Complexity of real-time Gaussian environments

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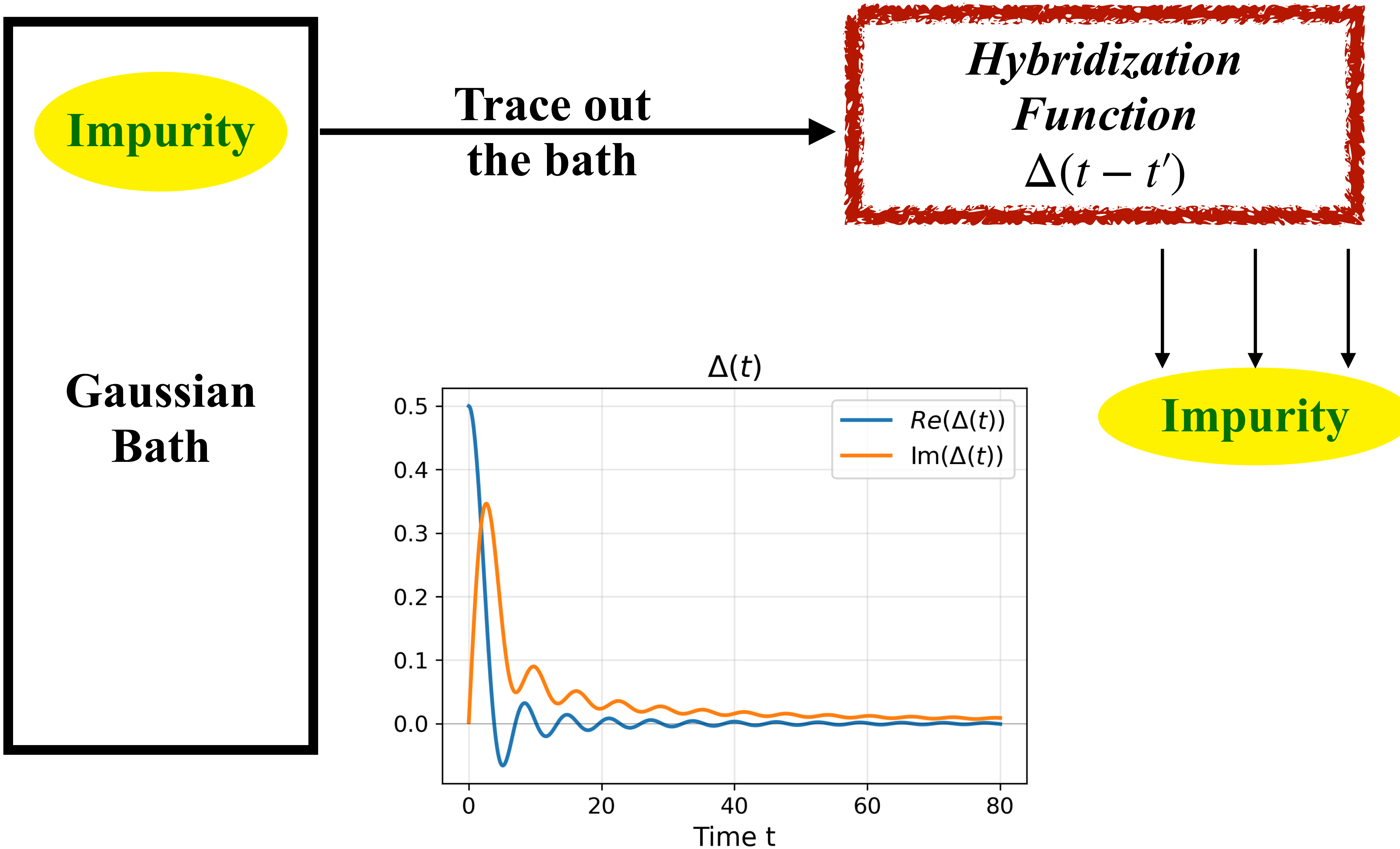
Gaussian bath and hybridization functions



