A Unified Description of System-Bath Coupling: Polaron Solution and Its Applications to Non-Equilibrium Transport (I)

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Outline

1. Back ground
2. Polaron frame method
    - Polaron transformation
    - Polaron Transformed Redfield Equation (PTRE)
3. Applications of polaron frame
    - Non-canonical distribution
    - Quantum heat engine
    - Heat transfer
    - Quantum coherent transport in disordered systems
4. Summary

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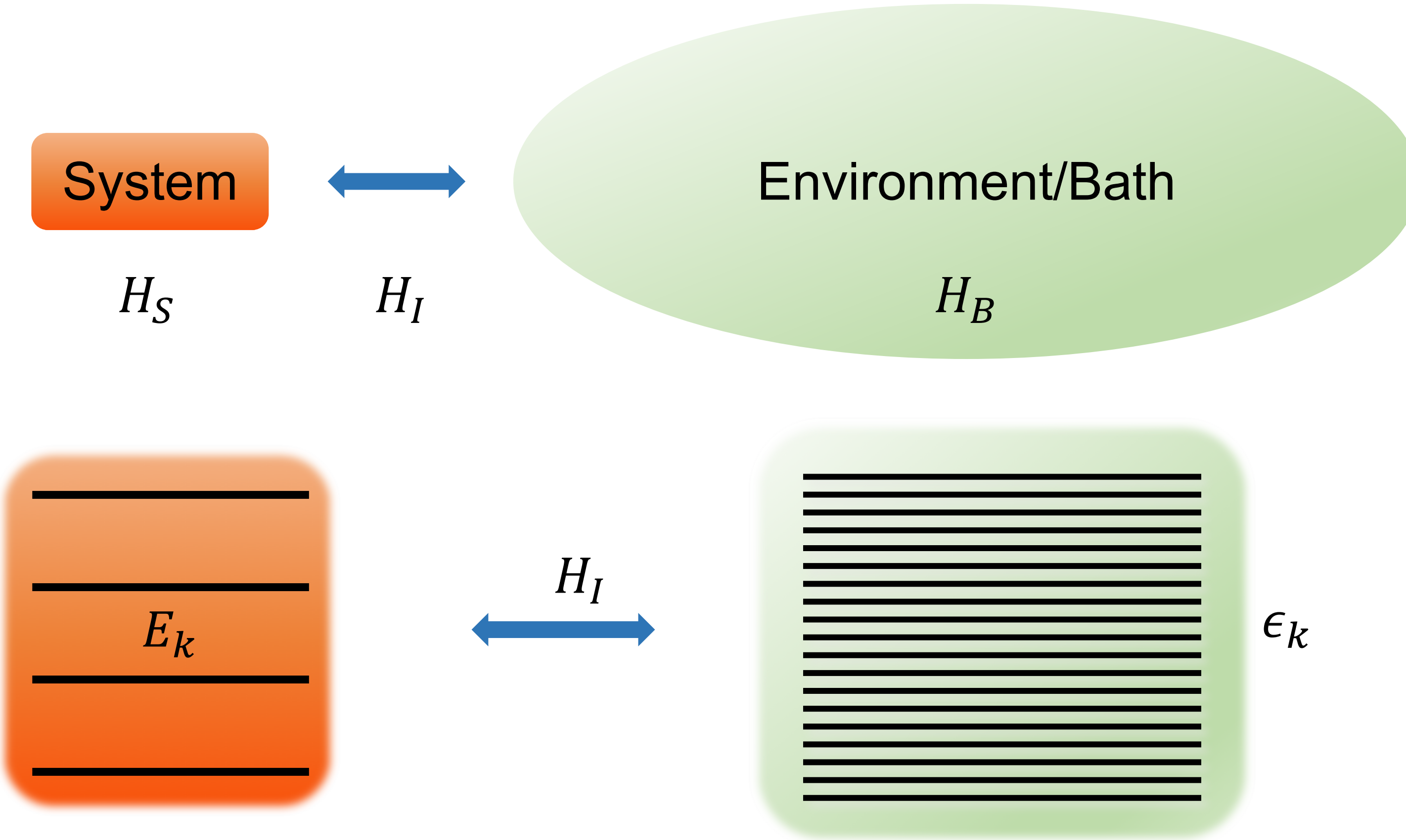
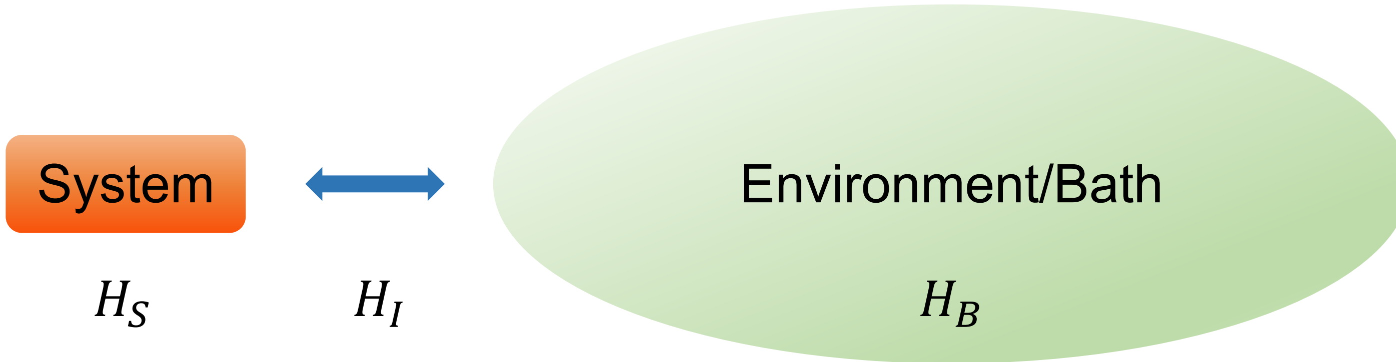
Open Quantum System



