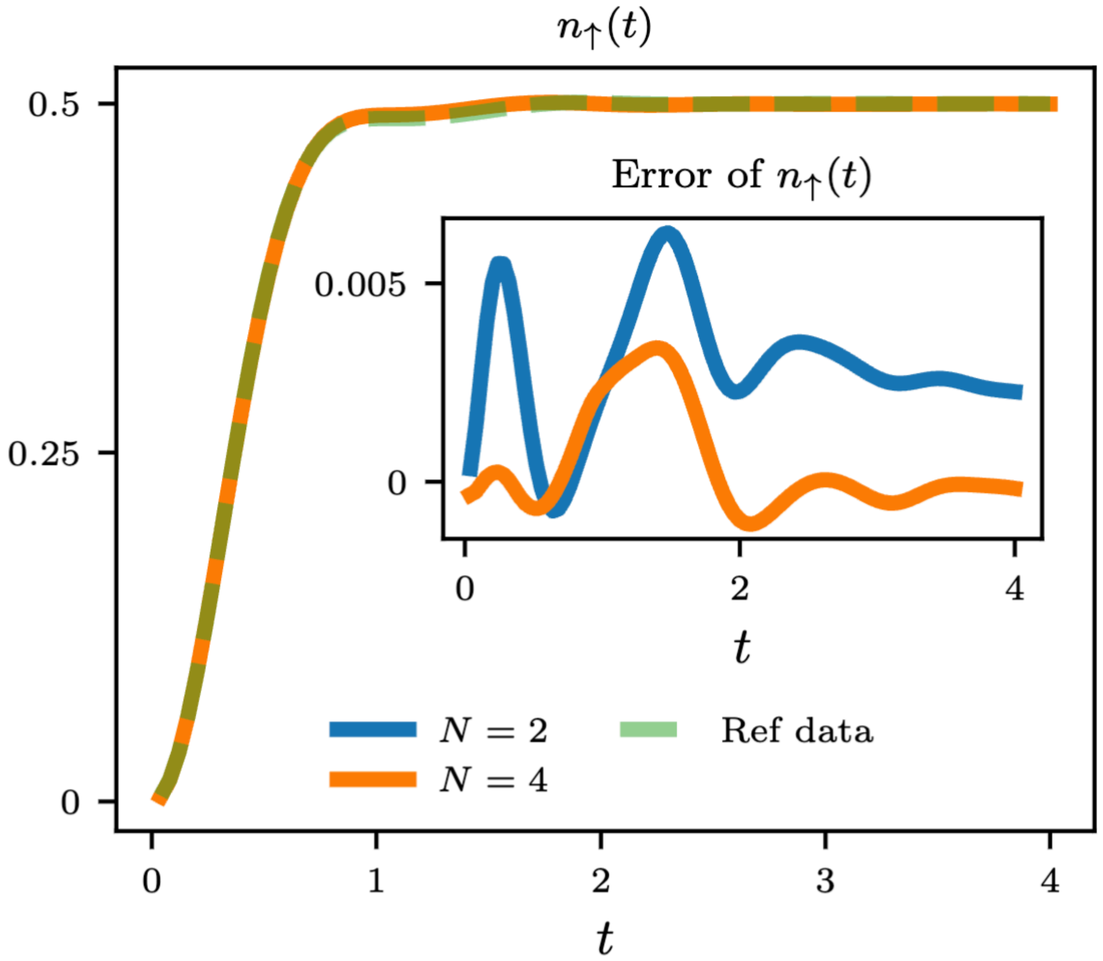
Efficient and *physical* pseudomode theory for non-Markovian open quantum systems



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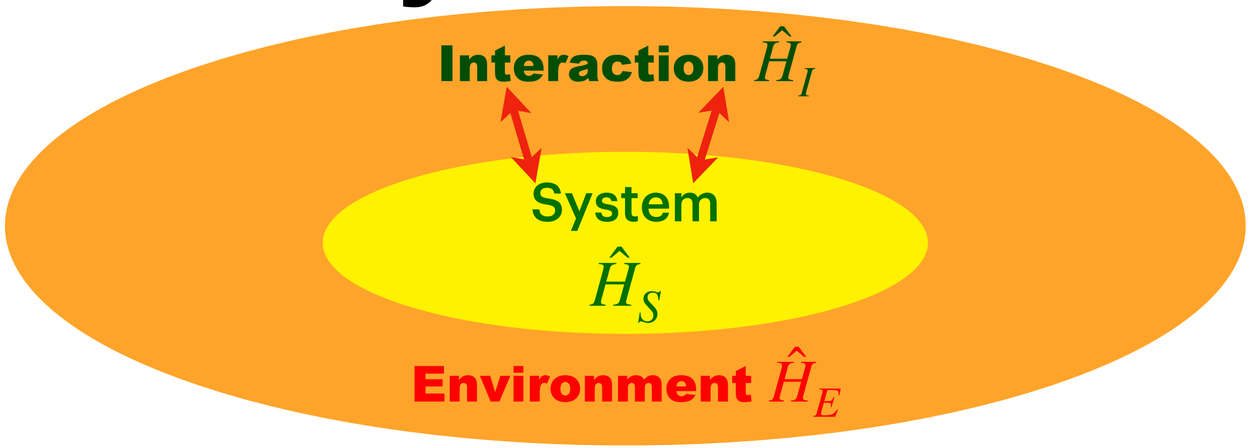
https://math.berkeley.edu/~hertz/

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, especially when Markovian approximation breaks down?
- Consider the usual set up:
  - Gaussian environment, with continuous degrees of freedom.
  - Linear system-bath coupling.

