Non-perturbative Treatment of Quantum Dissipation

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- Dynamics and Thermodynamics in the Polaron Frame
- Symmetry and Multiple Steady-states in Heat Transfer
- A Unified Stochastic Formalism of Quantum Dissipation

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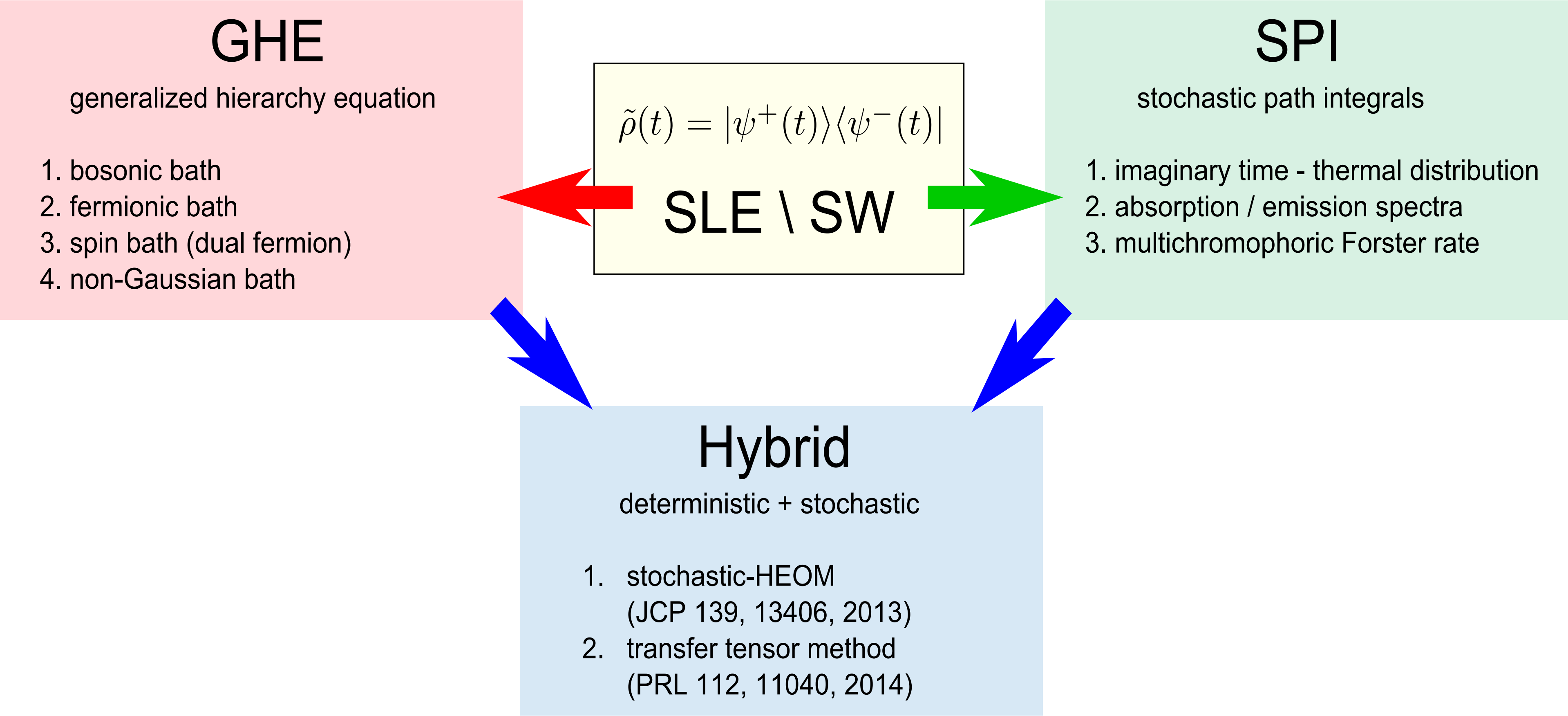
A Unified Stochastic Formalism of Quantum Dissipation

$$\frac{d\,\tilde{\rho}_s(t)}{dt} = -i[H_s, \tilde{\rho}_s] - iA\tilde{\rho}_s\,(t) f^+(t) + i\tilde{\rho}_s\,(t) A f^-(t)$$



$$\tilde{\rho}(t) = |\psi^+(t)\rangle\langle\psi^-(t)|$$

SLE \ SW

GHE

generalized hierarchy equation

1. bosonic bath
2. fermionic bath
3. spin bath (dual fermion)
4. non-Gaussian bath

SPI

stochastic path integrals

1. imaginary time - thermal distribution
2. absorption / emission spectra
3. multichromophoric Forster rate

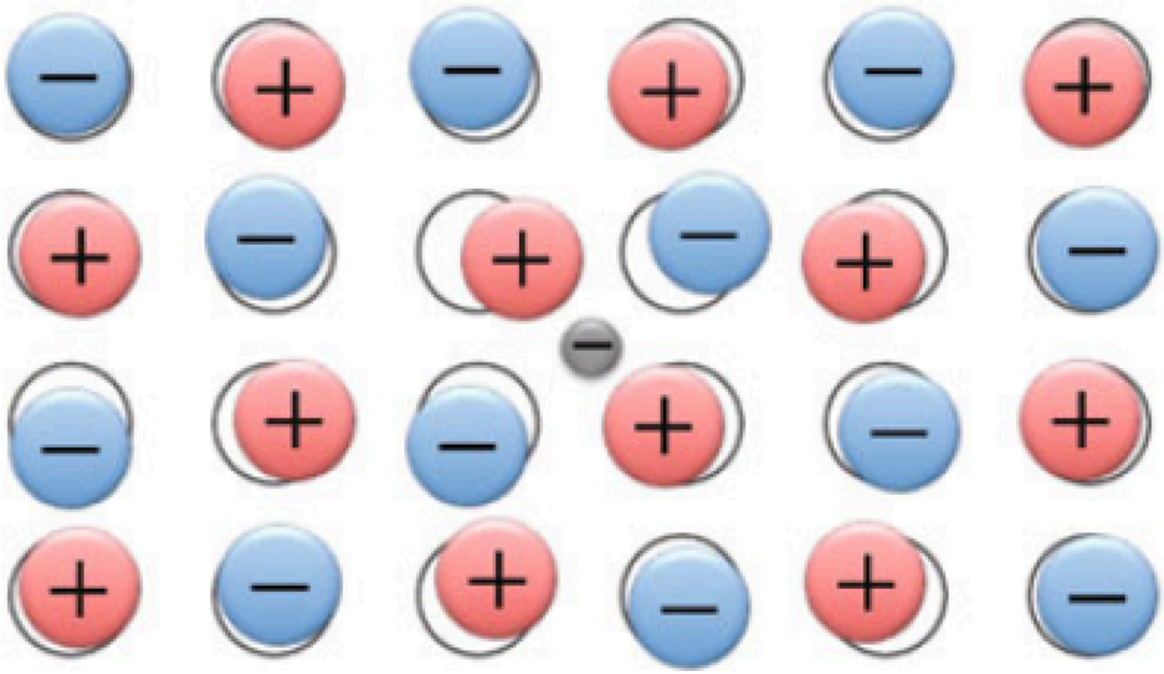
Hybrid

deterministic + stochastic

1. stochastic-HEOM
   (JCP 139, 13406, 2013)
2. transfer tensor method
   (PRL 112, 11040, 2014)

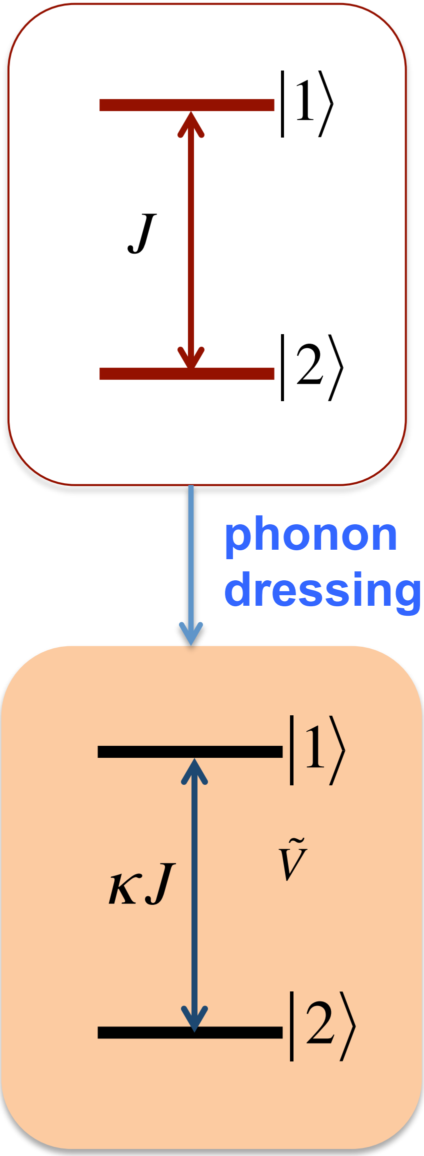
Hsieh and Cao, arXiv: 1701.05709

Polaron: Polarization of Lattice



- non-canonical thermal distribution
- polaron-transformed Redfield equation
- quantum diffusion in organic systems
- light-harvesting energy transfer
- heat transfer in NESB

Polaron transformation of the spin-boson model



$$H_e = \frac{\epsilon}{2}\sigma_z + \frac{J}{2}\sigma_x + \sum_k \omega_k b_k^\dagger b_k + \sigma_z \sum_k \left(f_k b_k^\dagger + \mathrm{H.c.} \right)$$

unitary polaron transformation

$$\tilde{H}_e = S H_e S^\dagger = \tilde{H}_S + \tilde{H}_B + \tilde{V}$$

$$S = \exp[\sigma_z B]$$

$$\kappa = \langle \cosh B \rangle \leq 1$$

$$B = \sum_k \frac{f_k}{\omega_k}\left(b_k^\dagger - b_k \right)$$

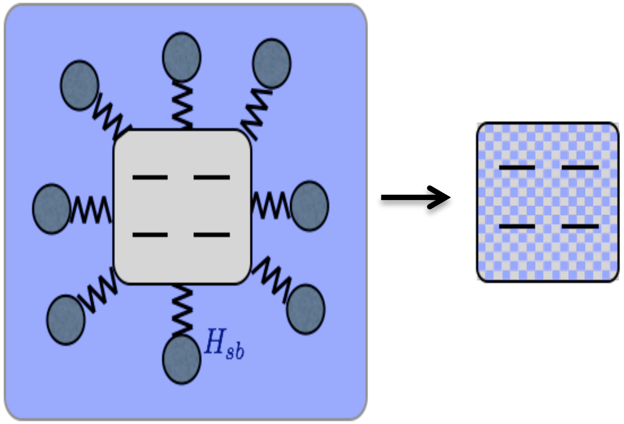
B is the phonon displacement

$$\tilde{H}_S = \frac{\varepsilon}{2}\sigma_z + \kappa \frac{J}{2}\sigma_x$$

$$\tilde{H}_B = \sum_k \omega_k b_k^\dagger b_k$$

$$\tilde{V} = \frac{J}{2}\left[\sigma_x (\cos B - \kappa) + \sigma_y \sin B \right]$$

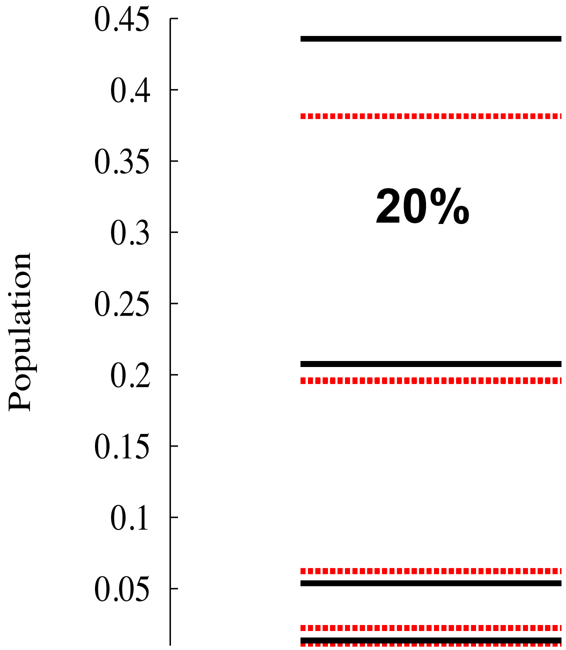
Deviation from Boltzmann



equilibrium reduced density matrix

$$\frac{1}{Z}\mathrm{Tr_b}e^{-\beta H} = e^{-\beta H_{eff}} \neq \frac{1}{Z}_s e^{-\beta H_s}$$

H_s and H_{SB} do not commute



Boltzmann/exact RDM

LH2 of purple bacteria at T_{room}

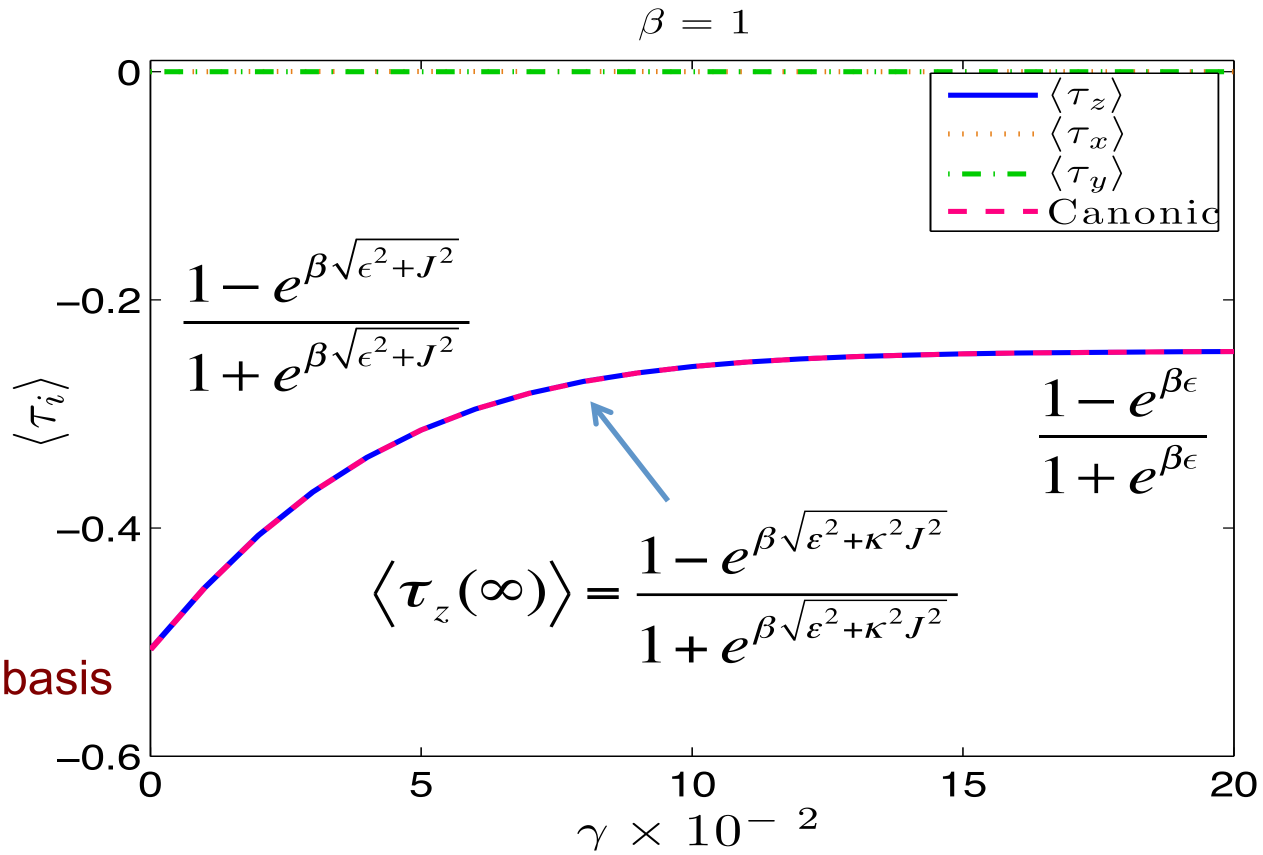
J Moix and J. Cao, PRB, 85, 115412, (2012): imaginary-time path integral calculations