- The energy spectrum of the system is much sparser than the heat bath.
- Usually, the coupling between the system and the bath is weak.

Perturbation Treatment of Open Quantum System



system-bath coupling strength α

Weak coupling $\alpha < 1$	Strong coupling $\alpha > 1$
H_I is perturbation	$V_S \in H_S$ is perturbation
Redfield/Lindblad equation	Fermi's Golden Rule/Marcus theory
Γ increases with α and T	Γ dreases with α and T
$\exp(-\beta H_S)$ in eigen basis	$\exp[-\beta(H_S - V_S)]$ in local basis

Weak system-bath coupling

$$\frac{d\rho_S(t)}{dt} = -\frac{1}{\hbar^2}\int_0^t d\tau \mathrm{Tr}_B\left[H_I(t), \left[H_I(\tau), \rho_S(\tau)\otimes\rho_B\right]\right]$$

Redfield equation (Born-Markovian approximation)

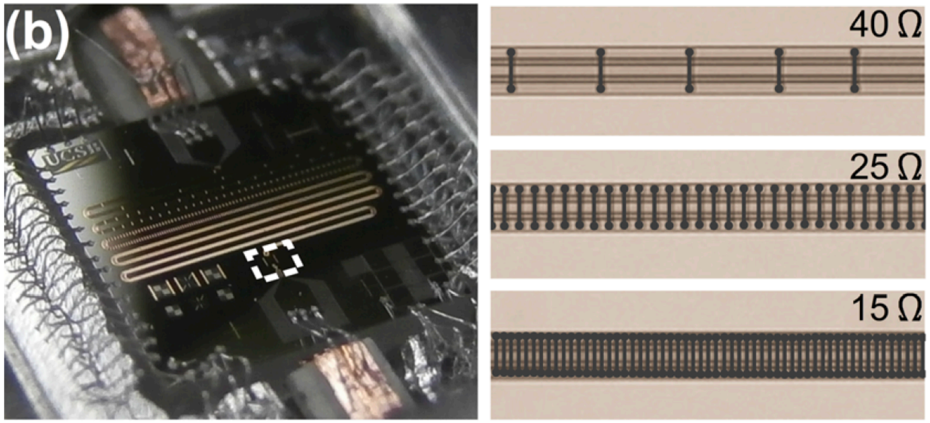
$$\begin{aligned}\frac{d}{dt}\rho_{ab} &= -i\omega_{ab}\rho_{ab} \\ &+ \frac{1}{\hbar^2}\sum_{\alpha\beta}\sum_{cd}\int_0^t d\tau\left[C_{\alpha\beta}(\tau)\left(e^{-i\omega_{ac}\tau}A^{\beta}_{ac}A^{\alpha}_{db} - \delta_{db}\sum_n e^{-i\omega_{nc}\tau}A^{\alpha}_{an}A^{\beta}_{nc}\right)\rho_{cd}\right. \\ &\left. + C^*_{\beta\alpha}(\tau)\left(e^{i\omega_{bd}\tau}A^{\beta}_{ac}A^{\alpha}_{db} - \delta_{ac}\sum_n e^{i\omega_{nd}\tau}A^{\alpha}_{dn}A^{\beta}_{nb}\right)\rho_{cd}\right]\end{aligned}$$

Lindblad equation (Born-Markovian approximation + secular approximation)

$$\frac{d}{dt}\rho(t) = -i\left[H_S, \rho(t)\right] + \frac{1}{2}\sum_j\left\{\left[L_j\rho(t), L_j^{\dagger}\right] + \left[L_j, \rho(t)L_j^{\dagger}\right]\right\}$$

