s_\alpha(t')\Delta_\alpha(t', t'')s_\alpha(t'')},
\] (26)

where
\[
\Delta_\alpha(t', t'') = \sum_k V_{\alpha k}^2 G_{\alpha k}(t', t'').
\] (27)

The generating functional \(\rho_d^{\xi_\alpha}(s^+_N)\) can be expressed as path integral as
\[
\rho_d^{\xi_\alpha}(s^+_N) = \left(\prod_\alpha Z_\alpha^{(0)}\right) \int \mathcal{D}[s]K[s]F[s]X_{\xi_\alpha}[s],
\] (28)

where
\[
X_{\xi_\alpha}[s] = e^{-i\xi_\alpha \int_0^t dt' s_\alpha(t')\Gamma_\alpha(t', t^-_N)}
\] (29)

with
\[
\Gamma_\alpha(t', t'') = \sum_k V_{\alpha k}^2 \omega_{\alpha k} G_{\alpha k}(t', t'').
\] (30)

Similarly, the generating functional \(\rho_d^{\chi_\alpha}(s^+_N)\) can be expressed as
\[
\rho_d^{\chi_\alpha}(s^+_N) = \left(\prod_\alpha Z_\alpha^{(0)}\right) \int \mathcal{D}[s]K[s]F[s]Y_{\chi_\alpha}[s],
\] (31)

where
\[
Y_{\chi_\alpha}[s] = e^{-i\chi_\alpha \int_0^t dt' s_\alpha(t')\Delta_\alpha(t', t^-_N)}.
\] (32)

Since \(\Delta_\alpha\) and \(\Gamma_\alpha\) are linear to \(G_\alpha\), they can be also split into four blocks as \(\Delta_\alpha^{\pm\pm}\) and \(\Gamma_\alpha^{\pm\pm}\).
3.2. Quasi-Adiabatic Propagator Path Integral Method

To be evaluated numerically, the path integral formalism \( F_\alpha[s] \), \( X_\xi_\alpha[s] \) and \( Y_\chi_\alpha[s] \) must be discretized. It should be noted that directly employing finite \( \delta t \) may cause a large deviation from the correct result, therefore an improved discretization scheme, which is called quasi-adiabatic propagator path integral (QUAPI) method \([13–15]\), need to be adopted.

The Feynman-Vernon influence functional can be written in a more specific form as \([25–27]\)

\[
F_\alpha[s] = e^{-\int_0^Tdt' \int_0^{t'}dt''[s_\alpha^+(t'-s_\alpha^-(t')][C_\alpha(t'-t'')s_\alpha^+(t'')-C_\alpha(t'-t'')s_\alpha^-(t'')]},
\]

where \( C_\alpha(t) \) is the autocorrelation function of \( \alpha \)th bath for which

\[
C_\alpha(t) = \int d\omega J_\alpha(\omega) \left[ \coth \left( \frac{\omega}{2T_\alpha} \right) \cos \omega t - i \sin \omega t \right],
\]

and \( \bar{C}_\alpha(t) \) is the complex conjugate. After the discretization, the double integral in exponential becomes a double summation as

\[
F_\alpha[s] = e^{-\sum_{j=0}^{N-1} \sum_{k=0}^{N-1} (s_\alpha^j - s_\alpha^k)(\eta_{jk}s_\alpha^k - \bar{\eta}_{jk} \bar{s}_\alpha^k)},
\]

where \( \eta_{jk} \) is a complex number and \( \bar{\eta}_{jk} \) is its complex conjugate. Here the path \( s_\alpha^j(t) \) is split into intervals of equal duration for which \( s_\alpha^j(t) = s_\alpha^j \) for \( (j - \frac{1}{2})\delta t < t < (j + \frac{1}{2})\delta t \). In this case we have for \( j \neq k \)

\[
\eta_{jk} = \int_{(j-\frac{1}{2})\delta t}^{(j+\frac{1}{2})\delta t} dt' \int_{(k-\frac{1}{2})\delta t}^{(k+\frac{1}{2})\delta t} dt'' C_\alpha(t' - t''),
\]

and for \( j = k \)

\[
\eta_{jj} = \int_{(j-\frac{1}{2})\delta t}^{(j+\frac{1}{2})\delta t} dt' \int_{(j-\frac{1}{2})\delta t}^{(j+\frac{1}{2})\delta t} dt'' C_\alpha(t' - t'').
\]

The source term \( X_\xi_\alpha[s] \) can be written in a specific form as

\[
X_\xi_\alpha[s] = e^{-i\xi_\alpha \int_0^T dt'[s_\alpha^+(t')\Gamma_\alpha^+(t'-t) - s_\alpha^-(t')\Gamma_\alpha^-(t'-t)]},
\]

which should also be discretized via QUAPI scheme. It should be emphasized that although the variable \( \xi_\alpha \) is only at a single time step \( t_N \), it in fact corresponds to the path segment \( s_N \). Therefore we need to replace it by a segment as

\[
\xi_\alpha \to \frac{1}{\delta t} \int_{(N-\frac{1}{2})\delta t}^{(N+\frac{1}{2})\delta t} \xi_\alpha(t') dt'
\]

with \( \xi_\alpha(t') = \xi_\alpha \). Otherwise, we would obtain wrong results which directly violate energy conservation expression \((17)\) and \((18)\). After the discretization we have

\[
X_\xi_\alpha[s] = e^{-i\xi_\alpha \sum_{j=0}^{N-1} (s_\alpha^j - s_\alpha^j)}
\]

where for \( j \neq N \)

\[
\gamma_{jN}^{\pm \pm} = \frac{1}{\delta t} \int_{(N-\frac{1}{2})\delta t}^{(N+\frac{1}{2})\delta t} dt' \int_{(j-\frac{1}{2})\delta t}^{(j+\frac{1}{2})\delta t} dt'' \Gamma_{\alpha}^{\pm \pm}(t'' - t'),
\]

and for \( j = N \)

\[
\gamma_{jN}^{\pm \pm} = \frac{1}{\delta t} \int_{(N-\frac{1}{2})\delta t}^{(N+\frac{1}{2})\delta t} dt' \int_{(N-\frac{1}{2})\delta t}^{t'} dt'' \Gamma_{\alpha}^{\pm \pm}(t'' - t').
\]
3.3. Time-Evolving Matrix Product Operators