Non-canonical distribution (I): polaron population

$$\tilde{H}_s = \frac{\varepsilon}{2}\sigma_z + \frac{\kappa J}{2}\sigma_x = \varepsilon_+ \left|+\right\rangle\left\langle+\right| + \varepsilon_- \left|-\right\rangle\left\langle-\right|$$

$$\left\langle\tau_z\right\rangle = -\tanh(\beta\sqrt{\varepsilon^2+\kappa^2 J^2}\,/\,2)$$

population distribution(energy gap) in the polaron basis



$$\frac{1-e^{\beta\sqrt{\epsilon^2+J^2}}}{1+e^{\beta\sqrt{\epsilon^2+J^2}}}$$

local basis

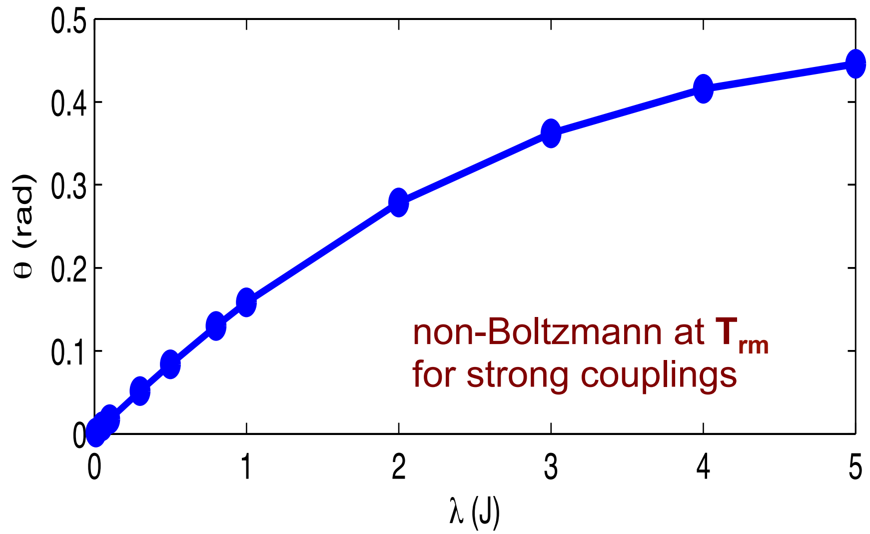
$$\frac{1-e^{\beta\epsilon}}{1+e^{\beta\epsilon}}$$

$$\left\langle\tau_z(\infty)\right\rangle = \frac{1-e^{\beta\sqrt{\varepsilon^2+\kappa^2J^2}}}{1+e^{\beta\sqrt{\varepsilon^2+\kappa^2J^2}}}$$

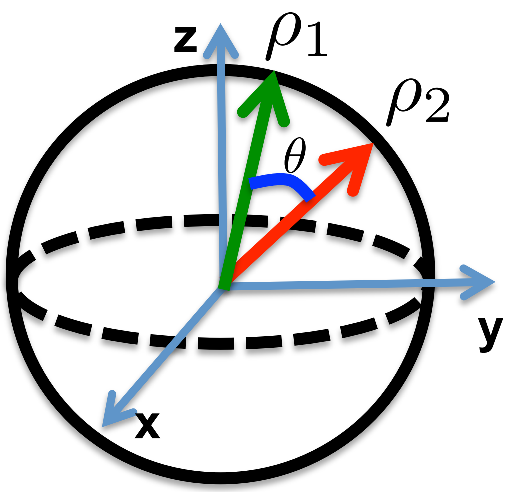
eigen basis

Lee, Cao, Gong, PRE 86, 021109 (2012)

Non-canonical distribution (II): basis set rotation

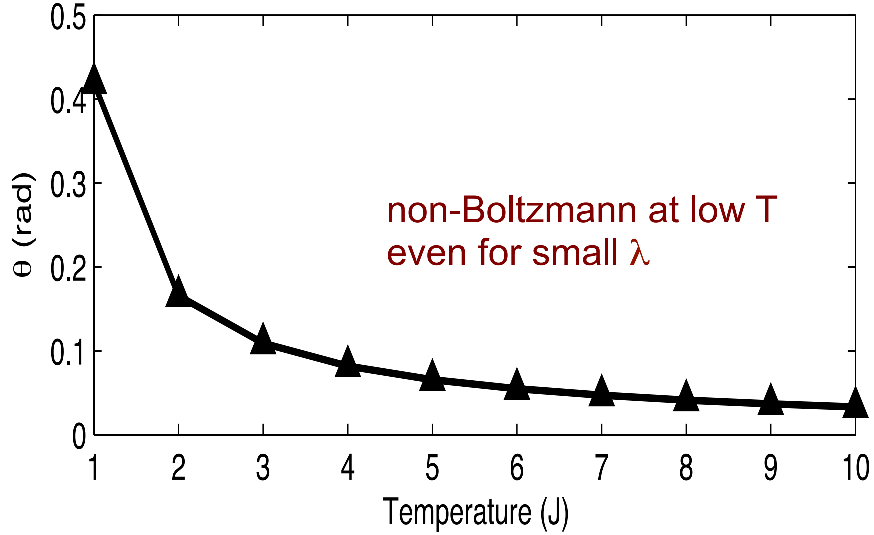


non-Boltzmann at **T**$_{\mathbf{rm}}$
for strong couplings

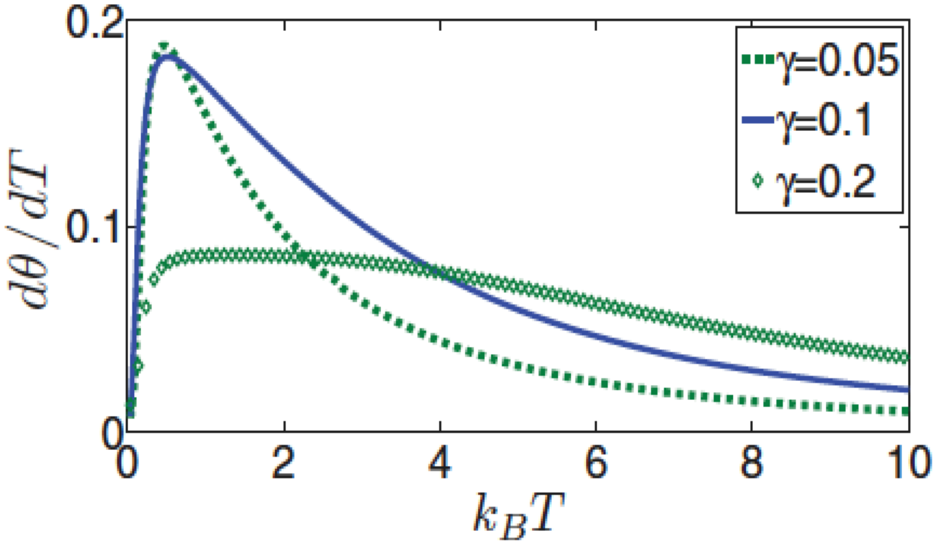


Bloch sphere

ρ_1: eigen
ρ_2: polaron
θ: deviation



non-Boltzmann at low T
even for small λ



Lee, Cao, and Gong, PRE, 86, 021109 (2012); Cerrillo and Cao, PRL 112, p110401 (2014) (TTM)

Master Equation in the Polaron Basis

$$\tilde{H}_S = \frac{\varepsilon}{2}\sigma_z + \kappa\frac{J}{2}\sigma \quad \tilde{H}_B = \sum_k \omega_k b_k^\dagger b_k \quad \tilde{V} = \frac{J}{2}\left[\sigma_x(\cos B - \kappa) + \sigma_y \sin B\right]$$

polaron basis

$$\varepsilon_\pm = \pm\frac{1}{2}\sqrt{\varepsilon^2 + \left(J\kappa\right)^2} \qquad \tan\theta = J\kappa/\varepsilon$$

$$|+\rangle = \cos\frac{\theta}{2}|1\rangle + \sin\frac{\theta}{2}|2\rangle, |-\rangle = \sin\frac{\theta}{2}|1\rangle - \cos\frac{\theta}{2}|2\rangle$$

$$\tau_z = |+\rangle\langle + | - |-\rangle\langle - |$$

$$\tau_+ = |+\rangle\langle - |, \tau_- = |-\rangle\langle + |$$

$$\Delta = \varepsilon_+ - \varepsilon_-$$

Master equation with Born-Markov approximation (Breuer and Petruccione)

$$\frac{d\tilde{\rho}(t)}{dt} = -i\left[\tilde{H}_s, \tilde{\rho}_e(t)\right] - \int_0^\infty d\tau \operatorname{Tr}_B\left[\tilde{V}_I(0), \left[\tilde{V}_I(-\tau), \tilde{\rho}(t)\rho_B\right]\right]$$

Polaron Dynamics: Silbey, Nazir, Schaller, Gelbwaser…

Polaron-Transformed Redfield-Bloch Equation (PTRE)

$$\frac{d}{dt}\begin{pmatrix}\langle\tau_z\rangle\\ \langle\tau_x\rangle\\ \langle\tau_y\rangle\end{pmatrix}=-\begin{pmatrix}\gamma_z & \gamma_{zx} & 0\\ \gamma_{xz} & \gamma_x & \Delta+\gamma_{xy}\\ \gamma_{yz} & -\Delta+\gamma_{yx} & \gamma_y\end{pmatrix}\begin{pmatrix}\langle\tau_z\rangle\\ \langle\tau_x\rangle\\ \langle\tau_y\rangle\end{pmatrix}+\begin{pmatrix}C_z\\ C_x\\ C_y\end{pmatrix}$$

Pauli operator in the polaron transformed basis

relaxation rate:

$$\gamma_z=\frac{J^2\kappa^2}{2}\int_0^\infty d\tau\cos(\Delta\tau)\left\{\cos^2\theta[\cosh\left[Q(\tau)\right]+\cosh\left[Q(-\tau)\right]-2]+\sinh\left[Q(\tau)\right]+\sinh\left[Q(-\tau)\right]\right\}$$

$$Q(\tau)=\int_0^\infty d\omega\frac{J(\omega)}{\pi\omega^2}\left(e^{i\omega\tau}n(\omega)+e^{-i\omega\tau}\left[1+n(\omega)\right]\right)$$

bath correlation function

$$\kappa=\exp\left[-\int_0^\infty d\omega\frac{J(\omega)}{\pi\omega^2}\left(n(\omega)+\frac{1}{2}\right)\right]=\exp[-\frac{1}{2}Q(0)]$$

Lee, Moix, and Cao JCP 142, p164103, (2015) Xu and Cao, Frontier of Physics 11(4),110308 (2016)

PTRE (I): Bridging Two Limits

Weak coupling limit $\kappa = \langle \cos B \rangle \rightarrow 1$

Redfield equation in eigen basis

$$\frac{d\rho_s^{++}}{dt} = -\Gamma\left[1+N\left(\Lambda_0\right)\right]\rho_s^{++} + \Gamma N\left(\Lambda_0\right)\rho_s^{--}$$

$$\frac{d\rho_s^{+-}}{dt} = -i\Lambda_0\rho_s^{+-} - \Gamma\left[\frac{1}{2}+N\left(\Lambda_0\right)\right]\rho_s^{+-}$$

Redfield relaxation rate: $\Gamma = \frac{1}{2}J\left(\Lambda_0\right)\sin^2\theta, \Lambda_0 = \sqrt{\Delta^2 + J^2}$

Strong coupling limit $\kappa \rightarrow 0$

Rate equation in local basis (no coherence)

$$\frac{d\rho_s^{11}}{dt} = -\Gamma_{11}\rho_s^{11} + \Gamma_{12}\rho_s^{22}$$

Fermi's Golden-rate rule: $\Gamma_{11} = \frac{1}{2}\kappa^2 J^2 \int_0^\infty d\tau \,\mathrm{Re}\left[e^{i\Delta\tau}\left(e^{Q(\tau)}-1\right)\right]$

Xu and Cao, Frontier of Physics 11(4),110308 (2016)

PTRE (II): Thermodynamic Consistency

Steady **s**tate solution

$$\frac{d\langle\vec{\tau}\rangle}{dt}=0 \Rightarrow \begin{pmatrix}\langle\tau_z(\infty)\rangle\\ \langle\tau_x(\infty)\rangle\\ \langle\tau_y(\infty)\rangle\end{pmatrix}=\begin{pmatrix}\gamma_z & \gamma_{zx} & 0\\ \gamma_{xz} & \gamma_x & \Delta+\gamma_{xy}\\ \gamma_{yz} & -\Delta+\gamma_{yx} & \gamma_y\end{pmatrix}^{-1}\begin{pmatrix}C_z\\ C_x\\ C_y\end{pmatrix}$$

population difference

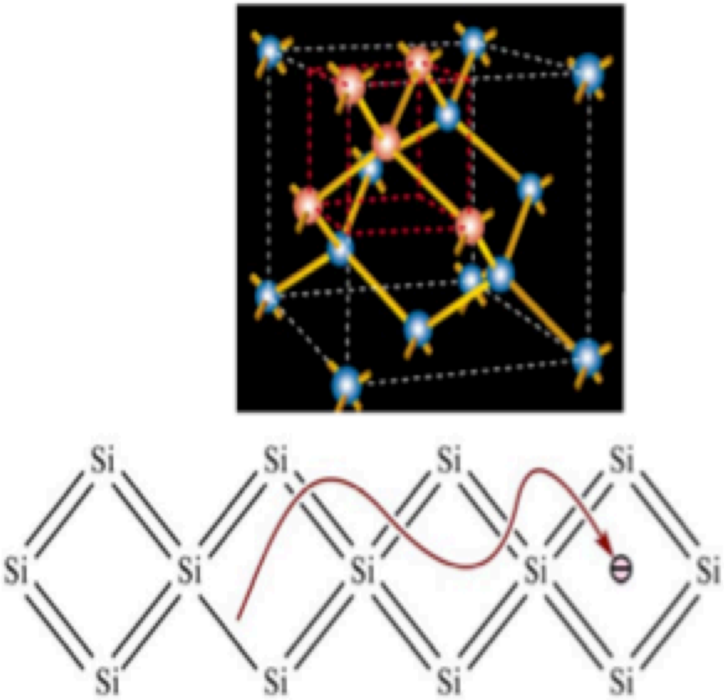
$$\langle\tau_z(\infty)\rangle = \frac{-2i\int_{-\infty}^{\infty} d\tau\sin(\Delta\tau)\eta^2 e^{Q(\tau)}}{\int_{-\infty}^{\infty} d\tau\cos(\Delta\tau)\eta^2\left\{e^{Q(\tau)}+e^{Q(-\tau)}\right\}} \approx \frac{1-e^{\beta\Delta}}{1+e^{\beta\Delta}}$$

canonical distribution in the polaron frame

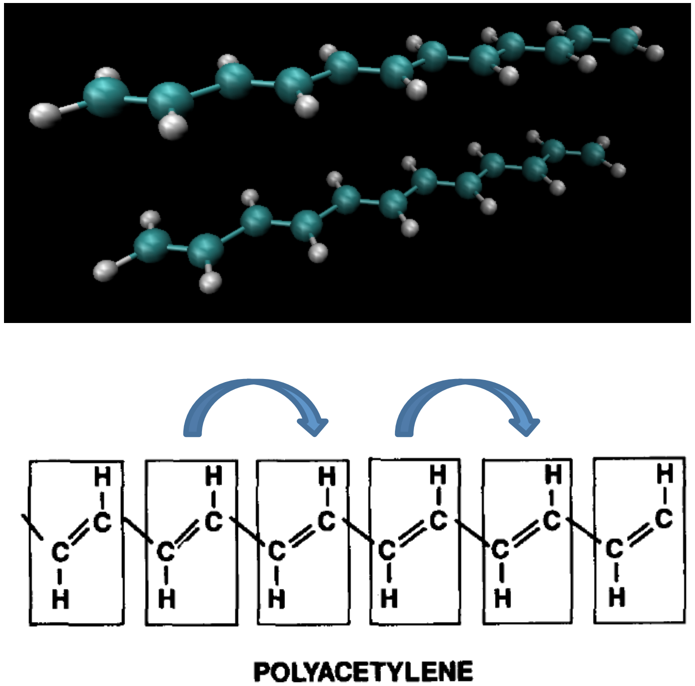
- Dynamical steady state and thermodynamic equilibrium state are consistent
- PTRE bridges smoothly the Redfield equation and Fermi-Golden-Rule rates
- Numerical comparison shows reliability in the relevant regime

