Exact simulation of non-Markovian quantum systems with reduced cost

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with Gunhee Park, Yuanran Zhu, Lin Lin, Chao Yang and Garnet K-L Chan

Physical formulation: G. Park, **Z. Huang**, Y. Zhu, L. Lin, C. Yang, G. K-L Chan**, Physics Review B, 110, 195148.**
Mathematical theory: Z. Huang, L. Lin, G. Park, Y. Zhu**, arXiv: 2411.08741**

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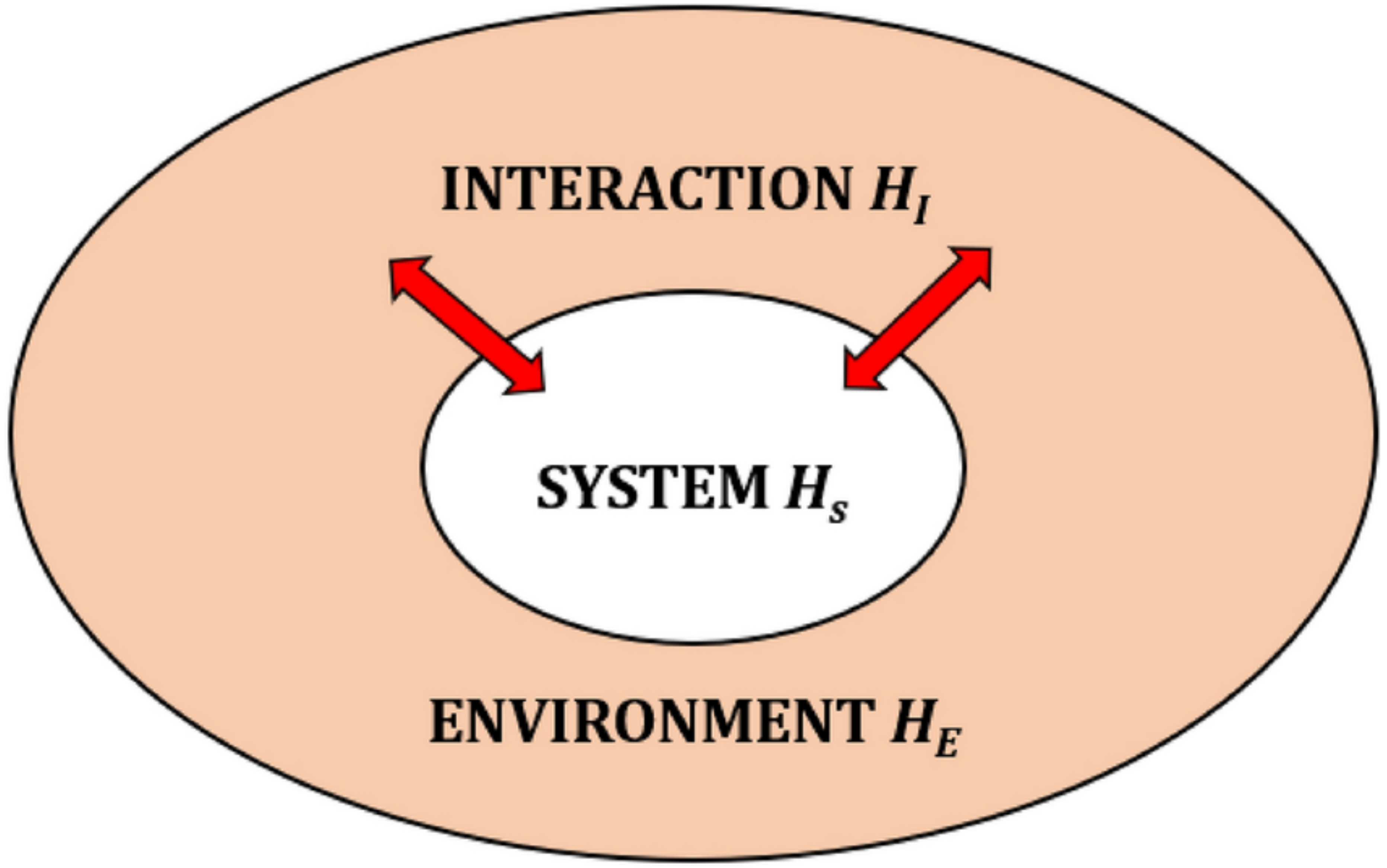
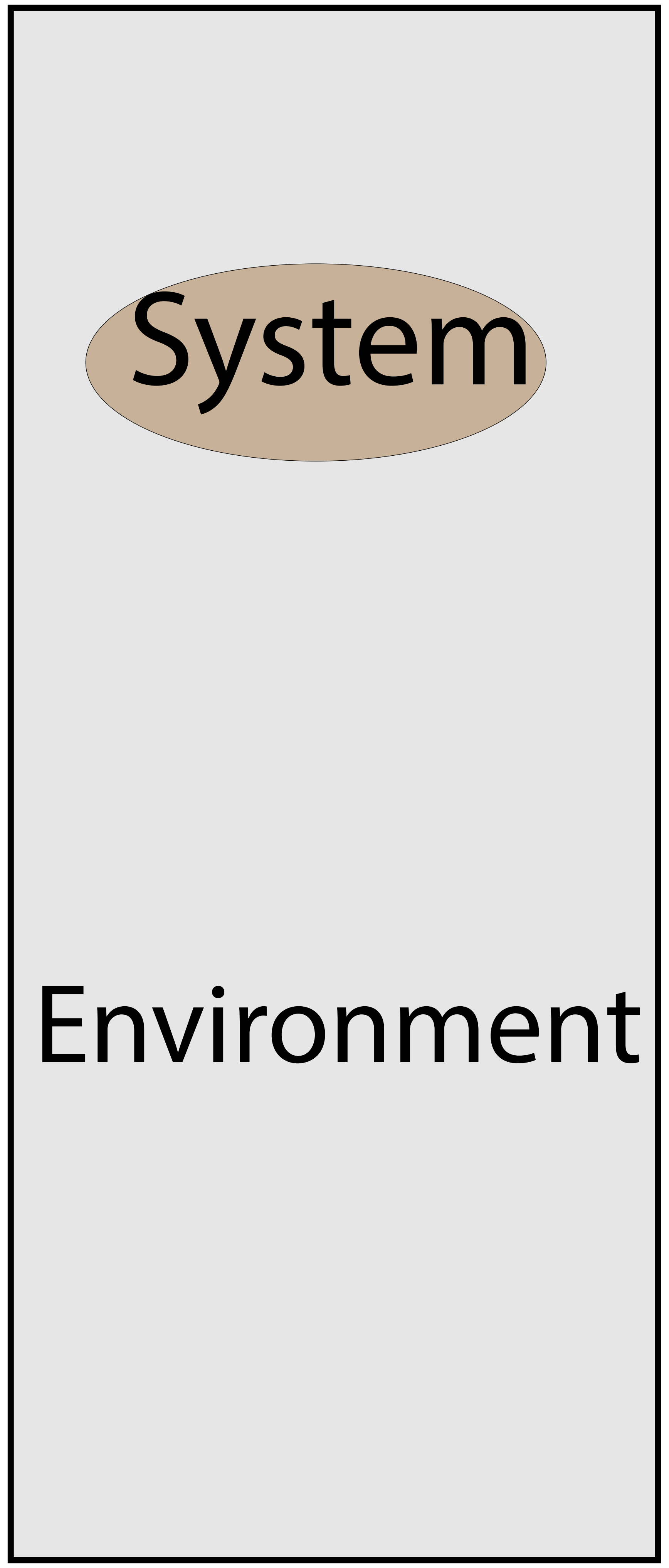
Open quantum systems