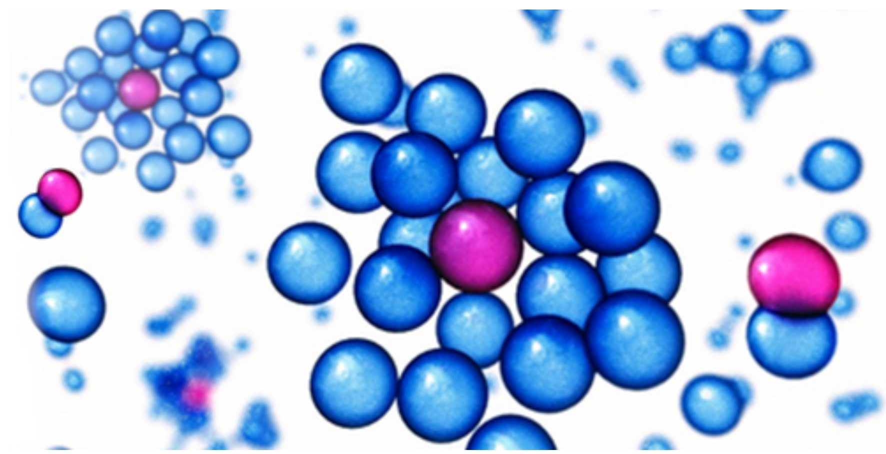
Applications

Light-matter coupling

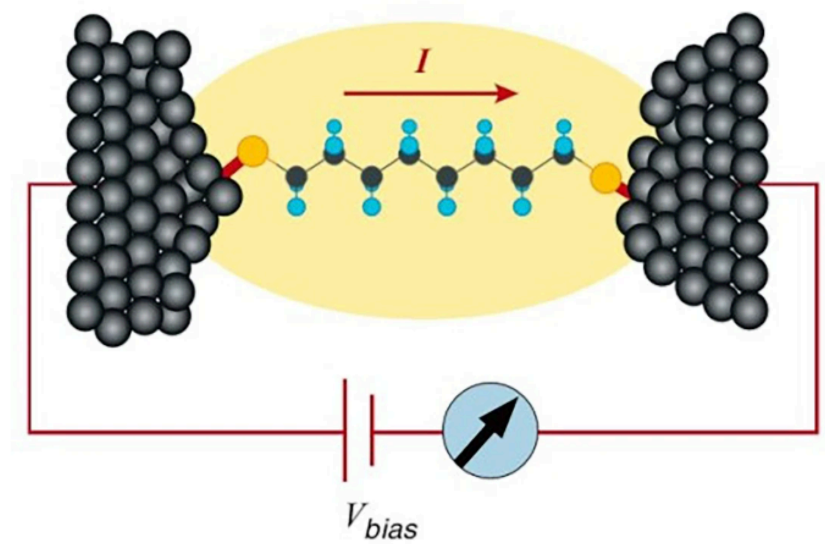
How strong is your light-matter coupling?