Xu and Cao, Frontier of Physics 11(4), 110308 (2016)

Two Models of Carrier Dynamics

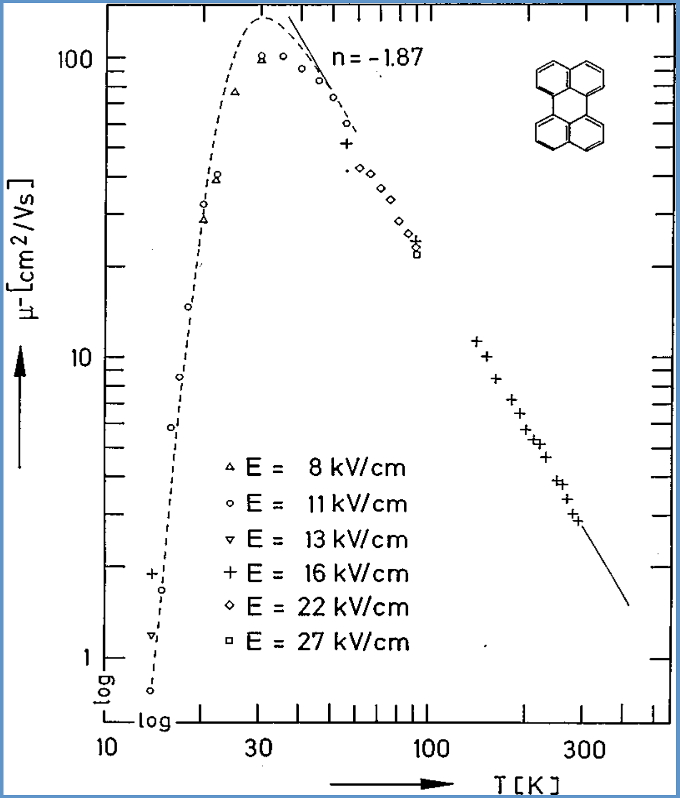


coherent band-like
(Redfield equation)



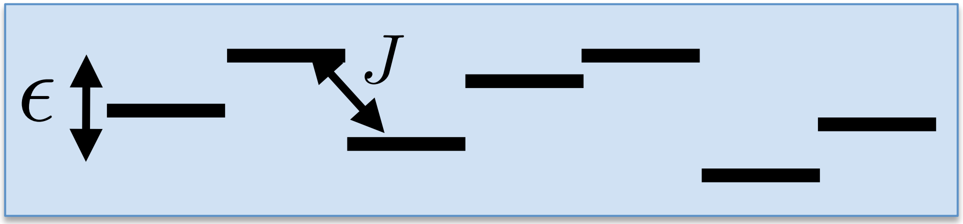
incoherent hopping
(Fermi's golden rule rate)

Fluctuating Anderson Model for Organic Solids



Optimal Temperature

disordered 1-D chain (Anderson model)



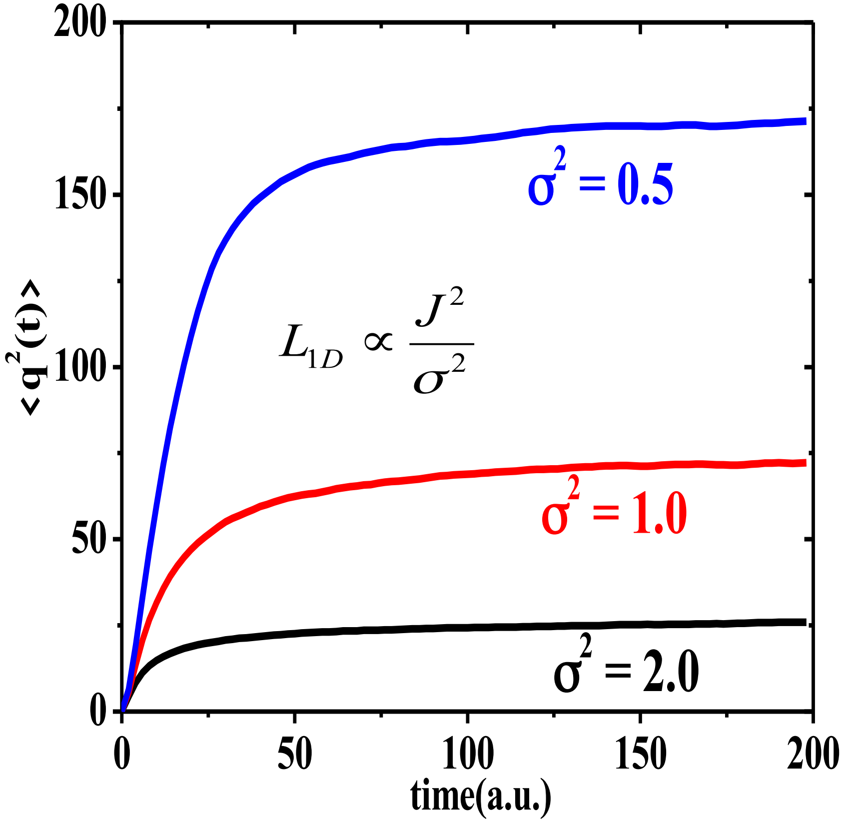
$$P(\epsilon) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\epsilon^2}{2\sigma^2}}$$

+ thermal fluctuations

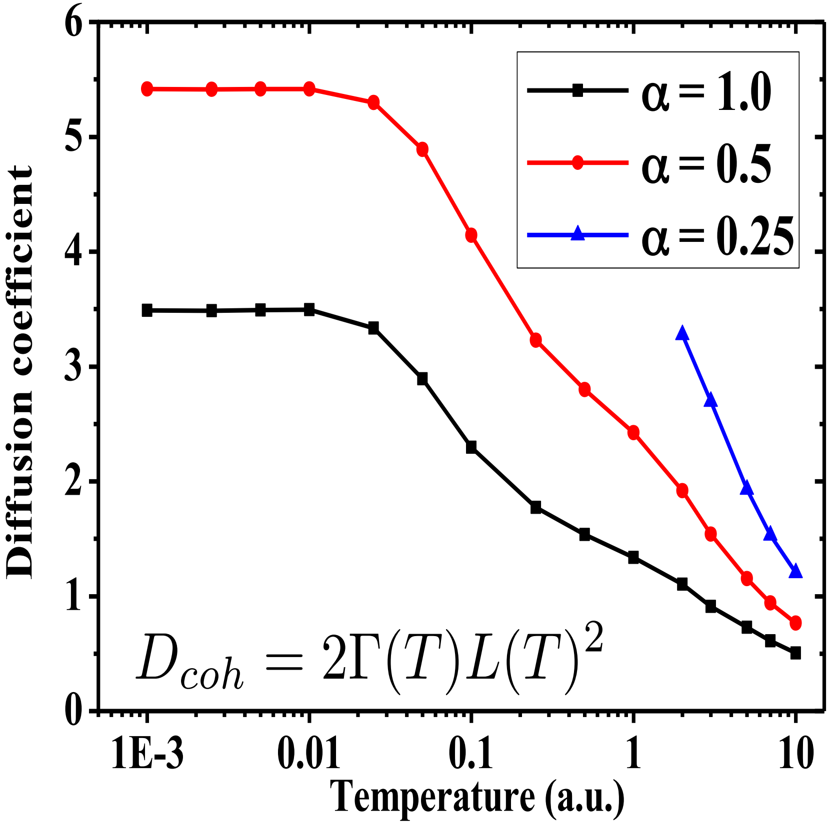
$$H(t) = H_s + \sum_i F_i(t)|i\rangle\langle i|$$

$$\left\langle F_i(t)F_j(t')\right\rangle_{QM} = \delta_{ij}C(t-t')$$

Two Limiting Cases

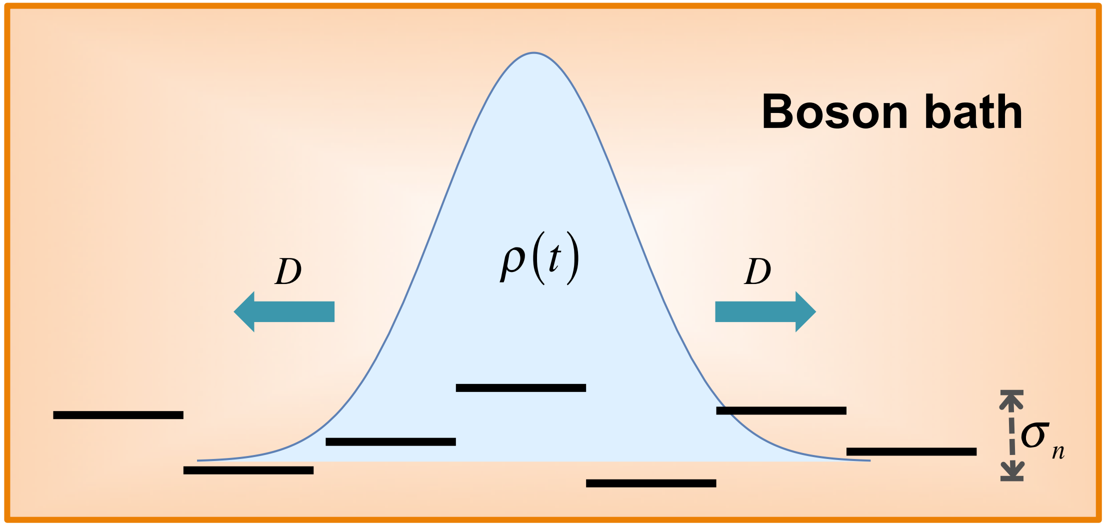


disordered chains: localization



homogeneous chains: polaron

T-dependence in Mobility: Quantized Phonon Bath

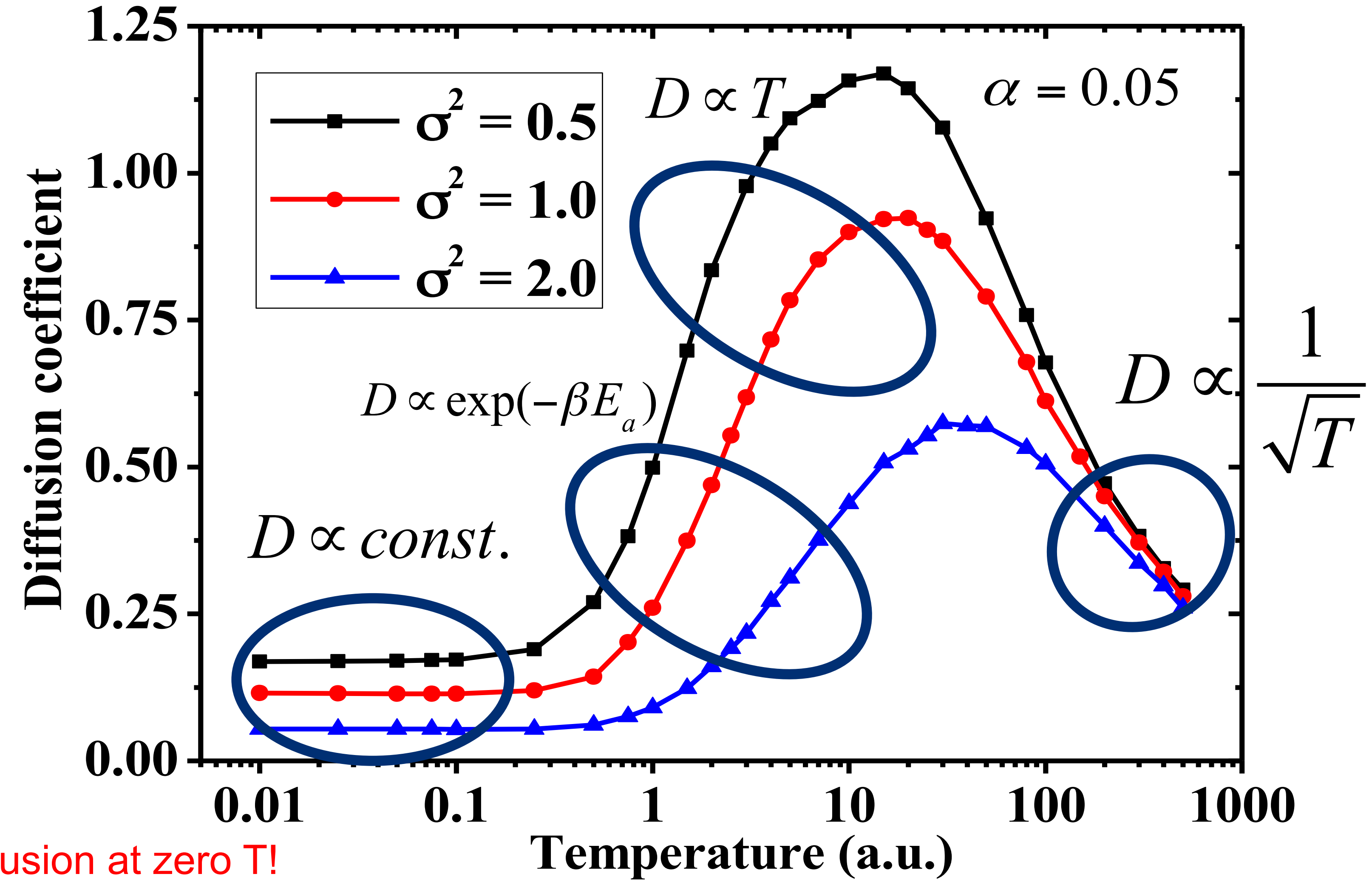


one-dimensional chain with 100-1000 sites
an independent quantum bath for each site
spin-boson model: 2 states and one bath

$$J(\omega) = \frac{\pi}{2}\alpha\omega e^{-\omega/\omega_c}$$

Redfield equation: weak coupling/low T (eigen-state basis)
Fermi’s golden rule rate: strong coupling/high T (site basis)

Diffusion Constant: Quantum Noise



diffusion at zero T!

Lee, Moix, and Cao (JCP 142, p164103, 2015)

Comparison with Measured Mobility

TABLE I: Mobility (in unit cm^2/Vs) of organic semiconductor materials at $T = 300K$ and $\sigma = 800cm^{-1}$.