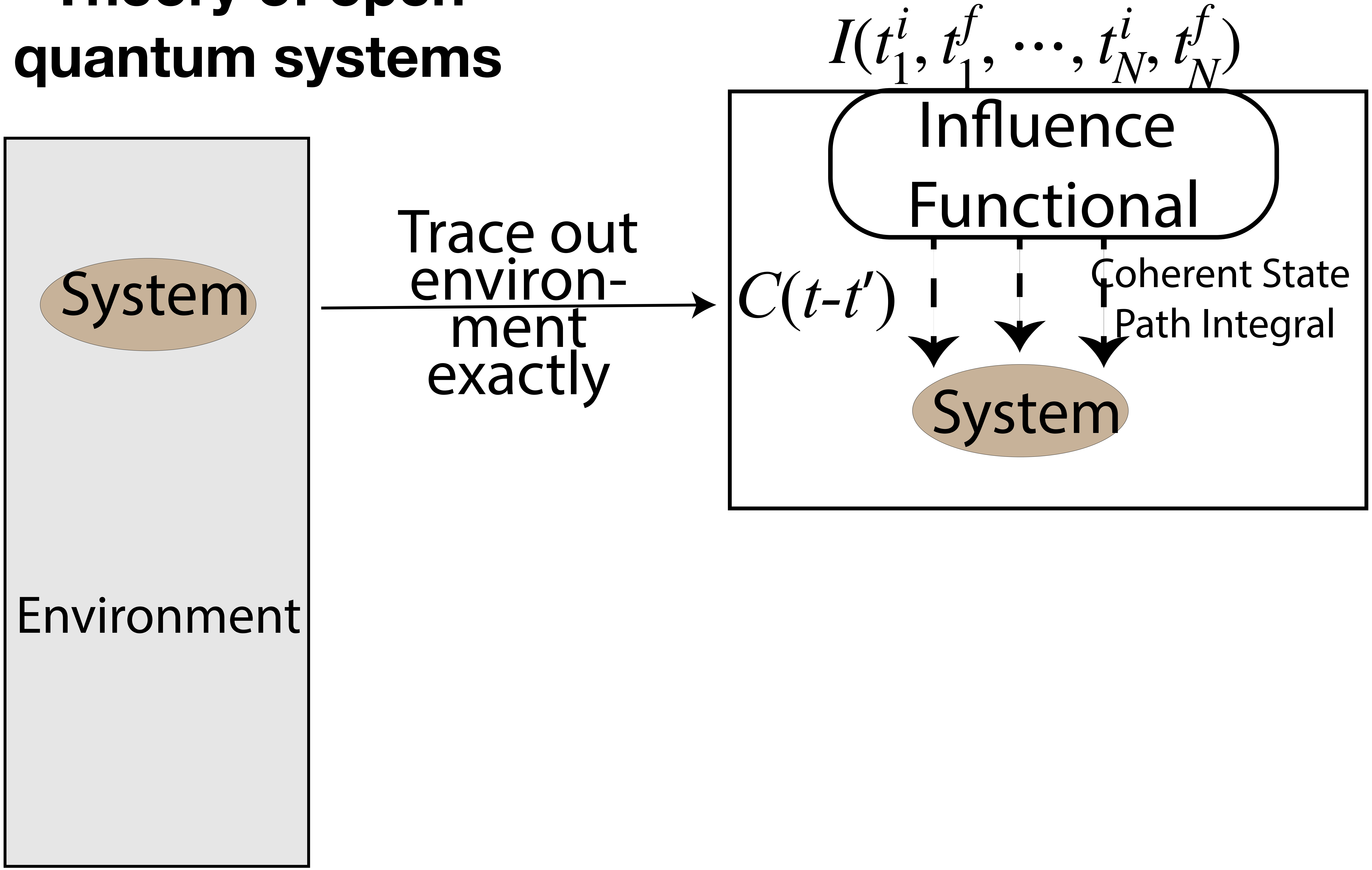


- Open quantum systems:
- $\partial_t \hat{\rho} = -\mathrm{i}[\hat{H}_S + \hat{H}_E + \hat{H}_I, \hat{\rho}]$,
- Goal: obtain $\hat{\rho}_S(t) = \mathrm{Tr}_E(\hat{\rho}(t))$.
- Making seperability assumption + truncation + secular approximation, one can obtain Markovian approximation, i.e. Lindblad equation.
- How to simulate the non-Markovian dynamics $\hat{\rho}_S(t)$ exactly?

