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A Unified theory of Quantum Dissipation in Three Classes of Bath

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Supported by NSF of China & RGC / UGC of Hong Kong S.A.R.

Open Quantum Systems

Unified Theory

Three classes of bath

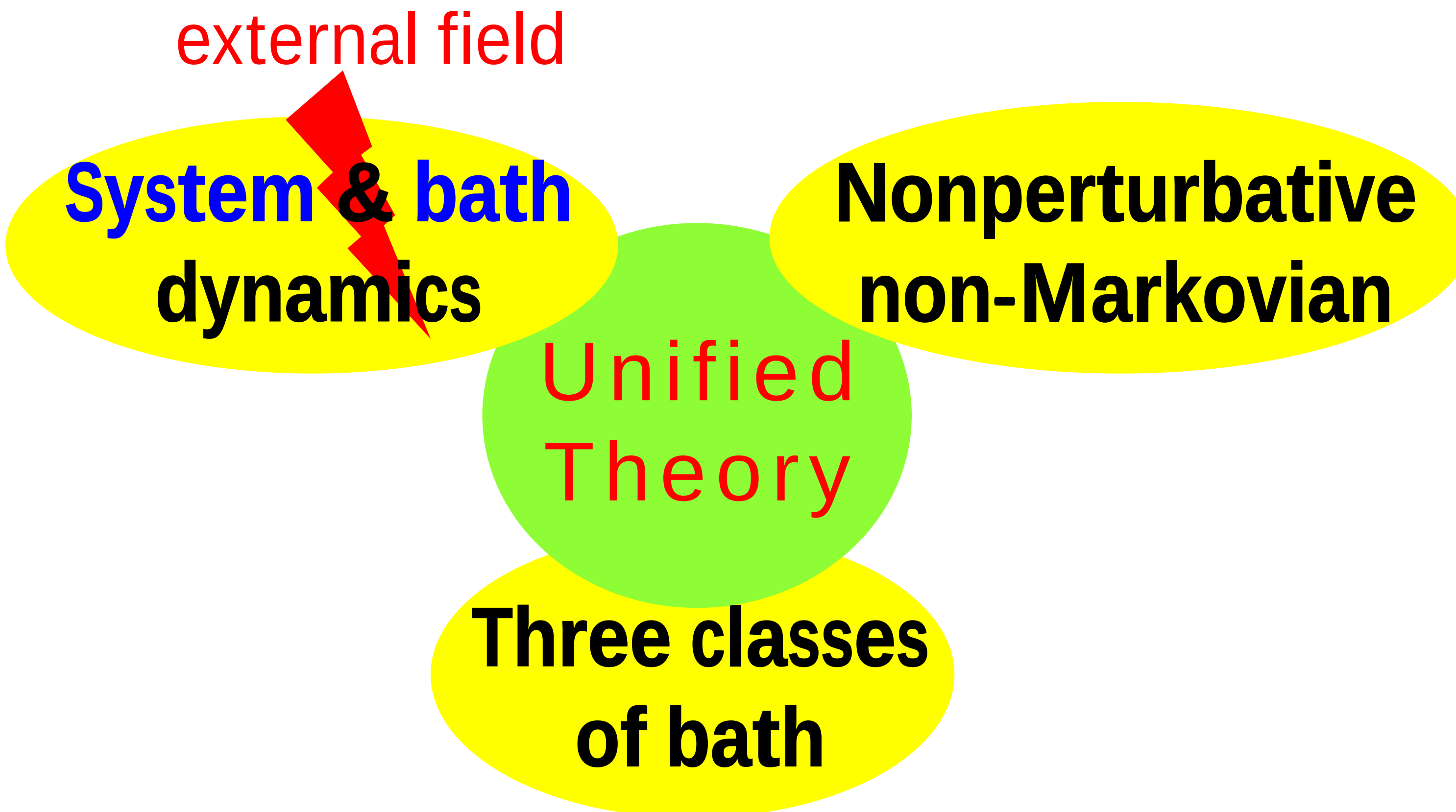
Bosonic (phonons)

Fermionic (electrons)

Excitonic (two-level spins)

Dissipaton Equation of Motion

YJY, JCP, 140, 054105 (2014)



Outline

- **Advancing quantum mechanics of open systems**
- Some benchmark evaluations
- Optimizing the unified formulation
- Concluding remarks

Quantum Mechanics of Open Systems: Basic Concepts

- **Density matrix:** $\rho(t) \equiv |\psi(t)\rangle\langle\psi(t)|$

$$|\psi(t)\rangle = \begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix}, \qquad \rho(t) = \begin{pmatrix} c_1 c_1^* & c_1 c_2^* & \cdots \\ c_2 c_1^* & c_2 c_2^* & \cdots \\ \vdots & \vdots & \vdots \end{pmatrix}$$

Isolated systems

Schrödinger eqn: $$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = (H_{\rm S} + h_{\rm B} + H_{\rm SB})|\psi(t)\rangle$$

Liouville-von Neuman equation:

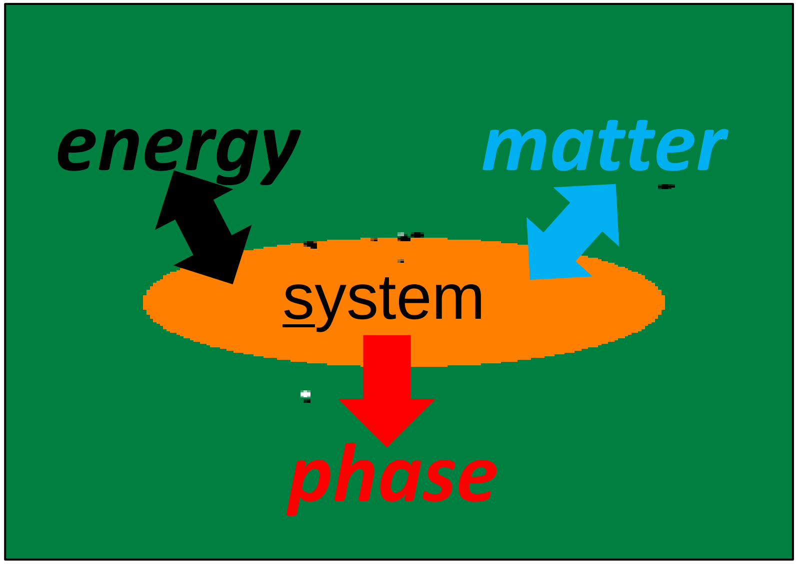
$$i\hbar\dot{\rho}_{\rm T}(t) = [H_{\rm S} + h_{\rm B} + H_{\rm SB}, \rho_{\rm T}(t)]$$

Quantum Mechanics of Open Systems: Basic Concepts

- **Reduced system density operator defined (≡) as**

$$\rho(t) \equiv \mathrm{tr}_{\mathrm{bath}}\, \rho_{\mathrm{Total}}(t)$$

Irreversibility (entropy & free-energy, ...)



Quantum Mechanics of Open Systems: Basic Concepts

- **Reduced system density operator defined** ($\equiv$) **as**

$$\rho(t) \equiv \mathrm{tr}_{\mathrm{bath}}\, \rho_{\mathrm{Total}}(t)$$

How does it evolve in time?

Quantum Mechanics of Open Systems:
Brief History of the Developments

Perturbative / Markovian Theories (phonon bath)

- Brownian motion (Einstein,1905) --

  Fluctuation-dissipation theorem
  (exact, by Callen & Welton, 1951)

- *Quantum master equation* ***(1950s--)***

- *Caldeira-Leggett equation (1983):* $\left(\delta(t), \dot{\delta}(t)\right)$ *-bath*

Quantum Mechanics of Open Systems: Brief History of the Developments

Exact Theories (for Gaussian bath)

➢ **Path integral influence functional formalism**

- **Bosonic (phonon) bath**
  Feynman-Vernon (1963)

- **Fermionic (electron) bath**
  Grassmann-Fermi-quantization (*early 70s*)

Quantum Mechanics of Open Systems: Brief History of the Developments

Exact Theories (for Gaussian bath)

- **Path integral influence functional formalism**

  Harmonic / noninteracting systems

- **Bosonic (phonon) bath**

  BL Hu, JP Paz, and Y Zhang, Phys. Rev. D **45**, 2843 (1992)

- **Fermionic (electron) bath**

  TMY Tu and WM Zhang, PRB 78, 235311 (2008)

Quantum Mechanics of Open Systems: Brief History of the Developments

Exact Theories (for Gaussian bath)

- **Path integral influence functional formalism**

- **HEOM formalism** (path integral based)

  - **Bosonic (phonon) bath**

    Y. Tanimura & R. Kubo (89); Y. Tanimura (90);
    R.X. Xu, ... & YJY (05); R.X. Xu & YJY (07)

  - **Fermionic (electron) bath**

    J.S. Jin, X. Zheng & YJY (08)

Quantum Mechanics of Open Systems: Brief History of the Developments

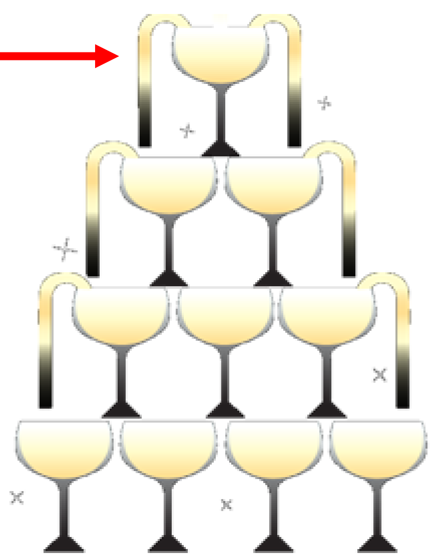
Exact Theories (for Gaussian bath)

- *Path integral influence functional formalism*

- **HEOM formalism** (path integral based)

Reduced **System** Density Operator

***Physical* meanings?**



Tier	
0	
1	master eqn.
2	

Quantum Mechanics of Open Systems: Brief History of the Developments

Exact Theories (for Gaussian bath)

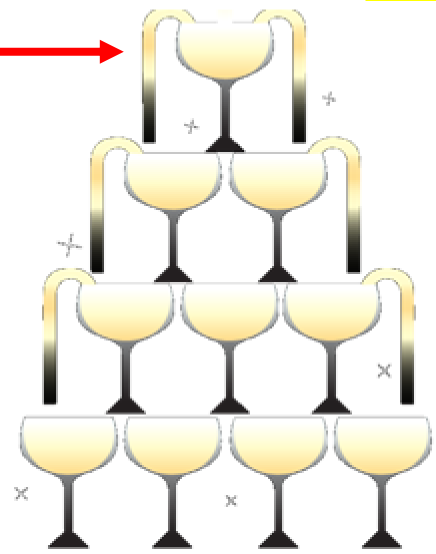
- **DEOM formalism** (quasi-particle algebra based)

YJY, J. Chem. Phys. **140**, 054105 (2014)

Reduced **System**
Density Operator

***Physical* meanings:**

Dissipatons
(bath)



# of dissipatons

0

1 **master eqn.**

2

Quantum Mechanics of Open Systems:
Dissipatons ?

(0) Liouville-von Neumann: $\dot{\rho}_{\rm T}(t) = -i[H_{\rm S} + h_{\rm B} + H_{\rm SB}, \rho_{\rm T}(t)]$

$$H_{\rm SB} = \sum_a \hat{Q}_a^{\rm S} \hat{F}_a^{\rm B}$$

$$\hat{F}_a^{\rm B} = \sum_k c_{ak}(\hat{b}_k^\dagger + \hat{b}_k)$$

$$h_{\rm B} = \sum_k \epsilon_k \hat{b}_k^\dagger \hat{b}_k$$

- ***Bath hybridizing function:***

$$J_{ab}(\omega) \equiv \frac{1}{2}\int_{-\infty}^{\infty} dt\, e^{i\omega t} \langle [\hat{F}_a^{\rm B}(t), \hat{F}_b^{\rm B}(0)]_{\mp} \rangle_{\rm B}$$

$$= \sum_k |c_{ak}|^2 \delta(\omega - \epsilon_k)$$

Quantum Mechanics of Open Systems: Dissipatons ?

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$-$: phonon bath	$+$: electron & exciton bath

(1) Parametrization of $J_{ab}(\omega)$ so that

$$\langle \hat{F}_a^{\rm B}(t)\hat{F}_b^{\rm B}(0)\rangle_{\rm B} = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t} J_{ab}(\omega)}{1 \mp e^{-\beta\omega}} = \sum_k \eta_k^{ab}\, e^{-\gamma_k^{ab} t}$$

Fluctuation-dissipation theorem

Quantum Mechanics of Open Systems:
Dissipatons !