The Feynman-Vernon influence functional (33) is nonlocal in time, and the nonlocality is characterized by the autocorrelation function (34), which corresponds to $\eta_{jk}$ in formula (35) after the discretization. For ohmic spectral function, it is shown that [27] in the limit $\Gamma_{\alpha} \to \infty$ the real part of the autocorrelation function behaves as the delta function $\delta(t)$ and its imaginary part behaves as $\delta'(t)$. In this case, the autocorrelation function is local in time and the dynamics is just Markovian. At finite temperature, the autocorrelation function becomes nonlocal but the nonlocality is finite even at low or zero temperature [14,28].

The finite nonlocality means that $\eta_{jk}$ can be truncated when $|j-k|$ is larger than a certain positive integer $N_s$. Based on such property, a numerically exact iterative tensor multiplication scheme based on QUAPI for long time dynamics of quantum dissipative systems is proposed [14,28]. The nonlocal interactions that arise from $T_{\alpha}^{\alpha-}$ and $T_{\alpha}^{\alpha--}$ also have finite range, which enables us to truncate $X_{\xi_{\alpha}}[s]$ and $Y_{\chi_{\alpha}}[s]$ in the same way.

In the original QUAPI algorithm, the computational cost scales exponentially with $N_s$. Typical simulations of QUAPI are restricted to $N_s < 20$ [32,58], and in fact when $N_s$ is greater than 10 it already becomes time consuming. In order to cover the nonlocality, we need $N_s\delta t \geq 4$, and in such a situation time interval $\delta t$ need often to be not less than a fairly large value 0.25.

Recently, it is shown that the QUAPI tensor multiplication scheme can be represented in terms of matrix product states (MPS) and matrix product operator (MPO) [43,44]. Then the iterative process is amenable to the standard MPS compression algorithm, thus the computational cost scaling becomes polynomially with $N_s$, which allows much larger $N_s$. This new algorithm is called time-evolving matrix product operators (TEMPO). The compression is achieved by performing singular value decomposition on each tensor in MPS and dispensing components with singular value below a threshold value. In this article, the threshold value is $\varepsilon S_{\text{max}}$, where $\varepsilon$ is the control parameter and $S_{\text{max}}$ is the largest singular value. There is also another approach for tensor network representation of discretized path integral [59,60].

We construct the tensor $K[s]F[s]$ as MPS using TEMPO method and naturally represent tensors $X_{\xi_{\alpha}}[s]$ and $Y_{\chi_{\alpha}}[s]$ as MPO, then formula (25), (28) and (31) can be easily evaluated. We set time interval $\delta t = 0.02$ and the truncation parameter $N_s = 200$ throughout this article. Here we choose a small value of $\delta t$, which already exceeds the demand of convergence, in order to obtain smooth curves in short time. The corresponding convergence analyses are shown in Appendix D.

4. Spin-Boson Model with A Single Bath

When evolution begins, system and bath start to correlate and interaction energy arises. Let us first consider an unbiased spin-boson model [26,61] with a single bath to demonstrate the details of this process. The system Hamiltonian is

$$\hat{H}_d = \frac{\Delta}{2} \hat{\sigma}_x,$$

where $\Delta$ is the tunneling amplitude between two states of the spin. Here we use $\Delta$ as the energy reference which fixes scales of other parameters, and set its value as $\Delta = 1$ for simplicity. The bath Hamiltonian and the coupling term are

$$\hat{H}_E = \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k, \quad \hat{H}_{de} = \hat{\sigma}_z \sum_k V_k (\hat{b}_k^\dagger + \hat{b}_k).$$

We set the spin to the $z$ direction at the initial time $t = 0$ for which

$$\rho_d(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \langle \hat{\sigma}_z(0) \rangle = 1, \quad \langle \hat{\sigma}_x(0) \rangle = 0.$$

There is only a single bath, and thus the heat that flows out from the bath flows into the system and system-bath coupling part. The directly evaluated quantities are the heat current out from the bath $I(t)$, the system
energy $E(t)$ and the interaction energy $W(t)$. The total heat that flows out from the bath is simply calculated numerically as $Q(t) = \sum_{i=0}^{N} I(t_i)\delta t$, and the change per unit time of the system energy is also evaluated simply as $\dot{E}(t_i) = [E(t_{i+1}) - E(t_i)]/\delta t$. The quantity $\dot{W}(t)$ is evaluated in the same way.

![Figure 2](image2.png)

**Figure 2.** The current $I(t)$ and time derivates $\dot{E}(t)$ and $\dot{W}(t)$ with coupling strength $\lambda = 0.1$ at temperature (a) $T = 1$ and (b) $T = 10$.

![Figure 3](image3.png)

**Figure 3.** The heat that flows out from bath $Q(t)$, the system energy $E(t)$ and interaction energy $W(t)$ with coupling strength $\lambda = 0.1$ at temperature (a) $T = 1$ and (b) $T = 10$.

Set the system-bath coupling strength $\lambda = 0.1$, the heat current $I(t)$, along with time derivate quantities $\dot{E}(t), \dot{W}(t)$ at different bath temperatures $T = 1$ and $T = 10$ are shown in Fig. 2. The heat that flows out from bath $Q(t)$, the system energy $E(t)$ and the interaction energy $W(t)$ are shown in Fig. 3.