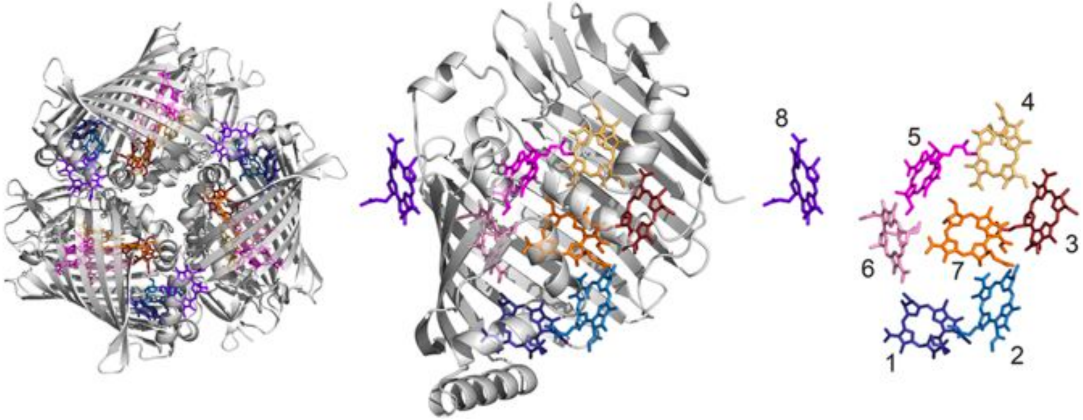
Strong system-bath coupling

Circuit-QED (Josephson parametric amplifier)



Applied Physics Letters **104**, 263513 (2014).

Photosynthesis complexes FMO



Nature (London) **434**, 625(2005);
Scientific Reports **6**, 31875 (2016).

Strong system-bath coupling

NIBA master equation

$$\begin{aligned}\frac{d}{dt}\rho_S^{ee} &= -\gamma(\epsilon)\rho_S^{ee} + \gamma(-\epsilon)\rho_S^{gg} \\ \frac{d}{dt}\rho_S^{gg} &= \gamma(\epsilon)\rho_S^{ee} - \gamma(-\epsilon)\rho_S^{gg}\end{aligned}$$

Fermi's golden rule rate

$$\gamma(\epsilon) = \left(\frac{\kappa\Delta}{2}\right)^2 \int_{-\infty}^{\infty} ds e^{i\epsilon s} \left(e^{Q(s)} - 1\right)$$

Beyond weak system-bath coupling: exact methods

Hierarchy equation of motion (HEOM)

Y. Tanimura and R. Kubo, *J. Phys. Soc. Jpn.* **58** 101 (1989).
Y. Yan, F. Yang, Y. Liu, and J. S. Shao, *Chem. Phys. Lett.* **395** 216 (2004).
R. X. Xu, P. Cui, X. Q. Li, Y. Mo, and Y. J. Yan, *J. Chem. Phys.* **122** 041103 (2005).
A.Ishizaki and Y. Tanimura, *J. Phys. Soc. Jpn.* **74** 3131 (2005).
C. -Y. Hsieh and J. Cao, J. Chem. Phys. **148**, 014103 (2018)

Quasi-adiabatic propagator path integral (QUAPI)

N. Makri and D. E. Makarov, *J. Chem. Phys*. **102**, 4600 (1995).

Multiconfiguration time-dependent Hartree approach

H.-D. Meyer, U. Manthe, and L. Cederbaum, *Chem. Phys. Lett.* **165**, 73 (1990).
M. Beck, A. Jckle, G. Worth, and H.-D. Meyer, *Phys. Rep*. **324**, 1 (2000).
M. Thoss, H. Wang, and W. H. Miller, *J. Chem. Phys*. **115**, 2991 (2001).

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Beyond weak system-bath coupling: PTRE

Polaron transformed Redfield equation (PTRE)

- Give correct result from weak to strong coupling regimes
- Both static and dynamic problems
- Both equilibrium and non-equilibrium systems
- Low computational costs, applicable for large system
- Convenient for analytical analysis

M. Grover and R. Silbey, J. Chem. Phys. **54**, 4843 (1971).
R. Silbey and R. A. Harris, J. Chem. Phys. **80**, 2615 (1984).
C. K. Lee, J. Moix, and J. Cao, J. Chem. Phys. **136**, 204120 (2012).
C. Wang, J. Ren and J. Cao, Scientific Reports **5**, 11787 (2015).
DZX, C. Wang, Y. Zhao, and J. S. Cao, New J. Phys. **18**, 023003 (2016).
DZX and J. S. Cao, Front. Phys. **11**, 110308 (2016).
C. Wang, J. Ren, and J.S. Cao, Phys. Rev. A **95**, 023610 (2017).

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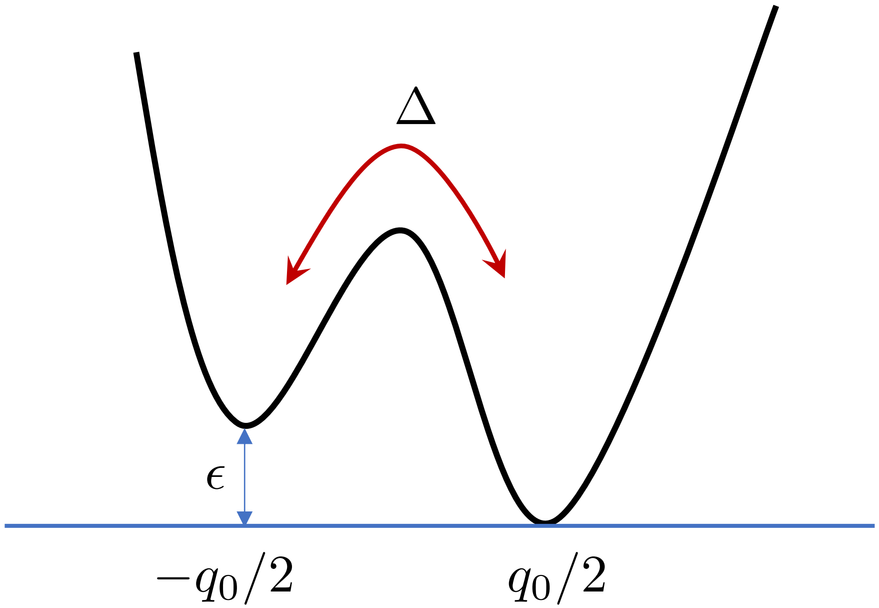
Spin-Boson Model