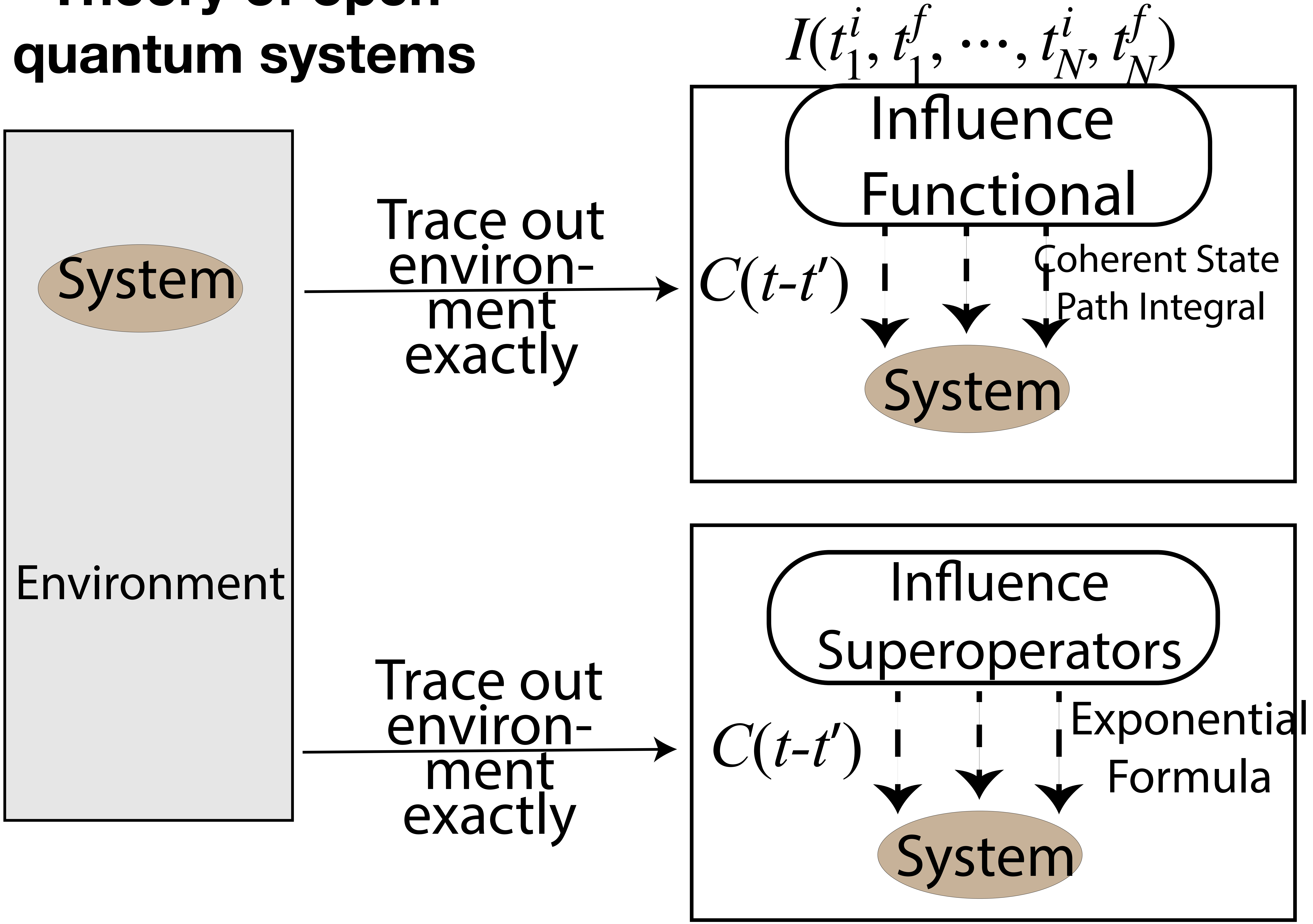
Theory of open quantum systems



Theory of open quantum systems

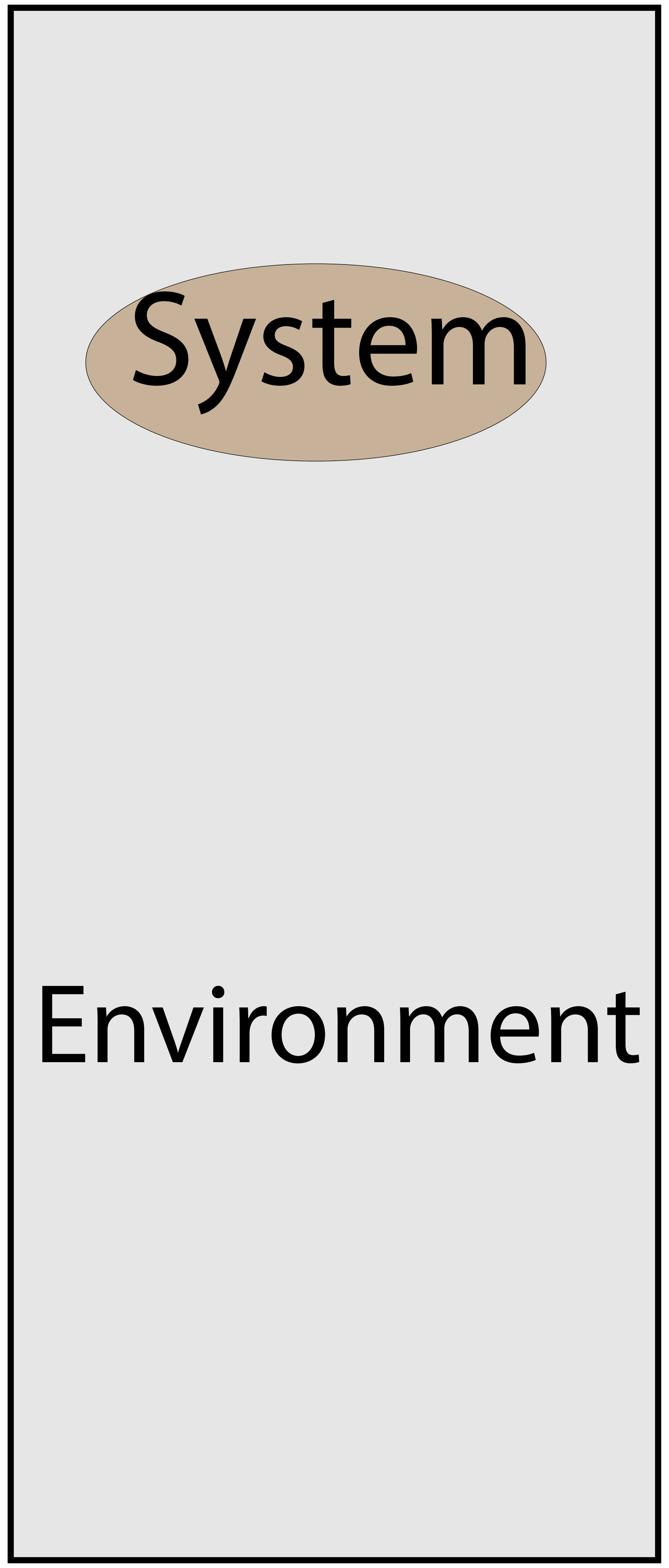


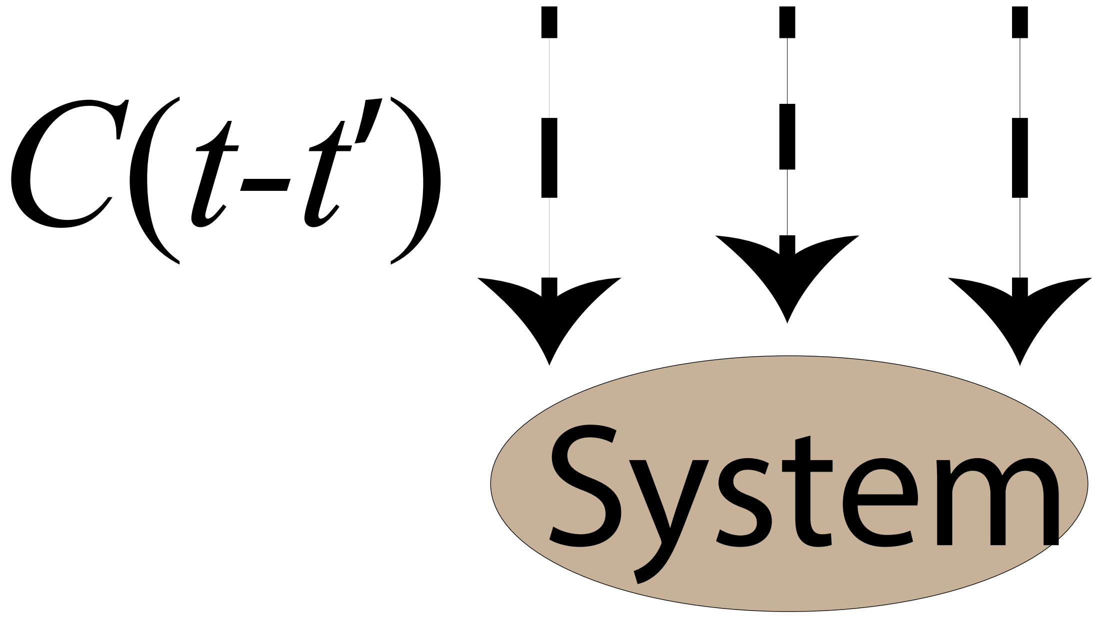
Theory of open quantum systems



Theory of open quantum systems
System
Environment
Trace out environ- ment exactly
$I(t_1^i, t_1^f, \cdots, t_N^i, t_N^f)$
Influence Functional
$C(t\text{-}t')$
Coherent State Path Integral
System
Quasi-adiabatic Path Integral method (QuAPI)
Hierarchial equation of motion (HEOM)
Tensor-network-based Methods
Methods based on approximating influence functional
Trace out environ- ment exactly
Influence Superoperators
$C(t\text{-}t')$
Exponential Formula
System