(2) Dissipaton decomposition of hybrid bath operator:

$$\hat{F}_a^{\rm B} = \sum_{b,k} \hat{f}_k^{ab}$$

$$j \equiv \{ab, k\}$$

$$\langle \hat{f}_j(t)\hat{f}_{j'}(0)\rangle_{\rm B} = 0; \quad \text{except for} \quad \langle \hat{f}_k^{ab}(t)\hat{f}_k^{ba}(0)\rangle_{\rm B} = \eta_k^{ab} e^{-\gamma_k^{ab} t}$$

Statistically Independent

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Quantum Mechanics of Open Systems:
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Statistically Independent

(3) Consequently,

$$H_{\mathrm{SB}} = \sum_a \hat{Q}_a \hat{F}^{\mathrm{B}}_a = \sum_{j=1}^{K} \hat{Q}_j \hat{f}_j$$

Quantum Mechanics of Open Systems: Dynamical Variables -- DDOs

(4) **Dissipaton density operators (DDOs)**

$$\rho_{\mathbf{j}}^{(n)}(t) \equiv \rho_{j_1\cdots j_n}^{(n)}(t) \equiv \mathrm{tr}_{\mathrm{B}}\left[\left(\hat{f}_{j_n}\cdots\hat{f}_{j_1}\right)^{\circ}\rho_{\mathrm{T}}(t)\right]$$

Set of n **irreducible** dissipatons

- Fermionic dissipatons: $(\hat{f}_j\hat{f}_{j'})^{\circ} = -(\hat{f}_{j'}\hat{f}_j)^{\circ}$
  (**electron bath**)
- Bosonic dissipatons: $(\hat{f}_j\hat{f}_{j'})^{\circ} = (\hat{f}_{j'}\hat{f}_j)^{\circ}$
  (**phonon bath**)
- Excitonic dissipatons: $(\hat{f}_j\hat{f}_{j'})^{\circ} = (1-\delta_{jj'})(\hat{f}_{j'}\hat{f}_j)^{\circ}$
  (**spin bath**)

Quantum Mechanics of Open Systems: DEOM: Derivation

(4) **Dissipaton density operators (DDOs)**

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Set of n **irreducible** dissipatons

(5) Applying $\dot{\rho}_{\mathrm{T}}(t) = -i[H_{\mathrm{S}} + h_{\mathrm{B}} + H_{\mathrm{SB}}, \rho_{\mathrm{T}}(t)]$ to (4) $\Rightarrow$

$$\dot{\rho}_{\mathbf{j}}^{(n)} = -\Big(i\mathcal{L}_{\mathrm{S}} + \sum_{r=1}^{n}\gamma_{j_r}\Big)\rho_{\mathbf{j}}^{(n)} - i\sum_{j}\mathcal{A}_{\bar{j}}\rho_{\mathbf{j}j}^{(n+1)} - i\sum_{r=1}^{n}\mathcal{C}_{j_r}\rho_{\mathbf{j}_r^-}^{(n-1)}$$

Quantum Mechanics of Open Systems: DEOM: Derivation

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(5) Applying $\dot{\rho}_{\mathrm{T}}(t) = -i[H_{\mathrm{S}} + h_{\mathrm{B}} + H_{\mathrm{SB}}, \rho_{\mathrm{T}}(t)]$ to (4) $\Rightarrow$

$$-i[\hat{f}_j, h_{\mathrm{B}}] = \Big(\frac{\partial}{\partial t}\hat{f}_j\Big)_{\mathrm{B}} = -\gamma_j \hat{f}_j$$

as dissipaton being of single exponential correlation function

$$\dot{\rho}_{\mathbf{j}}^{(n)} = -\Big(i\mathcal{L}_{\mathrm{S}} + \sum_{r=1}^{n}\gamma_{j_r}\Big)\rho_{\mathbf{j}}^{(n)} - i\sum_{j}\mathcal{A}_{\bar{j}}\rho_{\mathbf{j}j}^{(n+1)} - i\sum_{r=1}^{n}\mathcal{C}_{j_r}\rho_{\mathbf{j}_r^-}^{(n-1)}$$

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Set of *n* **irreducible** dissipatons

(5) Applying $\dot{\rho}_{\mathrm{T}}(t) = -i[H_{\mathrm{S}} + h_{\mathrm{B}} + H_{\mathrm{SB}}, \rho_{\mathrm{T}}(t)]$ to (4) $\Rightarrow$

Wick's Theorem:

$$\mathrm{tr}_{\mathrm{B}}\Big[\big(\hat{f}_{j_n}\cdots\hat{f}_{j_1}\big)^{\circ}\hat{f}_j\rho_{\mathrm{T}}(t)\Big]^{>} = \rho_{j\mathbf{j}}^{(n+1)} + \sum_{r=1}^{n}\langle\hat{f}_{j_r}\hat{f}_j\rangle_{\mathrm{B}}^{>}\rho_{\mathbf{j}_r^-}^{(n-1)}$$

$$\dot{\rho}_{\mathbf{j}}^{(n)} = -\Big(i\mathcal{L}_{\mathrm{S}} + \sum_{r=1}^{n}\gamma_{j_r}\Big)\rho_{\mathbf{j}}^{(n)} - i\sum_{j}\mathcal{A}_{\bar{j}}\rho_{\mathbf{j}j}^{(n+1)} - i\sum_{r=1}^{n}\mathcal{C}_{j_r}\rho_{\mathbf{j}_r^-}^{(n-1)}$$

Quantum Mechanics of Open Systems: DEOM: Derivation

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Quantum Mechanics of Open Systems: DEOM: Derivation

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η_{j_r}

$$\dot{\rho}_{\mathbf{j}}^{(n)} = -\left(i\mathcal{L}_{\mathrm{S}} + \sum_{r=1}^{n}\gamma_{j_r}\right)\rho_{\mathbf{j}}^{(n)} - i\sum_j \mathcal{A}_{\bar{j}}\rho_{\mathbf{j}j}^{(n+1)} - i\sum_{r=1}^{n}\mathcal{C}_{j_r}\rho_{\mathbf{j}_r^-}^{(n-1)}$$

Quantum Mechanics of Open Systems: DEOM

➢ Hybrid system and bath dynamics

$$\rho_{\mathbf{j}}^{(n)}(t) \equiv \rho_{j_1\cdots j_n}^{(n)}(t) \equiv \mathrm{tr}_{\mathrm{B}}\Big[\big(\hat{f}_{j_n}\cdots\hat{f}_{j_1}\big)^{\circ}\rho_{\mathrm{T}}(t)\Big]$$

Set of n **irreducible** dissipatons

$\rho^{(n=0)}(t)$: *reduced system dynamics*

$$H_{\mathrm{SB}} = \sum_a \hat{Q}_a \hat{F}_a^{\mathrm{B}} = \sum_{j=1}^{K} \hat{Q}_j \hat{f}_j$$

$$\dot{\rho}_{\mathbf{j}}^{(n)} = -\Big(i\mathcal{L}_{\mathrm{S}} + \sum_{r=1}^{n}\gamma_{j_r}\Big)\rho_{\mathbf{j}}^{(n)} - i\sum_j \mathcal{A}_{\bar{j}}\rho_{\mathbf{j}j}^{(n+1)} - i\sum_{r=1}^{n}\mathcal{C}_{j_r}\rho_{\mathbf{j}_r^-}^{(n-1)}$$

Quantum Mechanics of Open Systems: DEOM

- **Hybrid system and bath dynamics**

$$\rho_{\mathbf{j}}^{(n)}(t) \equiv \rho_{j_1\cdots j_n}^{(n)}(t) \equiv \mathrm{tr}_{\mathrm{B}}\Big[\big(\hat{f}_{j_n}\cdots\hat{f}_{j_1}\big)^{\circ}\rho_{\mathrm{T}}(t)\Big]$$

Set of n **irreducible** dissipatons

- **Unified theory for three classes of bath**

- **Linearity (DEOM-space) -- User friendly**

$$\dot{\rho}_{\mathbf{j}}^{(n)} = -\Big(i\mathcal{L}_{\mathrm{S}} + \sum_{r=1}^{n}\gamma_{j_r}\Big)\rho_{\mathbf{j}}^{(n)} - i\sum_{j}\mathcal{A}_{\bar{j}}\rho_{\mathbf{j}j}^{(n+1)} - i\sum_{r=1}^{n}\mathcal{C}_{j_r}\rho_{\mathbf{j}_r^-}^{(n-1)}$$

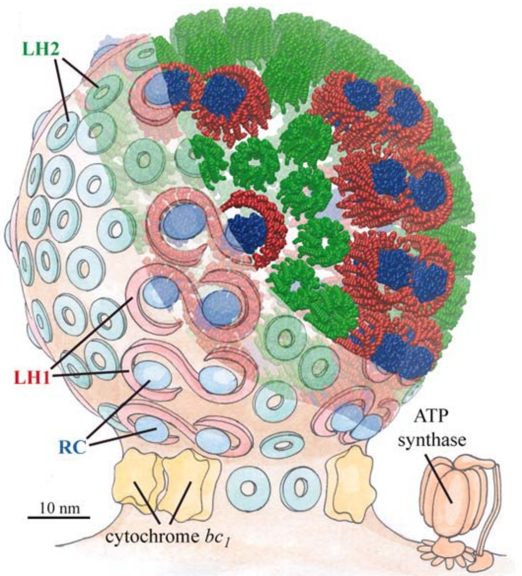
Outline

- Advancing quantum mechanics of open systems
- **Some benchmark evaluations**
- Optimizing the unified formulation
- Concluding remarks

system
bath

Open Quantum *Systems*

Nonlinear Response Functions



Excitation Energy Transfer

2D Spectroscopy

Bath: Bosonic (phonons)

Nonlinear Response Functions

Schrodinger Pictures

$$R^{(3)}(t_3, t_2, t_1) = i^3 \mathrm{Tr}[\boldsymbol{\mu}\hat{\mathcal{G}}(t_3)\mathcal{D}\hat{\mathcal{G}}(t_2)\mathcal{D}\mathcal{G}(t_1)\mathcal{D}\boldsymbol{\rho}(-\infty)]$$

2D Spectroscopy

Bath: Bosonic (phonons)

DEOM-based Evaluations

Nonlinear Response Functions

Mixed Heisenberg-Schrodinger Pictures

$$R^{(3)}(t_3, t_2, t_1) = i^3 \mathrm{Tr}[\boldsymbol{\mu}\hat{\mathcal{G}}(t_3)\mathcal{D}\hat{\mathcal{G}}(t_2)\mathcal{D}\mathcal{G}(t_1)\mathcal{D}\boldsymbol{\rho}(-\infty)]$$

detection ω_3 **excitation ω_1**

Excitation Energy Transfer

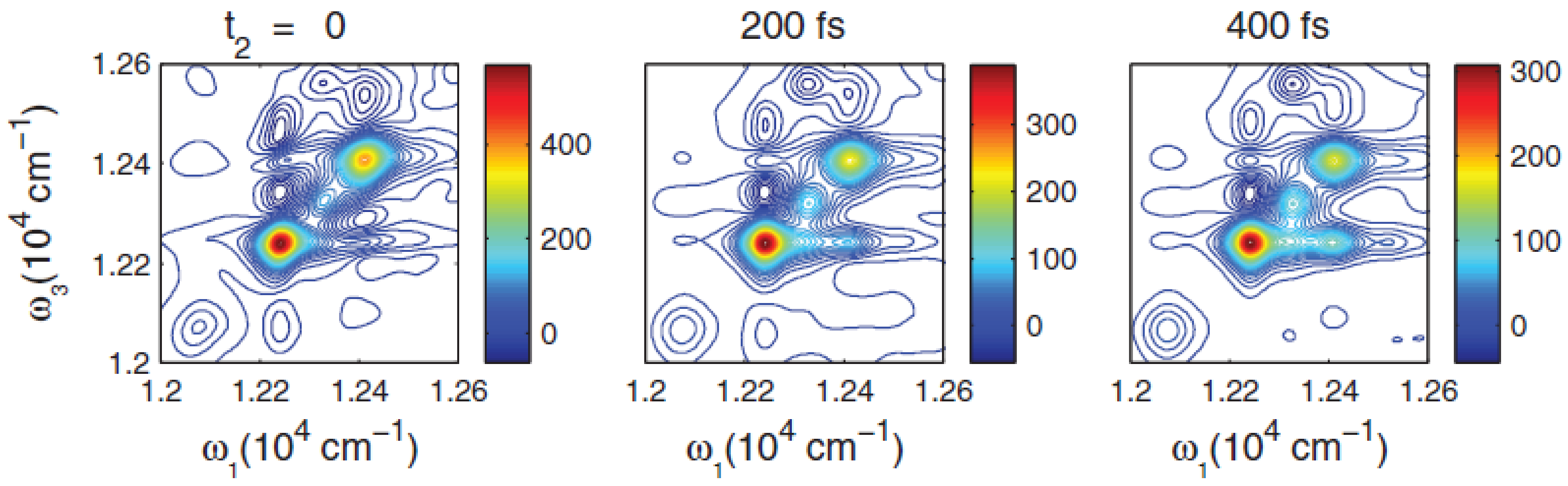
2D Spectroscopy

Bath: Bosonic (phonons)