It can be seen from Fig. 2 that at the beginning of the evolution, the current $I(t)$ and the quantity $\dot{W}(t)$ are both negative and their values are close. They reach a minimum soon, then tends to zero when approaching steady state. The magnitude of both $I(t)$ and $\dot{W}(t)$ is much larger than $\dot{E}(t)$, this means that the major energy change is not the
heat transfer between system and bath but the interaction energy change due to the correlation of system and bath. In the asymptotic limit, transport quantities $I(t), E(t)$ and $W(t)$ all tends to zero, as they should be.

The system energy is just $E(t) = \frac{1}{2}(\hat{\sigma}_x(t))$, and it tends to a negative value asymptotically at lower temperature $T = 1$, as shown in Fig. 3(a). In this case, the energy that flows out from the system becomes interaction energy and heat in the bath. Due to this amount of energy transfer, $\dot{W}(t)$ is slightly larger than $I(t)$, as shown in Fig. 2(a). At high temperature $T = 10$, the asymptotic value of $E(t)$ is close to zero [Fig. 3(b)], therefore there is not much energy flowing out from the system. In this case, $\dot{W}(t)$ and $I(t)$ almost coincide, as shown in Fig. 3(b).

5. Spin-Boson Model with Two Baths

It is clear that there would be no steady current with a single bath, thus it can be hardly called a transport problem. Now we consider a spin-boson model with two baths, in which the steady current exists when two baths are at different temperatures. Let us label two baths as 1st and 2nd. Correspondingly, the heat currents that flow out from the baths are denoted as $I_1(t)$ and $I_2(t)$, and the total heats that flow out from the baths are $Q_1(t)$ and $Q_2(t)$. The corresponding interaction energies are denoted as $W_1(t)$ and $W_2(t)$, and their time derivatives are $\dot{W}_1(t)$ and $\dot{W}_2(t)$.

We first consider the case where two baths are at different temperatures for which the 1st bath is at high temperature $T_1 = 10$ and 2nd bath is at lower temperature $T_2 = 1$. The coupling strengths between both baths are the same that $\lambda_1 = \lambda_2 = 0.1$. The results are shown in Fig. 4.

We denote steady state quantities as their asymptotic limit

$$\dot{E}, \dot{W}_1, \dot{W}_2, I_1, I_2 = \lim_{t \to \infty} E(t), W_1(t), W_2(t), I_1(t), I_2(t).$$ (46)

In steady state, the system energy remains constant and correspondingly $\dot{E} = 0$, therefore $E(t)$ and $\dot{E}(t)$ are not shown in the figure. It can be seen that in steady state, the interaction energies $W_1(t)$ and $W_2(t)$ are constant [Fig. 4(d)] and correspondingly $\dot{W}_1 = \dot{W}_2 = 0$ [Fig. 4(b)]. In this case, the heat that flows out from one bath all flows into another bath, which indicates that a steady heat current between the two baths is established.
Figure 4(a) shows that in steady state $I_1$ is positive while $I_2$ is negative. This means that heat flows out from 1st bath to 2nd bath, i.e., flows from the bath of higher temperature to the bath of lower temperature. We can also see in Fig. 4(a) that $I_1 + I_2 = 0$, which expresses the energy conservation in steady state.

Because of the existence of steady heat current, the total heat flows out from baths $Q_\alpha(t)$ would not become constant, which can be seen from Fig. 4(c). In the beginning, both $Q_1(t)$ and $Q_2(t)$ are negative, this is because that interaction energy and system energy flow into baths. When steady state is established, $Q_1(t)$ increases linearly with time and eventually becomes positive, while $Q_2(t)$ decreases linearly.

Figure 5 shows the results when two baths are at the same temperature but with different coupling strengths. The parameters are $\lambda_1 = 0.1$, $\lambda_2 = 0.01$ and $T_1 = T_2 = 1$. In this case, $\lambda_1$ is much larger than $\lambda_2$, and thus in the beginning the magnitude of $I_1(t)$ and $\dot{W}_1(t)$ are much larger than that of $I_2(t)$ and $\dot{W}_2(t)$ since much more energy can be extracted from $W_1(t)$. When arriving at steady state, both $I_1(t)$ and $I_2(t)$ tends to zero which shows that no steady current exists between two baths at the same temperature.

In a quantum transport problem with two baths, the observable of interesting is often the symmetrized current

$$I(t) = \frac{1}{2}[I_1(t) - I_2(t)].$$  \hspace{1cm} (47)

The steady state current is denoted as $I = \lim_{t \to \infty} I(t)$.

The steady current is determined by the temperature bias between two baths. For convenience, we denote $T = T_2$ as the base temperature and $\Delta T = T_1 - T_2$ as temperature bias. We set the coupling strengths of both baths to be equal for which $\lambda_1 = \lambda_2 = \lambda$. The steady currents beyond the linear response regime with different base temperatures $T = 1$ and $T = 2$ are shown in Fig. 6. Here we compare our results to that by standard Born-Markov master equation (BMME) [62], whose details refer to Appendix C. In the figure, the TEMPO results are shown in solid lines and the BMME results are shown in dashed lines. Fig. 6(a) shows currents with respect to $\Delta T/T$ with weak coupling ($\lambda = 0.01$), and Fig. 6(b) shows results with larger coupling $\lambda = 0.1$. In Fig. 6(c), the currents with respect to coupling strength $\lambda$ with $\Delta T/T = 10$ are shown.

Let us first look at Figs. 6(a) and 6(b). In a slightly nonequilibrium situation, i.e., linear response regime, the steady heat current is supposed to be proportional to $\Delta T/T$. It can be seen that it is indeed the case when $\Delta T/T$ is
small, while when $\Delta T/T$ becomes larger the linear response approximation fails. The magnitude of $I$ will saturate when $\Delta T/T$ is large enough. For both weak and larger coupling cases, BMME results with $T = 1$ and $T = 2$ almost coincide. This means that within the Markovian approximation, the steady current almost depends on only $\Delta T/T$ and the absolute value of $T$ is not important. On the contrary, TEMPO results, which fully take the non-Markovian effects, show that the steady currents with different base temperatures $T$ would deviate as $\Delta T/T$ increases.