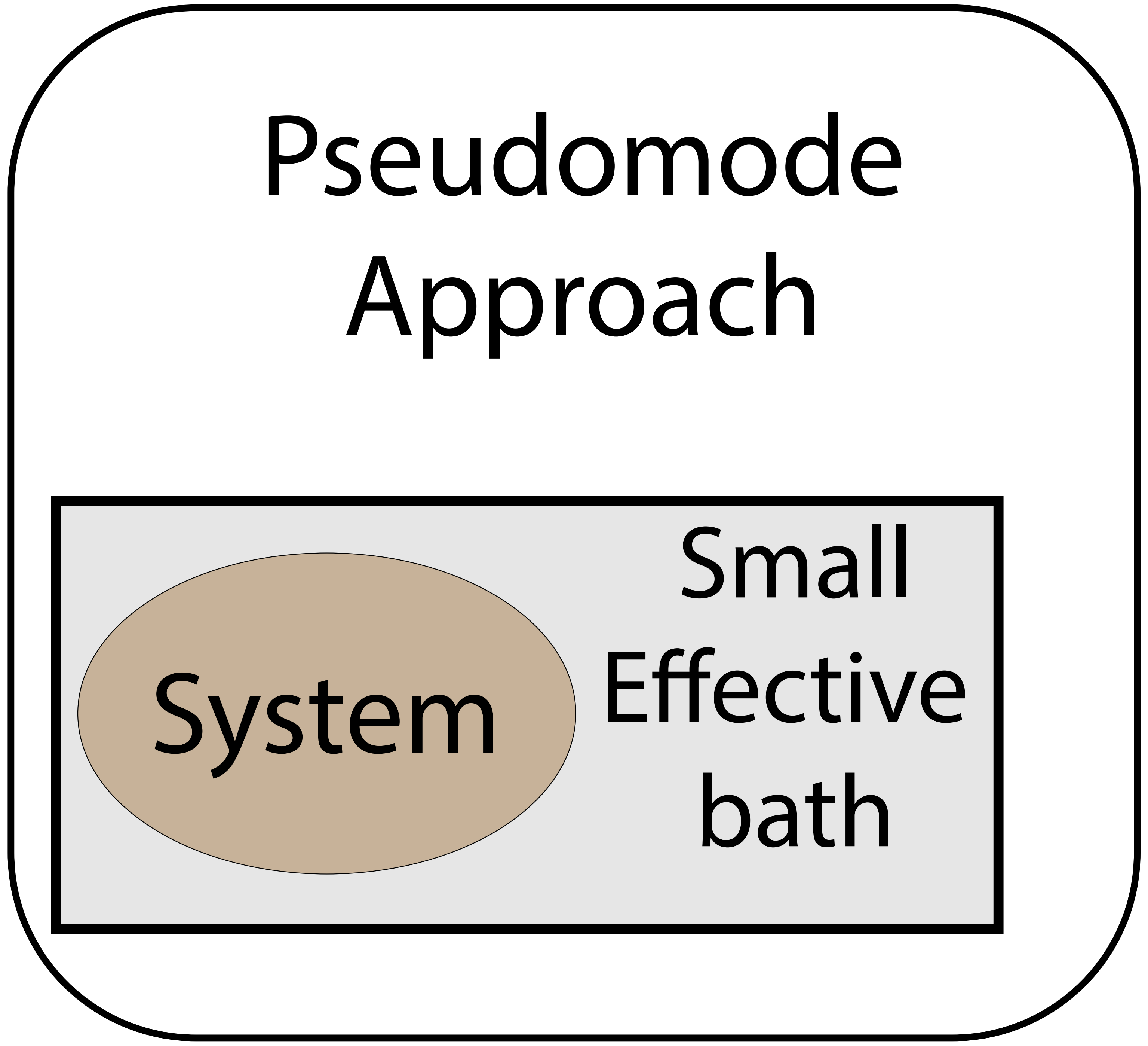
Theory of open quantum systems





The environment's influence on system is only through correlation function $C(t-t')$

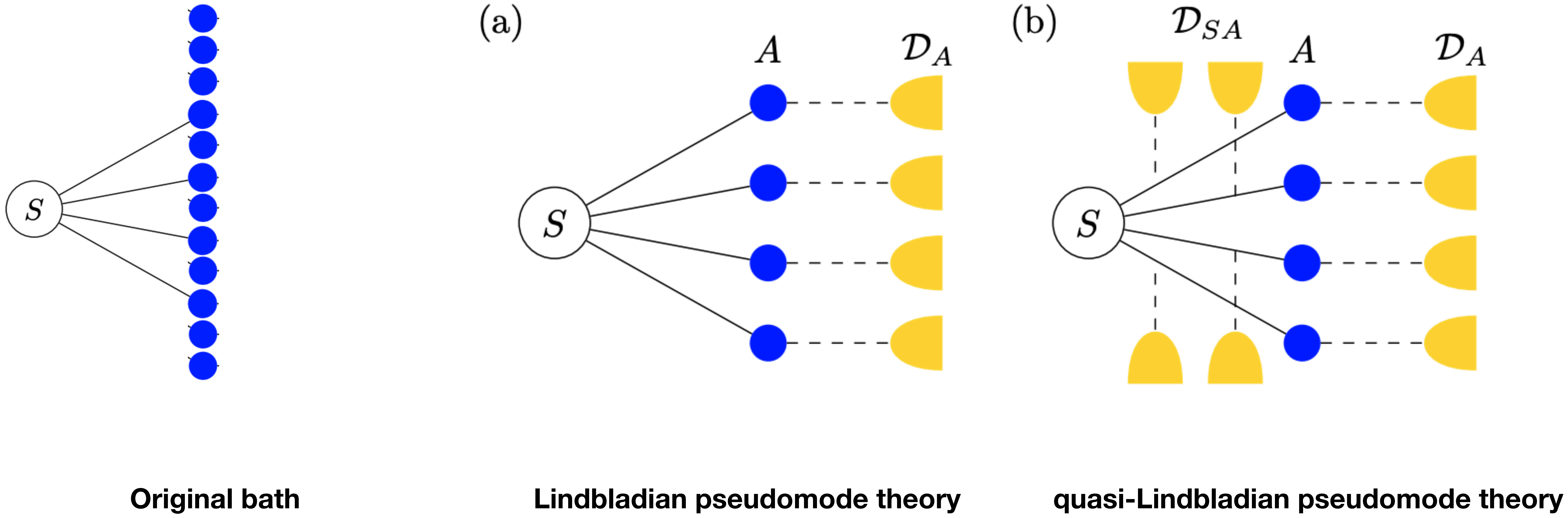
Our approach



Construct a small effective bath that has the same influence on the system dynamics.