Two-dimensional exciton spectroscopy of a biological light-harvesting (FMO) model system

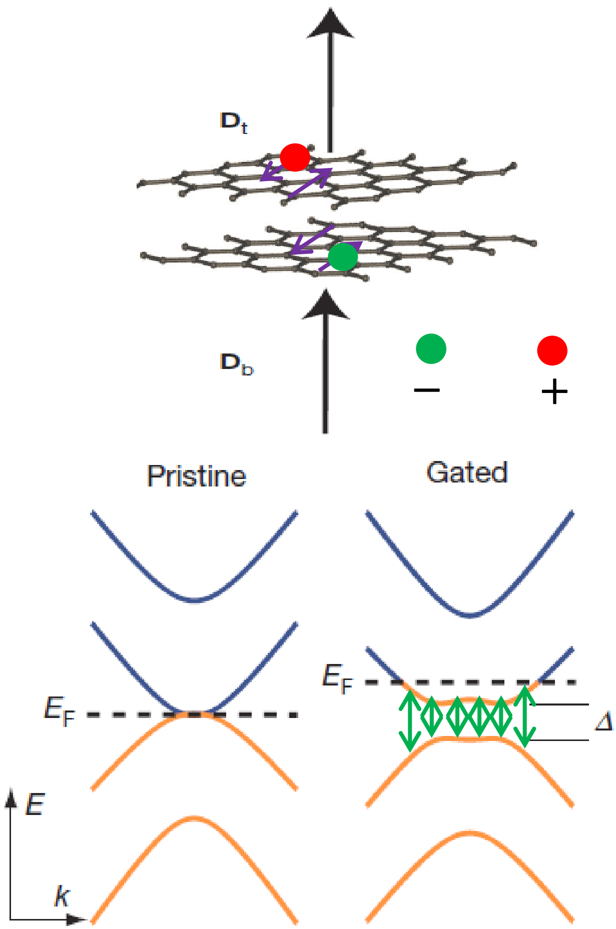
(1+7+21 = 29 system levels, converged with K = 14 and L = 4)

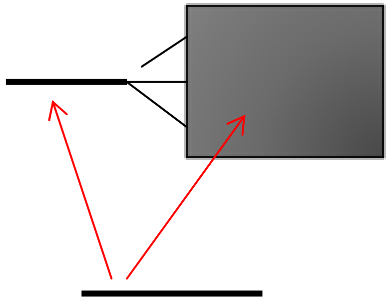
(single CPU: ~30 mins per frame)



J Xu, HD Zhang, RX Ru, YYJ, *J. Chem. Phys.* (2013) **138**:024106

Fano Interference in Double-Layer Graphene



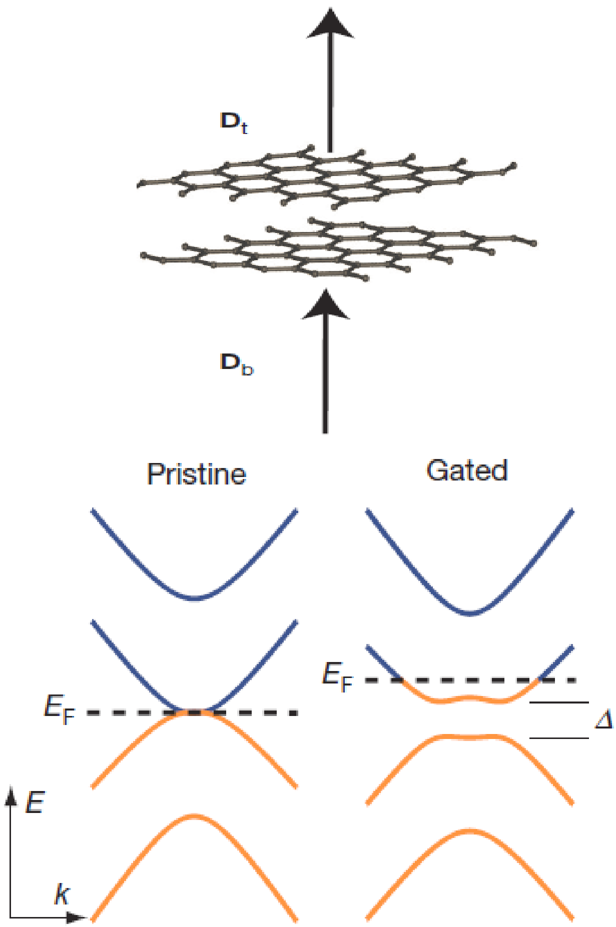


- System: Bi-layer lattice phonon (optically active, **discrete**)
- Bath: **Continuum excitonic** band-edge states that are also **optically active**

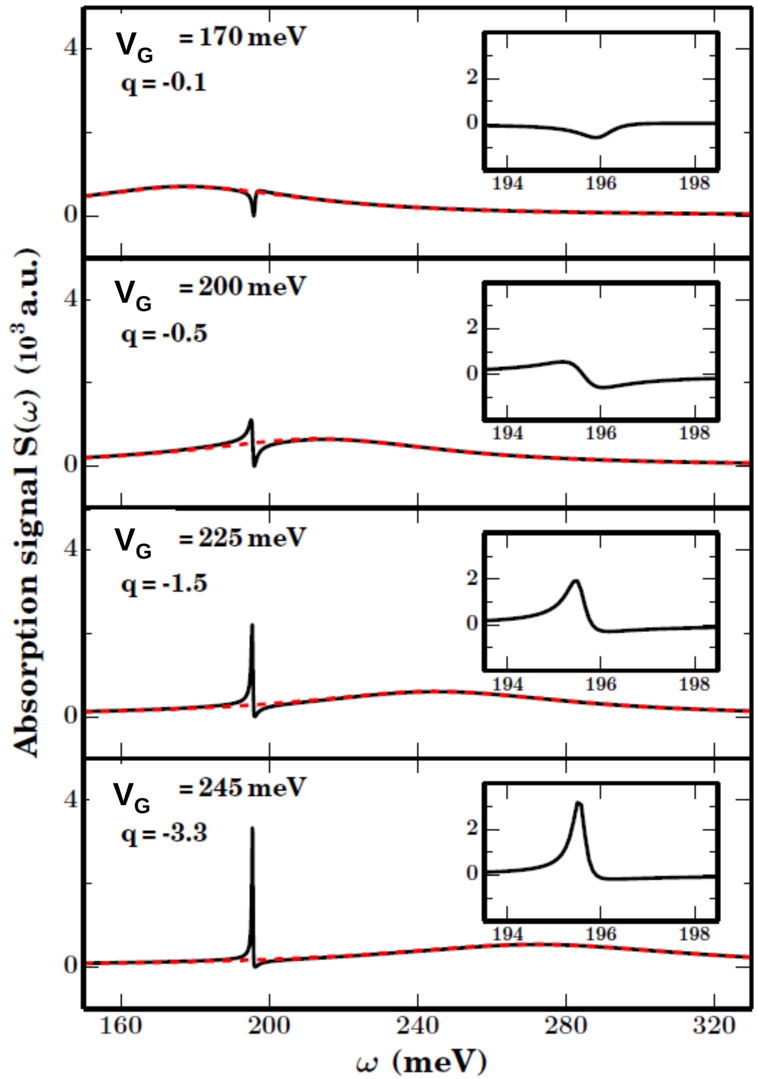
YB Zhang, et al, Nature (2009)

DEOM-based Evaluations

Fano Interference in Double-Layer Graphene



YB Zhang, et al, Nature (2009)

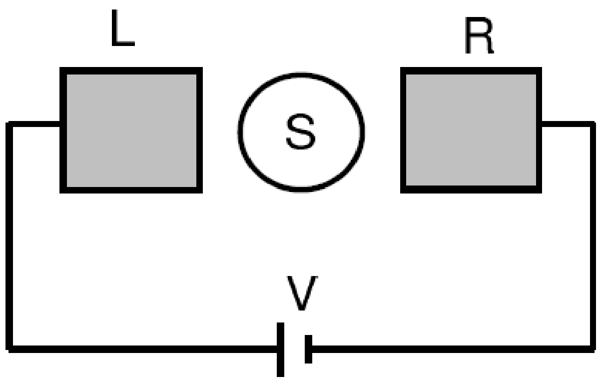


Fano turnover

(in preparation)

system
bath

Open Quantum *Systems*



- **Current $I(t)$**
- $\langle I(t)\, I(0) \rangle_{neq}$
- **Full counting statistics**

- **Kondo Physics (low T < T_K)**

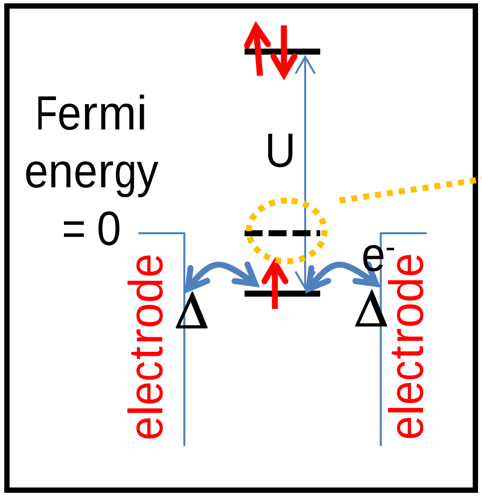
Strongly Correlated Systems

Bath: Fermionic (electrons)

DEOM-based Evaluations on SIAM

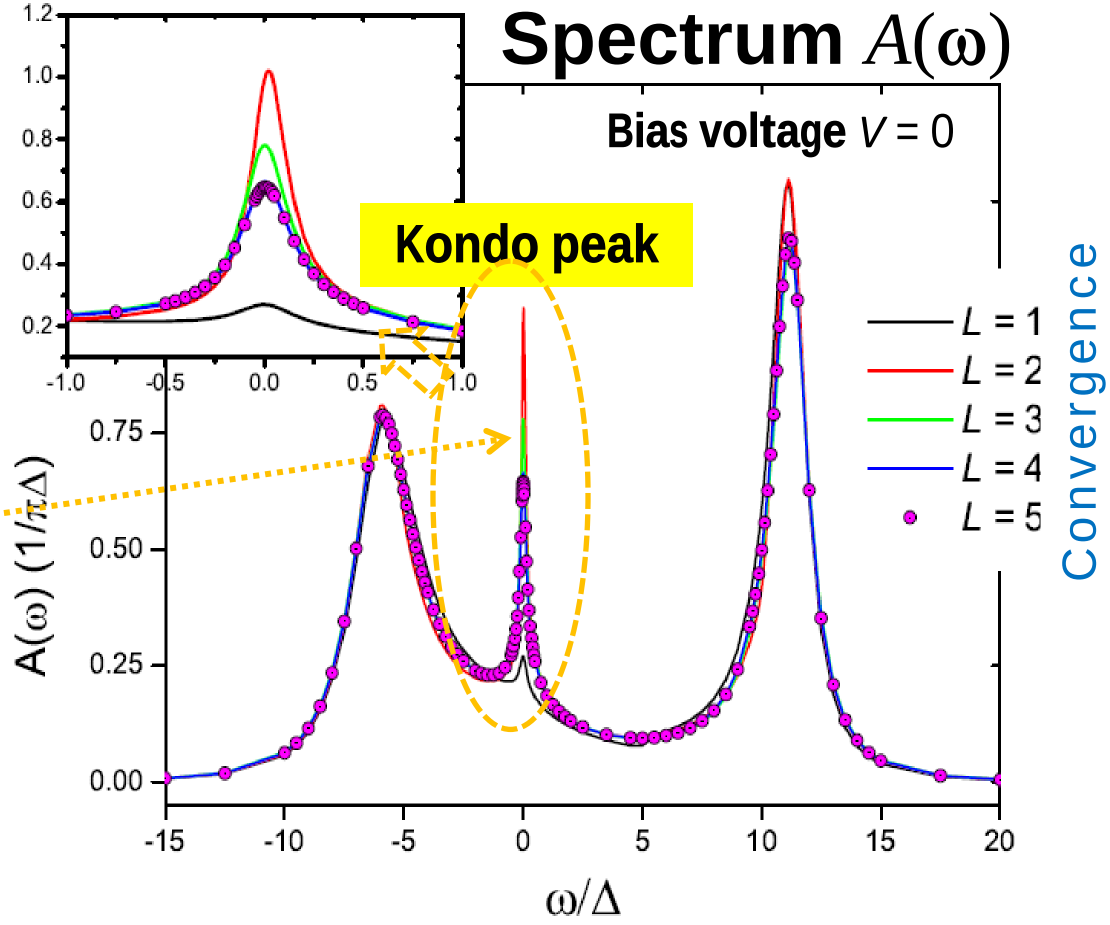
A standard model for strongly correlated electronic systems:

Single Impurity Anderson Model



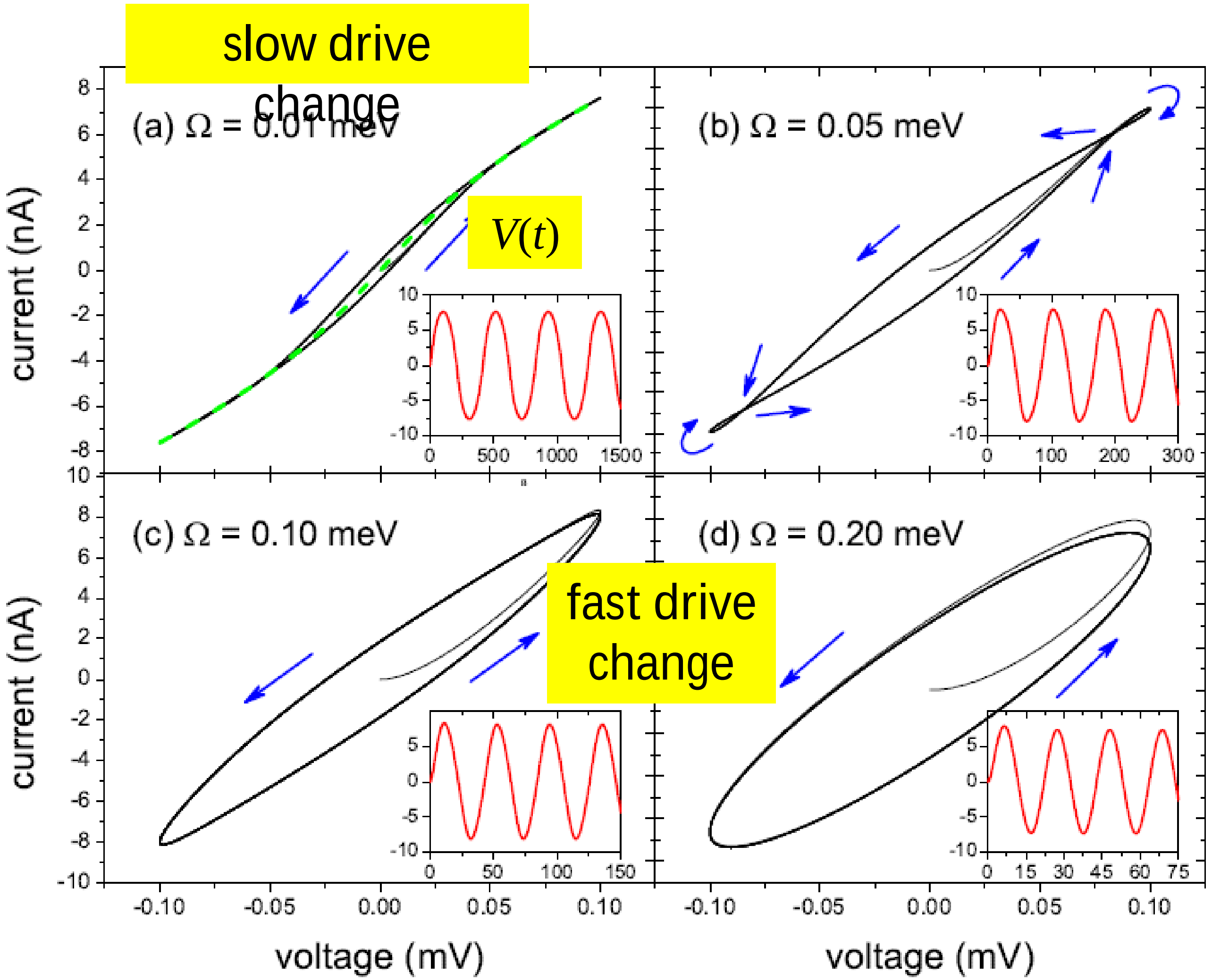
Δ: s-b coupling

U: Coulomb energy



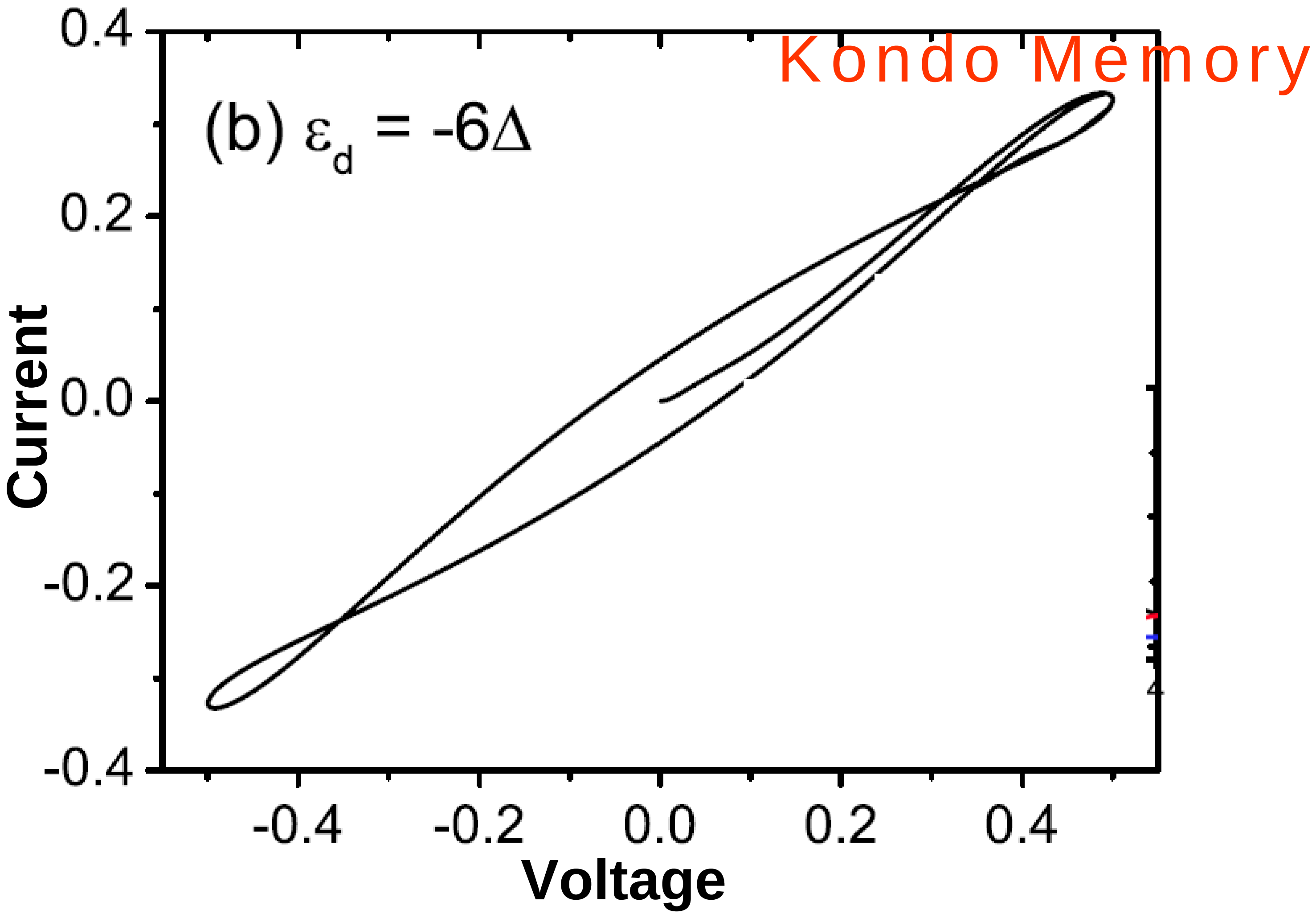
Kondo peak appears only when $U \neq 0$ and $T < T_K$ (Kondo temperature), with nonperturbative evaluation

Hysteresis Effect in
Single Impurity Anderson Model



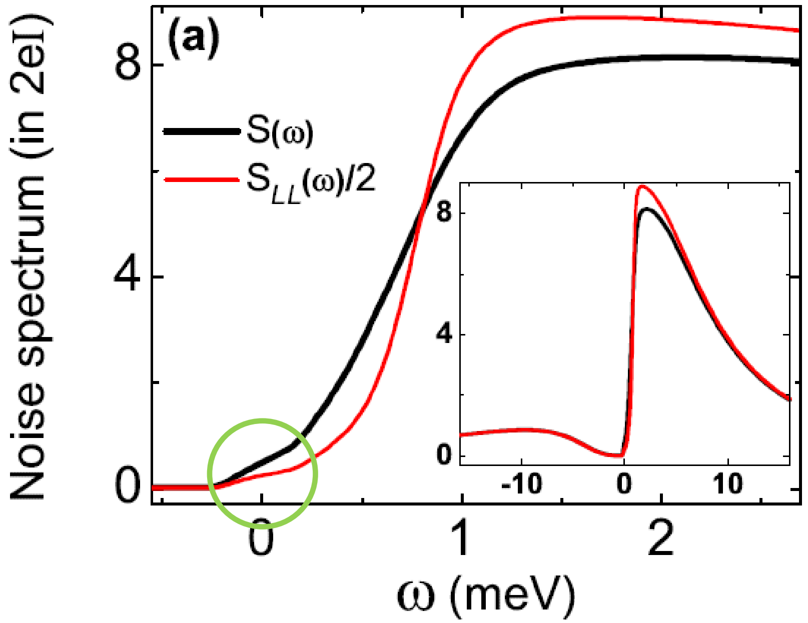
X Zheng, YJY, M. D. Ventra, *Phys. Rev. Lett.* (2013) **111**:086601

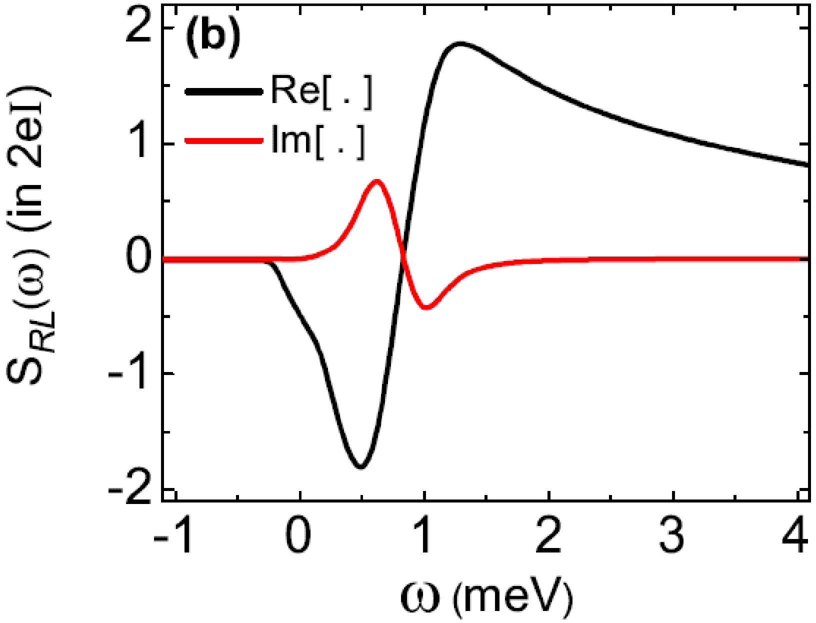
Hysteresis Effect in Single Impurity Anderson Model



X Zheng, YJY, M. D. Ventra, *Phys. Rev. Lett.* (2013) **111**:086601

Nonequilibrium
Current Noise Spectrum of SIAM





(To be published)