	PT-RE	Redfield	FGR	Experiment
Rubrene	11.1	41.2	0.33	3 to 15
Pentacene	0.73	2.0	0.045	0.66 to 2.3
PBI-F_2	2.2×10^{-5}	1.2×10^{-3}	2.0×10^{-5}	-
PBI-$(C_4F_9)_2$	0.61	104	0.25	-

our model **band-like** **hopping**

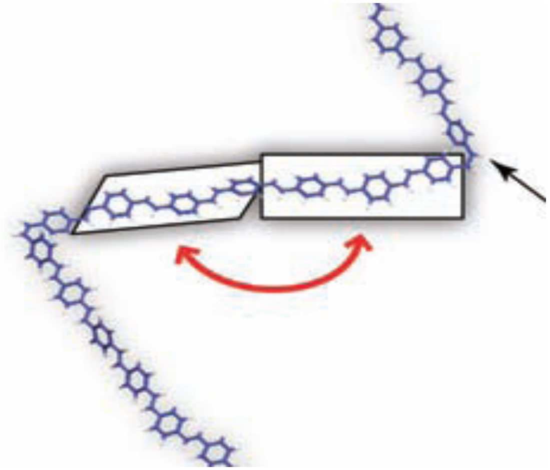
FGR: Fermi’s golden-rule rate (incoherent hopping transport)

Redfield: transitions between excitons (coherent band-like transport)

PT-RE: polaron-transformed Redfield Eq. (hopping between polarons)

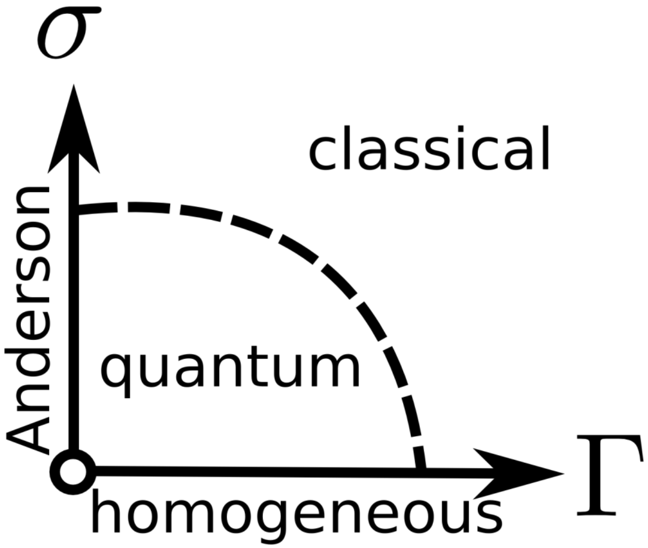
Quantum Diffusion

short-time localization
+ long-time hopping



quantum
speed-up

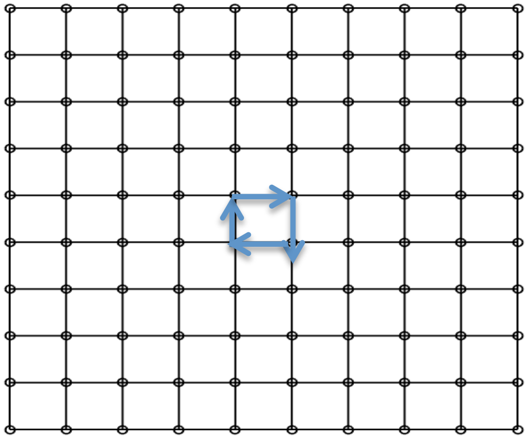
$$\frac{D_{coh}}{D_{incoh}} \approx L$$



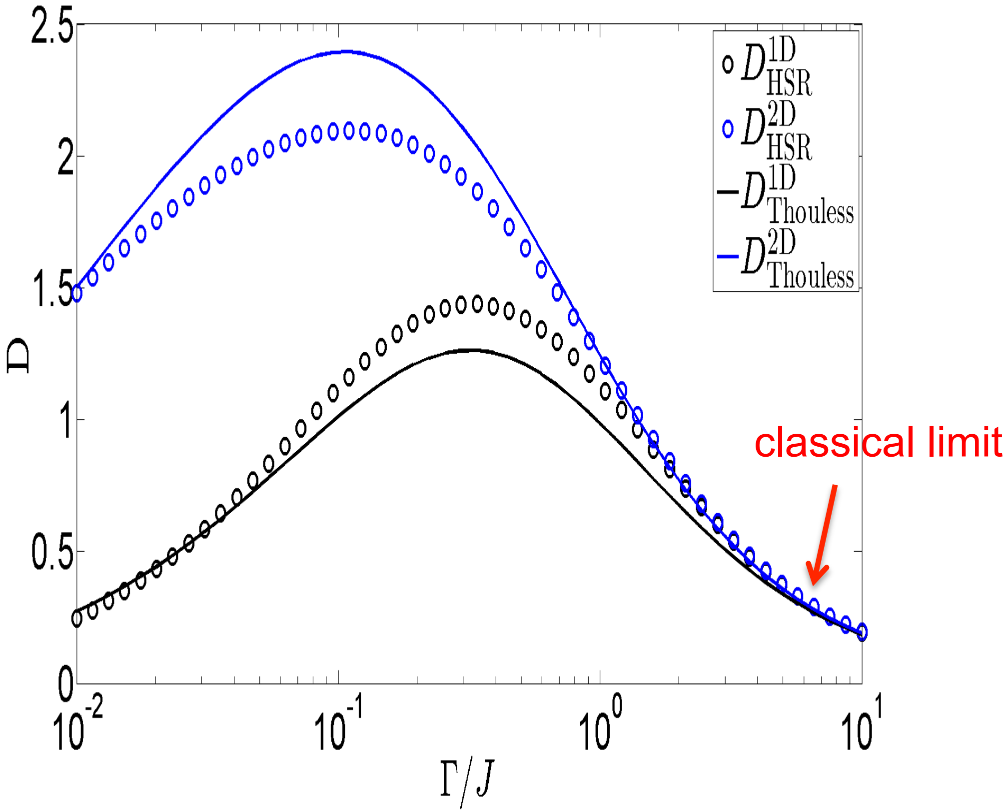
Moix, Khasin, and Cao (NJP 15, 085010, 2013)

From 1D Chains to 2D Films

$$L_{1D} \propto \frac{J^2}{\sigma^2}$$



$$L_{2D} \propto \frac{J^2}{\sigma^2}\exp(\frac{J^2}{\sigma^2})$$



Thouless Interpolation

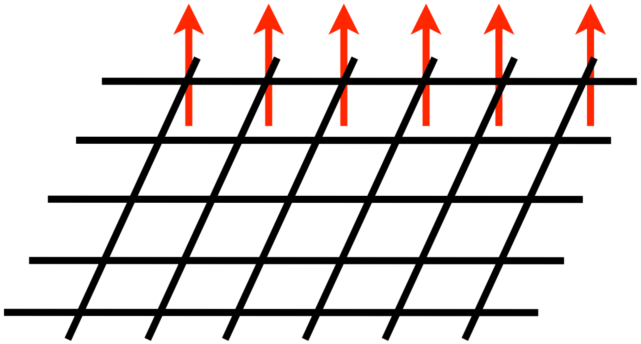
$$D \approx \left[\left(\frac{2J^2}{\Gamma + \sigma/2}\right)^{-1/2} + (\Gamma l^2)^{-1/2}\right]^{-2}$$

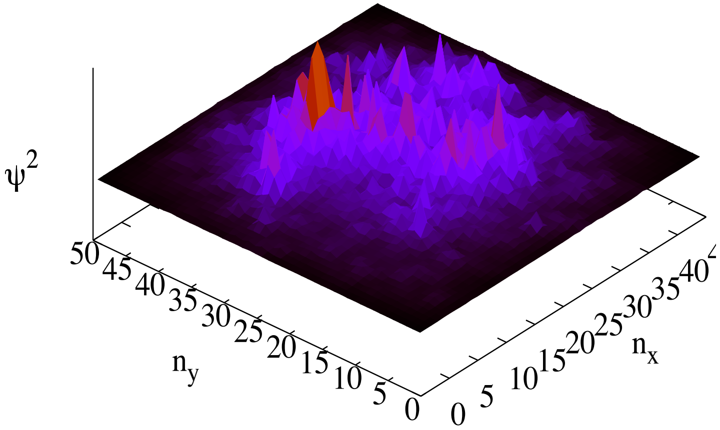
Chuang, Lee, Moix, Knoester, and Cao, PRL116, 196803, (2016)

Open Questions in Quantum Diffusion

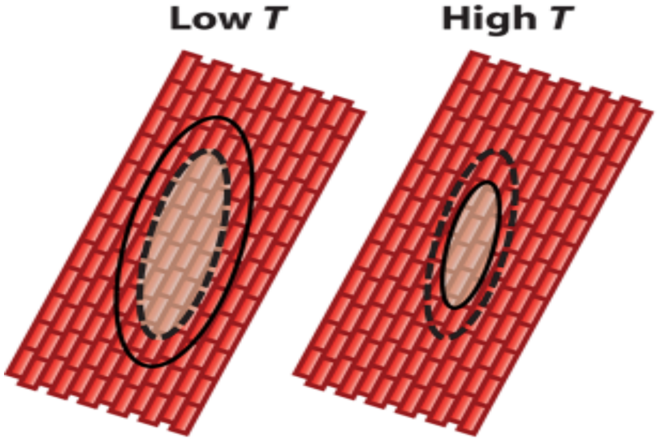
Anderson localization competes with the long-range dipolar interactions

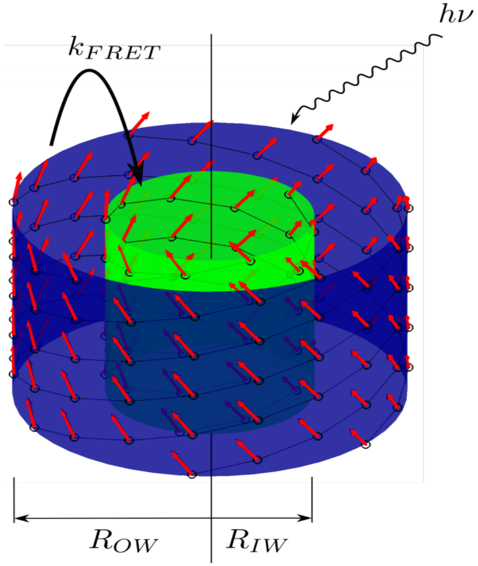
2D lattice with 3D dipoles (H-aggregates)



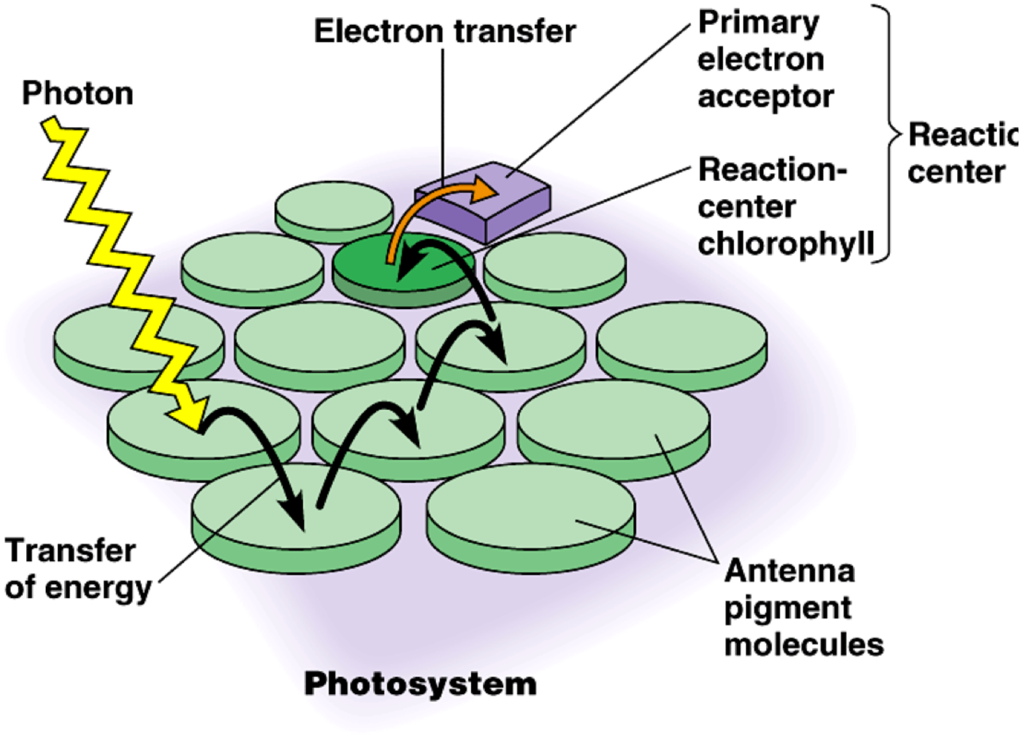


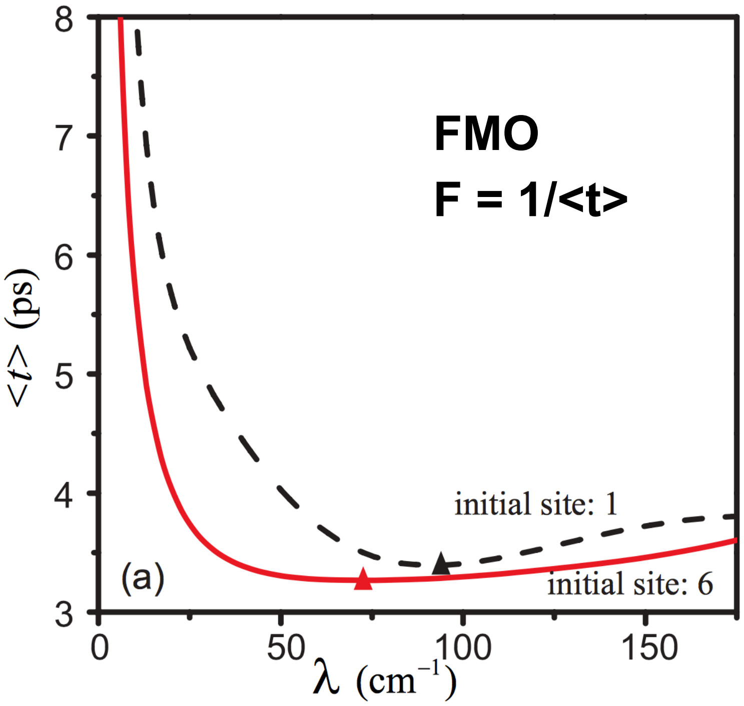
Anisotropic dipolar interactions (J-aggregates)





Energy transfer in photosystem: Optimal coupling



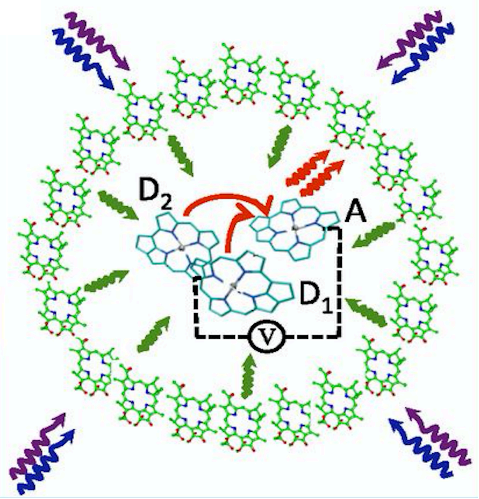


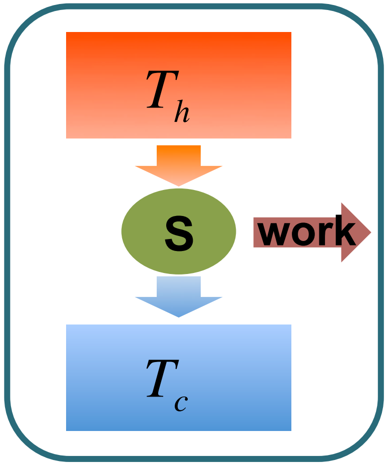
▲ ▲ optimal reorganization energy

intermediate system-bath coupling and temperature

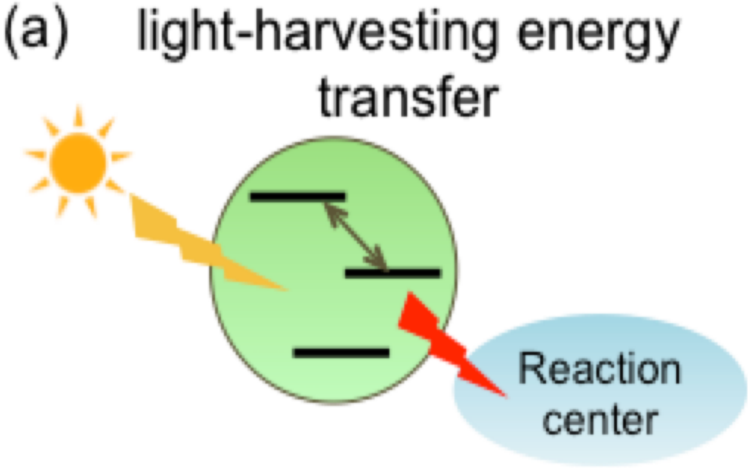
Wu, Silbey, and Cao, PRL 110, 200402 (2013); Wu, et al, NJP, 12, 105012 (2010)