Within the Markovian approximation, the dependence of current on temperature bias is always monotonic for which larger $\Delta T/T$ would induce larger current $I$. However, the $T = 2$ TEMPO result shows that with larger coupling strength $\lambda = 0.1$ [Fig. 6(b)], the steady current shows nonmonotonic dependence of temperature bias for which $I$ can even slightly decrease with increasing $\Delta T/T$. This is clearly a consequence of the non-Markovian effect.

In weak coupling case $\lambda = 0.01$ [Fig. 6(a)], the difference between TEMPO results and BMME results is small even with large $\Delta T/T$. This is not surprising since BMME should work in the weak coupling limit. When coupling strength is increased by 10 times that $\lambda = 0.1$ [Fig. 6(b)], the BMME currents also increase nearly 10 times. It can be seen from Fig. 6(c) that within Markovian approximation, the current is linear to system-bath coupling, therefore increasing coupling strength can significantly enhance the current. However, TEMPO results show that when considering non-Markovian effects, the enhancement by increasing coupling is not that significant for which the magnitude of current would saturate when $\lambda$ is large enough. This indicates that when designing nano devices the improvement of thermal conductivity by simply increasing the coupling strength is limited.

6. Conclusions

Iterative tensor multiplication based on path integral formalism is an important method to simulate reduced dynamics of quantum open systems. For fermionic environments, the corresponding tensor can be numerically obtained via the determinant formula [35–38]. For system linearly coupled to bosonic environments, the influence functional can be analytically represented by Feynman-Vernon formalism [25–27], and after discretization we obtain the corresponding tensor. The discretization scheme employed is usually the QUAPI method [13–15].

To handle quantum transport problems in path integral formalism, the knowledge of generating functional is
necessary. For fermionic environment, the generating functional can be obtained via the determinant formula and
the iterative tensor multiplication scheme, then the current is obtained by a numerical differentiation [39–42]. The
iterative tensor multiplication approach is numerical exact and fully non-Markovian, but its computational cost scales
exponentially. Such a problem can be resolved for the system linearly coupled to the bosonic environment by TEMPO
algorithm, where the tensor obtained via QUAPI is represented by MPS [43, 44].

In this article, we generalize TEMPO algorithm to nonequilibrium quantum transport problems. The generating
functional is evaluated as a tensor network via QUAPI and TEMPO method, and its numerical differentiation gives the
Corresponding heat current. A key point in this evaluation scheme is that the auxiliary variable in generating functional
needs to be handled in the same way as the system variable. That is, it should be treated as a path segment rather than
a single variable and needs to be also discretized via QUAPI scheme.

A part of the heat that flows out from one bath flows into the system and other baths, and the rest becomes
the interaction energy, i.e., the energy stored in the system-bath coupling part. The spin-boson model is used to
demonstrate the details of such heat flowing. In addition, steady currents between two baths at different temperatures
beyond the linear response regime are demonstrated.

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Appendix A. Derivation of Path Integral Formalism

Here we give a detailed derivation of the path integral formalism. For simplicity, let us first consider the situation with
a single bath consisting of a single boson mode. The generalization to continuous boson modes and multiple baths is
straightforward. In this case, the bath Hamiltonian and the system-bath coupling are

\[ \hat{H}_{E} = \omega \hat{b}^\dagger \hat{b}, \quad \hat{H}_{\text{dE}} = \sigma_z V (\hat{b}^\dagger + \hat{b}). \]  

(A.1)

The bath can be described by boson coherent states [57, 63] which is defined as the eigenstate of \( \hat{b} \)
\[ \hat{b} |\varphi\rangle = \varphi |\varphi\rangle, \quad \langle \varphi | \hat{b}^\dagger = \langle \varphi | \bar{\varphi}, \]  

(A.2)

where \( \varphi \) is a complex number and \( \bar{\varphi} \) is its complex conjugate. The identity operator in bath Hilbert space can be
expressed in terms of coherent states as

\[ \int \frac{d\bar{\varphi} d\varphi}{2\pi i} e^{-\bar{\varphi}\varphi} |\varphi\rangle\langle \varphi|. \]  

(A.3)

Accordingly, the trace over the bath can be written as

\[ \text{Tr}_{E}[\cdots] = \int \frac{d\bar{\varphi} d\varphi}{2\pi i} e^{-\bar{\varphi}\varphi} \langle \varphi | \cdots | \varphi\rangle. \]  

(A.4)

Suppose states \(|s\rangle\) spans the Hilbert space of the system, i.e., \( \sum_s |s\rangle s\rangle \) is the identity operator in system Hilbert space,
then the trace over the system can be expressed as

\[ \text{Tr}_{d}[\cdots] = \sum_s \langle s | \cdots | s\rangle. \]  

(A.5)

Correspondingly, the identity operator in the whole Hilbert space can be written as

\[ 1 = \sum_s \int \frac{d\bar{\varphi} d\varphi}{2\pi i} e^{-\bar{\varphi}\varphi} |s\varphi\rangle\langle s\varphi|. \]  

(A.6)
Heat Current in Non-Markovian Open Systems

Insert the above identity operator every time step in (19) and employ the first order Trotter-Suzuki decomposition [64, 65] that
\[ e^{i\delta t \hat{H}} = e^{i\delta t \hat{H}_d} e^{i\delta t \hat{H}_b} e^{i\delta t \hat{H}_d} e^{i\delta t \hat{H}_b}, \] (A.7)
and we have
\[ \langle s_{\alpha+1}^+ | e^{-i\delta t \hat{H}_d} | s_{\alpha}^+ \rangle = \langle s_{\alpha+1}^+ | e^{-i\delta t \hat{H}_d} \rangle e^{\alpha \bar{\varphi}_{\alpha+1}^+ \varphi_{\alpha+1}^- - i\delta t V(s_{\alpha+1}^+ \bar{\varphi}_{\alpha+1}^+ + s_{\alpha}^+ \varphi_{\alpha+1}^+), \] (A.8)
and
\[ \langle s_{\alpha}^- \varphi_{\alpha}^- | e^{i\delta t \hat{H}_d} | s_{\alpha+1}^- \varphi_{\alpha+1}^- \rangle = \langle s_{\alpha}^- \varphi_{\alpha}^- | e^{i\delta t \hat{H}_d} \rangle e^{\alpha \bar{\varphi}_{\alpha}^- \varphi_{\alpha}^- + i\delta t V(s_{\alpha}^- \bar{\varphi}_{\alpha}^- + s_{\alpha+1}^- \varphi_{\alpha+1}^-). \] (A.9)