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

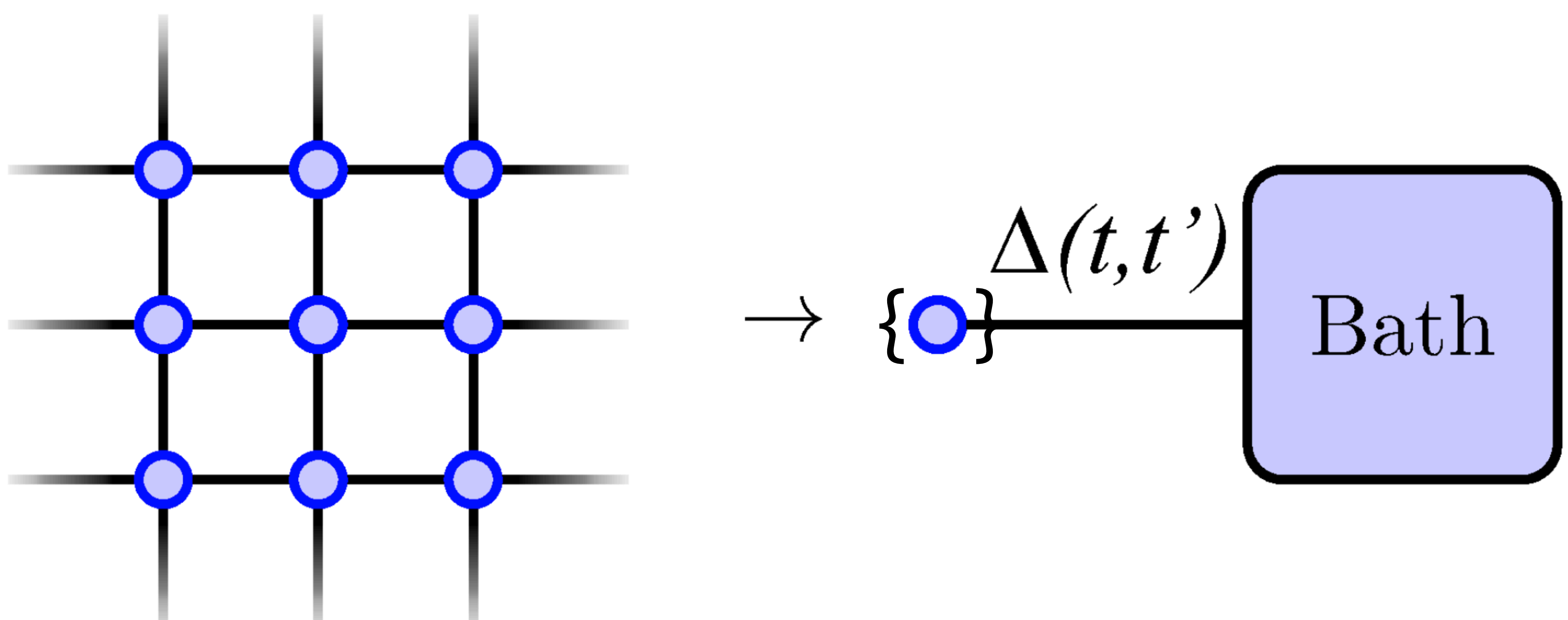
Quantum impurities



Molecular junctions



Dynamical mean-field theory (DMFT)



The problem of real-time bath fitting

Find w_k and z_k such that:

$$\Delta(t) \approx \sum_{k=1}^{N} w_k \mathrm{e}^{-\mathrm{i} z_k t}, \; w_k, z_k \in \mathbb{C}, \text{ with accuracy } \varepsilon \text{ on } [0, T].$$

Question:

How many terms is needed? (What is N?)

a.k.a.

How complicated is my Gaussian bath?

Or

How complicated could a sum-of-exponential problem be?

Recall known results on imaginary-time hybridization functions

$$\Delta(\tau) = \int_{\mathbb{R}} K_\beta(\tau,\omega) J(\omega) \mathrm{d}\omega, \quad \tau \in [0,\beta], \quad K_\beta(\tau,\omega) = \frac{\mathrm{e}^{-\tau\omega}}{1+\mathrm{e}^{-\beta\omega}}.$$

Exponentially decaying kernel in imaginary time.

Compared to $K(t,\omega) = \mathrm{e}^{-i\omega t}$ in real-time. **Oscillatory**.

Fri. March 20, 8:36 — 8:48 a.m.
Convention Center, Meeting Room 605

Block-sparse evaluation of imaginary-time strong-coupling Feynman diagrams

Part of MAR-Y45 Precision Many-Body Physics V: Techniques in Precision Many-body Physics

We present an algorithm for the evaluation of imaginary-time Feynman diagrams in the strong-coupling expansion of the Anderson impurity model that makes use of sparse linear algebra to accelerate existing deterministic methods. A symmetry i...