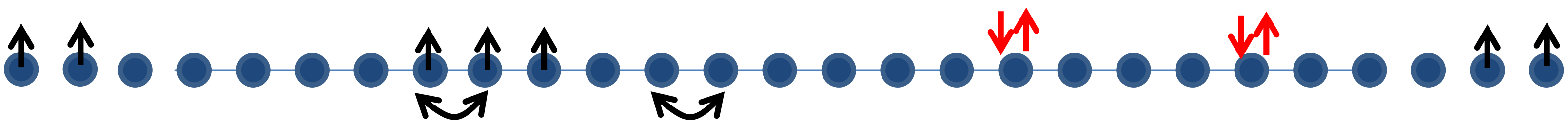
Strongly Correlated Systems

"The term *strong correlation* refers to behavior of electrons in solids that is not well-described (often not even in a qualitatively correct manner) by simple one-electron theories such as the Local Density Approximation (LDA) of density functional theory or Hartree-Fock theory" -- Wikipedia

Also for phonons and excitons

Strongly Correlated Systems

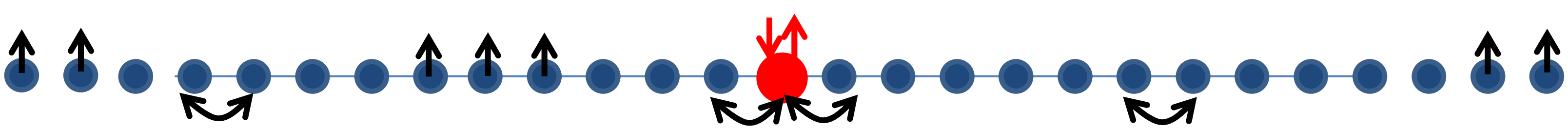
Hubbard Model (1963)



tight-binding (t) + **Coulomb** (U)

Dynamical Mean-Field Theory **(1992)**

Impurity Anderson Model (1961)

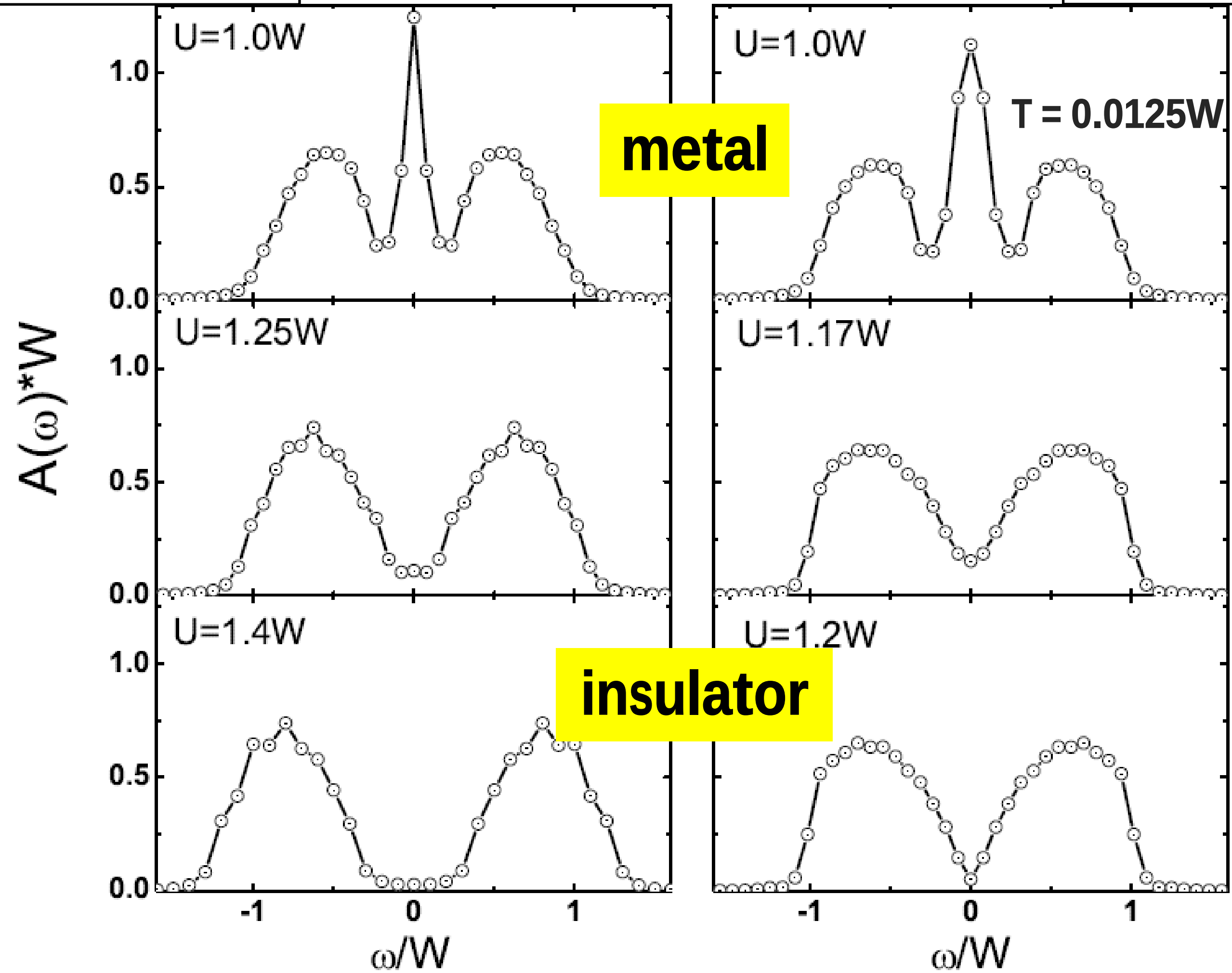


tight-binding (t) + **Coulomb** (U)

Mott Transition: DEOM+DMFT

$A_0^{\mathrm{h}}(\epsilon) = \frac{1}{\tilde{t}\sqrt{2\pi}} \exp(-\frac{\epsilon^2}{2\tilde{t}^2})$ **hypercubic**

Bethe $A_0^{\mathrm{B}}(\epsilon) = \frac{1}{2\pi\tilde{t}^2}\sqrt{4\tilde{t}^2 - \epsilon^2}$



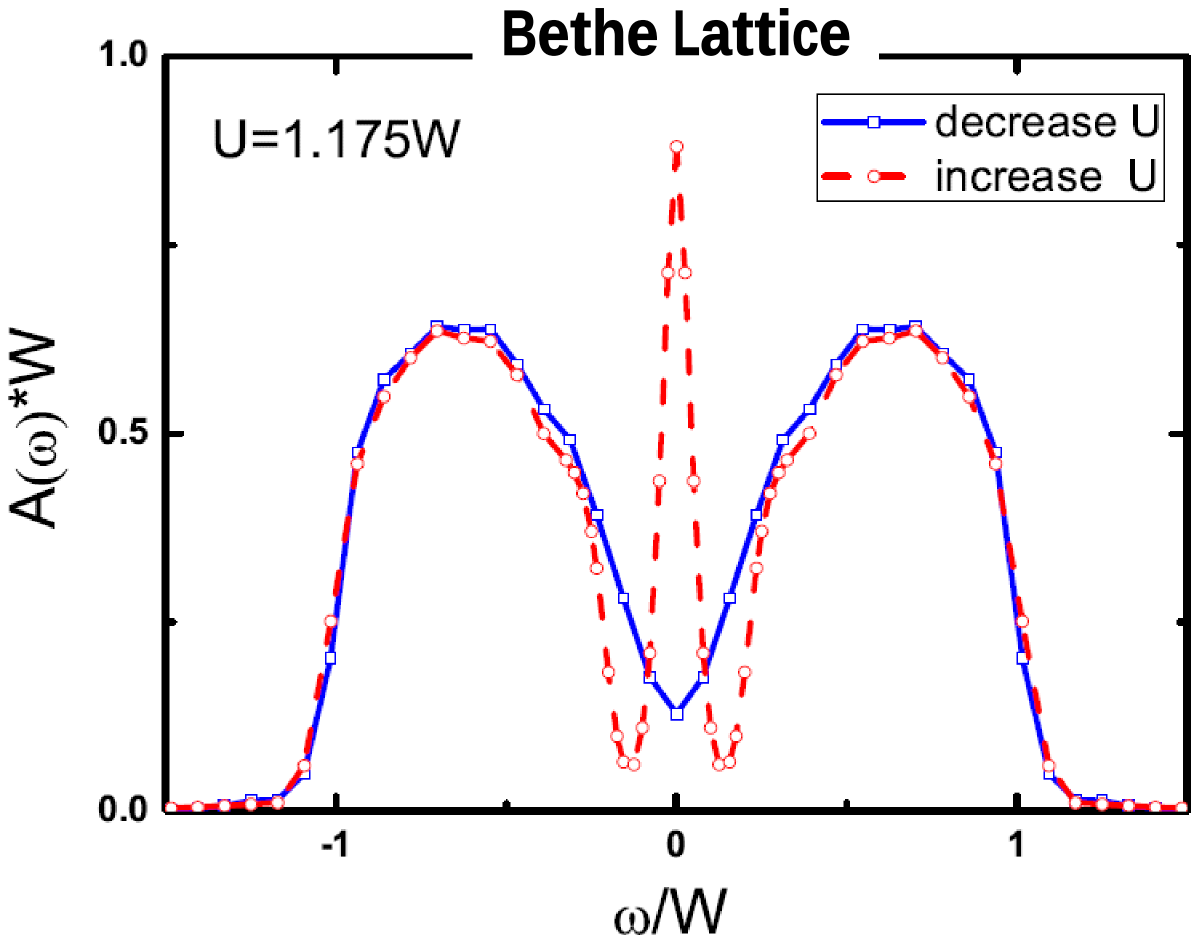
$T_C = 0.02W$

Bank width:
W=4*t*
(half-fill)

(submitted)

Mott Transition: DEOM+DMFT

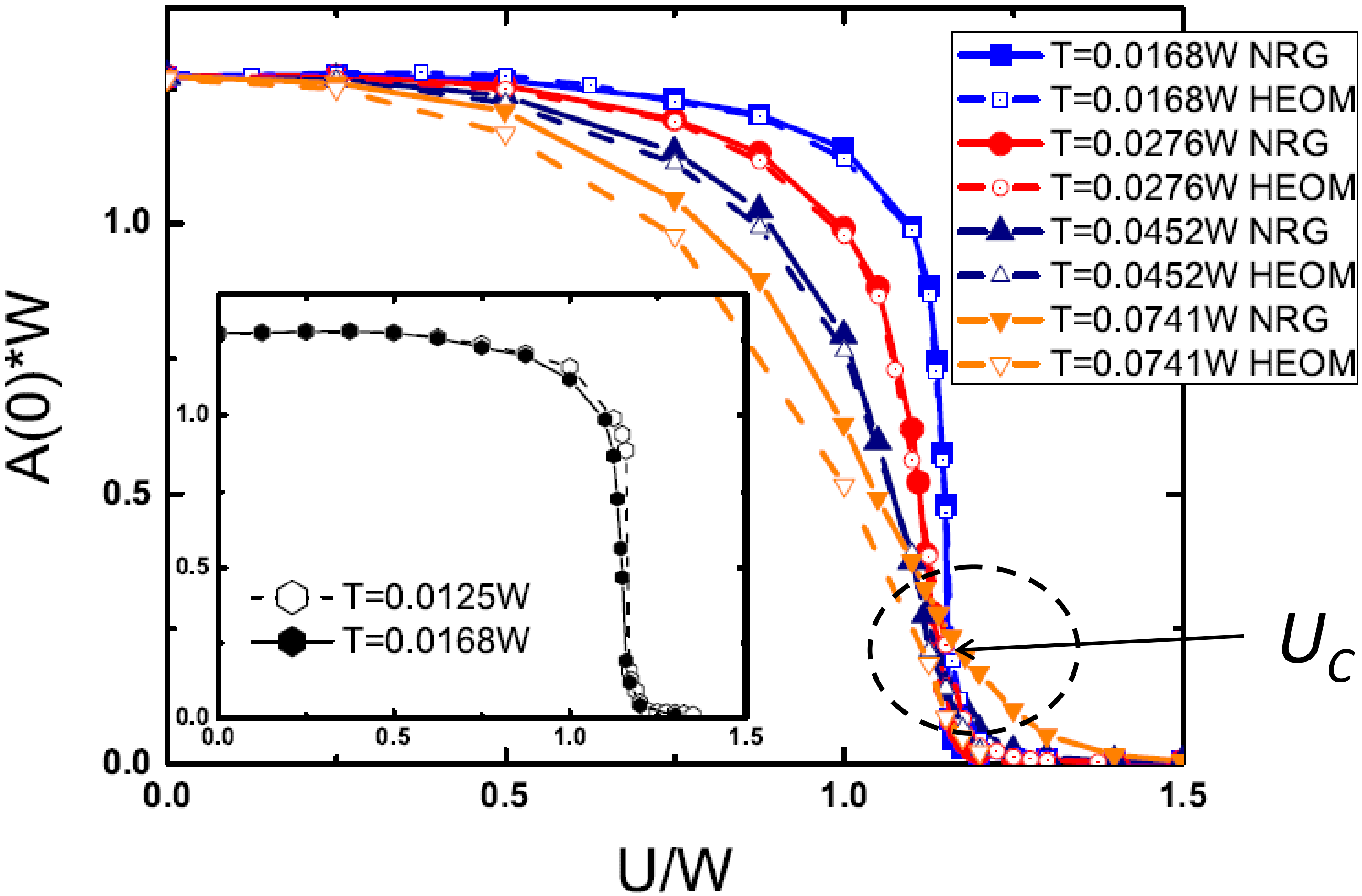
Bi-stability at certain $T<T_C$



(submitted)