The element of the reduced density matrix is then
\[ \rho_d(s_N^+) = \sum_{s_0^+, \ldots, s_{N-1}^+} K(s_0^+, \ldots, s_N^+)^F(s_0^+, \ldots, s_N^+), \] (A.10)
where \( K(s_0^+, \ldots, s_N^+) \) is the bare system propagator
\[ K(s_0^+, \ldots, s_N^+) = \langle s_N^+ | e^{-i\delta t \hat{H}_d} | s_{N-1}^+ \rangle \cdots \langle s_0^+ | e^{i\delta t V} | s_0^- \rangle \cdots \langle s_{N-1}^- | e^{i\delta t \hat{H}_d} | s_N^- \rangle. \] (A.11)

Define two vectors of \( 2N - 1 \) elements as
\[ \bar{\zeta} = (s_0^+, \ldots, s_{N-1}^+, s_N^-, s_{N-1}^-, \ldots, s_0^-), \] (A.12)
and
\[ \zeta = (s_0^+, \ldots, s_{N-1}^+, s_N^-, s_{N-1}^-, \ldots, s_0^-). \] (A.13)

Note that here \( \bar{\zeta} \) is not the Hermitian conjugate of \( \zeta \), the bar over \( \bar{\zeta} \) is just a symbol for convenience. Besides, we define a time interval operator on the contour \( \delta t \) as \( \delta t \) when acting on \( s \) on the forward branch and \( -\delta t \) on the backward branch. Due to the trace over the bath, we have \( \varphi(t_N^+) = \bar{\varphi}_N \) and \( \varphi(t_N^-) = \varphi_N \). Denote a vector \( \varphi = (\varphi_0^+, \ldots, \varphi_{N-1}^+, \varphi_N, \varphi_{N-1}^-, \ldots, \varphi_0^-) \) and \( \bar{\varphi} \) as its Hermitian conjugate, the influence functional \( F(s_0^+, \ldots, s_N^+) \) can be written as
\[ \int D[\bar{\varphi}\varphi] e^{-\sum_{j=0}^{2N-1} \sum_{k=0}^{2N-1} \bar{\varphi}_j S_{jk} \varphi_k - i\delta t V \sum_{k=0}^{2N-1} (\bar{\varphi}_k \varphi_k + \bar{\varphi}_k \varphi_k)}, \] (A.14)
where
\[ D[\bar{\varphi}\varphi] = \prod_{k=1}^{2N-1} \frac{d\bar{\varphi}_k d\varphi_k}{2\pi i}. \] (A.15)
This expression can be written in a more compact form as
\[ \int D[\bar{\varphi}\varphi] e^{-\bar{\varphi} S \varphi - i\delta t V (\bar{\varphi} \varphi + \varphi \bar{\varphi})}, \] (A.16)
where \( S \) is a \( (2N - 1) \times (2N - 1) \) matrix
\[ S = \begin{pmatrix}
1 & e^{-\omega/T} & & \\
-\bar{a} & 1 & & \\
& -\bar{a} & 1 & \\
& & -\bar{a} & 1
\end{pmatrix}, \] (A.17)
where \( a = e^{-i\delta t\omega} \) and \( \bar{a} = e^{i\delta t\omega} \). The expression (A.16) can carried out via Gaussian integral as
\[
F(s_0, \ldots, s_N) = |\text{det } S|^{-1} e^{-V^2 dt \bar{s}^{-1} dt c}.
\]
(A.18)
The determinant of \( S \) is just \( 1 - e^{-\omega/T} \) and then \( |\text{det } S|^{-1} \) gives the partition function of the free bath. The element of inverse matrix \( S^{-1} \) is just the contour Green’s function for which
\[
S^{-1}_{ij} = G(t_i, t_j),
\]
(A.19)
where \( G(t_i, t_j) = \langle T_C \hat{b}(t_i) \hat{b}^\dagger(t_j) \rangle_0 \). Therefore in the continuous limit, the influence functional can be written as
\[
F[s] = e^{-\int_C dt' \int_C dt'' s(t') \Delta(t', t'')} s(t''),
\]
(A.20)
where
\[
\Delta(t', t'') = V^2 G(t', t'').
\]
(A.21)
Now let us evaluate the generating functional
\[
\hat{\rho}^\omega(t) = \text{Tr}_E[\hat{\rho}(t)e^{V \omega b}],
\]
(A.22)
With such an extra source term, the influence functional (A.16) before Gaussian integral becomes
\[
\int D[\bar{\varphi}, \varphi] e^{-\int_C dt \bar{s}(t) \bar{\varphi}(t) - i d t V (\bar{\varphi}(t) + s(t)) + \xi V \omega \varphi_N},
\]
(A.23)
then after the Gaussian integral we have an extra term
\[
X_\xi[s] = e^{-i\xi \int_C dt' s(t') \Gamma(t', t_N)},
\]
(A.24)
where \( \Gamma(t', t'') = \omega V^2 G(t', t'') \). For generating functional \( \hat{\rho}^\omega(t) = \text{Tr}_E[\hat{\rho}(t)e^{V \omega b}] \), we can apply the same procedure and obtain an extra term
\[
Y_\xi[s] = e^{-i\xi \int_C dt' s(t') \Delta(t', t_N)},
\]
(A.25)
Now let us turn to the situation with a single bath consisting of continuous boson modes. In this case, the bath Hamiltonian and the system-bath coupling are same to (44). Following the same procedure, we shall find that the influence functional now writes \( F[s] = \prod_k F_k[s] \), where
\[
F_k[s] = e^{-\int_C dt' \int_C dt'' s(t') \Delta_k(t', t'')} s(t'')
\]
(A.26)
with \( [G_k(t', t'') = \langle T_C \hat{b}(t') \hat{b}^\dagger_k(t'') \rangle_0] \)
\[
\Delta_k(t', t'') = V_{kk}^2 G_k(t', t'').
\]
(A.27)
Therefore
\[
F[s] = e^{-\sum_k \int_C dt' \int_C dt'' s(t') \Delta_k(t', t'')} s(t'') = e^{-\int_C dt' \int_C dt'' s(t') \Delta(t', t'') s(t'')},
\]
(A.28)
where
\[
\Delta(t', t'') = \sum_k V_{kk}^2 G_k(t', t'') = \int d\omega J(\omega) G_\omega(t', t'').
\]
(A.29)
Here \( G_\omega(t', t'') \) is \( G_k(t', t'') \) when \( \omega_k = \omega \). Similarly, we have
\[
X_\xi[s] = e^{-i\xi \int_C dt' s(t') \Gamma(t', t_N)},
\]
(A.30)
where