$$H = \frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sigma_z \frac{q_0}{2}\sum_k c_k x_k + \frac{1}{2}\sum_k \left(\frac{p_k^2}{2m_k} + m_k \omega_k^2 x_k^2\right)$$



A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, *Rev. Mod. Phys*. **59**, 1 (1987).

U. Weiss, Quantum Dissipative Systems (World Scientific, Singapore, 2008).

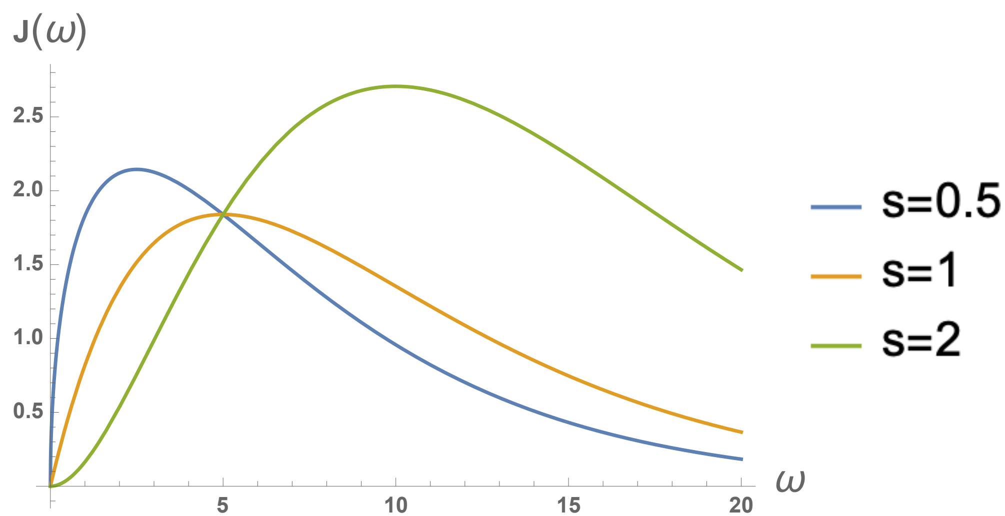
Spectral density

The system-environment coupling is characterized by the spectral density function $J(\omega)$

$$J(\omega) = \frac{\pi}{2} \sum_k \frac{c_k^2}{m_k \omega_k} \delta(\omega - \omega_k)$$

Usually we assume the $J(\omega)$ has a power-law form with an exponential cutoff ω_c

$$J(\omega) = \pi \alpha \omega^s \omega_c^{1-s} e^{-\omega/\omega_c} \quad \begin{cases} 0 < s < 1, & \text{sub-Ohmic} \\ s = 1, & \text{Ohmic} \\ s > 1, & \text{super-Ohmic} \end{cases}$$



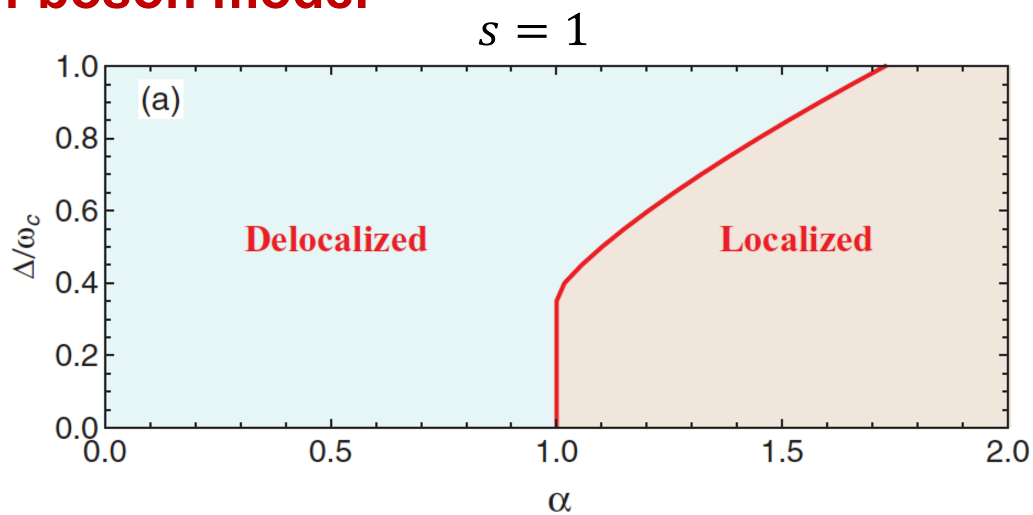
Important parameters for spin-boson model