Mott Transition: DEOM+DMFT

(*vs.* NRG)



(submitted)

Outline

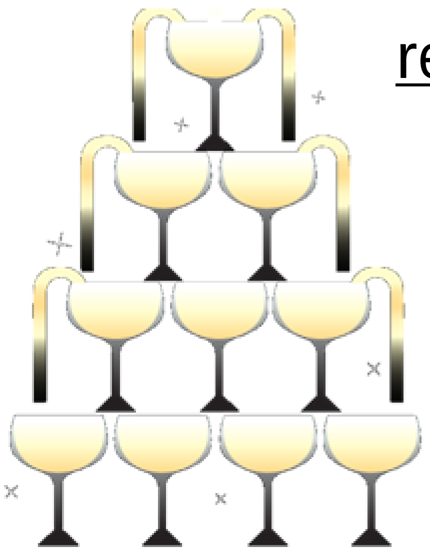
- Advancing quantum mechanics for open systems
- Examples of DEOM-based evaluations
- Optimizing the unified formulation
- Concluding remarks

DEOM

" **Full** (bath) **Configuration Interaction** "

- DEOM expression completely dictated with

$$\langle \hat{F}^{+}_{\alpha\mu}(t)\hat{F}^{-}_{\alpha\nu}(0)\rangle_{\rm B} = \int_{-\infty}^{\infty} d\omega\, \frac{e^{i\omega t} J_{\alpha\mu\nu}(\omega)}{1+e^{\beta(\omega-\mu_\alpha)}} \simeq \sum_k \eta_{\alpha\mu\nu k} \exp(-\gamma_{\alpha\mu\nu k}\, t)$$



reduced system Density Operator (DO)

***K* number of single-dissipaton DOs**

***L*-dissipaton effect**

***Total # of* DOs: combinatory law on (*K*, *L*)**

Minimizing the # of DOs

Optimizing the Formulations

Minimizing the # of DOs

- Minimizing value of ***K*** (# of distinct exponents)

$$\langle \hat{F}^{+}_{\alpha\mu}(t)\hat{F}^{-}_{\alpha\nu}(0)\rangle_{\mathrm{B}} = \int_{-\infty}^{\infty} d\omega \frac{e^{i\omega t} J_{\alpha\mu\nu}(\omega)}{1+e^{\beta(\omega-\mu_\alpha)}} \simeq \sum_k \eta_{\alpha\mu\nu k} \exp(-\gamma_{\alpha\mu\nu k}\, t)$$

Sum-over-poles (SOP)

Fermi function:

$$\frac{1}{1+e^x} = \frac{1}{2} - \frac{1}{2}\frac{\sinh(x/2)}{\cosh(x/2)} \equiv \frac{1}{2} - x\Phi(x^2)$$

poles *in math*.

Matsubara:

$$\Phi(x^2) \approx \sum_{k=1}^{N} \frac{2\eta_k}{x^2+\zeta_k^2}$$

with $\eta_k = 1$, $\zeta_k = (2k+1)\pi$

- Minimizing *effect* ***L*$_{\mathbf{eff}}$** value

Minimizing the # of DOs

- Minimizing value of ***K*** (# of distinct exponents)

$$\langle \hat{F}^{+}_{\alpha\mu}(t)\hat{F}^{-}_{\alpha\nu}(0)\rangle_{\mathrm{B}} = \int_{-\infty}^{\infty} d\omega \frac{e^{i\omega t} J_{\alpha\mu\nu}(\omega)}{1+e^{\beta(\omega-\mu_\alpha)}} \simeq \sum_k \eta_{\alpha\mu\nu k} \exp(-\gamma_{\alpha\mu\nu k}\, t)$$

Sum-over-poles (SOP)

Fermi function:

$$\frac{1}{1+e^x} = \frac{1}{2} - \frac{1}{2}\frac{\sinh(x/2)}{\cosh(x/2)} \equiv \frac{1}{2} - x\Phi(x^2)$$

Matsubara:

$$\Phi(x^2) \approx \sum_{k=1}^{N} \frac{2\eta_k}{x^2+\zeta_k^2} \equiv \frac{P_M(x^2)}{Q_N(x^2)}$$

$y = x^2$

$$\frac{p_0 + p_1 y + \cdots + p_M y^M}{1 + q_1 y + \cdots + q_M y^N}$$

Minimizing the # of DOs

- Minimizing value of ***K*** (# of distinct exponents)

$$\langle \hat{F}^{+}_{\alpha\mu}(t)\hat{F}^{-}_{\alpha\nu}(0)\rangle_{\mathrm{B}} = \int_{-\infty}^{\infty} d\omega \frac{e^{i\omega t} J_{\alpha\mu\nu}(\omega)}{1+e^{\beta(\omega-\mu_\alpha)}} \simeq \sum_k \eta_{\alpha\mu\nu k} \exp(-\gamma_{\alpha\mu\nu k}\, t)$$

Sum-over-poles (SOP)

Fermi function:

$$\frac{1}{1+e^x} = \frac{1}{2} - \frac{1}{2}\frac{\sinh(x/2)}{\cosh(x/2)} \approx \frac{1}{2} - x\frac{P_M(x^2)}{Q_N(x^2)}$$

[M/N] Padé the best

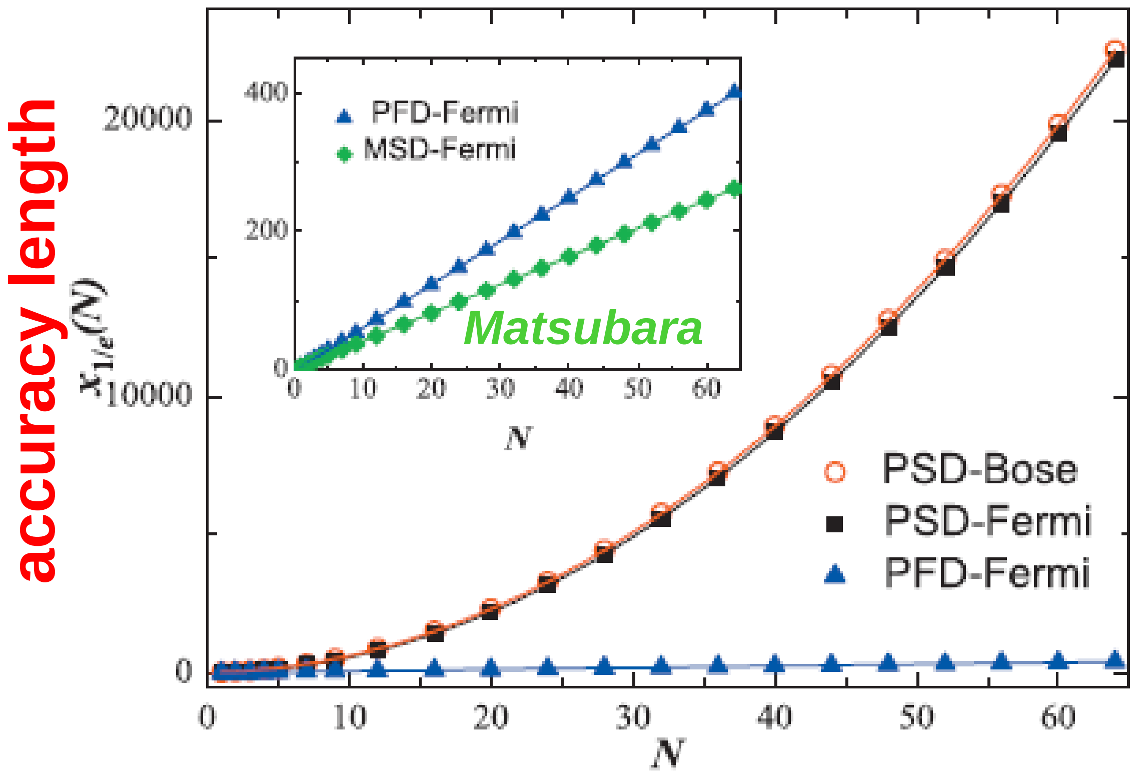
M = ***N*–1**, ***N***, and ***N*+1**

Padé Spectrum Decomposition (PSD) for high precision pole-coefficient evaluation

JCP **133**:101106 (2010); **134**:244106 (2011)

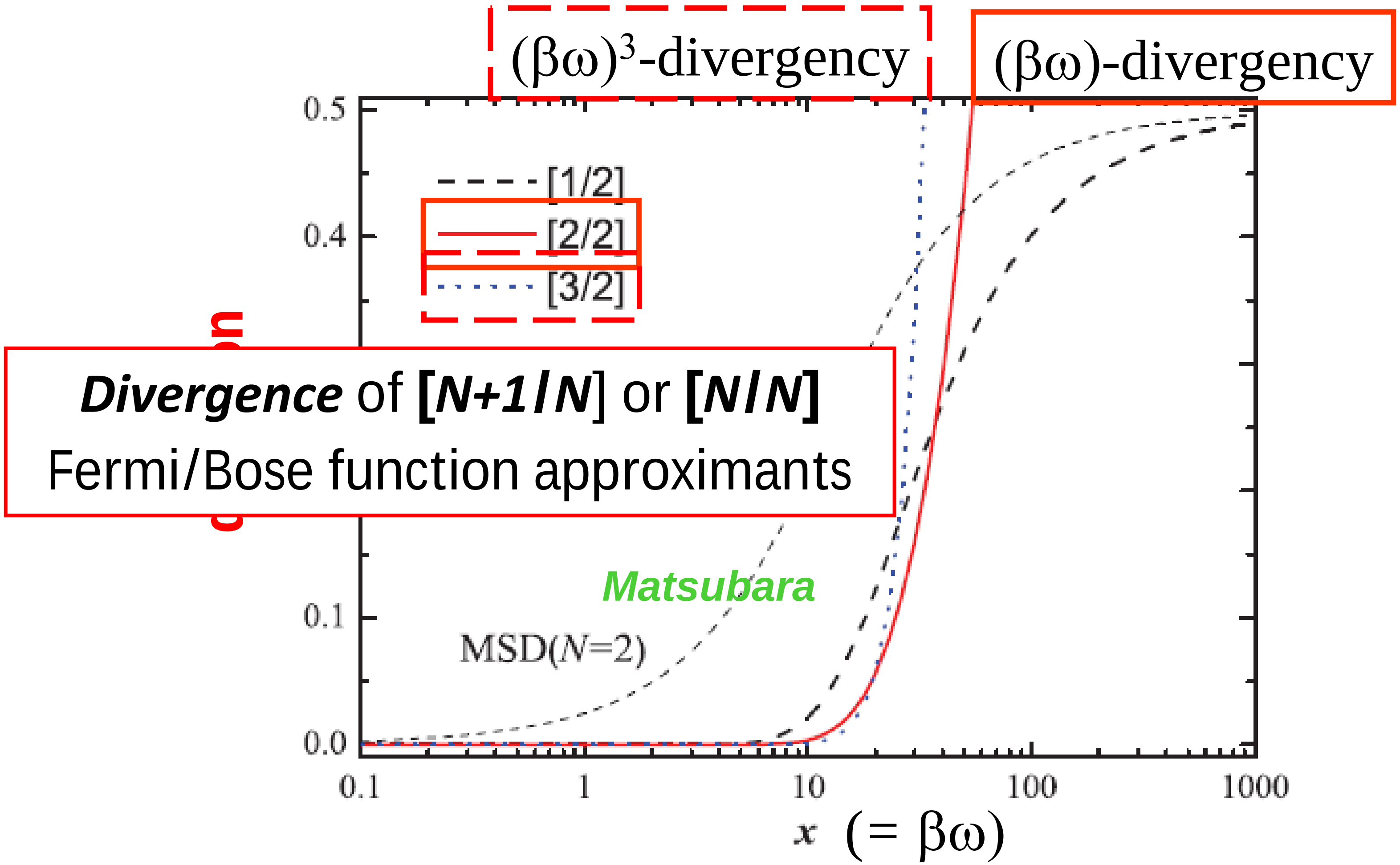
Accuracy length analysis

$(x = \beta\omega)$



JCP **133**:101106 (2010)