Examples

Light-matter coupling:

Lednev, García-Vidal, Feist, PhysRevLett.132.106902

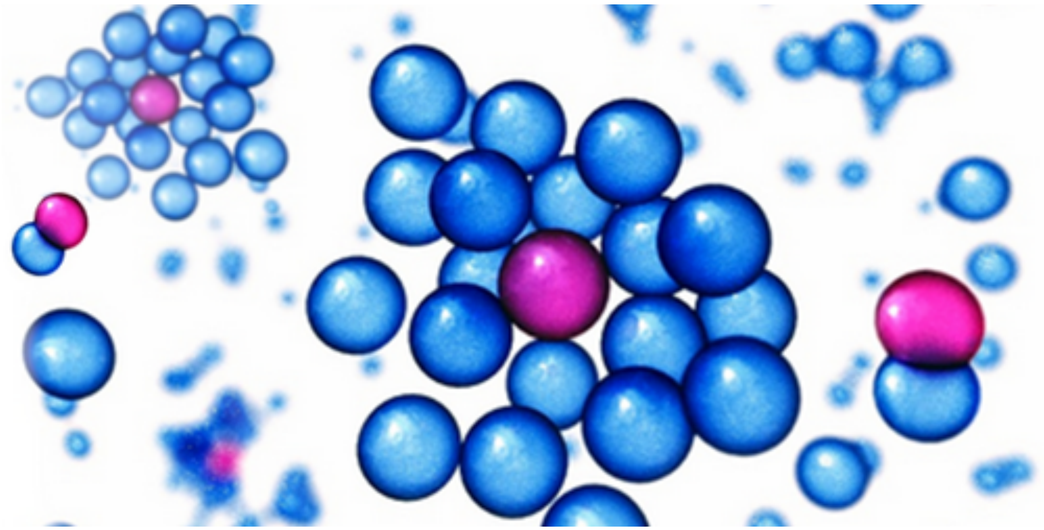
Slides from Prof. Kono's talk

How strong is your light-matter coupling?

$g > (\gamma + \kappa)/4$	**Strong**
$g > 0.1\omega_0$	**Ultrastrong**
$g > \omega_0$	**Deep Strong**
$g > \Delta\omega$	**Superstrong**
$g > \mathrm{Ry}^*$	**Very Strong**
...	

https://online.kitp.ucsb.edu/online/qoelectrons-c25/kono/

Quantum impurities



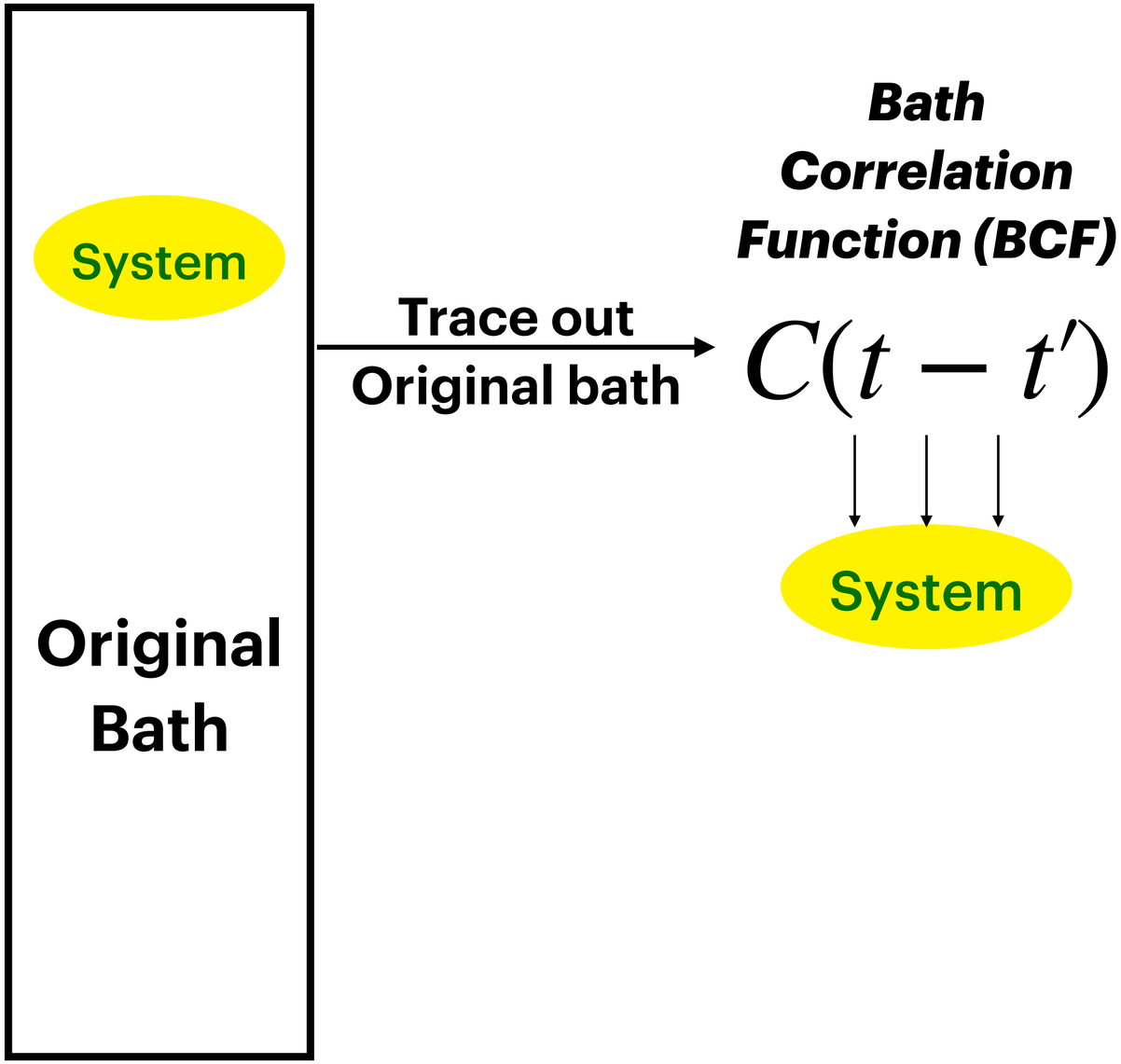
Electronic transport
Kondo physics
Quantum embedding theories
.....