α: system coupling strength

ω_c: bath cutoff frequency.
Determine how fast the bath can follow the motion of the system

Δ: bare tunnelling matrix element

T: temperature



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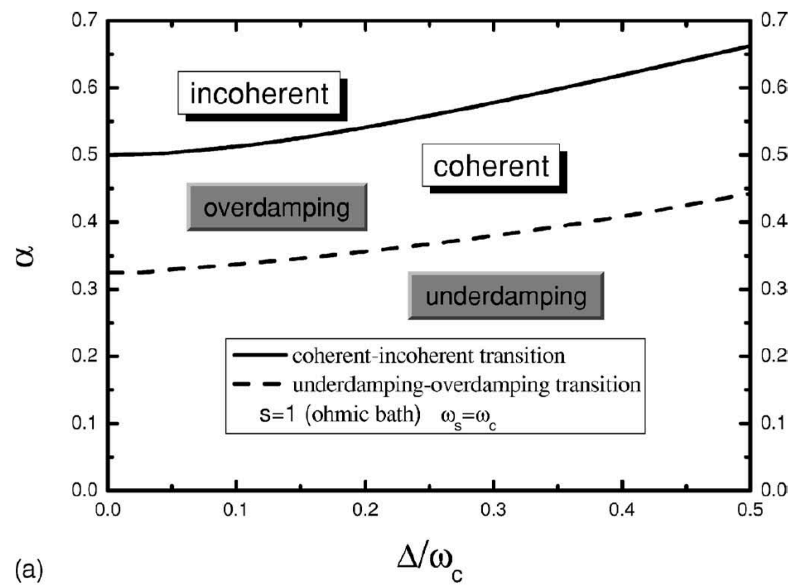

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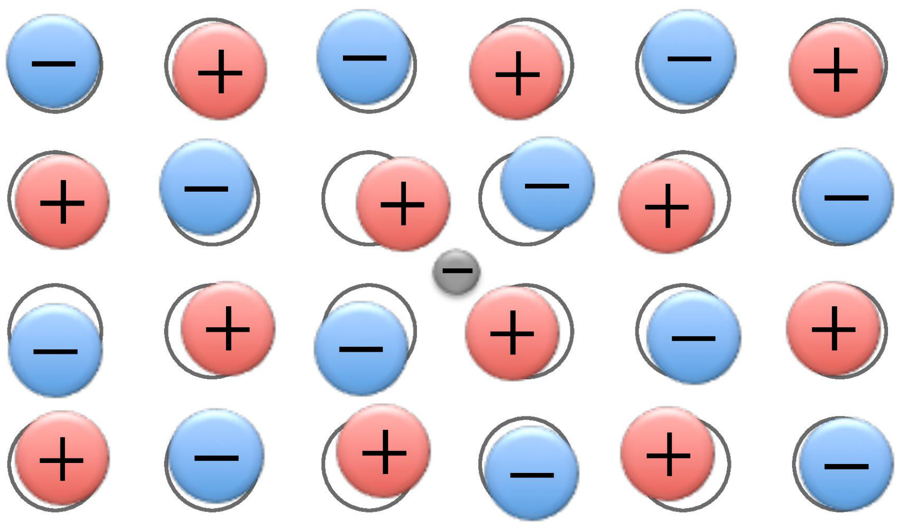
H. B. Wang and M. Thoss, New J. Phys. **10**, 115005 (2008)
A. Chin and M. Turlakov, Phys. Rev. B **73**, 075311 (2011)
C. Duan, Z. Tang, J. Cao, and J. Wu, Phys. Rev. B **95**, 214308 (2017)

Polaron transformation

Polaron: a quasiparticle describing an electron moving in a dielectric crystal where the atoms move from their equilibrium positions to effectively screen the charge of an electron



L. D. Landau, Über die Bewegung der Elektronen in Kristallgitter. *Phys. Z. Sowjetunion* **3,** 644 (1933).
T. D. Lee, F. E. Low, and D. Pines, *Phys. Rev.* **90,** 297 (1953).