Quality of [*M*/*N*]-PSD Approximants



JCP **134**:244106 (2011)

Minimizing the # of DOs

➢ Minimizing value of ***K*** (**# of distinct exponents**)

$$\langle \hat{F}^{+}_{\alpha\mu}(t)\hat{F}^{-}_{\alpha\nu}(0)\rangle_{\rm B} = \int_{-\infty}^{\infty} d\omega\, \frac{e^{i\omega t} J_{\alpha\mu\nu}(\omega)}{1+e^{\beta(\omega-\mu_\alpha)}} \simeq \sum_k \eta_{\alpha\mu\nu k} \exp(-\gamma_{\alpha\mu\nu k}\, t)$$

+ residue

$\big(\delta(t), \dot{\delta}(t)\big)$
Caldeira-**L**eggett type

Divergence of **[*N+1*/*N*]** or **[*N*/*N*]**
Fermi/Bose function approximants

- **CL-residue can be incorporated into DEOM formalism**
- **CL-residue is accuracy controllable**

Optimized DEOM with *K minimized*

JCP **135**:164107 (2011); **140**:054105 (2014)]

Minimizing the # of DOs

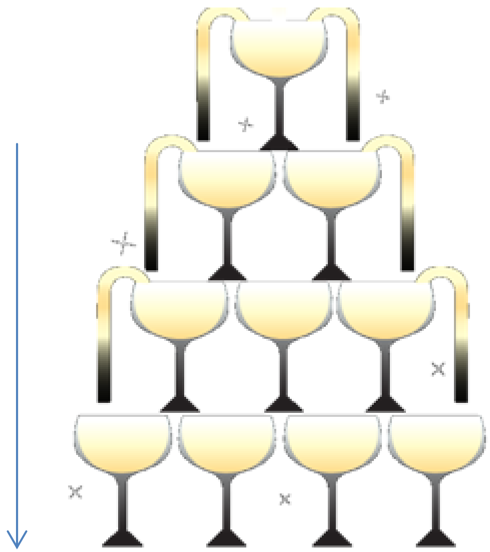
Same technique can also be used in **minimizing *individual L_{eff}***

- **CL-residue can be incorporated into DEOM formalism**
- **CL-residue is accuracy controllable**

→ **Optimized DEOM with *K minimized***

JCP **135**:164107 (2011); **140**:054105 (2014)]

Optimizing DEOM: Summary



***L*-dissipaton effect**

***K* number of single-dissipaton DOs**

Exploit the Caldeira-Leggett Markov construction for *residues* in both *K* and *individual L* directions

Summary

- Fundamental theory of open quantum systems, for hybrid system and bath dynamics via

$$\rho^{(n)}_{j_1\cdots j_n}(t) \equiv \mathrm{tr}_{\mathrm{bath}}\left[\left(\hat{f}_{j_n}\cdots\hat{f}_{j_1}\right)^{\circ}\rho_{\mathrm{total}}(t)\right]$$

- Universal and user friendly

- Accurate and Efficient (**finite temperatures**)

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Prof. ZHENG Xiao (USTC)
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Mr. ZHANG Houdao (HKUST) – Fano resonance (graphene)
Dr. HOU Dong (USTC / HKUST) – Strong correlations

Prof. Ninghua Tong (Renmin Univ. Beijing, China)
(NRG, Quantum MC, etc. for comparison)

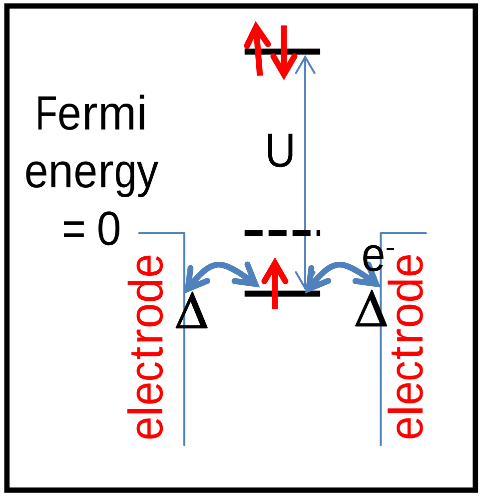
GRC of Hong Kong SAR & NSF of China

Thanks

DEOM-based Evaluations on SIAM

A standard model for strongly correlated electronic systems:

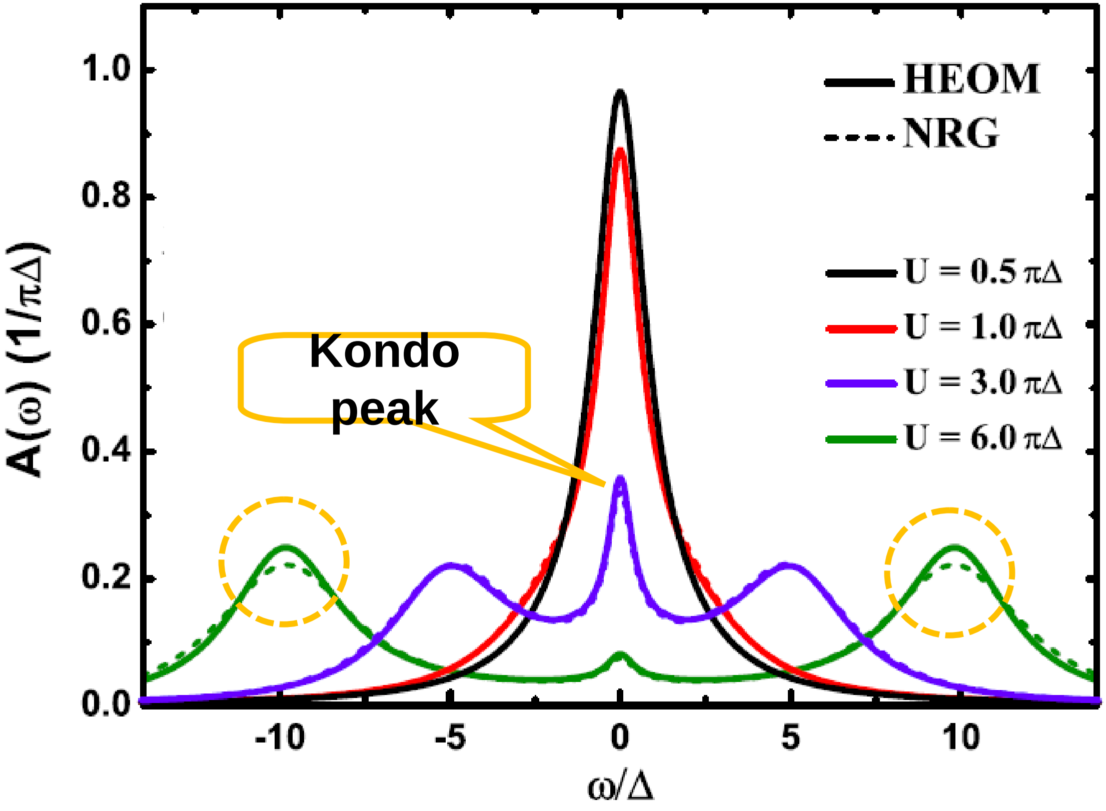
Single Impurity Anderson Model



Δ: s-b coupling

U: Coulomb energy

Comparison to NRG evaluation on symmetric SIAM at a finite *T*



Often more accurate & efficient than conventional methods

DEOM-based Evaluations

Correlation functions

$$\langle \hat{A}(t)\hat{B}(0)\rangle = \mathrm{Tr}_{\mathrm{T}}[\hat{A}e^{-i\mathcal{L}_{\mathrm{T}}t}(\hat{B}\rho^{\mathrm{st}}_{\mathrm{T}})] \equiv \mathrm{Tr}_{\mathrm{T}}[\hat{A}\rho_{\mathrm{T}}(t;\hat{B})]$$

with $\rho_{\mathrm{T}}(t;\hat{B}) = e^{-i\mathcal{L}_{\mathrm{T}}t}\rho_{\mathrm{T}}(0;\hat{B});\qquad \rho_{\mathrm{T}}(0;\hat{B}) \equiv \hat{B}\rho^{\mathrm{st}}_{\mathrm{T}}$

(i) $$\rho^{(n);\mathrm{st}}_{j_1\cdots j_n} \equiv \mathrm{tr}_{\mathrm{B}}\Big[\big(\hat{f}_{j_n}\cdots\hat{f}_{j_1}\big)^{\circ}\rho^{\mathrm{st}}_{\mathrm{T}}\Big]$$

steady-state solution to DEOM

DEOM-based Evaluations

Correlation functions

$$\langle \hat{A}(t)\hat{B}(0)\rangle = \mathrm{Tr}_{\mathrm{T}}[\hat{A}e^{-i\mathcal{L}_{\mathrm{T}}t}(\hat{B}\rho_{\mathrm{T}}^{\mathrm{st}})] \equiv \mathrm{Tr}_{\mathrm{T}}[\hat{A}\rho_{\mathrm{T}}(t;\hat{B})]$$

with $\rho_{\mathrm{T}}(t;\hat{B}) = e^{-i\mathcal{L}_{\mathrm{T}}t}\rho_{\mathrm{T}}(0;\hat{B})$; $\rho_{\mathrm{T}}(0;\hat{B}) \equiv \hat{B}\rho_{\mathrm{T}}^{\mathrm{st}}$

(i) $$\rho^{(n);\mathrm{st}}_{j_1\cdots j_n} \equiv \mathrm{tr}_{\mathrm{B}}\Big[\big(\hat{f}_{j_n}\cdots\hat{f}_{j_1}\big)^{\circ}\rho_{\mathrm{T}}^{\mathrm{st}}\Big]$$

(ii) Express $$\rho^{(n)}_{j_1\cdots j_n}(0;\hat{B}) \equiv \mathrm{tr}_{\mathrm{B}}\Big[\big(\hat{f}_{j_n}\cdots\hat{f}_{j_1}\big)^{\circ}\hat{B}\rho_{\mathrm{T}}^{\mathrm{st}}\Big]$$

in terms of steady-state MDDOs, using e.g., the underlying contraction relations

DEOM-based Evaluations

Correlation functions

$$\langle \hat{A}(t)\hat{B}(0)\rangle = \mathrm{Tr}_{\mathrm{T}}[\hat{A}e^{-i\mathcal{L}_{\mathrm{T}}t}(\hat{B}\rho_{\mathrm{T}}^{\mathrm{st}})] \equiv \mathrm{Tr}_{\mathrm{T}}[\hat{A}\rho_{\mathrm{T}}(t;\hat{B})]$$

with $\rho_{\mathrm{T}}(t;\hat{B}) = e^{-i\mathcal{L}_{\mathrm{T}}t}\rho_{\mathrm{T}}(0;\hat{B})$; $\quad \rho_{\mathrm{T}}(0;\hat{B}) \equiv \hat{B}\rho_{\mathrm{T}}^{\mathrm{st}}$

(i) $$\rho_{j_1\cdots j_n}^{(n);\mathrm{st}} \equiv \mathrm{tr}_{\mathrm{B}}\Big[\big(\hat{f}_{j_n}\cdots\hat{f}_{j_1}\big)^{\circ}\rho_{\mathrm{T}}^{\mathrm{st}}\Big]$$

(ii) Express $\rho_{j_1\cdots j_n}^{(n)}(0;\hat{B}) \equiv \mathrm{tr}_{\mathrm{B}}\Big[\big(\hat{f}_{j_n}\cdots\hat{f}_{j_1}\big)^{\circ}\hat{B}\rho_{\mathrm{T}}^{\mathrm{st}}\Big]$

(iii) DEOM propagation to obtain $\{\rho_{j_1\cdots j_n}^{(n)}(t;\hat{B})\}$

DEOM-based Evaluations

Correlation functions

$$\langle \hat{A}(t)\hat{B}(0)\rangle = \mathrm{Tr}_{\mathrm{T}}[\hat{A}e^{-i\mathcal{L}_{\mathrm{T}}t}(\hat{B}\rho^{\mathrm{st}}_{\mathrm{T}})] \equiv \boxed{\mathrm{Tr}_{\mathrm{T}}[\hat{A}\rho_{\mathrm{T}}(t;\hat{B})]}$$

with $\rho_{\mathrm{T}}(t;\hat{B}) = e^{-i\mathcal{L}_{\mathrm{T}}t}\rho_{\mathrm{T}}(0;\hat{B})$; $\quad \rho_{\mathrm{T}}(0;\hat{B}) \equiv \hat{B}\rho^{\mathrm{st}}_{\mathrm{T}}$