Model setup

- Spin-boson model
  - $\hat{H}_S$ is the spin Hamiltonian.
  - $\hat{H}_B = \int \omega \hat{b}_\omega^\dagger \hat{b}_\omega \mathrm{d}\omega.$
  - $\hat{H}_{SB} = \sum_i \hat{S}_i \int f_i(\omega)\hat{b}_i + \overline{f_i(\omega)}\hat{b}_i^\dagger \mathrm{d}\omega\,.$
  - BCF:
    $C(t) = \int J(\omega)\left(\coth(\beta\omega)\cos(\omega t) - \mathrm{i}\sin(\omega t)\right)\mathrm{d}\omega$
  - Bath spectral density (BSD):
    $J(\omega) = f_i(\omega)\overline{f_j(\omega)}.$

- Fermionic impurity model
  - $\hat{H}_S(\hat{a}_i, \hat{a}_i^\dagger)$ is the impurity Hamiltonian.
  - $\hat{H}_B = \int \omega \hat{c}_\omega^\dagger \hat{c}_\omega \mathrm{d}\omega\,.$
  - $\hat{H}_{SB} = \sum_i \int f_i(\omega)\hat{a}_i^\dagger \hat{c}_\omega \mathrm{d}\omega + h\,.\,c\,.$
  - BCF: $C^{>}(t) = \int J(\omega) f_{FD}^{\beta}(\omega)\mathrm{e}^{-\mathrm{i}\omega t}\mathrm{d}\omega,$
    $C^{<}(t) = \int J(\omega)(1 - f_{FD}^{\beta}(\omega))\mathrm{e}^{-\mathrm{i}\omega t}\mathrm{d}\omega.$
  - BSD: $J(\omega)f_{FD}^{\beta}(\omega), J(\omega)(1 - f_{FD}^{\beta}(\omega))\,.$
    $J(\omega) = f_i(\omega)\overline{f_j(\omega)}.$
    $f_{FD}^{\beta}(\omega)$ is the Fermi-Dirac function.

Pseudomode theory



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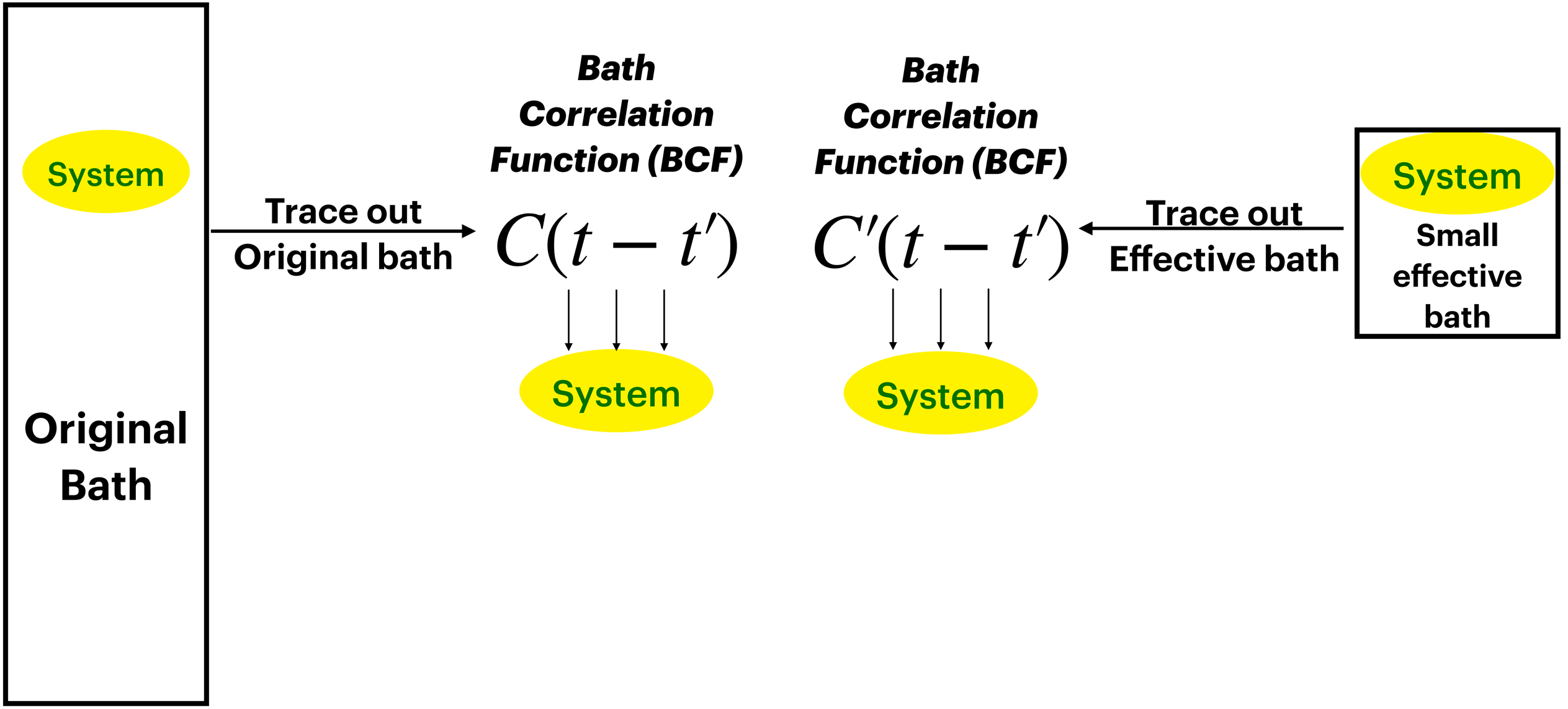