$$
\Gamma(t', t'') = \sum_k \omega_k V_k^2 G_k(t', t'') = \int d\omega \omega J(\omega) G_\omega(t', t''),
$$

(A.31)

and

$$
Y_\chi[s] = e^{-ix_\chi \int d't' s(t') \Delta(t', t_N)}.
$$

(A.32)

The extension to multiple baths is the same as what we have done above, and finally we shall obtain the path integral formulas shown in Sec. 3.1.

**Appendix B. Discretization Scheme**

Here we represent the details of the discretization scheme of the path integral formalism. The specific form of the contour ordered Green’s function are

$$
G_{\alpha k}^{++}(t' - t'') = \begin{cases} 
(1 + n_{\alpha k})e^{-i\omega_{\alpha k}(t' - t'')}, & t' \geq t'', \\
n_{\alpha k}e^{-i\omega_{\alpha k}(t' - t'')}, & t' < t''
\end{cases}
$$

(B.1)

$$
G_{\alpha k}^{--}(t' - t'') = \begin{cases} 
n_{\alpha k}e^{-i\omega_{\alpha k}(t' - t'')}, & t' \geq t'', \\
(1 + n_{\alpha k})e^{-i\omega_{\alpha k}(t' - t'')}, & t' < t''
\end{cases}
$$

(B.2)

$$
G_{\alpha k}^{+-}(t' - t'') = n_{\alpha k}e^{-i\omega_{\alpha k}(t' - t'')},
$$

(B.3)

$$
G_{\alpha k}^{-+}(t' - t'') = (1 + n_{\alpha k})e^{-i\omega_{\alpha k}(t' - t'')},
$$

(B.4)

where $n_{\alpha k} = (e^{\omega_{\alpha k}/T_\alpha} - 1)^{-1}$ is the Bose-Einstein distribution function. Substituting the above specific form of $G$ into (26) and noticing that the area integral $\int_0^t dt' \int_0^{t'} dt''$ can be split as $\int_{t' \geq t''} dt' dt''$ and $\int_{t' < t''} dt' dt''$, we shall obtain a specific form of $F_\alpha[s]$ as (33). In order to discretize the influence functional $F_\alpha[s]$, we need to discretize the autocorrelation function (34) according to formula (36) and (37).

Now let us turn to the generating functional term $X_\chi_\alpha[s]$, whose path integral formalism is (29). The second argument in $\Gamma_\alpha(t', t_N)$ is fixed at the starting point of the backward branch, therefore when $t'$ is on the forward branch we have $\Gamma_\alpha^{+-}$ and when $t'$ is on the backward branch we have $\Gamma_\alpha^{-+}$. The contour integral in (29) is thus

$$
\int_C dt' s_\alpha(t') \Gamma_\alpha(t', t_N) = \int_0^t dt' \left[ s_\alpha^+(t') \Gamma_\alpha^{+-}(t', t) - s_\alpha^-(t') \Gamma_\alpha^{-+}(t', t) \right].
$$

(B.5)

Applying QUAPI scheme to above formula, we shall obtain the discretization formula (40).

Similar to the situation of $X_\chi_\alpha[s]$, the contour integral in $Y_\chi_\alpha[s]$, whose path integral formalism is (32), is

$$
\int_C dt' s_\alpha(t') \Delta_\alpha(t', t_N) = \int_0^t dt' \left[ s_\alpha^+(t') \Delta_\alpha^{+-}(t', t) - s_\alpha^-(t') \Delta_\alpha^{-+}(t', t) \right].
$$

(B.6)

Therefore after the discretization, we have

$$
Y_\chi_\alpha[s] = e^{-ix_\chi \sum_{j=0}^{N-1} s_\alpha^j \sum_{j=0}^{N-1} s_\alpha^j \zeta_{jN}^+ - s_\alpha^j \zeta_{jN}^-},
$$

(B.7)

where for $j \neq N$

$$
\zeta_{jN}^{+-} = \frac{1}{\delta t} \int_{(N-\frac{1}{2})\delta t}^{(N+\frac{1}{2})\delta t} dt' \int_{(j-\frac{1}{2})\delta t}^{(j+\frac{1}{2})\delta t} dt'' \Delta_\alpha^{+-}(t'' - t'),
$$