(i) $$\rho^{(n);\mathrm{st}}_{j_1\cdots j_n} \equiv \mathrm{tr}_{\mathrm{B}}\Big[\big(\hat{f}_{j_n}\cdots\hat{f}_{j_1}\big)^{\circ}\rho^{\mathrm{st}}_{\mathrm{T}}\Big]$$

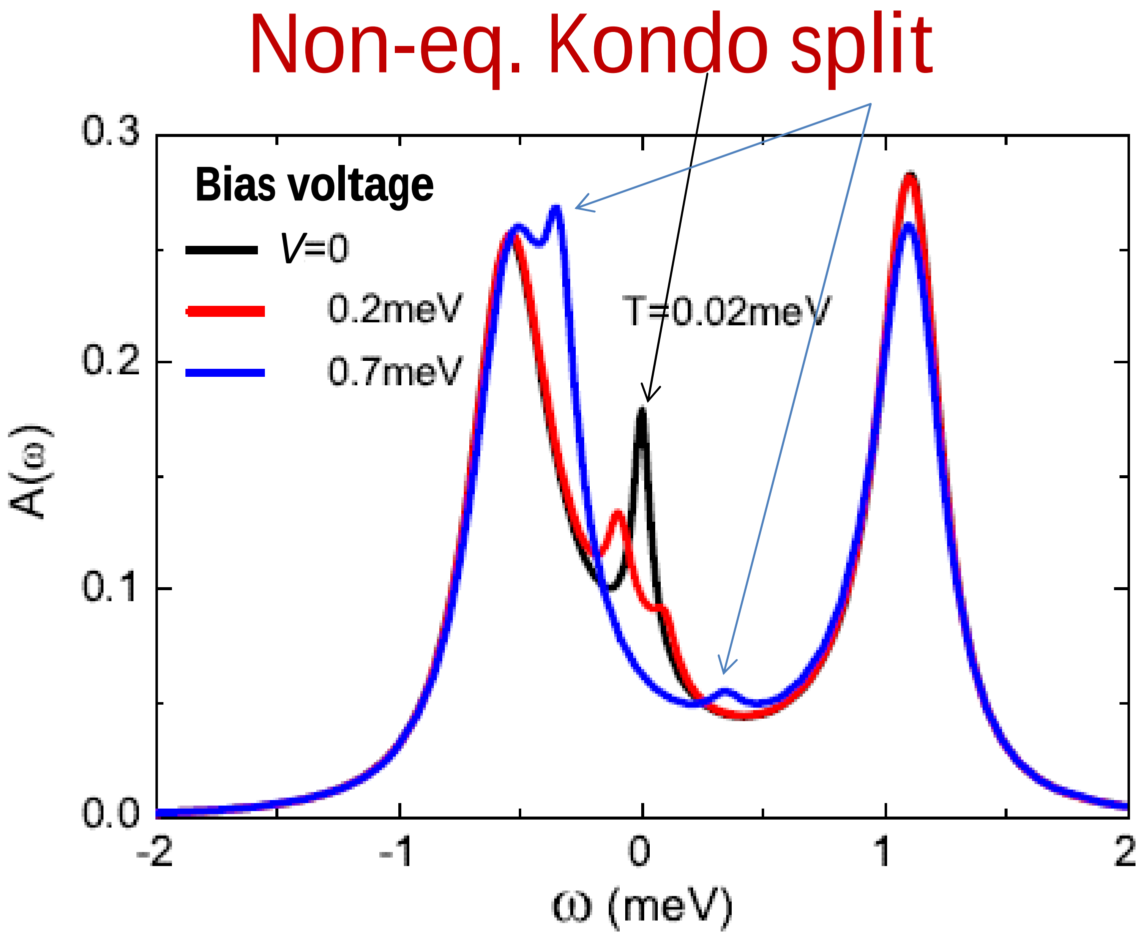
(ii) Express $\rho^{(n)}_{j_1\cdots j_n}(0;\hat{B}) \equiv \mathrm{tr}_{\mathrm{B}}\Big[\big(\hat{f}_{j_n}\cdots\hat{f}_{j_1}\big)^{\circ}\hat{B}\rho^{\mathrm{st}}_{\mathrm{T}}\Big]$

(iii) DEOM propagation to obtain $\big\{\rho^{(n)}_{j_1\cdots j_n}(t;\hat{B})\big\}$

(iv) Evaluate $\langle \hat{A}(t)\hat{B}(0)\rangle$ via $\boxed{\mathrm{tr}_{\mathrm{S}}\Big\{\mathrm{tr}_{\mathrm{B}}\Big[\big(\hat{f}_{j_n}\cdots\hat{f}_{j_1}\big)^{\circ}\hat{A}\rho_{\mathrm{T}}(t;\hat{B})\Big]\Big\}}$

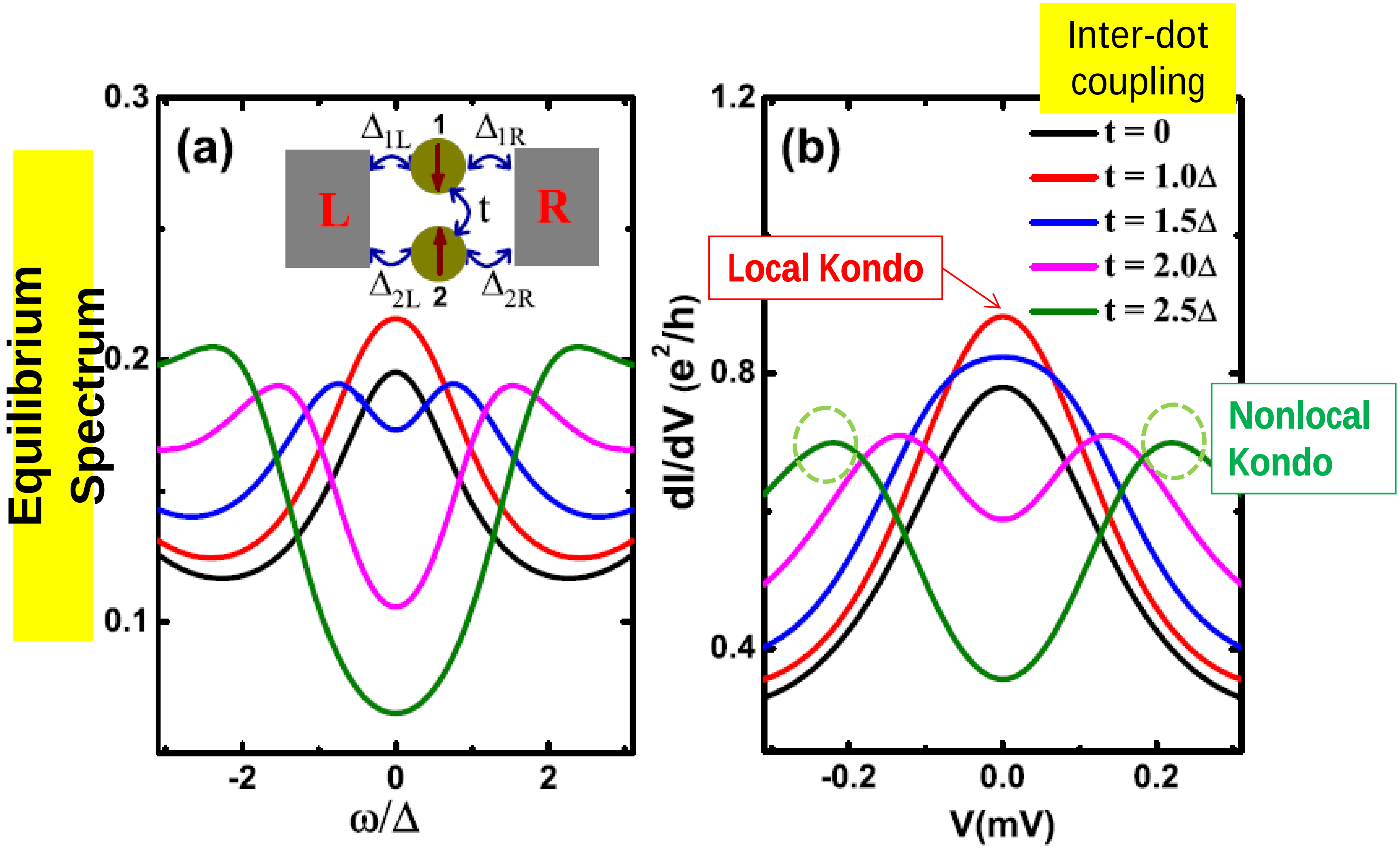
in terms of MDDOs of (iii)

Asymmetric SIAM under Finite Bias Voltage



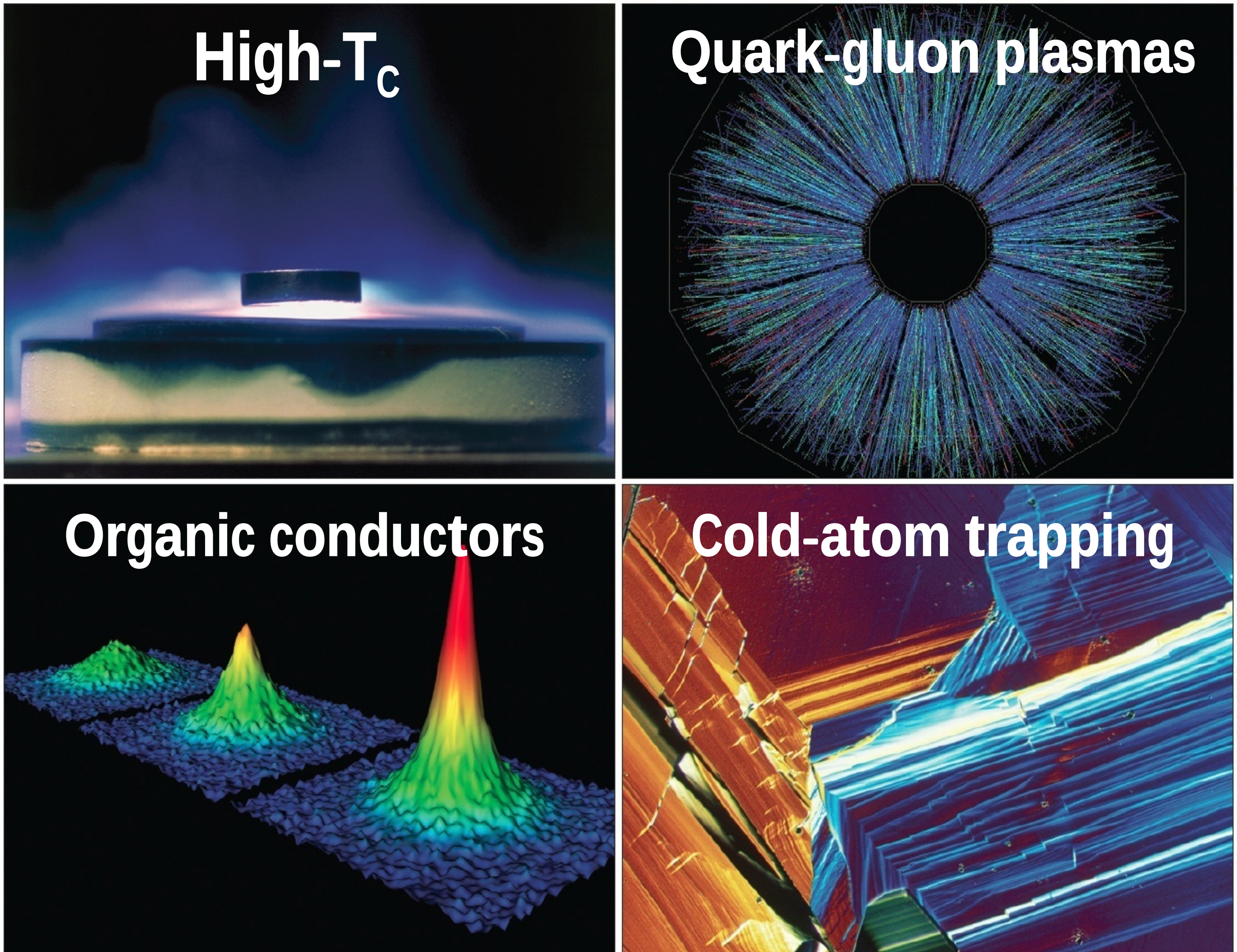
Shikuan Wang, Xiao Zheng, Jinshuang Jin, YJY, *Phys. Rev.* B **88**, 035129 (2013)

Transition of Kondo Singlet in Double-dots



Z Li, NH Tong, X Zheng, D Hou, JH Wei, J Hu, YJY, *Phys. Rev. Lett.* (2012) **109**:266403

Strongly Correlated Systems



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