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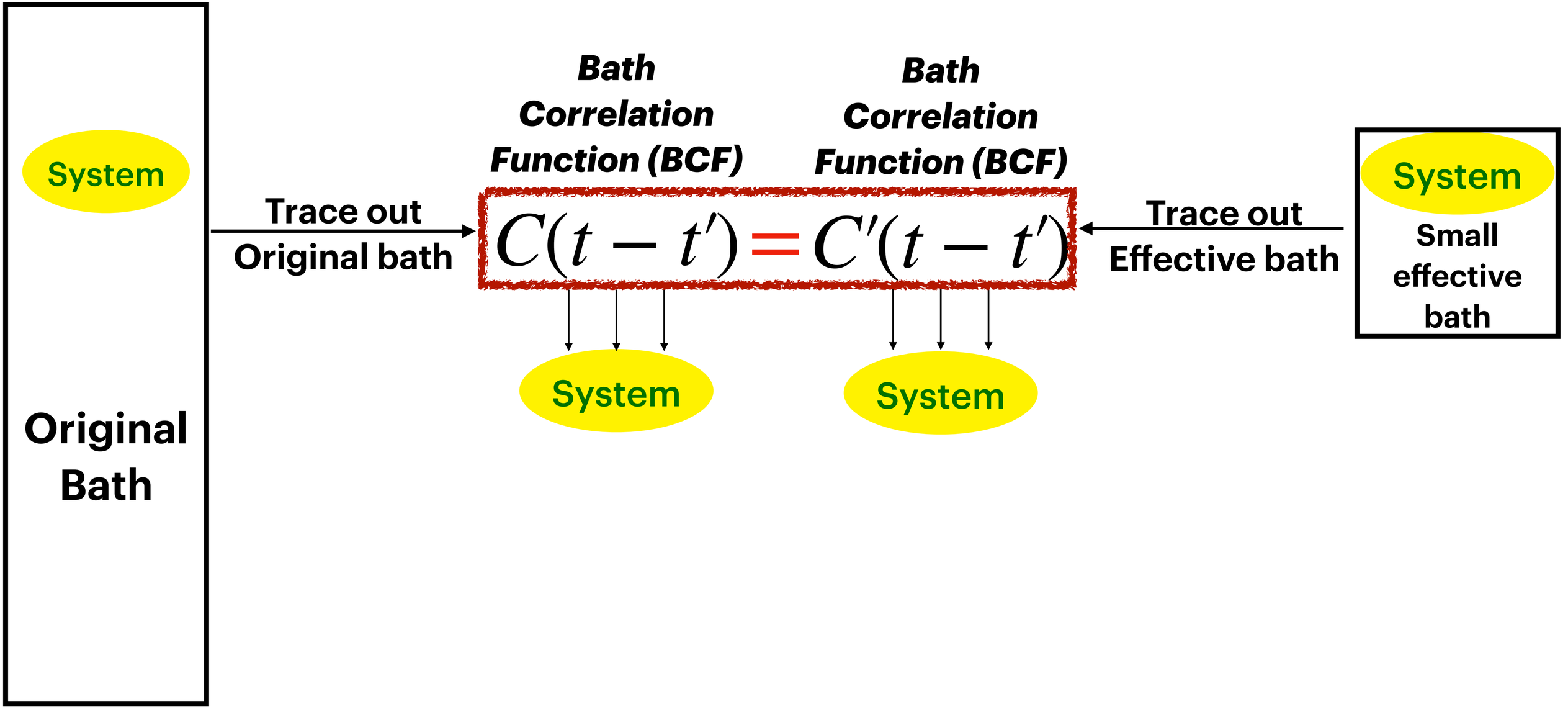