(B.8)
\[ \zeta^N_{jN} = \frac{1}{\delta t} \int_{(N-\frac{1}{2})\delta t}^{(N+\frac{1}{2})\delta t} dt' \int_{(j-\frac{1}{2})\delta t}^{(j+\frac{1}{2})\delta t} dt'' \Delta^-_{\alpha}(t'' - t'), \quad \text{(B.9)} \]

and for \( j = N \)

\[ \zeta^N_{NN} = \frac{1}{\delta t} \int_{(N-\frac{1}{2})\delta t}^{(N+\frac{1}{2})\delta t} dt' \int_{(N-\frac{1}{2})\delta t}^{(N+\frac{1}{2})\delta t} dt'' \Delta^-_{\alpha}(t'' - t'), \quad \text{(B.10)} \]

\[ \zeta^-_{NN} = \frac{1}{\delta t} \int_{(N-\frac{1}{2})\delta t}^{(N+\frac{1}{2})\delta t} dt' \int_{(N-\frac{1}{2})\delta t}^{(N+\frac{1}{2})\delta t} dt'' \Delta^-_{\alpha}(t'' - t'). \quad \text{(B.11)} \]

Note that here \( t' \) is always not greater than \( t \), according to (30) the specific form of \( \Gamma^+_\alpha \) and \( \Gamma^-_\alpha \) are

\[ \Gamma^+_\alpha(t' - t) = \int d\omega J(\omega) n_\alpha(\omega) e^{-i\omega(t' - t)}, \quad \text{(B.12)} \]

and

\[ \Gamma^-_\alpha(t' - t) = \int d\omega J(\omega)[1 + n_\alpha(\omega)] e^{-i\omega(t' - t)}, \quad \text{(B.13)} \]

where \( n_\alpha(\omega) = (e^{\omega/T_\alpha} - 1)^{-1} \) is the Bose-Einstein distribution function for \( \alpha \) th bath. Similarly, according to (27), the specific form of \( \Delta^+_\alpha \) and \( \Delta^-_\alpha \) are

\[ \Delta^+_\alpha(t' - t) = \int d\omega J(\omega)n_\alpha(\omega)e^{-i\omega(t' - t)}, \quad \text{(B.14)} \]

and

\[ \Delta^-_\alpha(t' - t) = \int d\omega J(\omega)[1 + n_\alpha(\omega)]e^{-i\omega(t' - t)}. \quad \text{(B.15)} \]

At last, we list explicit formulas for these coefficients after the discretization as

\[ \eta_{jk} = 2 \int_0^\infty d\omega \frac{J_\alpha(\omega)}{\omega^2} \left[ \coth \frac{\omega}{2T_\alpha} \cos[\omega(j - k)\delta t] - i \sin \omega(j - k)\delta t \right] (1 - \cos \omega \delta t), \quad j \neq k; \quad \text{(B.16)} \]

\[ \eta_{jj} = \int_0^\infty d\omega \frac{J_\alpha(\omega)}{\omega^2} \left[ \coth \frac{\omega}{2T_\alpha} (1 - \cos \omega \delta t) - i(\omega \delta t - \sin \omega \delta t) \right], \quad \text{(B.17)} \]

\[ \gamma^+_{jN} = 2 \int_0^\infty d\omega \frac{J_\alpha(\omega)}{\omega} n_\alpha(\omega)e^{-i\omega(j - N)\delta t}(1 - \cos \omega \delta t), \quad j \neq N, \quad \text{(B.18)} \]

\[ \gamma^-_{jN} = 2 \int_0^\infty d\omega \frac{J_\alpha(\omega)}{\omega} [1 + n_\alpha(\omega)]e^{-i\omega(j - N)\delta t}(1 - \cos \omega \delta t), \quad j \neq N, \quad \text{(B.19)} \]

\[ \gamma^+_{NN} = \int_0^\infty d\omega \frac{J_\alpha(\omega)}{\omega} n_\alpha(\omega)[(1 + i\omega \delta t) - e^{i\omega \delta t}], \quad \text{(B.20)} \]

\[ \gamma^-_{NN} = \int_0^\infty d\omega \frac{J_\alpha(\omega)}{\omega} [1 + n_\alpha(\omega)][(1 + i\omega \delta t) - e^{i\omega \delta t}], \quad \text{(B.21)} \]

\[ \zeta^+_{jN} = 2 \int_0^\infty d\omega \frac{J_\alpha(\omega)}{\omega^2} n_\alpha(\omega)e^{-i\omega(j - N)\delta t}(1 - \cos \omega \delta t), \quad j \neq N, \quad \text{(B.22)} \]
\[
\begin{align*}
\zeta_{NN}^+ &= 2 \int_0^\infty d\omega \frac{J_{\alpha}(\omega)}{\omega^2} [1 + n_{\alpha}(\omega)] e^{-i\omega(j-N)\delta t}(1 - \cos \omega \delta t), \quad j \neq N, \\
\zeta_{NN}^- &= \int_0^\infty d\omega \frac{J_{\alpha}(\omega)}{\omega^2} n_{\alpha}(\omega)[(1 + i\omega \delta t) - e^{i\omega \delta t}], \\
\zeta_{NN}^- &= \int_0^\infty d\omega \frac{J_{\alpha}(\omega)}{\omega^2} [1 + n_{\alpha}(\omega)][(1 + i\omega \delta t) - e^{i\omega \delta t}] + 1.
\end{align*}
\]

Appendix C. Born-Markov Master Equation

In Sec. 5 we use Born-Markov master equation to benchmark our steady current results. For the spin-boson model with two baths in this article, the Born-Markov master equation can be written as [62]

\[
\frac{\partial}{\partial t} \hat{\rho}_d(t) = -i[\hat{H}_d, \hat{\rho}_d(t)] + D_1[\hat{\rho}(t)] + D_2[\hat{\rho}(t)],
\]

where \(D_\alpha\) is the dissipator of \(\alpha\)th bath for which

\[
D_\alpha[\hat{\rho}_d(t)] = -\int_0^\infty [\hat{\sigma}_z, \hat{\sigma}_z(-\tau)\hat{\rho}_d(t)] C_\alpha(\tau) d\tau + \int_0^\infty [\hat{\sigma}_z(\hat{\rho}_d(t)\hat{\sigma}_z(-\tau)] C_\alpha(-\tau) d\tau.
\]