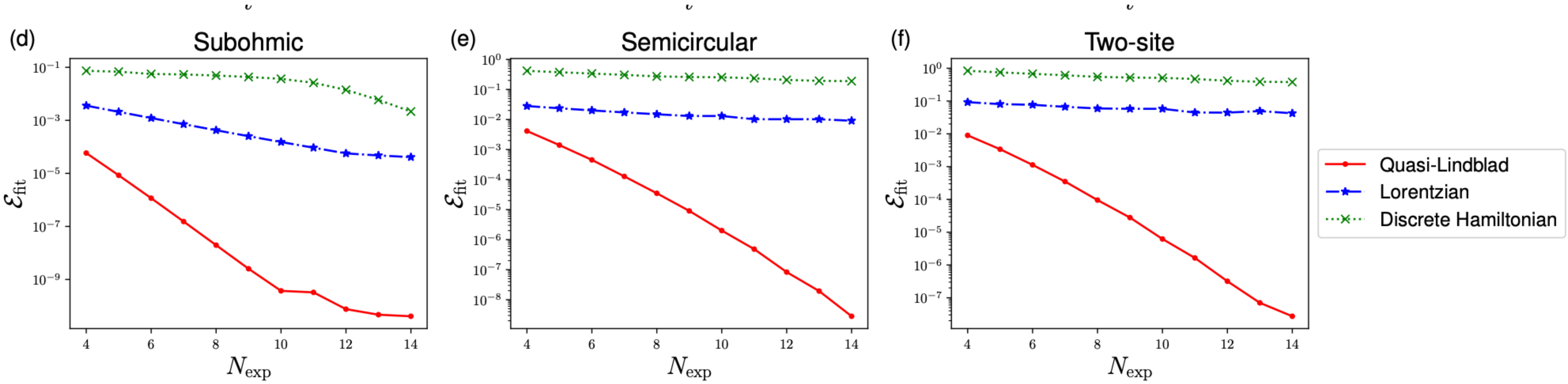
Pseudomode theory

- Pseudomode theory: construct a fictious/auxiliary bath to replace the original bath.
- Unitary case: discrete the continuous spectrum in some way: equidistance grid, Gauss-Legendre, adaptive quadrature, …
- Lorentzian pseuodomode theory: replace the unitary bath with diagonal Lindbladian bath.
- Quasi-Lindbladian pseuodomode theory: replace the unitary bath with Lindbladian bath, replace the unitary system-bath coupling with Lindbladian coupling.
- Conditions for exact simulation: make sure correlation functions are the same!



S
(a)
A
$\mathcal{D}_A$
S
(b)
$\mathcal{D}_{SA}$
A
$\mathcal{D}_A$
S
Original bath
Lindbladian pseudomode theory
quasi-Lindbladian pseudomode theory

Number of baths required for getting accurate correlation functions



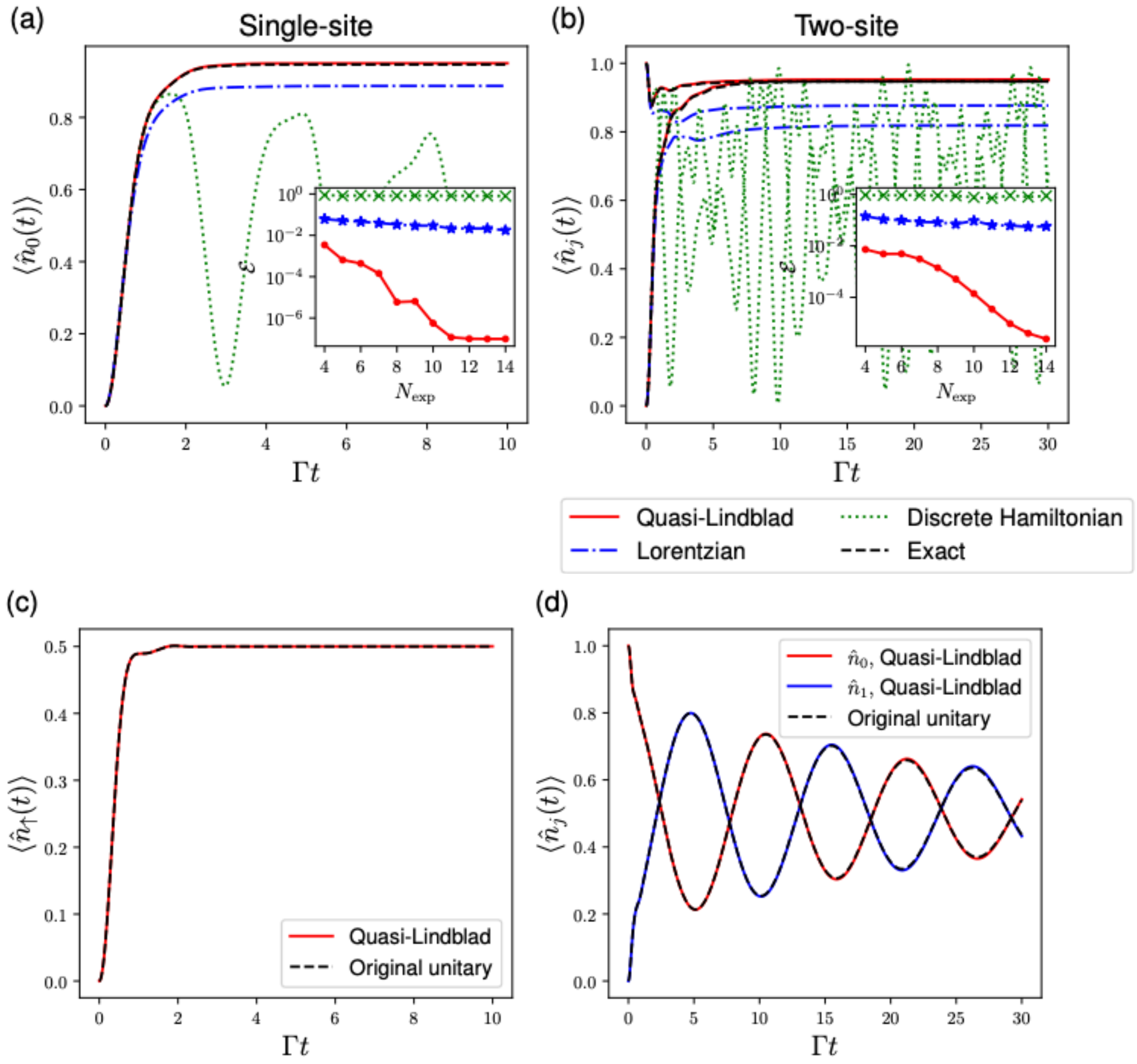
- Number of bath required is much smaller in quasi-Lindblad pseudocode theory, compared to Lorentzian and unitary.
- Similar things, known in the HEOM community (Free pole HEOM).