Authors: Francisco Rilloraza (presenter), Jason Kaye, Hugo Strand, Zhen Huang, Denis Golez

Fri. March 20, 8:48 — 9:00 a.m.
Convention Center, Meeting Room 605

The TRIQS arbirary X-Crossing Approximation impurity solver (triqs_xca)

Part of MAR-Y45 Precision Many-Body Physics V: Techniques in Precision Many-body Physics

The triqs_xca solver is the latest quantum impurity solver addition to the Toolbox for Research on Interacting Quantum Systems (TRIQS) based on the bold hybridization expansion, a.k.a. the X:th order Crossing Approximation (XCA). Using the sum-of-...

Authors: Hugo Strand (presenter), Paco Rilloraza, Zhen Huang, Nils Wentzell, Denis Golez, Jason Kaye

- IR, DLR, modified AAA. **See also talks Friday Room 605 8:36am - 9am.**

Exciting progress in imaginary-time multi-orbital impurity solvers.

Recall known results on imaginary-time hybridization functions

$$\Delta(\tau) = \int_{\mathbb{R}} K_\beta(\tau,\omega)J(\omega)\mathrm{d}\omega, \quad \tau \in [0,\beta], \quad K_\beta(\tau,\omega) = \frac{\mathrm{e}^{-\tau\omega}}{1+\mathrm{e}^{-\beta\omega}}.$$

Exponentially decaying kernel in imaginary time.

Compared to $K(t,\omega) = \mathrm{e}^{-\mathrm{i}\omega t}$ in real-time. **Oscillatory**.

- Imaginary-time bath fitting: $\Delta(\tau) \approx \sum_{k=1}^{N} w_j \mathrm{e}^{-z_j\tau}, z_j \in \mathbb{R}$,
  - $N \sim O(\log(\beta W/\varepsilon))$.
  - Efficient algorithms:

    Kaye, **Huang**, Strand, Golež, Physics Review X, 14, 031034 (2024)

    Huang, Golež, Strand, Kaye, SciPost Phys. 19, 121 (2025)

    - IR, DLR, modified AAA. **See also talks Friday Room 605 8:36am - 9am.**
    - Additional constraints on $\omega_j \geq 0$ for causality. **Huang**, Gull, Lin, Phys. Rev. B 107, 075151 (2023)

What could be the contributing factors to complexity of real-time bath fitting?

$$\Delta(t) = \int_{\mathbb{R}} J(\omega) f_{FD}(\omega) \mathrm{e}^{-\mathrm{i}\omega t} \mathrm{d}\omega, \quad f_{FD}(\omega) = \frac{1}{1 + \mathrm{e}^{\beta(\omega - \mu)}}.$$

- Accuracy ε?
- Maximum time T?
- Temperature β? Bandwidth W?
- Smoothness of J?

- Previous analysis:
  - Strong assumptions on analyticity of J. Showing $N \sim \log^2(T/\varepsilon)$.

Singularities of spectral density

- Generally unreasonable to assume analyticity in practice!

PHYSICAL REVIEW VOLUME 89, NUMBER 6 MARCH 15, 1953

The Occurrence of Singularities in the Elastic Frequency Distribution of a Crystal

LÉON VAN HOVE
Institute for Advanced Study, Princeton, New Jersey
(Received December 5, 1952)