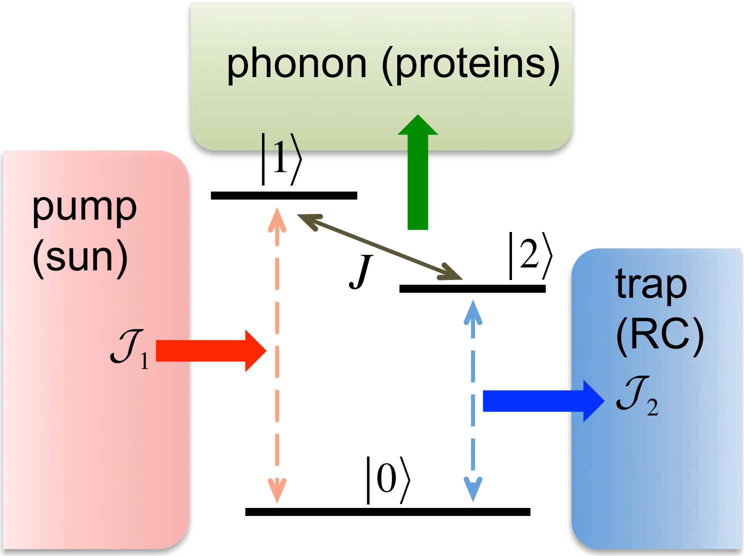
Three-level Light-Harvesting Model





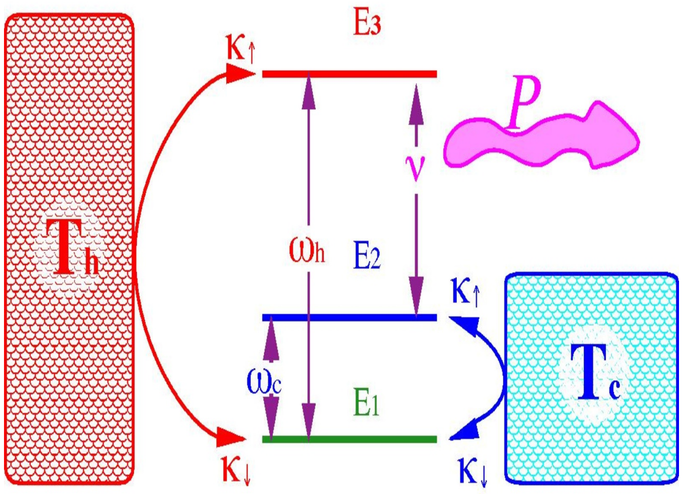
Scully, et al.
PNAS (2011)





Three-level Quantum Heat Engine and Heat Pump

quantum heat engine

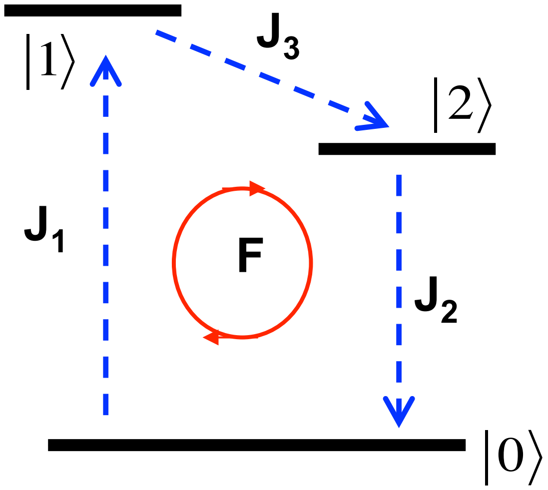


maser efficiency (kinetic Limit)

$$\boxed{\eta_{\mathrm{SSD}} = \frac{\nu}{\varepsilon_h} \leq \eta_C}$$

Scovil and Schulz-DuBois Limit
Phys. Rev. Lett. 2 262 (1959)

light-harvesting (heat pump)



strong coupling (Re[ρ_{12}]=0)

$J_i = \varepsilon_i F \quad \eta_{\mathrm{SSD}} = \varepsilon_2/\varepsilon_1$

F is the exciton population flux

Xu, Wang, Cao, NJP 023003 (2016)

Energy flux and quantum coherence

Time evolution of the light-harvesting system

$$\frac{d\rho_s(t)}{dt} = -i[H_S, \rho_s(t)] + \underbrace{\mathcal{L}_{pump}[\rho_s] + \mathcal{L}_{trap}[\rho_s]}_{\text{Redfield-Lindblad form}} + \underbrace{\mathcal{L}_{phonon}[\rho_s]}_{\text{polaron approach}}$$

Energy flux

$$\mathcal{J} = \mathrm{Tr}_s\left[\frac{d\rho}{dt} H_s\right] = \mathrm{Tr}_s\left[\mathcal{L}_{pump}[\rho] H_s\right] + \mathrm{Tr}_s\left[\mathcal{L}_{trap}[\rho] H_s\right] + \mathrm{Tr}_s\left[\mathcal{L}_{phonon}[\rho] H_s\right]$$

$$\mathcal{J}_2 = \mathrm{Tr}_s[\mathcal{L}_{trap}\rho_s H_s] = -\epsilon_2\gamma_2\left[(n_2+1)\rho_{22} - n_2\rho_{gg}\right] - \frac{J\gamma_2}{2}(n_2+1)\mathrm{Re}[\rho_{12}]$$

$$\mathcal{J}_1 = \mathrm{Tr}_s[\mathcal{L}_{pump}\rho_s H_s] = -\epsilon_1\gamma_1[(n_1+1)\rho_{11} - n_1\rho_{gg}] - \frac{J\gamma_1}{2}(n_1+1)\mathrm{Re}[\rho_{12}]$$

population term

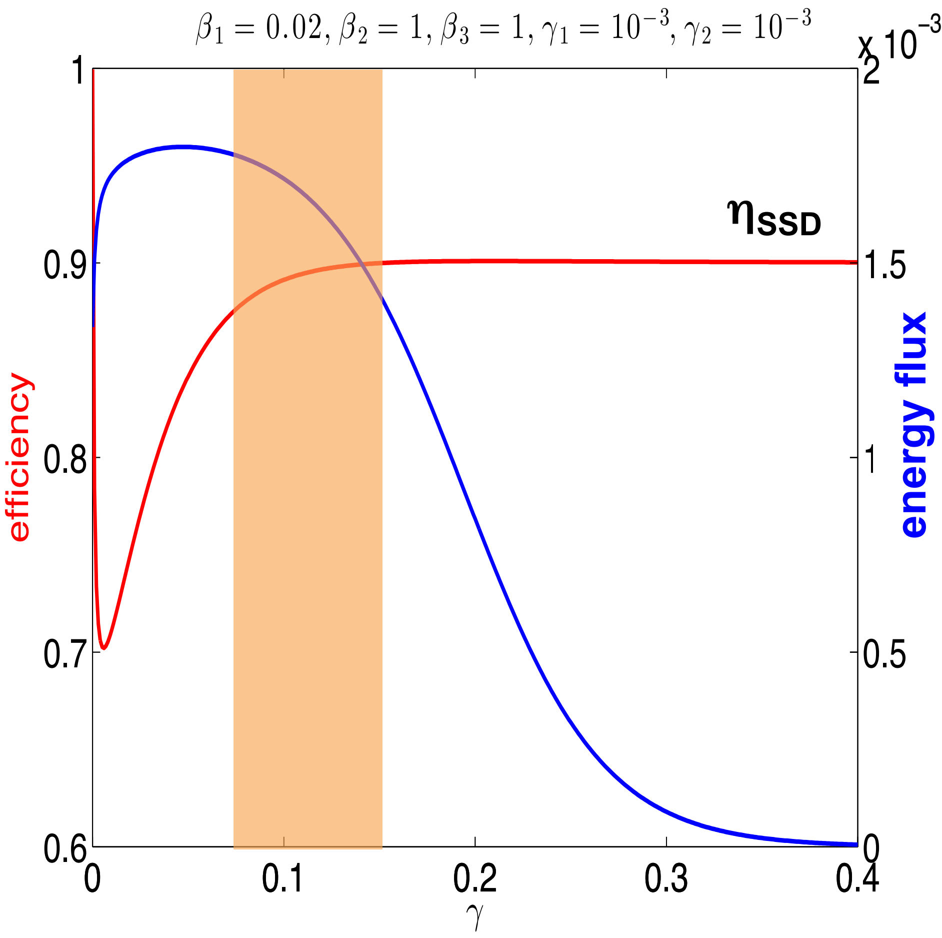
coherence term: Re[ρ_{12}]

Efficiency

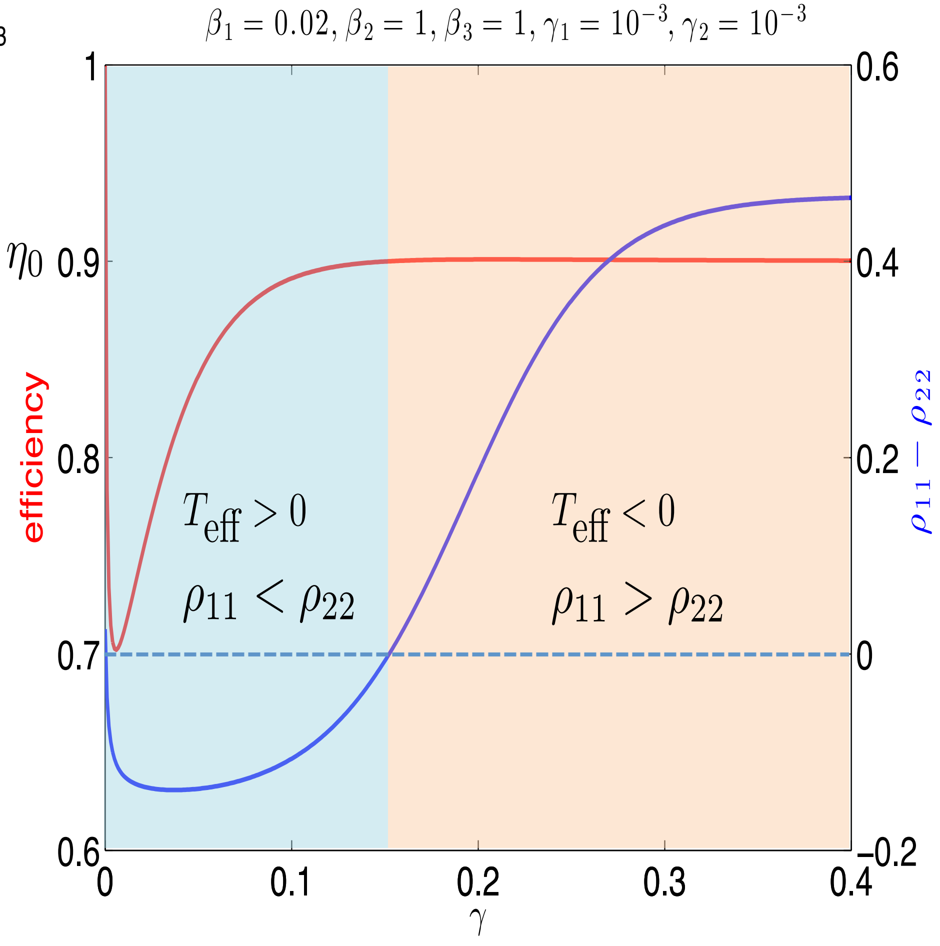
$$\boxed{\eta_{eff} = -\frac{\mathcal{J}_2}{\mathcal{J}_1}}$$

Without coherence, Re[ρ_{12}]=0, then $J_j=\varepsilon_j F$ and $\boldsymbol{\eta_{SSD} = \varepsilon_2/\varepsilon_1}$

Optimal performance, coherence, and population inversion



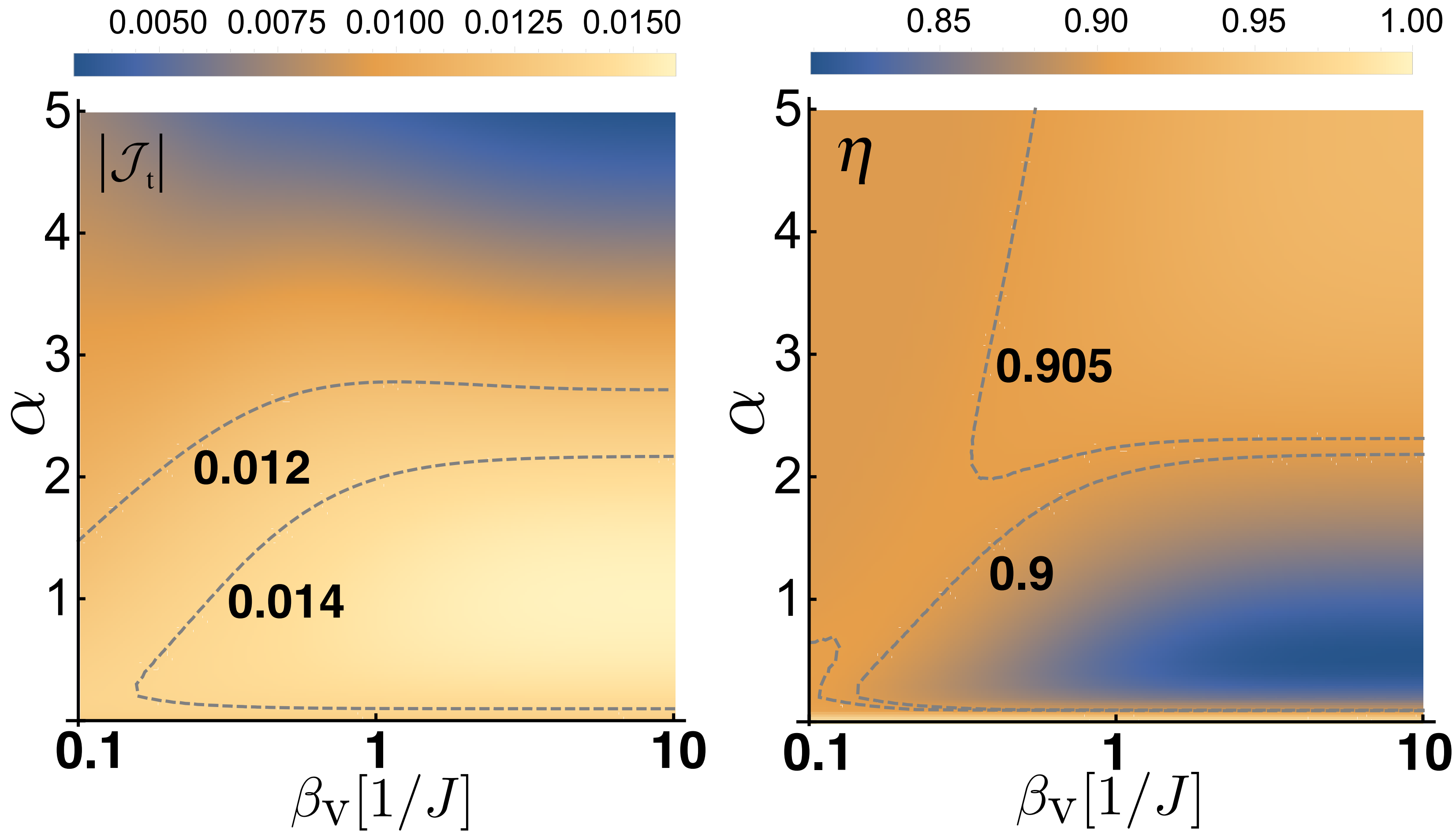
optimal coupling (maximal coherence)