Quasi-Lindblad theory for spin-boson model

- Original unitary dynamics: $\hat{H}_{\text{phy}} = \hat{H}_S + \hat{H}_B + \hat{H}_{SB} = \hat{H}_S + \int d\omega\ \omega\ \hat{c}_\omega^\dagger \hat{c}_\omega + \sum_j \hat{S}_j \hat{B}_j$
- Bath correlation functions: $C^B_{jj'}(t,t') = \mathrm{Tr}_B\left[\hat{B}_j(t)\hat{B}_{j'}(t')\hat{\rho}_B(0)\right]$
- Quasi-Lindblad Pseudomode theory:
- $\partial_t \hat{\rho} = -\mathrm{i}[\hat{H}_{aux}, \hat{\rho}] + D_A(\hat{\rho}) + D_{SA}(\hat{\rho}),$ $\quad \hat{H}_{\text{aux}} = \hat{H}_S + \hat{H}_A + \hat{H}_{SA}$
- $\mathcal{D}_A \bullet = 2\sum_{kk'} \Gamma_{kk'} \left(\hat{F}_{k'} \bullet \hat{F}_k^\dagger - \frac{1}{2}\{\hat{F}_k^\dagger \hat{F}_{k'}, \bullet\}\right),$ $\quad \mathcal{D}_{SA}\bullet = \sum_j \hat{L}'_j \bullet \hat{S}_j + \hat{S}_j \bullet \hat{L}'^\dagger_j - \frac{1}{2}\{\hat{S}_j \hat{L}'_j + \hat{L}'^\dagger_j \hat{S}_j, \bullet\},$
- Let $L_{SA}(\hat{\rho}) = -\mathrm{i}[\hat{H}_{SA}, \hat{\rho}] + D_{SA}(\hat{\rho}), L_A(\hat{\rho}) = -\mathrm{i}[\hat{H}_A, \hat{\rho}] + D_A(\hat{\rho})$.
- L_{SA} has the decomposition $\quad \mathcal{L}_{SA} = -i\sum_j \mathcal{S}_j \mathcal{F}_j + i \sum_j \widetilde{\mathcal{S}}_j \widetilde{\mathcal{F}}_j,$
- Then BCF is $C^A_{jj'}(t,t') = \mathrm{Tr}_A\left[\mathcal{F}_j e^{\mathcal{L}_A(t-t')} \mathcal{F}_{j'} e^{\mathcal{L}_A t'} \hat{\rho}_A(0)\right].$
- Matching condition: $C^B_{jj'}(t,t') = C^A_{jj'}(t,t')$.

Result

- Single-site and two-site fermonic Anderson impurity model.



Mathematical foundations (1): Error analysis beyond Gronwall

Lemma 1.1 (Gronwall-type error bound for system observables). Let $C(t-t')$ and $C'(t-t') = C(t-t') + \delta C(t-t')$ be two-point BCFs corresponding to two different environments, and for a bounded system operator $\hat{O}_S$, let $O_S(t)$, $O'_S(t)$ be the system observables corresponding to the two environments. Then, we have

$$|O_S(t) - O'_S(t)| \le \|\hat{O}_S\| \epsilon_1 t e^{\mathcal{M}_1 t} \quad \text{for } t \in [0,T] \qquad T_0 \sim O\left(\frac{1}{M_1}\log(1/\epsilon_1)\right)$$

Here, $\epsilon_1 = \|\delta C\|_{L^1[0,T]}$, $\mathcal{M}_1 = \|C\|_{L^1[0,T]}$ (see Eq. (2.31)), $\|\hat{O}_S\|$ is the operator norm of $\hat{O}_S$, and $\|\cdot\|_{L^1[0,T]}$ is the L^1 norm of a function on $[0,T]$.

Theorem 1.1 (Main theorem, for system observables). Let $C(t-t')$, $C'(t-t')$, $O_S(t)$, $O'_S(t)$ and ϵ_1 be the same as in Lemma 1.1. Then, we have

$$|O_S(t) - O'_S(t)| \le \|\hat{O}_S\| (e^{\epsilon_1 t} - 1), \quad \text{for } t \in [0,T] \qquad T \sim O(1/\epsilon_1)$$

Mathematical foundations (2): Stability analysis

- The quasi-Lindblad equation breaks the positivity condition. Yet it appears stable in practice. WHY?

- Turns out this is a coherent-induced stability.

- Recall $\hat{H}_{SA} = \sum_{i \in sys} \sum_{j \in bath} \nu_{ij} \hat{a}_i^\dagger \hat{c}_j + h.c.$

- Theorem (informal): (with some technical assumption), there exists constant m, if $|\nu| \geq m$, the dynamics is stable.

- Rigorous proved for quasi-free case (quadratic Hamiltonian, linear jump).

- Ongoing work: proof for general case.

Pseudomode theory could be unstable

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On stability issues of the HEOM method

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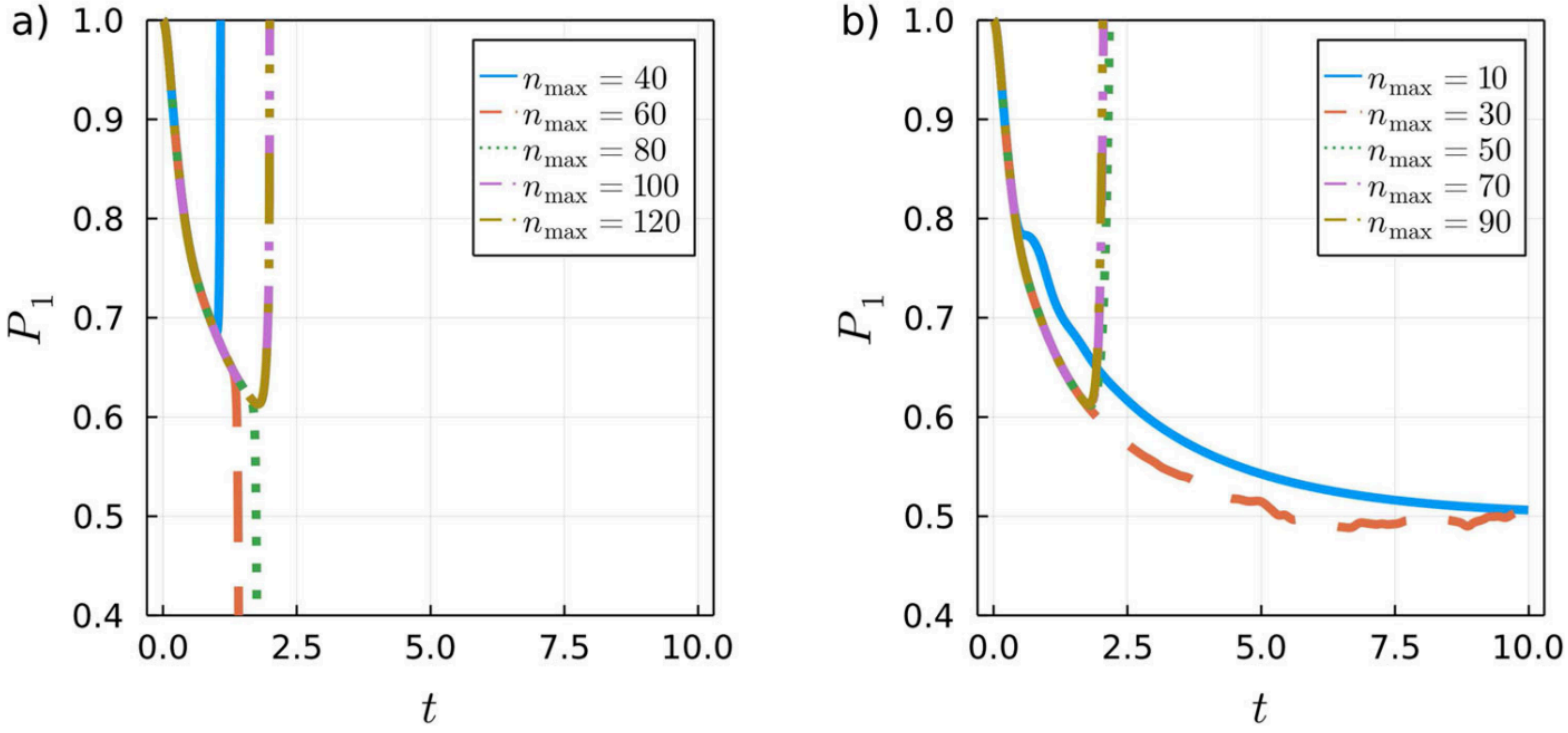