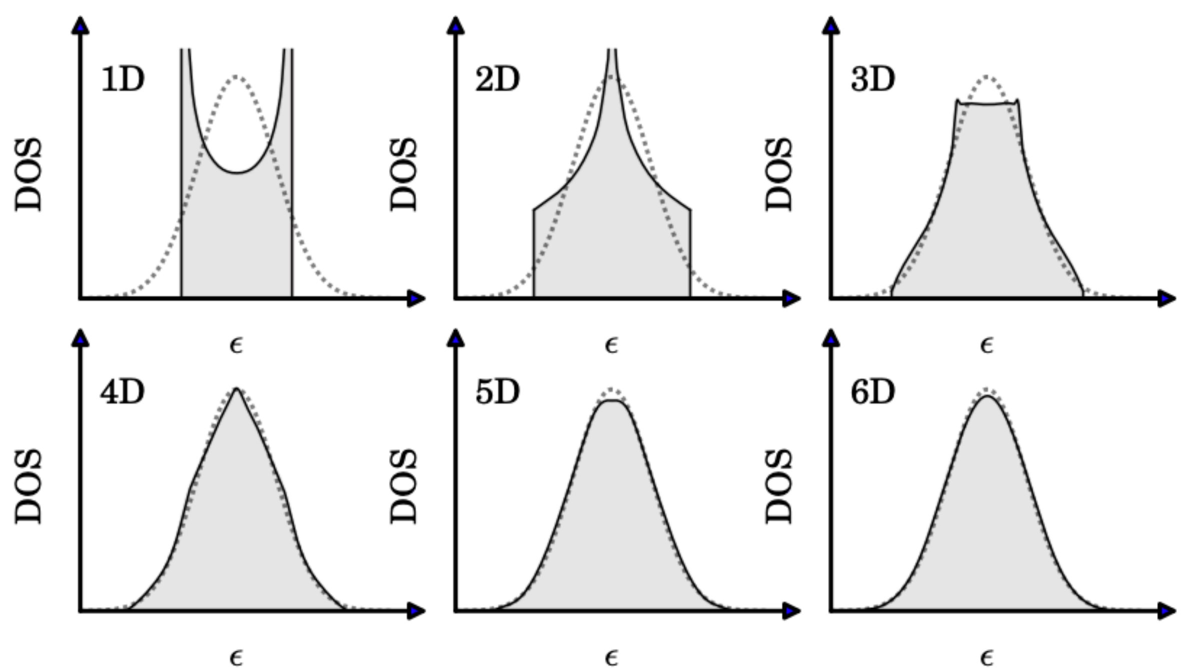


Figure 2.2: Density of states for the square lattice in 1 to 6 dimensions (solid lines and gray shaded areas) compared with the infinite dimensional limit (gray dotted line), inspired by [17].

Define singularity order α:

$$J(\omega) \sim (\omega - \omega_0)^\alpha$$

Our result: clarifying the origin of the T dependence

Huang, Ding, Wang, Kaye, Li, Lin, in preparation, 2026

Define singularity order α:
$J(\omega) \sim (\omega - \omega_0)^\alpha$

- Informal statement of our theorem:
  - If the effective spectral density is continuous ($\alpha > 0$), then $N \sim O(\log^2(1/\varepsilon_1))$
    Independent of T.
  - If the effective spectral density is discontinuous ($\alpha \leq 0$) in ω, then:
    - $N \sim O(\log^2(T/\varepsilon_1))$ for $\alpha < 0$;
    - $N \sim O(\log(T/\varepsilon_1)\log((\log T)/\varepsilon_1))$ for $\alpha = 0$.
- In all cases, independent of β!

- A square-root singularity is **not STRONG enough** to create a T dependence.