quantum coherence $\sigma_x = \kappa \tan(\theta) \sigma_z$

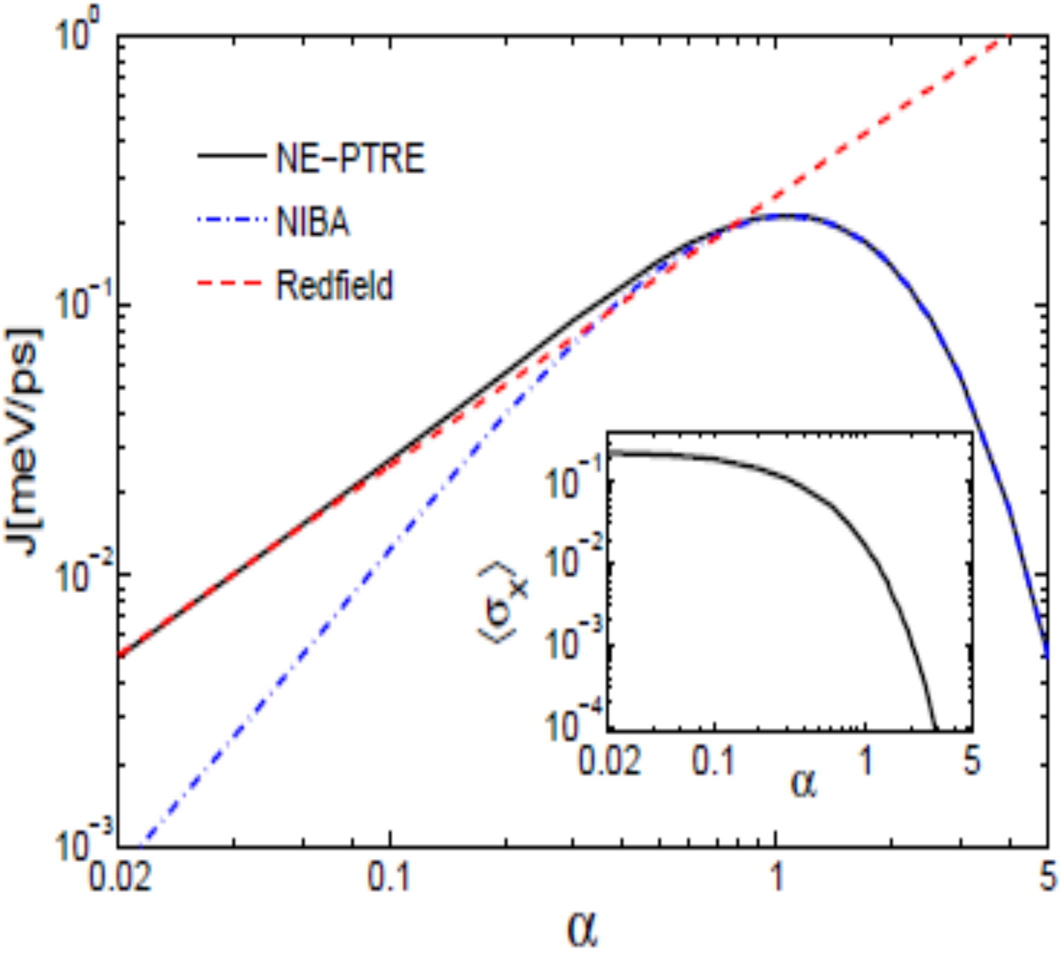
D. Xu, C Wang, Y Zhao, J Cao, NJP18, 023003 (2016)

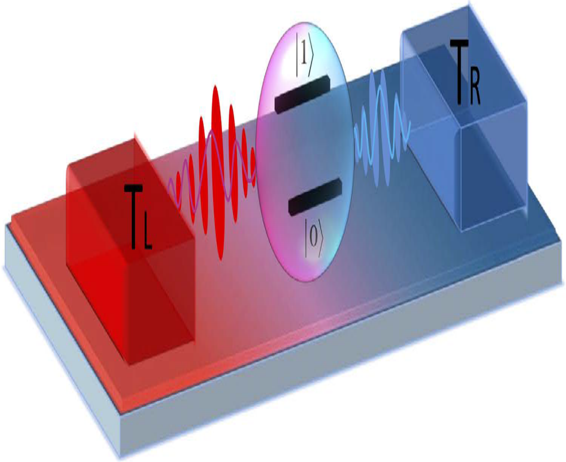
Dependence on temperature and coupling strength



- The high efficiency is not correlated with high energy output
- The optimal regime is intermediate coupling and temperature
- These observations are consistent with LH

Heat transfer in non-equilibrium spin-boson model





differential thermal conductivity
Berry phase in heat pumping
current fluctuations (FDR)

Wang, Ren and Cao, Sci. Rep. 5, 11787(2015) & PRA 95 0236610 (2017)

Non-perturbative Treatment of Quantum Dissipation

Jianshu Cao

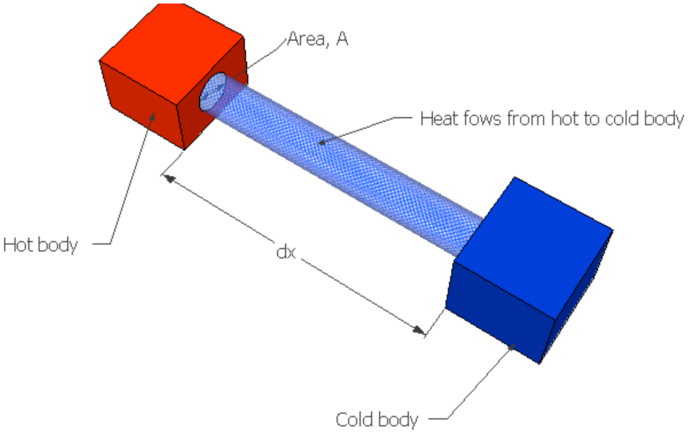
Department of Chemsitry, MIT

- Dynamics and Thermodynamics in the Polaron Frame

  non-canonical thermal distribution
  polaron-transformed Redfield equation
  charge mobility in organic systems
  light-harvesting energy transfer
  heat transfer in NESB

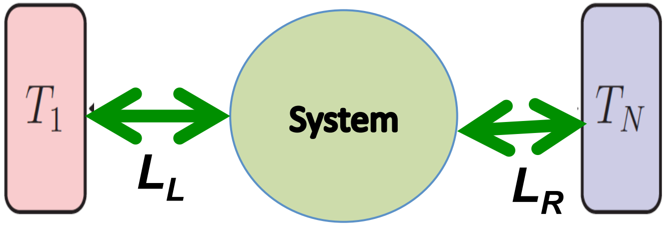
- Symmetry and Multiple Steady-states in Heat Transfer

Heat Transfer and Fourier Law



unique steady state $\vec{J} = \kappa \nabla T$

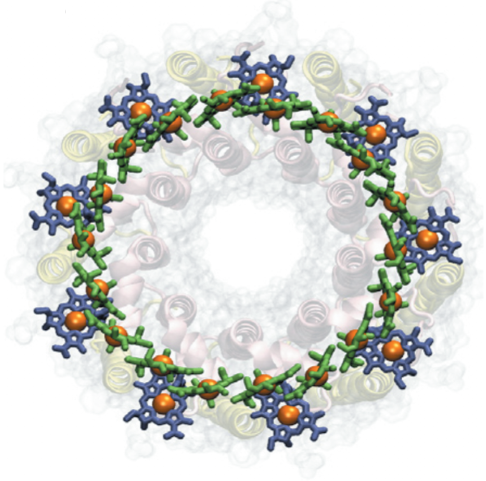
Joseph Fourier (1768 –1830)



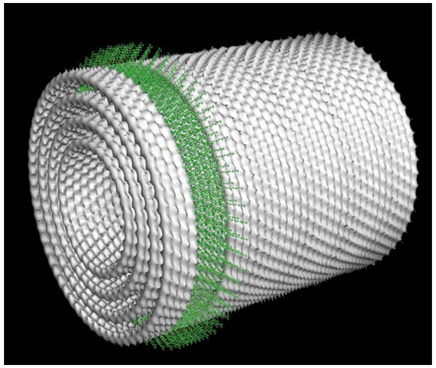
$$\dot{\rho} = -i\left[H_s, \rho\right] + \hat{L}_{\mathrm{L}}\rho + \hat{L}_{\mathrm{R}}\rho \qquad J_{st} = Tr(H_s L_L \rho) = -Tr(H_s L_R \rho)$$

The Liouvillian equation for the quantum system predicts the steady state flux J

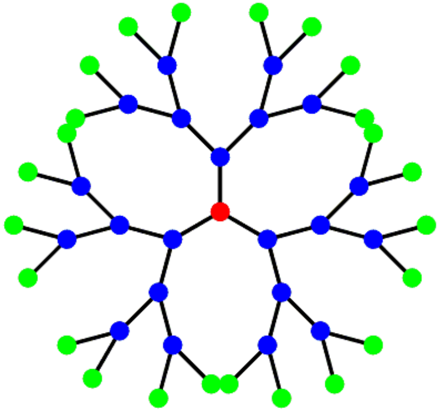
Symmetric Molecular Structures



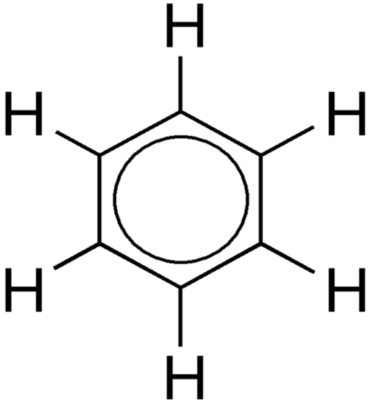
LH2
Cleary, Chen, Silbey, Cao, PNAS 110, 8537 (2013)



Chlorosome
Chuang, Moix, Knoester, Cao, PRL 116, 196803 (2016)

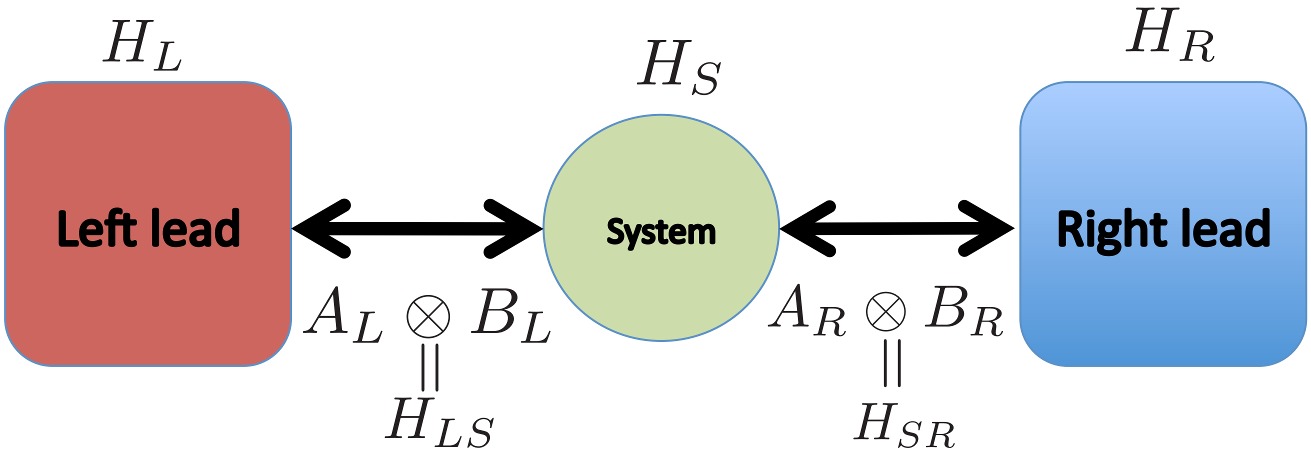


Dendrimer
Wu, Silbey and Cao, PRL 110, 200402 (2013)



Benzene
Thingna, Manzano and Cao, Sci. Rep. 6, 28027 (2016)

Symmetries and Multiple Steady-states



If there exists a unitary operator Π such that:

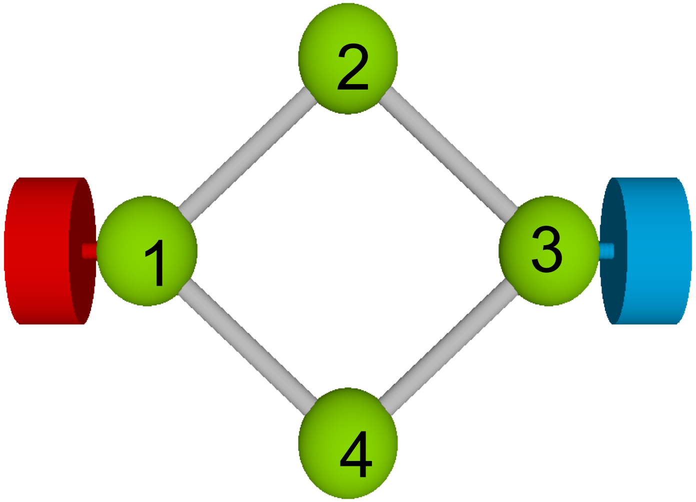
$$[\Pi, H_S] = [\Pi, A_\alpha] = 0$$

$\Longrightarrow$ Multiple steady-states

# of steady states = # of independent symmetry operators + 1

Buča and Prosen, NJP. 14, 073007 (2012); Thingna, Manzano, and J. Cao, Sci Rep. 6, 28027 (2016)

Symmetry and Steady-states of 4-Site Model



mirror symmetry: two steady states

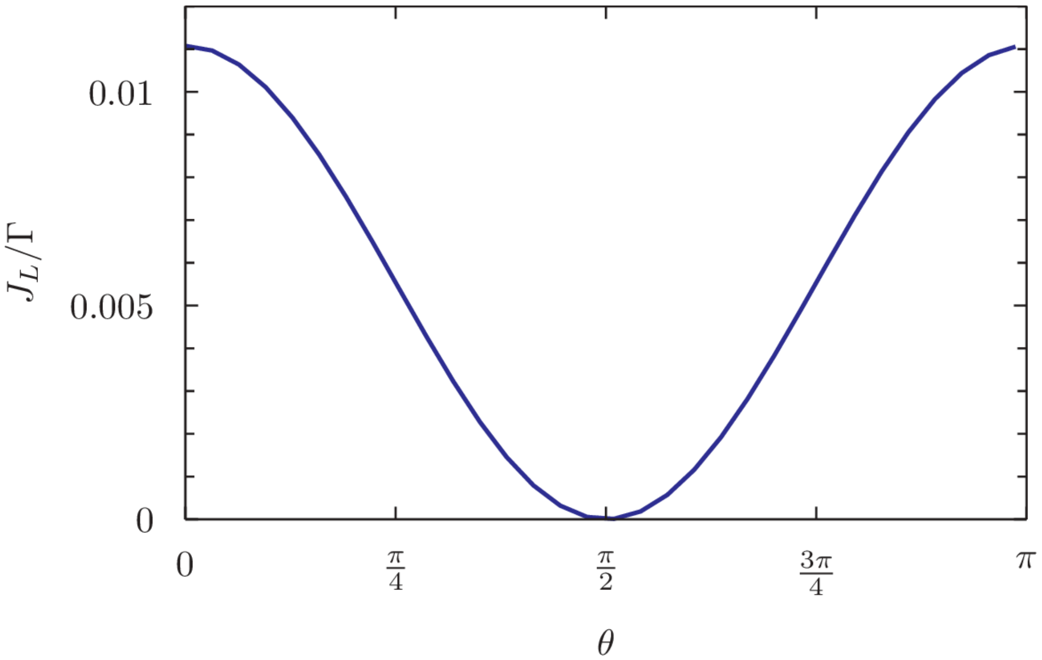
ρ_1: mixed state of even symmetry and non-zero current J_{st}