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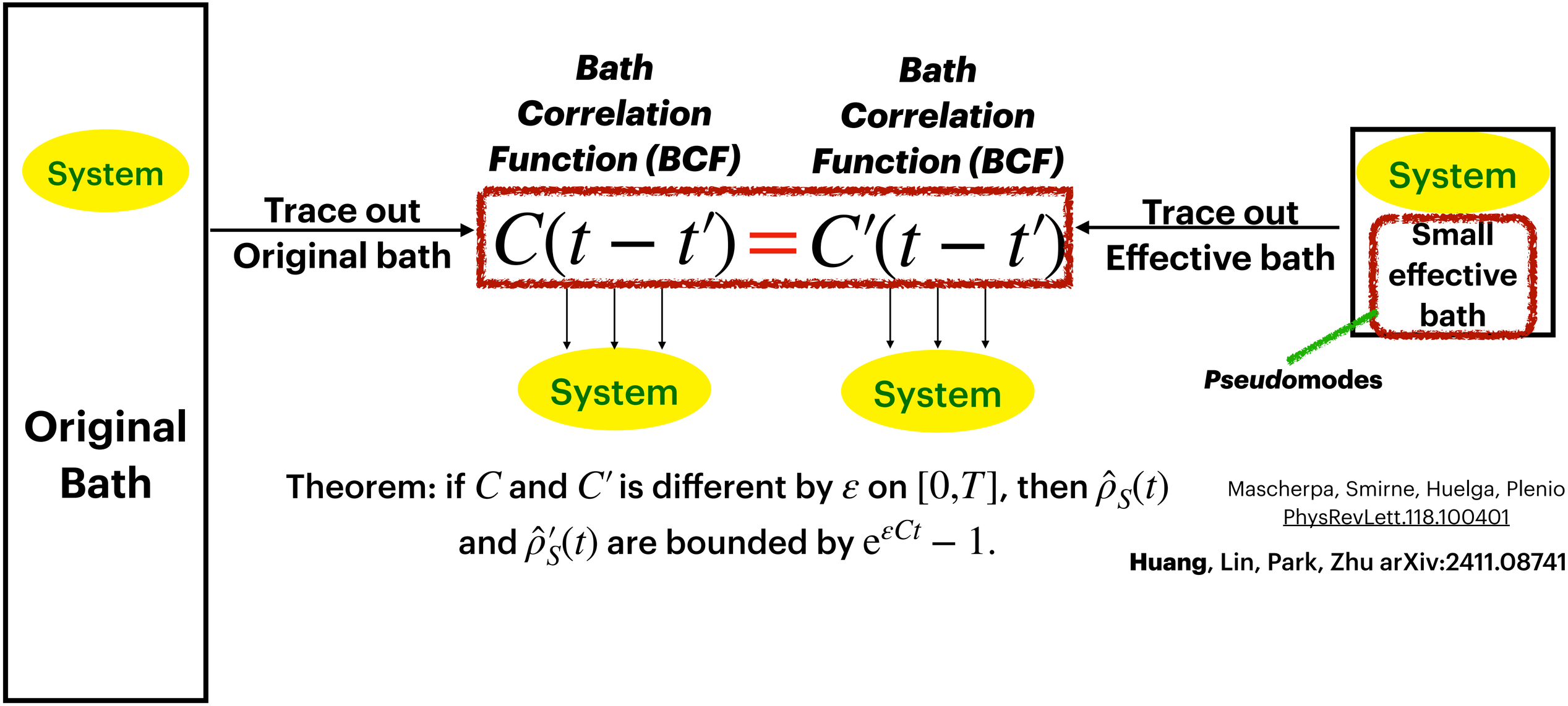
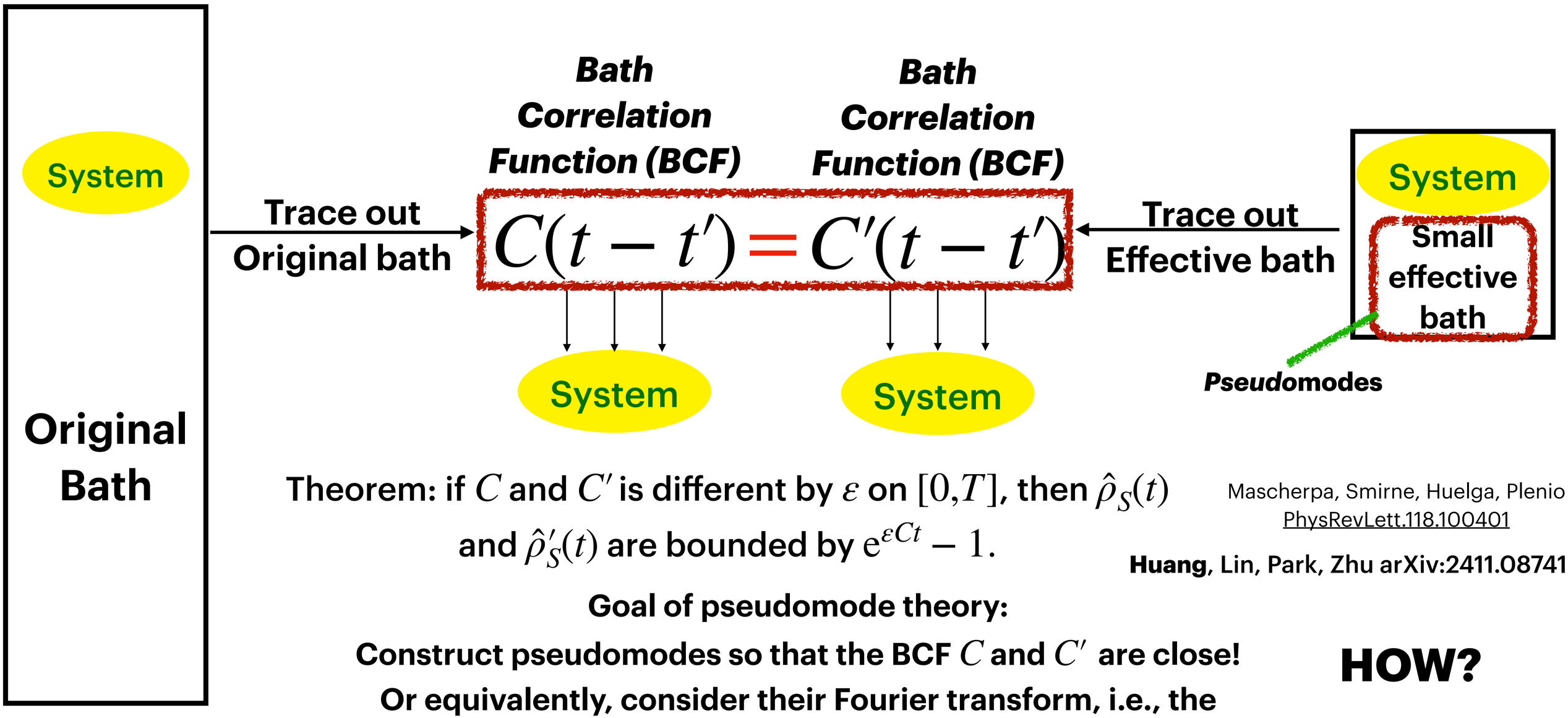


Theorem: if C and C' is different by ε on $[0,T]$, then $\hat{\rho}_S(t)$ and $\hat{\rho}'_S(t)$ are bounded by $\mathrm{e}^{\varepsilon C t} - 1$.

Mascherpa, Smirne, Huelga, Plenio PhysRevLett.118.100401

Huang, Lin, Park, Zhu arXiv:2411.08741

Pseudomode theory



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Goal of pseudomode theory:

Construct pseudomodes so that the BCF C and C' are close!

Or equivalently, consider their Fourier transform, i.e., the bath spectral density $J(\omega), J'(\omega)$.

HOW?

Review of Pseudomode theory

Goal: reproduce BCF $C(t)$ with pseudomodes, on $[0,T]$, with ε error.