- The instability is not improvable by increasing the truncation dimension.

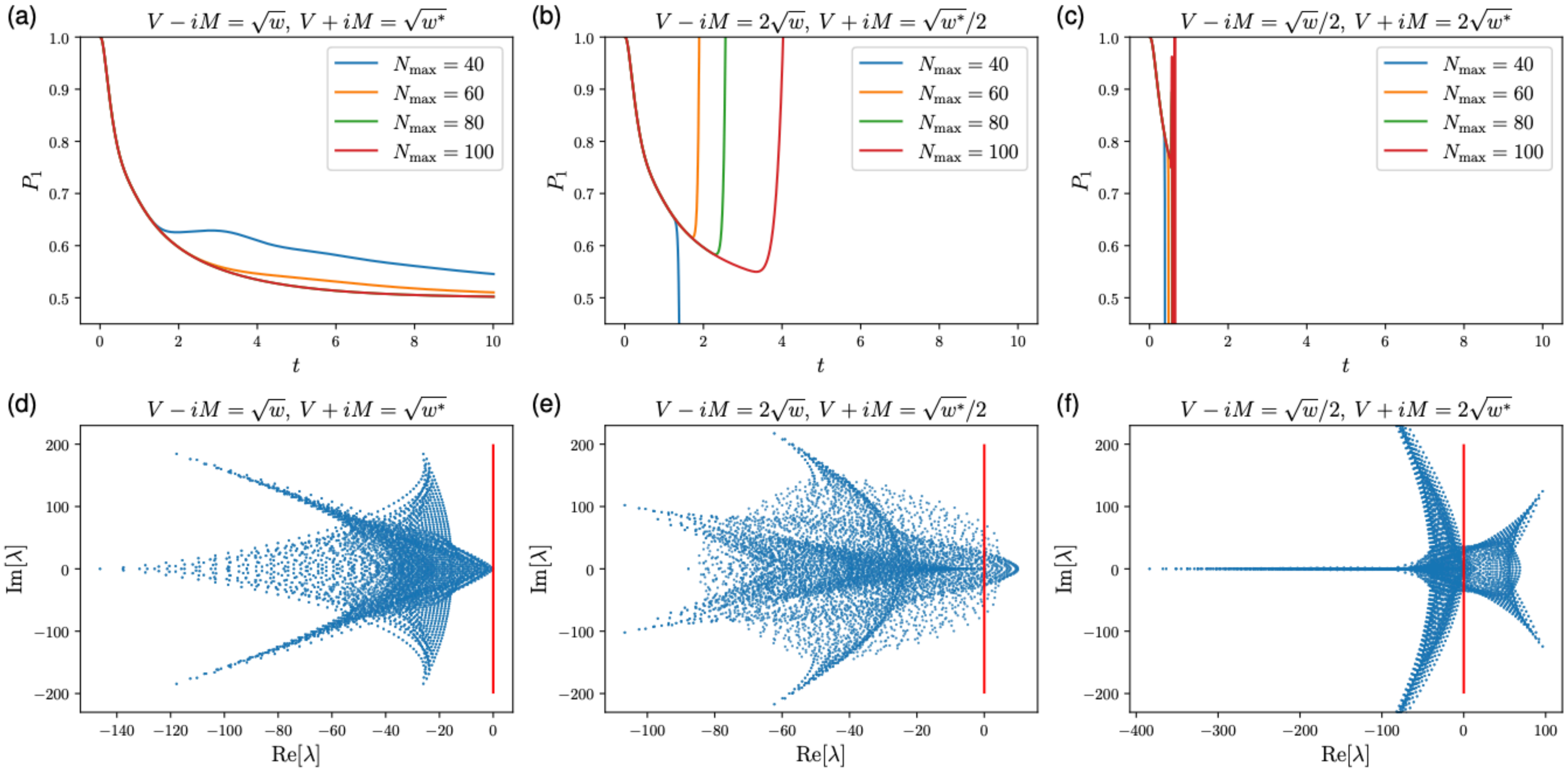
Pseudomode theory

- Various pseudomode theories that break positivity to gain computational advantage.
- Comparison? (Using same parameter settings as the previous HEOM experiment)

Our pseudomode theory

Observables

Eigenvalues of Liouvillians



Discussions

- Mathematics:
  - Stability.
  - Error bound analysis.
- Numerics:
  - Algorithms for solving quasi-Lindblad equations.
- Applications:
  - Nonequilibrium dynamics of density, non-equilibrium Green’s function, …