ρ_2: pure state with zero current J=0

$$\rho_2 = |\psi_2\rangle\langle\psi_2| \quad \psi_2 = \frac{1}{\sqrt{2}}(e_2 - e_4)$$

$$H_S = \begin{pmatrix} e_g & 0 & 0 & 0 & 0 \\ 0 & e_1 & J_1 & 0 & J_1 \\ 0 & J_1 & e_2 & J_2 & 0 \\ 0 & 0 & J_2 & e_3 & J_2 \\ 0 & J_1 & 0 & J_2 & e_2 \end{pmatrix} \Longrightarrow \Pi = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}.$$

Coherent Control of Steady-State Current

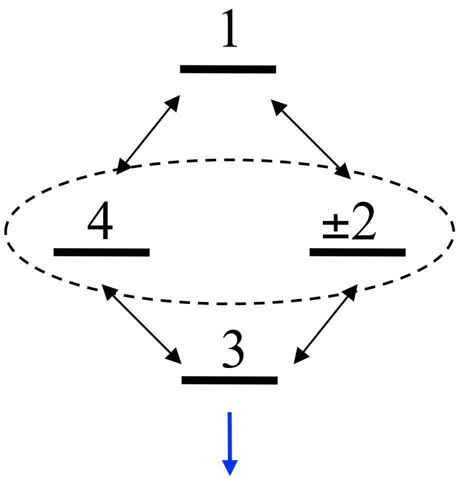


$$\rho(0) = \cos^2(\theta)\rho_1 + \sin^2(\theta)\rho_2$$

$$\theta \equiv \text{Mixing angle}$$

control of steady-state current

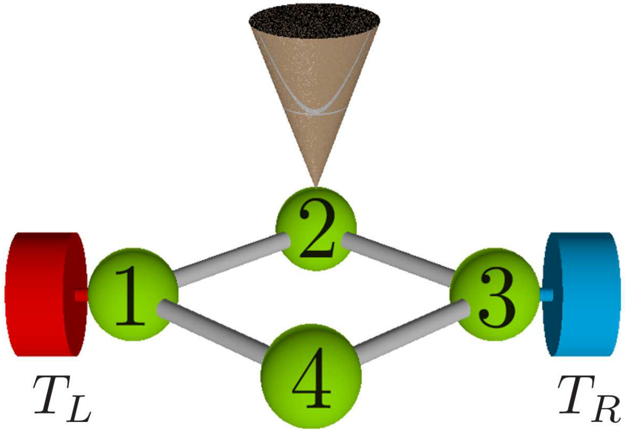
double-slit experiment



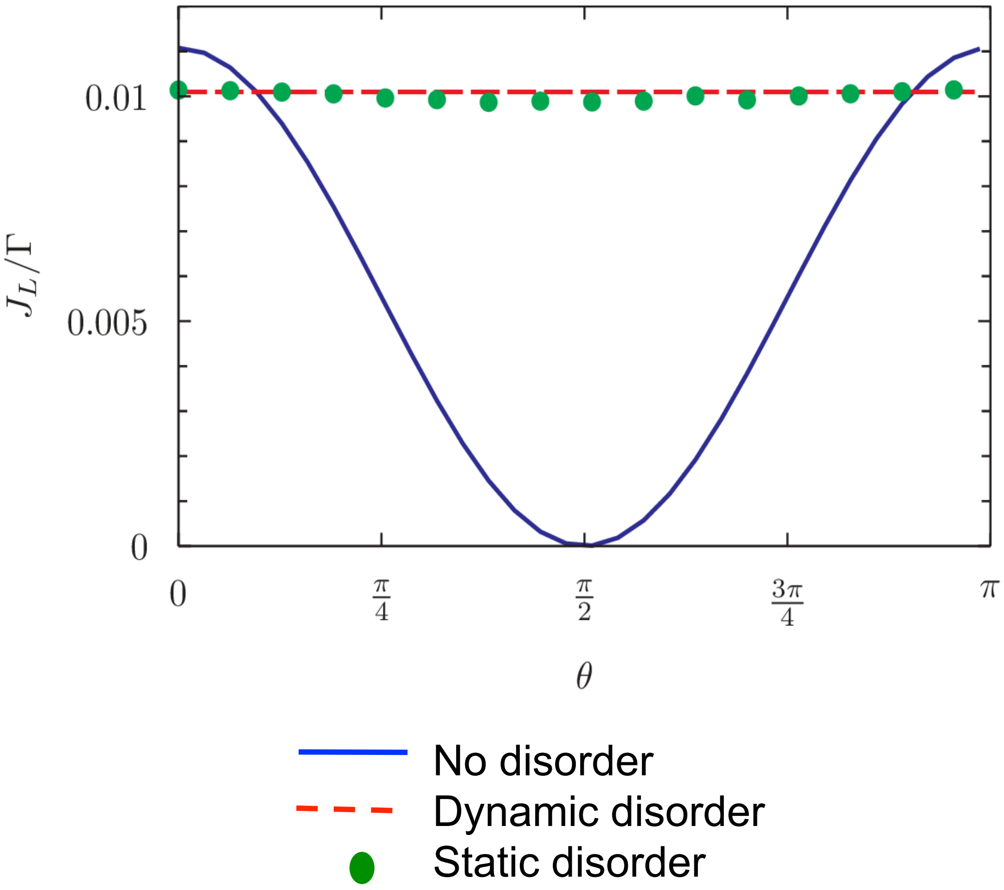
ρ_1 (+) constructive, $J=J_M$
ρ_2 (-) destructive, $J=0$
$0 < J < J_M$

Thingna, Manzano, and Cao, Scientific Reports 6, 28027 (2016)

Broken Symmetry and Unique Steady-State



Buttiker probe



- one unique steady-state.
- quasi steady-state

How to detect symmetry in the presence of disorder?
(steady-state / transient current)

Master Equation and Transient Current

$$\frac{d\rho}{dt} = -\mathrm{i}[H_S, \rho] + \mathcal{L}_P[\rho] + \sum_{\substack{\alpha=L,R\\ i=p,d}}^{\alpha} \mathcal{L}_i^{\alpha}[\rho],$$

The dissipative Liouvillians are given by,

$$\mathcal{L}_i^{\alpha}[\rho] = A_i^{\alpha}\rho A_i^{\alpha\dagger} - \frac{1}{2}\left\{A_i^{\alpha\dagger}A_i^{\alpha}, \rho\right\},$$

$$\mathcal{L}_P[\rho] = \int_0^{\infty} d\tau [S, \rho S(\tau)]C(\tau) - [S, S(\tau)\rho]C(-\tau).$$

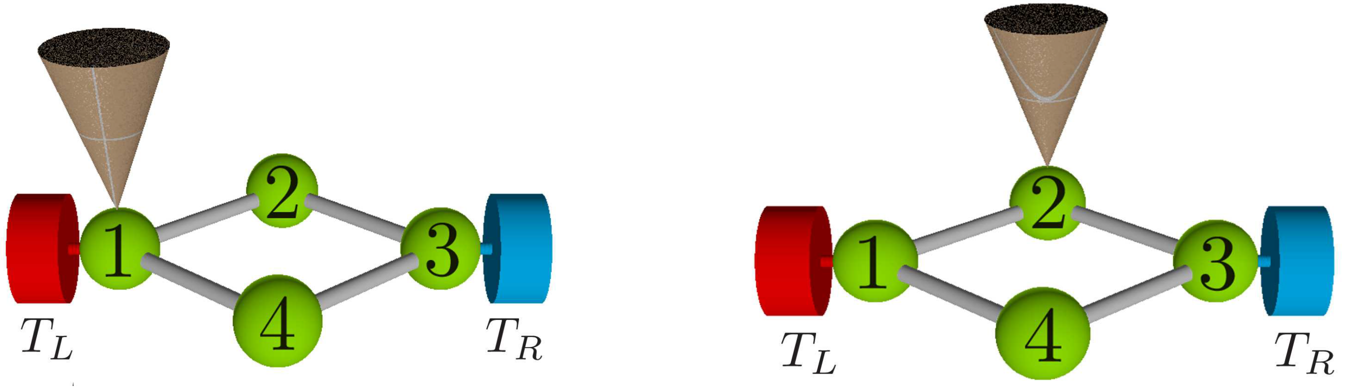
Above S breaks the symmetry, i.e., $[S, \Pi] \neq 0$

$$J(\omega) = \frac{\gamma\omega}{\left[1 + \left(\frac{\omega}{\omega_D}\right)^2\right]}; \quad C(\tau) = \int_0^{\infty} \frac{d\omega}{\pi} J(\omega)\left[\coth\left(\frac{\beta\omega}{2}\right)\cos(\omega\tau) - \mathrm{i}\sin(\omega\tau)\right]$$

The excitonic current

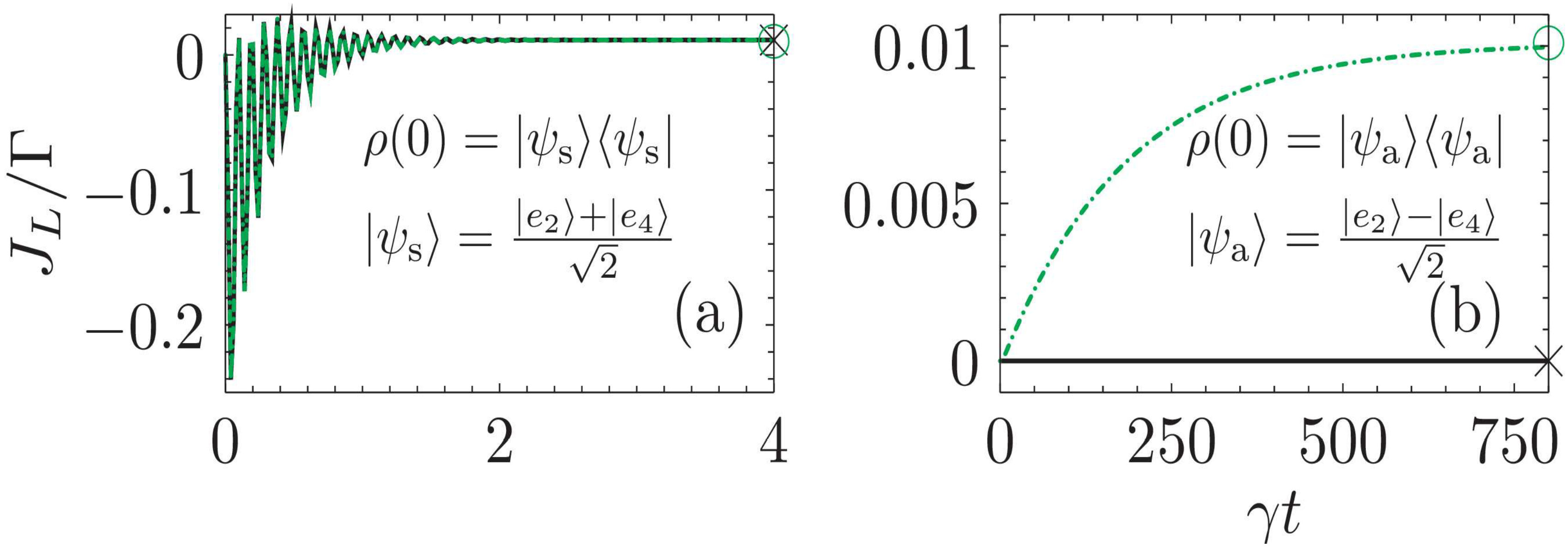
$$J_x^{\mathrm{in}} = \mathrm{Tr}\left(A_p^{L\dagger}A_p^{L}\rho(t)\right) - \mathrm{Tr}\left(A_d^{L\dagger}A_d^{L}\rho(t)\right)$$

Effects of Buttiker Probe



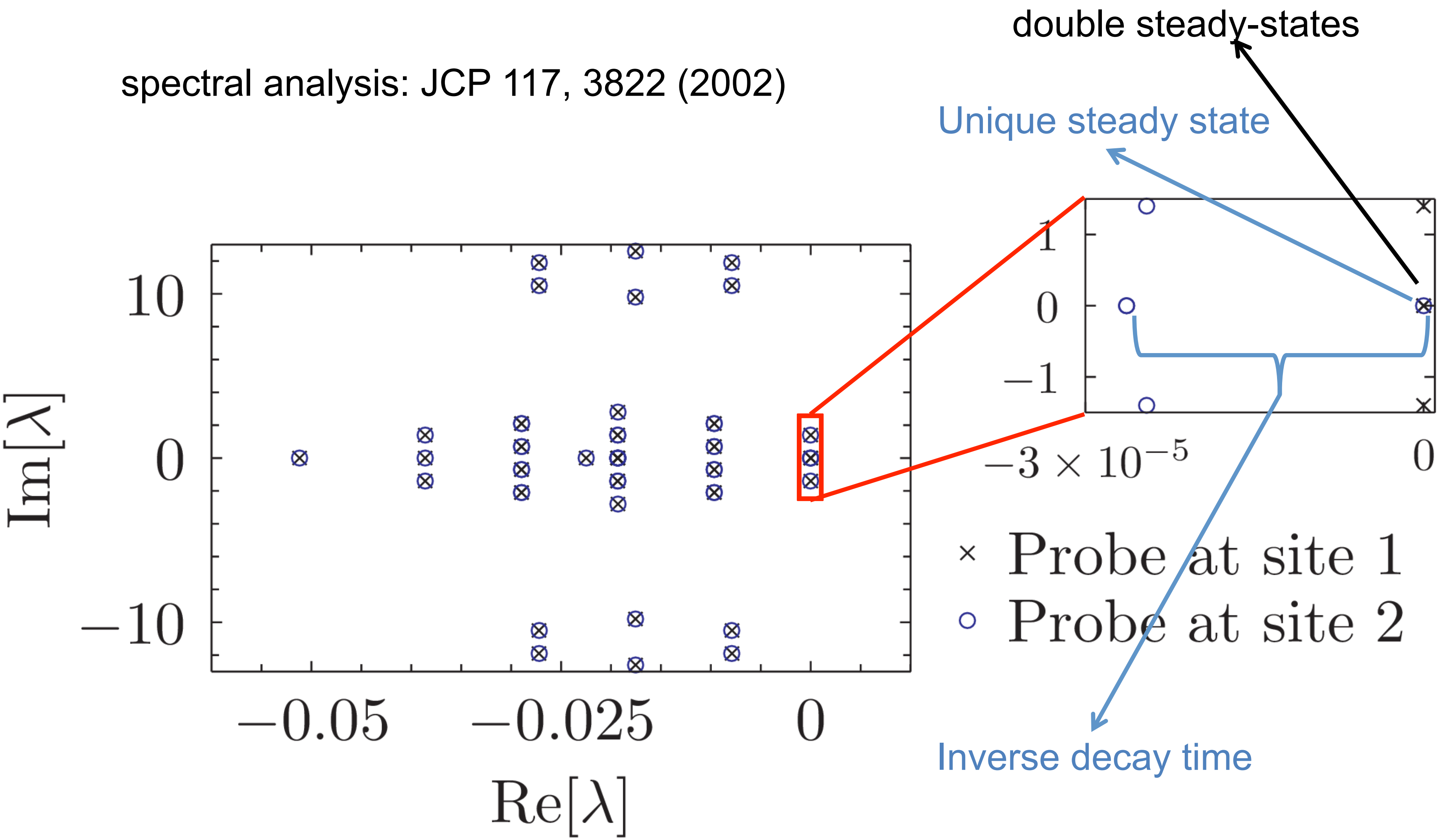
Black solid lines ▬ site 1

Green dashed lines ▬ site 2



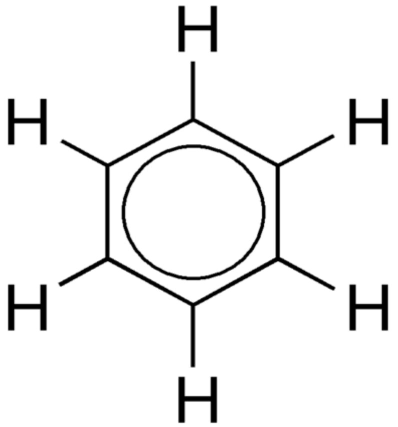
Eigen-spectrum of Open Systems

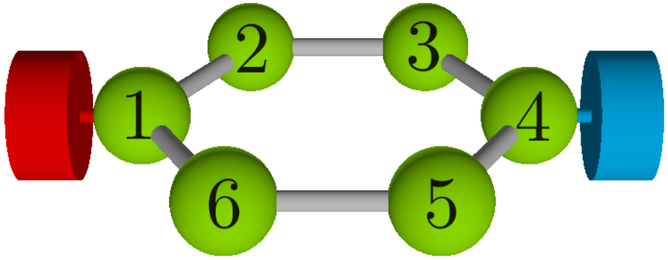
spectral analysis: JCP 117, 3822 (2002)