	BCF formalism	Pseudomode Dynamics	Complexity: Number of pseudomodes required
Unitary pseudomode theory	$\sum_{k=1}^{N} \lvert g_k \rvert^2 \mathrm{e}^{-\mathrm{i}\omega_k t}$	$-\mathrm{i}\left[\hat{H}_{\mathrm{S}} + \hat{H}_{\mathrm{A}}^{\mathrm{diag}} + \hat{H}_{\mathrm{SA}}, \cdot\right]$	$O(\mathrm{poly}(T)\mathrm{polylog}(\varepsilon^{-1}))$
Lorentzian pseudomode theory	$\sum_{k=1}^{N} \lvert g_k \rvert^2 \mathrm{e}^{(-\mathrm{i}\omega_k - \gamma_k)t}$	$-\mathrm{i}\left[\hat{H}_{\mathrm{S}} + \hat{H}_{\mathrm{A}}^{\mathrm{diag}} + \hat{H}_{\mathrm{SA}}, \cdot\right] + \boldsymbol{D}_{\mathrm{A}}^{\mathrm{diag}}(\cdot)$	$O(\mathrm{poly}(T\varepsilon^{-1}))$
Quasi-Lindblad pseudomode theory	$\sum_{k=1}^{N} (g_k - \mathrm{i}\alpha_k)^2 \mathrm{e}^{(-\mathrm{i}\omega_k - \gamma_k)t}$	$-\mathrm{i}\left[\hat{H}_{\mathrm{S}} + \hat{H}_{\mathrm{A}}^{\mathrm{diag}} + \hat{H}_{\mathrm{SA}}, \cdot\right] + \boldsymbol{D}_{\mathrm{A}}^{\mathrm{diag}}(\cdot) + \boldsymbol{D}_{\mathrm{SA}}(\cdot)$	$O(\mathrm{poly}\,\log(T\varepsilon^{-1}))$

- Physical, but ***not efficient***
- Efficient, but ***not physical***

Guaranteed stability

Can we have a pseudomode theory that is both **Efficient** and **Physical**?

Efficiency and physicality

Coupled Lindblad pseudomode theory

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = -\mathrm{i}[\hat{H}_\mathrm{S} + \hat{H}_\mathrm{A} + \hat{H}_\mathrm{SA}, \cdot] + \boldsymbol{D}_\mathrm{A}(\cdot),$$

$$\hat{H}_\mathrm{A} = \sum_{k,l=1}^{N} h_{kl}\hat{b}_k^\dagger \hat{b}_l, \quad \hat{H}_\mathrm{SA} = \sum_{k=1}^{N} \hat{S}\left(g_k \hat{b}_k + \overline{g_k}\hat{b}_k^\dagger\right),$$

$$\boldsymbol{D}_\mathrm{A}(\cdot) = \sum_{k,l=1}^{N} \Gamma_{kl}\left(2\hat{b}_k \cdot \hat{b}_l^\dagger - \left\{\hat{b}_l^\dagger \hat{b}_k, \cdot\right\}\right).$$

- Coupled Lindblad modes:
  - Both bath Hamiltonian and dissipation matrices h and Γ are full matrices.

$$C(t) = g^\dagger \mathrm{e}^{(-\mathrm{i}H-\Gamma)t} g\,.$$

Efficiency and physicality

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Coupled Lindblad modes itself is *not* new!

PRL 132.106902, 2024

For example, Lednev et al considers coupled modes motivated by the artificial pumping problem in simulation of light -matter coupling.

Efficiency and physicality

Coupled Lindblad pseudomode theory

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = -\mathrm{i}[\hat{H}_\mathrm{S} + \hat{H}_\mathrm{A} + \hat{H}_\mathrm{SA}, \cdot] + \boldsymbol{D}_\mathrm{A}(\cdot),$$

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- Coupled Lindblad modes:
  - Both bath Hamiltonian and dissipation matrices h and Γ are full matrices.

$$C(t) = g^\dagger \mathrm{e}^{(-\mathrm{i}H-\Gamma)t} g\,.$$

- What's new in this work:
  - Establish the efficiency ($O(polylog(T/\varepsilon))$ scaling) of this approach:
  - Efficient and robust construction of coupled modes.

Efficiency of coupled Lindblad pseudomode theory: Feasibility condition

- Quasi-Lindblad pseudomode theory is efficient. ($O(polylog(T/\varepsilon))$ scaling)

$$C^{\mathrm{q}}(t) = \sum_{k=1}^{N} (g_k^{\mathrm{q}} - \mathrm{i}\alpha_k^{\mathrm{q}})^2 \mathrm{e}^{(-\mathrm{i}\omega_k^{\mathrm{q}} - \gamma_k^{\mathrm{q}})t}$$

- If the following feasibility condition holds, one could construct a coupled Lindblad pseudomode of the same size as the quasi-Lindblad pseudo modes.
- Therefore the scaling automatically carries over!

Let $\Lambda = \mathrm{diag}(\boldsymbol{\omega}^{\mathrm{q}} - \mathrm{i}\boldsymbol{\gamma}^{\mathrm{q}})$, and $\boldsymbol{u}_{\pm} = \boldsymbol{g}^{\mathrm{q}} \pm \mathrm{i}\boldsymbol{\alpha}^{\mathrm{q}}$. Then the feasibility condition is as follows:

Definition (Feasibility condition)**.** There exists $n \times n$ positive definite matrix Y such that:

$$Y\boldsymbol{u}_- = \boldsymbol{u}_+, \quad \mathrm{i}(Y\Lambda - \Lambda^\dagger Y) \succeq 0.$$