Physical implications (1): bosons

Sub-ohmic, ohmic and super-ohmic baths

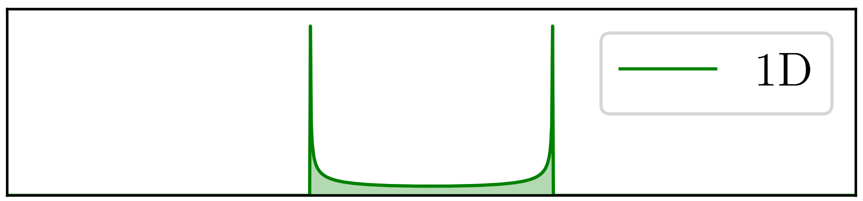
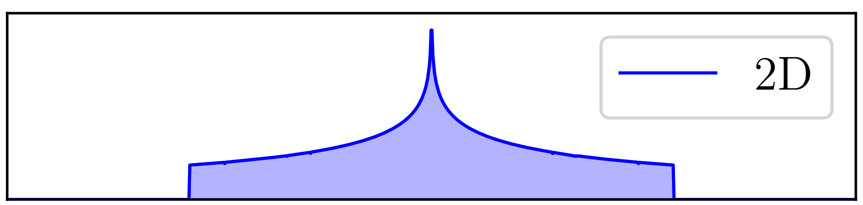
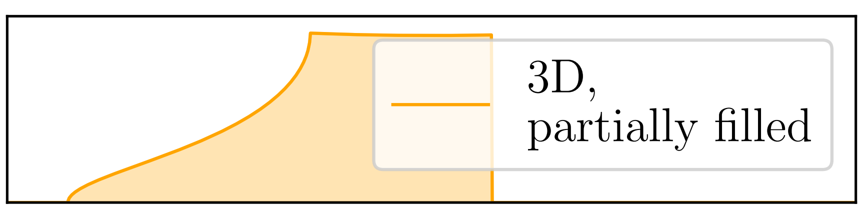
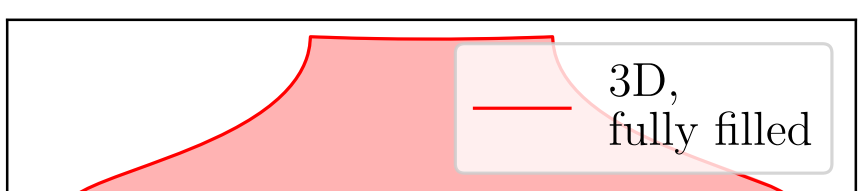
- For bosonic bath, $J(\omega) \sim \omega^\gamma$ near $\omega = 0$. $\gamma > 0$.
- Finite temperature (fixed accuracy):

$0 < \gamma < 1$	$\gamma = 1$	$\gamma > 1$
Sub Ohmic	**Ohmic**	**Super Ohmic**
$N \sim O(\log^2 T)$	$O(\log T \log\log T)$	$N \sim O(1)$

- Zero temperature:
  - $N \sim O(1)$.
- Qualitative differences!

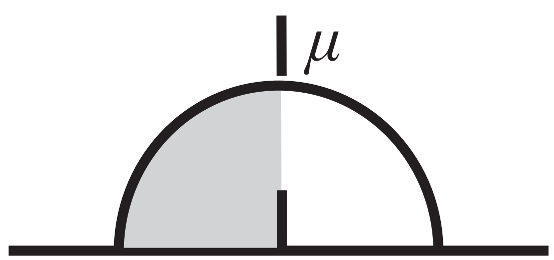
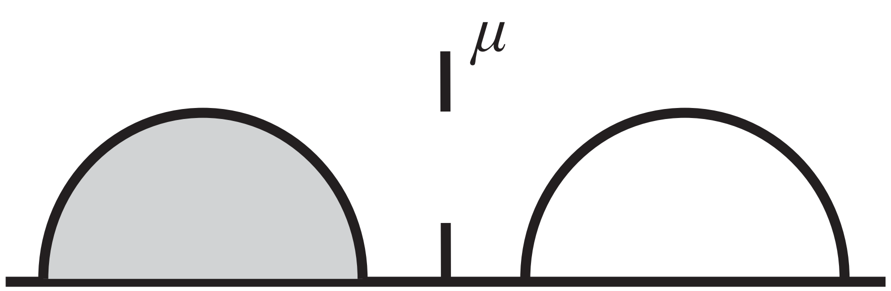
Physical implications (2)

Van Hove singularities

DOS	Singularity	N v.s. T
	Inverse square root $\alpha = -\frac{1}{2}$	$O(\log^2 T)$
	Logarithmic $\alpha = 0$	$O(\log T \cdot \log\log T)$
	Step discontinuity $\alpha = 0$	$O(\log T \cdot \log\log T)$
	Continuous (Non-smooth) $\alpha = \frac{1}{2}$	$O(1)$

Physical implications (3)

Gapped v.s. gapless baths

DOS	Singularity	N v.s. T
	$\alpha = 0$ Step discontinuity	$O(\log T \cdot \log\log T)$
	Continuous (Non-smooth) $\alpha > 0$	$O(1)$

- “When can we stop worrying about bath fitting, and focus on ***real*** physics?” — Informal comment from someone in this room, May 2025.