Here \(\hat{\sigma}_z(t)\) is the interaction picture operator

\[
\hat{\sigma}_z(t) = e^{i\hat{H}_d t} \hat{\sigma}_z e^{-i\hat{H}_d t} = \begin{pmatrix} \cos \Delta t & -i \sin \Delta t \\ i \sin \Delta t & -\cos \Delta t \end{pmatrix},
\]

and \(C_\alpha(t)\) is the autocorrelation function of \(\alpha\)th bath

\[
C_\alpha(t) = \int J(\omega)\{n_{\alpha}(\omega) e^{i\omega t} + [1 + n_{\alpha}(\omega)] e^{-i\omega t}\} d\omega.
\]

The energy change of the system is

\[
\dot{E}(t) = \text{Tr}_d[\hat{H}_d \frac{\partial \hat{\rho}_d(t)}{\partial t}]
= -i \text{Tr}_d[\hat{H}_d \dot{\hat{\rho}}_d(t)] + \text{Tr}_d[\dot{\hat{H}}_d D_1(\hat{\rho}_d(t))] + \text{Tr}_d[\dot{\hat{H}}_d D_2(\hat{\rho}_d(t))].
\]

Here the first term is zero, and the last two terms correspond to the energy change due to baths, i.e., the currents flow into the system from the baths. Therefore we have \(I_n(t) = \text{Tr}_d[\dot{\hat{H}}_d D_\alpha(\hat{\rho}_d(t))]\).

Within Born-Markov approximation, there is no interaction energy \(\dot{W}(t)\) since the density matrix is always decoupled into system and bath parts, and thus we only consider the steady state currents. In steady state, the system energy change \(\dot{E} = 0\) and then we have \(I_1 + I_2 = 0\).

For evaluation of master equation, we define a quantity

\[
C_\alpha(E) = \int_0^\infty e^{iEt} C_\alpha(t) dt
= \pi \{J_\alpha(-E)n_{\alpha}(-E) + J_\alpha(E)[1 + n_{\alpha}(E)]\} + i P \int J_\alpha(\omega) \left[ \frac{n_{\alpha}(\omega)}{E + \omega} + \frac{1 + n_{\alpha}(\omega)}{E - \omega} \right] d\omega. \tag{C.6}
\]
where $P$ denotes the Cauchy principal value. Here we have employed the relation
\[
\int_0^\infty e^{\pm iEt} \, dt = \pi \delta(E) \pm i P \frac{1}{E}.
\] (C.7)

Then we have
\[
\int_0^\infty \cos \Delta t C_\alpha(t) \, dt = \frac{1}{2} [C_\alpha(\Delta) + C_\alpha(-\Delta)], \quad i \int_0^\infty \sin \Delta t C_\alpha(t) \, dt = \frac{1}{2} [C_\alpha(\Delta) - C_\alpha(-\Delta)].
\] (C.8)

Therefore the dissipator can be written as
\[
D_\alpha[\hat{\rho}_d(t)] = -[\hat{s}_z, \hat{A}_\alpha \hat{\rho}_d(t)] + \hat{A}_\alpha(t) \hat{\Lambda}_\alpha, \quad \hat{A}_\alpha = \frac{1}{2} \begin{bmatrix} C_\alpha(\Delta) + C_\alpha(-\Delta) & C_\alpha(\Delta) - C_\alpha(-\Delta) \\ C_\alpha(-\Delta) - C_\alpha(\Delta) & -C_\alpha(\Delta) - C_\alpha(-\Delta) \end{bmatrix}.
\] (C.9)

Appendix D. Convergence Analysis

![Figure D1](image_url)

**Figure D1.** (a) The current $I(t)$ with $\delta t = 0.02$, $N_s = 200$ and different $\varepsilon$. (a) The current $I(t)$ with $\varepsilon = 10^{-8}$, no $N_s$ and different time step $\delta t$. (b) The current with $\delta t = 0.02$ and different $N_s$.

The convergence is controlled by parameters $\delta t$, $N_s$, and $\varepsilon$. Here we use the single bath spin-boson model given in Sec. 4 to show the convergence test. Here we demonstrate the case with a large coupling strength $\lambda = 0.5$ and the temperature is $T = 1$. We first set a small $\delta t = 0.02$ and a fairly large $N_s = 200$ to find a proper SVD truncation parameter $\varepsilon$, the results are shown in Fig. D1(a) where the current flows out from the bath $I(t)$ with different $\varepsilon$ are shown. The value $\varepsilon = 10^{-4}$ is too coarse that the curve is not even smooth, and with $\varepsilon = 10^{-6}$ the convergence is already archived. In this article, we adopt a much finer value $\varepsilon = 10^{-8}$ which is also used in Ref. [66]. In Ref. [67], a looser value $\varepsilon = 10^{-6.5}$ is used.

In Fig. D1(b), the current with no $N_s$ and different time step $\delta t$ are shown. It can be seen that the convergence can be archived with fairly large $\delta t$. In order to show smooth details at short time scale, we choose a smaller $\delta t = 0.02$. In Fig. D1(c), the current with $\delta t = 0.02$ and different $N_s$ are shown. It can be seen that small $N_s$ may cause discontinuity of $I(t)$, see $N_s = 40$ case. In this case, we have $N_s \delta t = 0.8$, therefore a discontinuity arises at $t = 0.8$. Similarly, when $N_s = 60$ we have a discontinuity at $t = 1.2$. The presence of discontinuity is a sign that $N_s$ is not
large enough. When $N_s$ is large enough, the discontinuity would disappear and we obtain convergent results. It can be seen that $N_s = 120$ is already large enough and in this article we adopt a even larger value $N_s = 200$. Basically, the model used in this article is not difficult to converge, and for safety we have adopted stricter parameters.

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