Construction of coupled modes

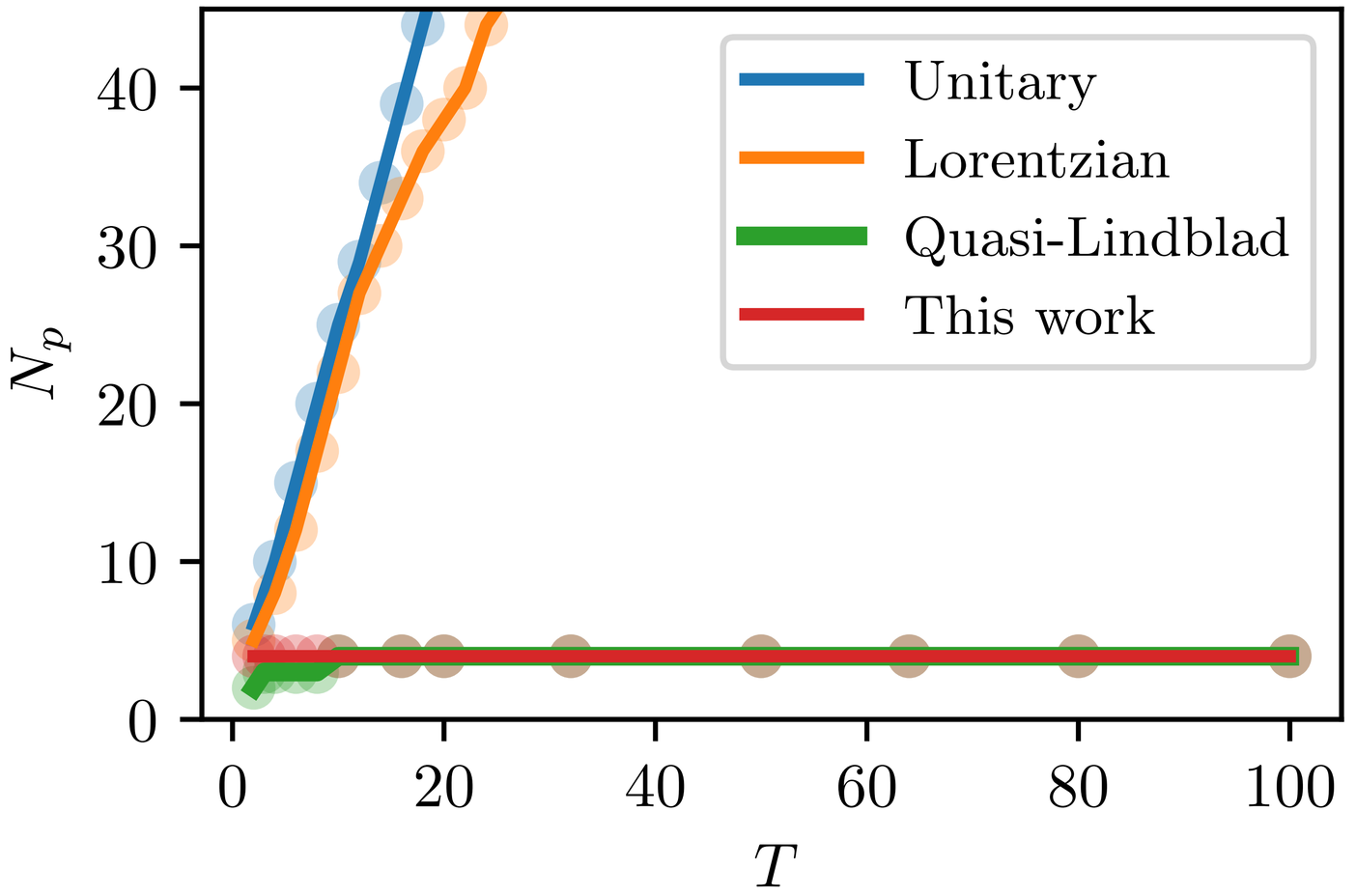
$$C(t) = g^\dagger \mathrm{e}^{(-\mathrm{i}H-\Gamma)t} g \Leftrightarrow J(\omega) = \frac{1}{\pi} Im(g^\dagger (H - \mathrm{i}\Gamma - \omega)^{-1} g)\,.$$

- Naive method: direct optimization.
- Highly nonconvex! Very ineffective
- Method 1: using the feasibility condition, construct coupled modes based on quasi-Lindblad modes.
  - Error accumulation, due to the intermediate quasi-Lindblad fitting step.
- Method 2: inspired by realization problem in control theory.
  - Realization problem: given $f(\omega)$, find l, r, T such that $f(\omega) = l^\dagger (\omega - T)^{-1} g\,.$
  - Nontrivial generalization of the realization problem to coupled modes.

Benchmarking complexity

Model: single impurity Anderson model. Calculate observable $n_{imp}(t)$.

Number of pseudomodes required v.s. time T, so that $n_{imp}(t)$ reaches 10^{-2} accuracy on $[0,T]$.