Polaron Transformation

Spin-boson model

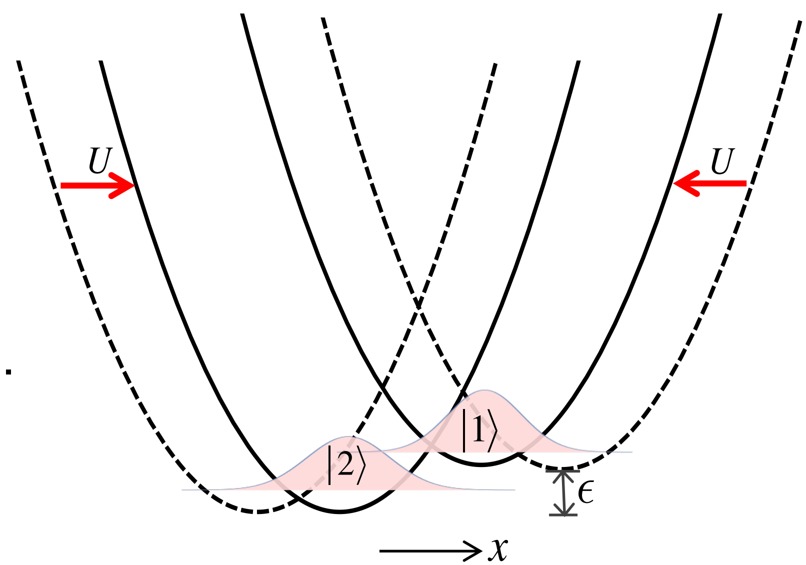
$$H_{tot} = \frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sigma_z \sum_k (g_k b_k^\dagger + g_k^* b_k) + \sum_k \omega_k b_k^\dagger b_k$$

Polaron transformation

$$U = \exp\left(\frac{i}{2}\sigma_z B\right)$$

$$B = 2i \sum_k \left(\frac{f_k}{\omega_k} b_k^\dagger - \frac{f_k^*}{\omega_k} b_k\right)$$

f_k: the variational parameter
$f_k = 0$, the displacement is zero;
$f_k = g_k$, is called full polaron transformation.



Polaron transformation

$$\tilde{H}_{tot} = U^\dagger H_{tot} U = e^{\sigma_z \sum_k \left(\frac{f_k}{\omega_k} b_k^\dagger - \frac{f_k^*}{\omega_k} b_k \right)} H_{tot} e^{-\sigma_z \sum_k \left(\frac{f_k}{\omega_k} b_k^\dagger - \frac{f_k^*}{\omega_k} b_k \right)}$$

$$= U^\dagger \left[\frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sigma_z \sum_k (g_k b_k^\dagger + g_k^* b_k) + \sum_k \omega_k b_k^\dagger b_k \right] U$$

$$\frac{\Delta}{2}(\sigma_x \cos B + \sigma_y \sin B)$$

$$\sigma_z \sum_k \left(g_k b_k^\dagger + g_k^* b_k \right) - \sum_k \frac{1}{\omega_k} (g_k f_k^* + g_k^* f_k)$$

$$\sum_k \left[\omega_k b_k^\dagger b_k - \sigma_z \left(f_k b_k^\dagger + f_k^* b_k \right) + \frac{|f_k|^2}{\omega_k} \right]$$

Polaron transformed system-bath coupling

$$\tilde{H}_{tot} = \frac{\epsilon}{2}\sigma_z + \sum_k \omega_k b_k^\dagger b_k + \sum_k \frac{1}{\omega_k}\left(|f_k|^2 - g_k f_k^* - g_k^* f_k\right)$$
$$+\frac{\Delta}{2}\left(\cos B\sigma_x + \sin B\sigma_y\right) + \sigma_z \sum_k \left[\left(g_k - f_k\right) b_k^\dagger + h.c.\right]$$

- Including transvers system-bath coupling (σ_x and σ_y terms)

- Including high order phonon terms

$$\cos B = 1 - \frac{B^2}{2!} + \frac{B^4}{4!} + \cdots$$
$$\sin B = B - \frac{B^3}{3!} + \frac{B^5}{5!} + \cdots$$

Consider the thermal averages of H_I

x-direction

$$\begin{aligned}\kappa &\equiv \langle \cos B \rangle_{\tilde{H}_B} \\ &= \mathrm{Tr}\left[\frac{\exp\left(-\beta \sum_k \omega_k b_k^\dagger b_k\right)}{\mathcal{Z}_B}\cos B\right] \\ &= \exp\left[-2\sum_k \frac{f_k^2}{\omega_k^2}\coth\left(\frac{\beta\omega_k}{2}\right)\right]\end{aligned}$$

Laguerre polynomial $L_n(x)$

$$L_n(x) = \sum_{k=0}^{n} C_n^k \frac{(-1)^k}{k!} x^k$$

$$\sum_{n=0}^{\infty} \lambda^n L_n(x) = \frac{1}{1-\lambda}\exp\left(-\frac{\lambda x}{1-\lambda}\right)$$

y-direction

$$\langle \sin B \rangle_{\tilde{H}_B} = 0$$

z-direction

$$\left\langle \sum_k \left[(g_k - f_k)\, b_k^\dagger + h.c.\right] \right\rangle_{\tilde{H}_B} = 0$$