Thingna, Manzano, and Cao, Scientific Reports 6, 28027 (2016)

Symmetry Structure of Benzene

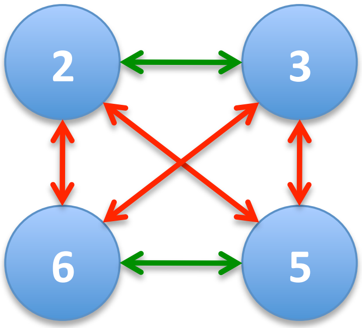




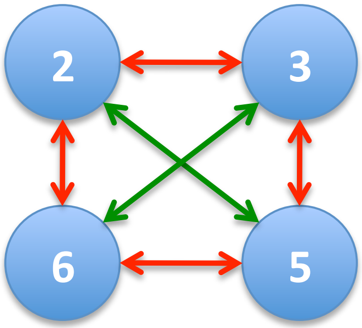
Para-benzene has 2 exchange symmetries and 3 steady-states

1 NESS with even symmetry and steady-state current (ρ_1)

2 pure states with zero steady state current (ρ_2 and ρ_3)



$$\rho_2 = |\psi_2\rangle\langle\psi_2|$$



$$\rho_3 = |\psi_3\rangle\langle\psi_3|$$

↔ symmetric exchange

↔ antisymmetric exchange

Perturbation Analysis

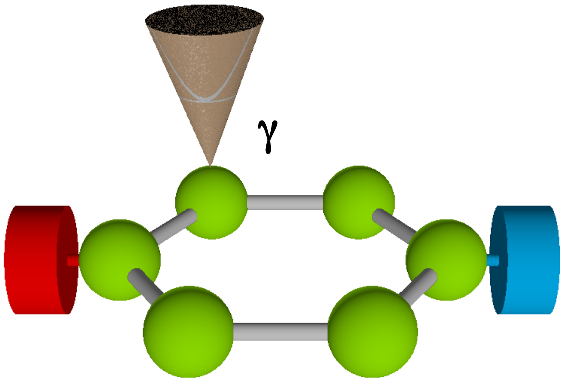
- Para-Benzene molecule has 3 steady-states.
- The application of the probe perturbs the Liouvillian breaking the degeneracy of the 3 steady-states.
- The eigenvalues of the perturbation matrix should give the longest time-scale of the perturbed dynamics.

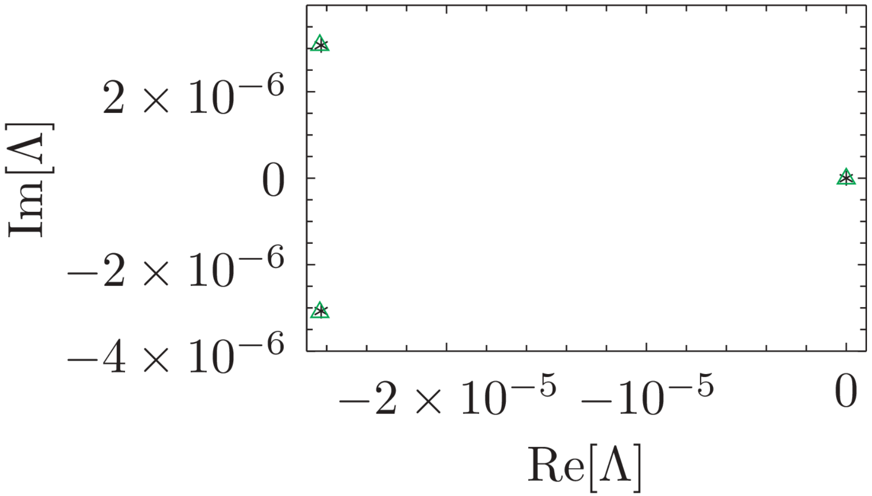
$$L = L_0 + \delta L \qquad \delta L = \begin{pmatrix} \theta_0 & \sigma_1 & \sigma_2 \\ \theta_1 & R_{11} & R_{12} \\ \theta_2 & R_{21} & R_{22} \end{pmatrix}$$

R's are Redfield tensors resulting from the probe
R_{12} ~ 0 because of detailed balance
$R_{21} = 0$ for a single site probe (complex conjugate eigen-values)
R_{21} is non-zero for a double site probe (real eigen-values)

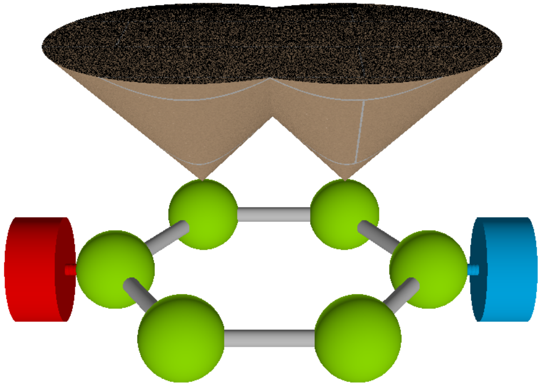
Effects of Probe Location

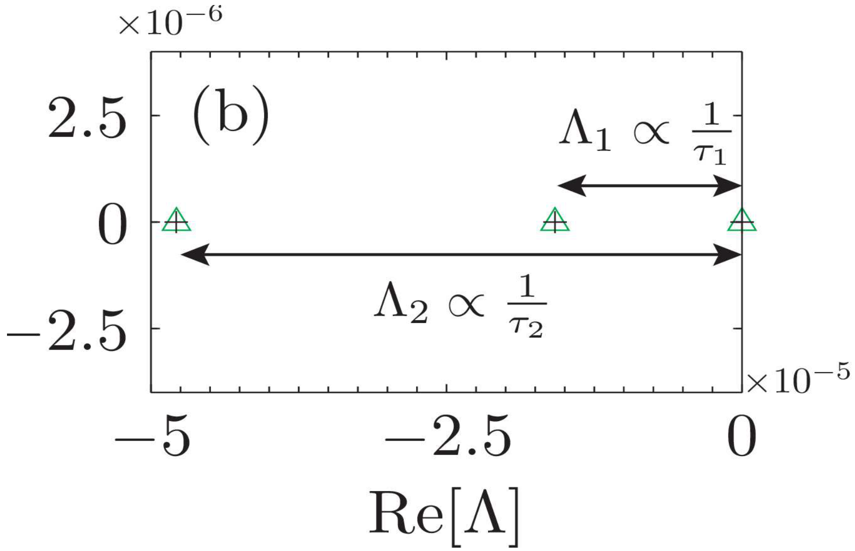
Single site probe



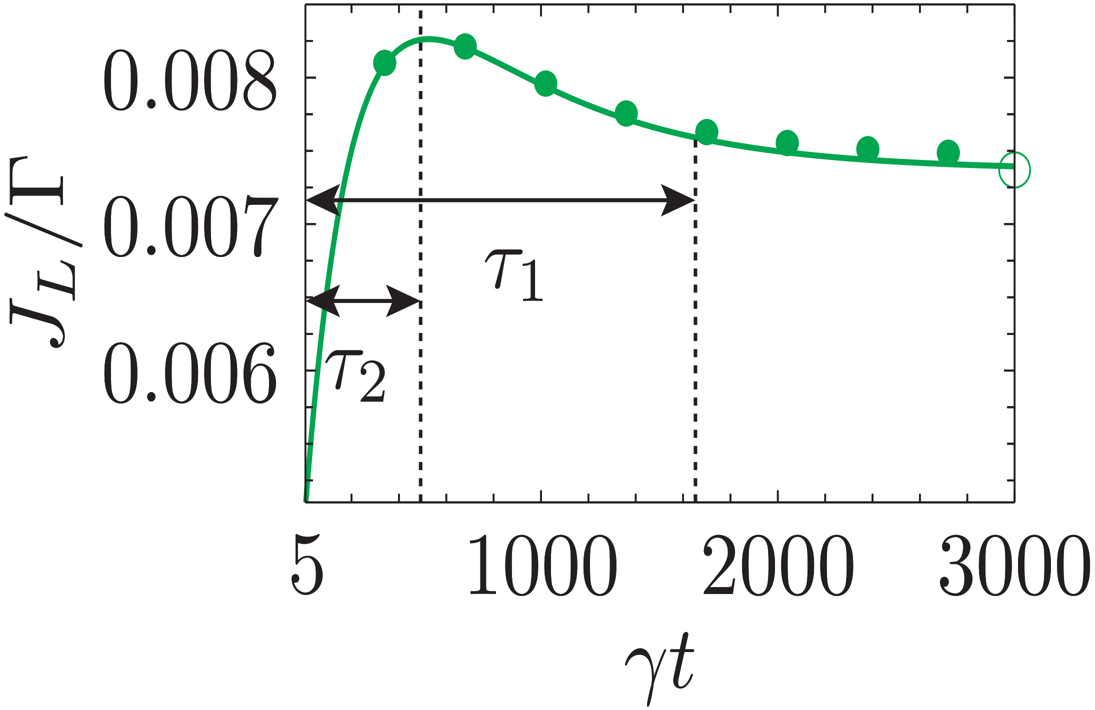


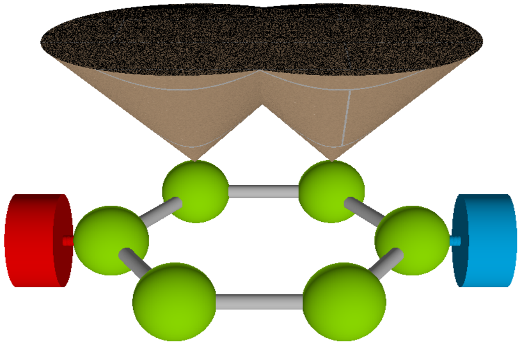
Double site probe





Bi-exponential Relaxation

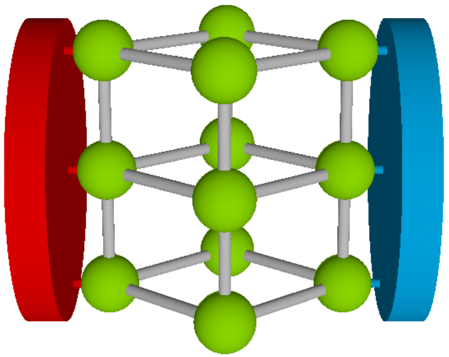




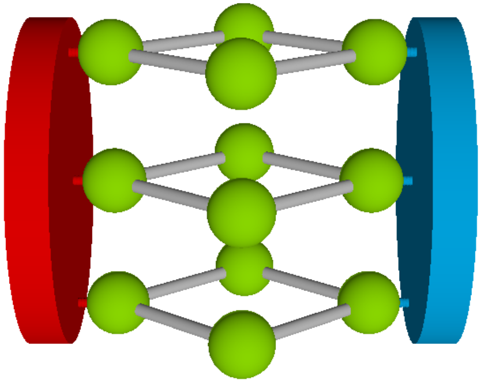
- Buttiker probe breaks the symmetries i.e. the degeneracy
- number of exponents = number of symmetries
- dynamical control of current is robust against static disorder

Thingna, Manzano, and Cao, Scientific Reports 6, 28027 (2016)

Systems of Interest

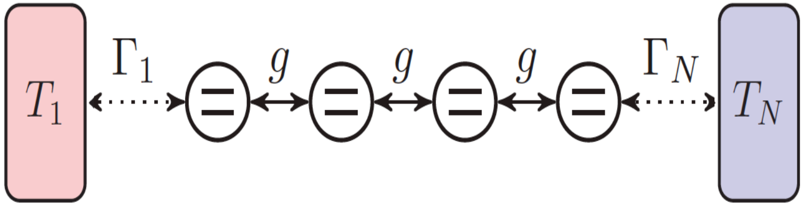


ladder of rings

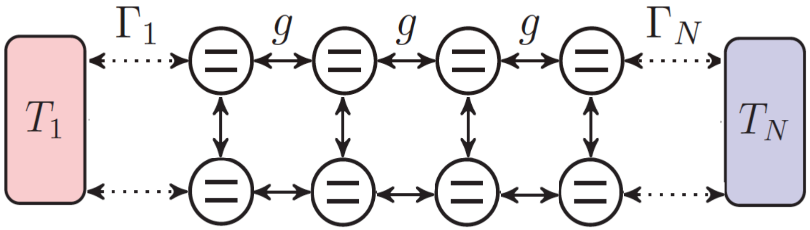


stacked rings

$g\sigma^{+}_{k}\sigma^{-}_{k+1}$ + cc



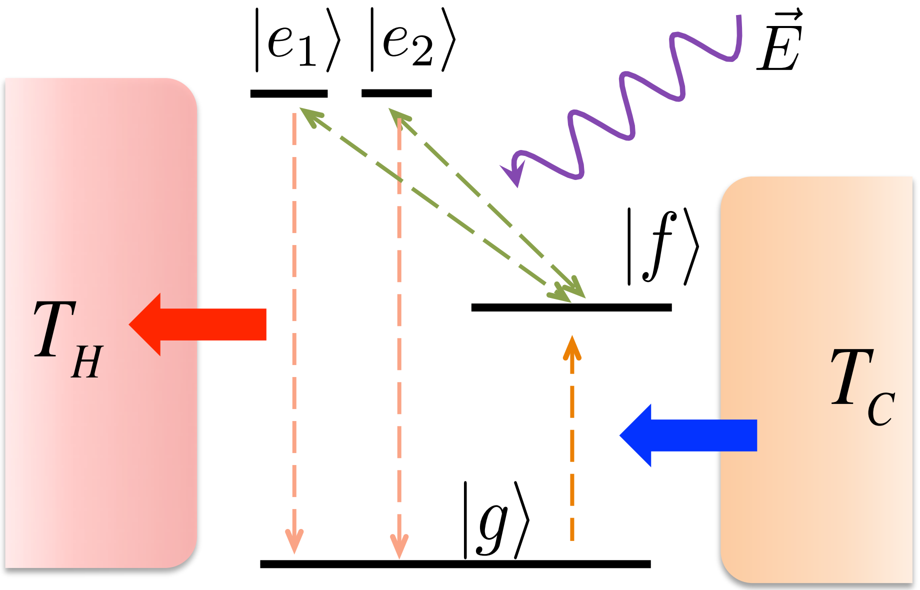
ballistic
spin chain



diffusive
spin ladder

Manzano, Chern, and Cao, NJP 18, 043044 (2016)

Degenerate Heat Engines



Use degeneracy to control coherence and thus energy flux

B=$|e_1>+|e_2>$ is bright, $J < 4J_{single}$ $\eta = \eta_{single}$,

D=$|e_1>-|e_2>$ is dark to the phonon baths but can be bright to photons

Non-equilibrium systems with symmetry will be further explored

Summary

- Dynamics and thermodynamics in the polaron frame
- Symmetry and multiple steady-states

coherent control of steady-state current

dynamical signatures of hidden symmetry

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polaron dynamics: C. Lee, C. Wang, D. Xu
multiple steady-states: J. Thingna, D. Manzano
transfer tensor method (TTM): J Cerrillo
energy transfer in FMO: J. Wu

Funding: NSF and SMART

Thank you for your attention!