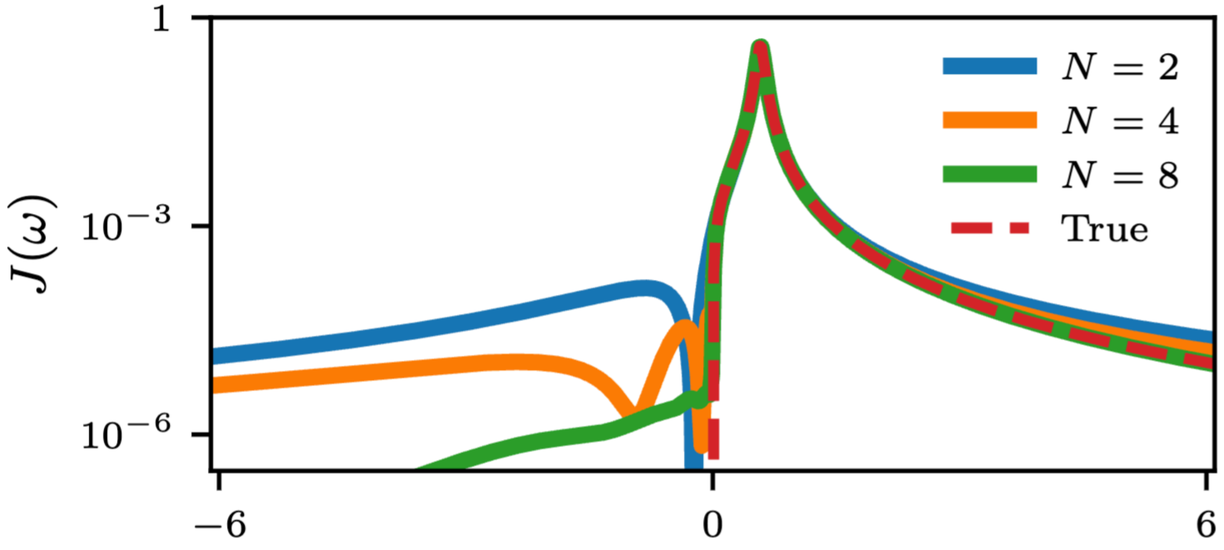


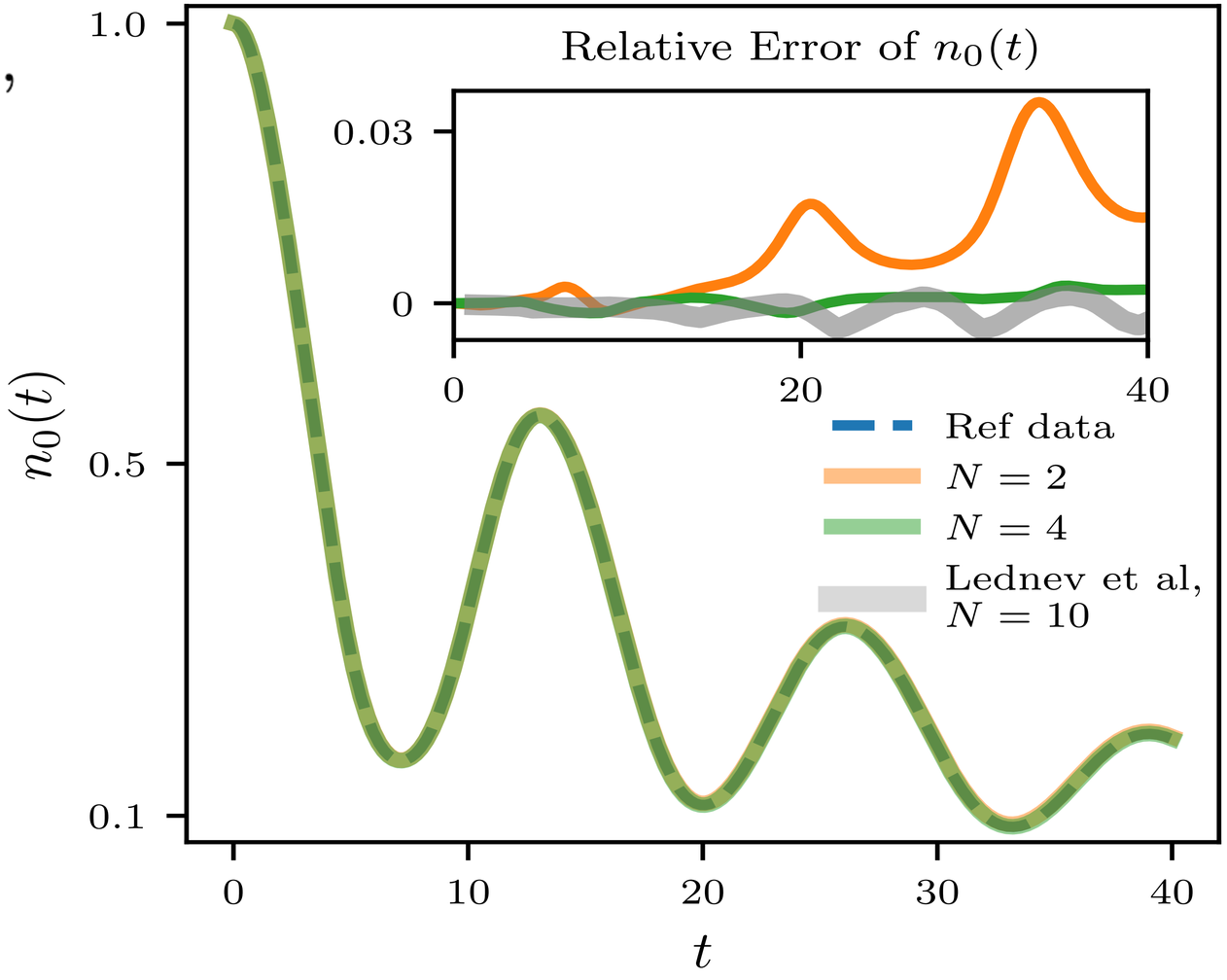
Example: ultra-strong light-matter coupling

Lednev, García-Vidal, Feist, PhysRevLett.132.106902

$$H = \frac{\omega_e}{2}\sigma_z + \int_{-\infty}^{\infty} (\omega a_\omega^\dagger a_\omega + \sqrt{J(\omega)}(a_\omega^\dagger + a_\omega)\sigma_x)\mathrm{d}\omega,$$

$$J_{\mathrm{sm}}(\omega) = \theta(\omega)\frac{2g^2}{\pi}\frac{\kappa\omega_c\omega}{(\omega_c^2-\omega^2)^2+\kappa^2\omega^2},$$



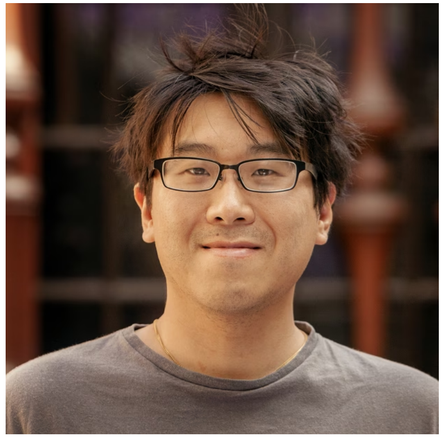


Conclusions

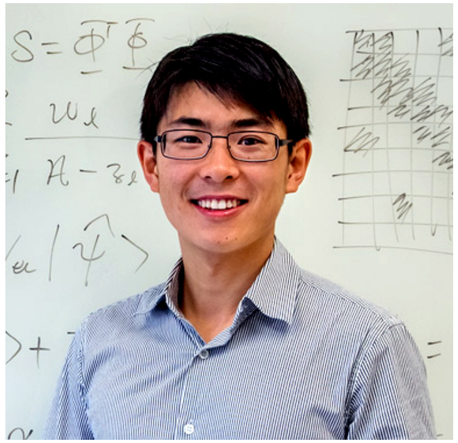
- Physical and efficient pseudomode theory
- Robust construction of the pseudomodes
- Applications
  - Dynamics of reduced system density.
  - Correlation functions (Green's functions), spectrum.
  - Real-time quantum impurity solvers, towards non-equilibrium dynamical mean-field theory.

Acknowledgement

Gunhee Park, Caltech



Garnet K.-L. Chan, Caltech



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