Polaron transformed system-bath coupling

$$\begin{aligned}\tilde{H}_{tot} &= \frac{\epsilon}{2}\sigma_z + \sum_k \omega_k b_k^\dagger b_k + \sum_k \frac{1}{\omega_k}\left(|f_k|^2 - g_k f_k^* - g_k^* f_k\right) \\ &+ \frac{\Delta}{2}\left(\cos B\sigma_x + \sin B\sigma_y\right) + \sigma_z \sum_k \left[\left(g_k - f_k\right) b_k^\dagger + h.c.\right] \\ &\equiv H_0 + H_I \equiv H_S + H_B + H_I\end{aligned}$$

$$H_S = \frac{\epsilon}{2}\sigma_z + \frac{\kappa\Delta}{2}\sigma_x + \sum_k \frac{1}{\omega_k}\left(|f_k|^2 - g_k f_k^* - g_k^* f_k\right)$$

$$H_I = \sigma_x V_x + \sigma_y V_y + \sigma_z V_z$$

$$\begin{aligned}V_x &= \frac{\Delta}{2}\left(\cos B - \kappa\right), \\ V_y &= \frac{\Delta}{2}\sin B, \\ V_z &= \sum_k \left[\left(g_k - f_k\right) b_k^\dagger + h.c.\right].\end{aligned}$$

In this arrangement, $\langle H_I \rangle_{H_B} = 0$, thus can be considered as a perturbation.

Variational polaron transformation (Equilibrium)

In order to fix the variational parameters f_k, we minimize the upper bound of the free energy given by the Gibbs-Bogoliubov-Feynman inequality

$$F \leq F_0 + \langle H_I \rangle_{H_0} \equiv A_B$$

R. P. Feynman, *Statistical Mechanics. A set of lectures* (Addison Wesley, Longman, 1998)

F is the free energy of the total system $\widetilde{H}_{tot}$, F_0 is the free energy of only the free Hamiltonian $\widetilde{H}_0$.

$$\begin{aligned} F &= -\frac{1}{\beta} \ln \mathrm{Tr}\left[e^{-\beta \tilde{H}_{tot}}\right] \\ F_0 &= -\frac{1}{\beta} \ln \mathrm{Tr}\left[e^{-\beta H_0}\right] \end{aligned}$$

$$\langle H_I \rangle_{H_0} = \mathrm{Tr}[\frac{e^{-\beta H_0}}{\mathcal{Z}_0} H_I] = 0$$

To minimize the upper bound of free energy, the following equation needs to be solved

$$\frac{dA_B}{df_k} = 0 \quad \Rightarrow \quad f_k = g_k \xi\left(\omega_k\right),$$

where $$\xi\left(\omega_k\right) = \left[1 + \frac{\kappa^2 \Delta^2}{\omega_k \Lambda} \coth\left(\frac{\beta \omega_k}{2}\right) \tanh\left(\frac{\beta \Lambda}{2}\right)\right]^{-1}$$

$$\Lambda = \sqrt{\epsilon^2 + \kappa^2 \Delta^2}$$

$$\kappa = \exp\left[-2 \sum_k \frac{g_k^2}{\omega_k^2} \xi^2\left(\omega_k\right) \coth\left(\frac{\beta \omega_k}{2}\right)\right]$$

$\xi(\omega)$ is a function of κ, and κ is also a function of $\xi(\omega)$, thus the above equation must be solved self-consistently.

R. Silbey and R. A. Harris, J. Chem. Phys. **80**, 2615 (1984).

Spectral density $J\left(\omega\right) = 4\pi \sum g_k^2 \delta\left(\omega - \omega_k\right)$

$$\kappa = \exp\left[-\int_0^\infty \frac{d\omega}{2\pi}\frac{J\left(\omega\right)}{\omega^2}\xi\left(\omega\right)^2 \coth\left(\frac{\beta\omega}{2}\right)\right]$$

$$\xi\left(\omega_k\right) = \left[1 + \frac{\kappa^2\Delta^2}{\omega_k\Lambda}\coth\left(\frac{\beta\omega_k}{2}\right)\tanh\left(\frac{\beta\Lambda}{2}\right)\right]^{-1}$$

1. $\omega_c \ll \Delta$ or $\alpha \ll 1, \Longrightarrow \xi(\omega) \approx 0,\ f_k \approx 0.$

   Bath is too slow to follow the motion of system, the polaron effect almost vanishes.

2. $\omega_c \gg \Delta$ or $\alpha \gg 1, \Longrightarrow \xi(\omega) \approx 1,\ f_k \approx g_k.$

   Full polaron limit, which applies for fast bath or strong system-bath coupling.

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Polaron Transformed Redfield Equation (PTRE)

Full polaron ($f_k = g_k$) transformed Hamiltonian

$$
\begin{aligned}
H_S &= \frac{\epsilon}{2}\sigma_z + \frac{\kappa\Delta}{2}\sigma_x \\
H_B &= \sum_k \omega_k b_k^\dagger b_k \\
H_I &= \sigma_x V_x + \sigma_y V_y
\end{aligned}
$$