- For real-time bath fitting, now we know both **how to** (previous works) and **how good it is** (this work).

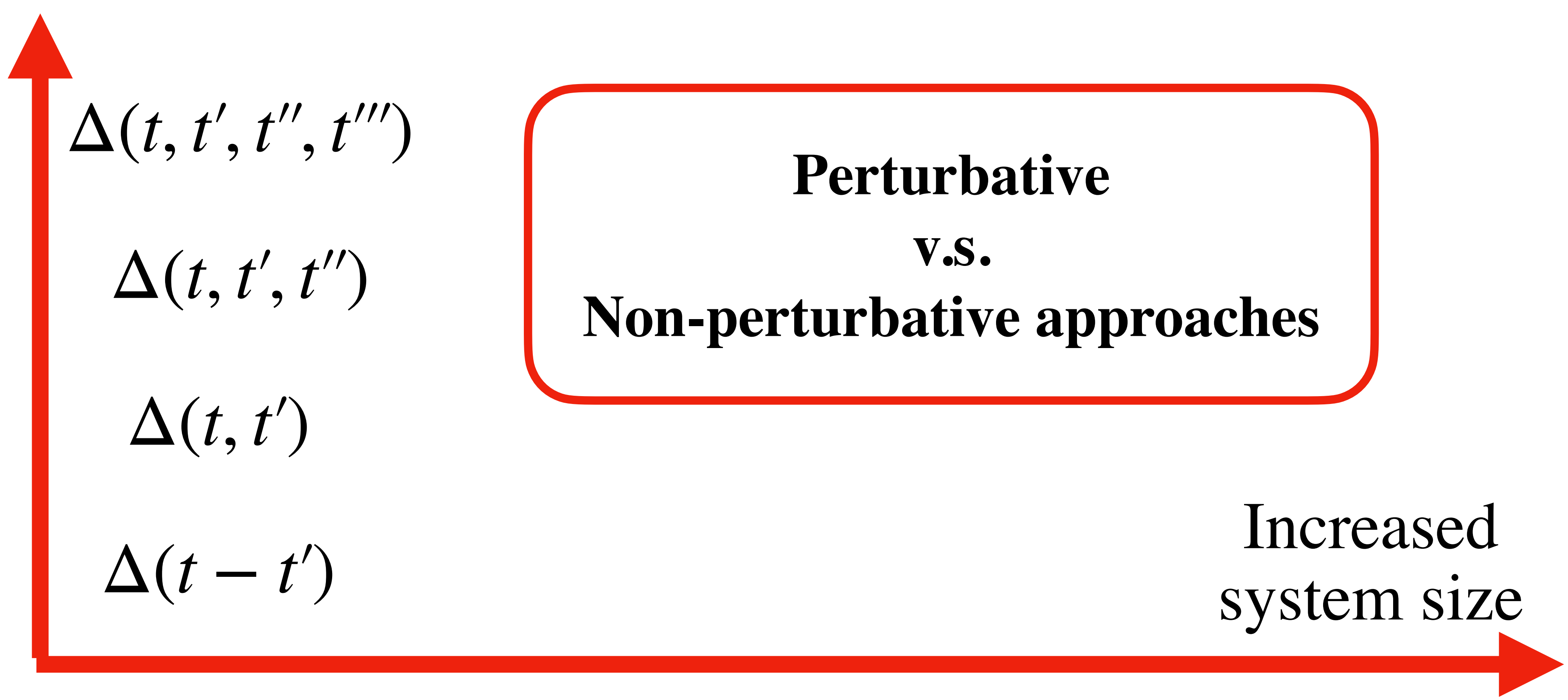
  - Efficiency: quasi-Lindblad.

    Park, **Huang**, Zhu, Yang, Chan, Lin, *Phys. Rev. B* 110, 195148 (2024)

  - Efficiency + physicality guarantee: coupled-Lindblad.

- What’s next?

  Huang, Park, Chan, Lin, *Phys. Rev. Letter* 136, 090403 (2026)



Thank you for your attention!

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