PTRE is derived in the eigen representation of H_S

$$H_S|\pm\rangle = \pm\sqrt{\epsilon^2 + \kappa^2\Delta^2}|\pm\rangle \equiv \pm\Lambda|\pm\rangle$$

$$
\begin{aligned}
|+\rangle &= \cos\frac{\theta}{2}\,|e\rangle + \sin\frac{\theta}{2}\,|g\rangle\,, \\
|-\rangle &= \sin\frac{\theta}{2}\,|e\rangle - \cos\frac{\theta}{2}\,|g\rangle\,.
\end{aligned}
$$

$$\tan\theta = \kappa\Delta/\epsilon$$

In the interaction picture, $\hat{A}(t) \equiv e^{iH_0 t} A e^{-iH_0 t}$, the density matrix of total open system $\hat{\rho}_{tot}(t)$ satisfies

$$\frac{d}{dt}\hat{\rho}_{tot}(t) = -i\left[\hat{H}_I(t), \hat{\rho}_{tot}(t)\right] \tag{1}$$

Formally integration

$$\Rightarrow \quad \hat{\rho}_{tot}(t) = \hat{\rho}_{tot}(0) - i\int_0^t ds\left[\hat{H}_I(s), \hat{\rho}_{tot}(s)\right] \tag{2}$$

Take (2) into (1),

with the fact $\mathrm{Tr}_B\left[\hat{H}_I(t), \hat{\rho}_{tot}(0)\right] = 0$ and Born approximation

$$\hat{\rho}_{tot}(s) = \hat{\rho}_S(s) \otimes \rho_B$$

$$\Rightarrow \quad \frac{d}{dt}\hat{\rho}_S(t) = -\int_0^t ds \mathrm{Tr}_B\left[\hat{H}_I(t), \left[\hat{H}_I(s), \hat{\rho}_S(s) \otimes \rho_B\right]\right]$$

$$\frac{d}{dt}\hat{\rho}_S\left(t\right) = -\int_0^t ds \mathrm{Tr}_B\left[\hat{H}_I\left(t\right), \left[\hat{H}_I\left(s\right), \hat{\rho}_S(s) \otimes \rho_B\right]\right]$$

Markov approximation: 1) $\hat{\rho}_S(s) \to \hat{\rho}_S(t)$;
2) $s \to t - s$;
3) $\int_0^t \to \int_0^\infty$.

Born-Markov master equation:

➡ $$\frac{d}{dt}\hat{\rho}_S\left(t\right) = -\int_0^\infty ds \mathrm{Tr}_B\left[\hat{H}_I\left(t\right), \left[\hat{H}_I\left(t-s\right), \hat{\rho}_S(t) \otimes \rho_B\right]\right]$$

Transform back to the Schrodinger picture:

$$\frac{d\rho_S(t)}{dt} = -i[H_S, \rho_S(t)] - \int_0^\infty ds \mathrm{Tr}_B\left\{\left[H_I, \left[\hat{H}_I(-s), \rho_S(t) \otimes \rho_B\right]\right]\right\}$$

$$\hat{H}_I(t) = \hat{\sigma}_x(t)\,\hat{V}_x(t) + \hat{\sigma}_y(t)\,\hat{V}_y(t)$$

⬇

$$\frac{d\rho_S(t)}{dt} = -i[H_S, \rho_S(t)] - \sum_{i,j=x,y} \int_0^\infty ds \langle V_i V_j(-s) \rangle_B \left[\sigma_i, \sigma_j(-s)\rho_S(t)\right] + \text{H.c.}$$

Bath correlation functions:

$$\begin{aligned}
\langle V_x V_x(-s)\rangle_B &= (\frac{\kappa\Delta}{2})^2 \left(\cosh\left[Q(s)\right] - 1\right) \\
\langle V_y V_y(-s)\rangle_B &= (\frac{\kappa\Delta}{2})^2 \sinh\left[Q(s)\right] \\
\langle V_x V_y(-s)\rangle_B &= \langle V_y V_x(-s)\rangle_B = 0
\end{aligned}$$

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

average phonon number $n(\omega) = 1/[\exp(\beta\omega) - 1]$

Pauli operators in the eigen representation

$$\begin{aligned}\tau_z &= \left|+\right\rangle\left\langle+\right| - \left|-\right\rangle\left\langle-\right|, \\ \tau_+ &= \left|+\right\rangle\left\langle-\right|, \\ \tau_- &= \left|-\right\rangle\left\langle+\right|.\end{aligned}$$

The system operators can be written as

$$\begin{aligned}\hat{\sigma}_x(t) &= \sin\theta\tau_z - \cos\theta\left(\tau_+ e^{i\Lambda t} + \tau_- e^{-i\Lambda t}\right) \equiv \sum_{i=z,\pm} c_i^x e^{-i\omega_i t}\tau_i \\ \hat{\sigma}_y(t) &= i\tau_+ e^{i\Lambda t} - i\tau_- e^{-i\Lambda t} \equiv \sum_{i=z,\pm} c_i^y e^{-i\omega_i t}\tau_i\end{aligned}$$

PTRE:

$$\frac{d\rho_S(t)}{dt} = -i[H_S, \rho_S(t)] - \sum_{k=x,y}\sum_{i,j=z,\pm} c_i^k c_j^k \Gamma_k(\omega_j)\left[\tau_i, \tau_j\rho_S(t)\right] + \mathrm{H.c.}$$

$$\Gamma_k(\omega) = \int_0^\infty ds e^{i\omega s}\langle V_k V_k(-s)\rangle_B$$

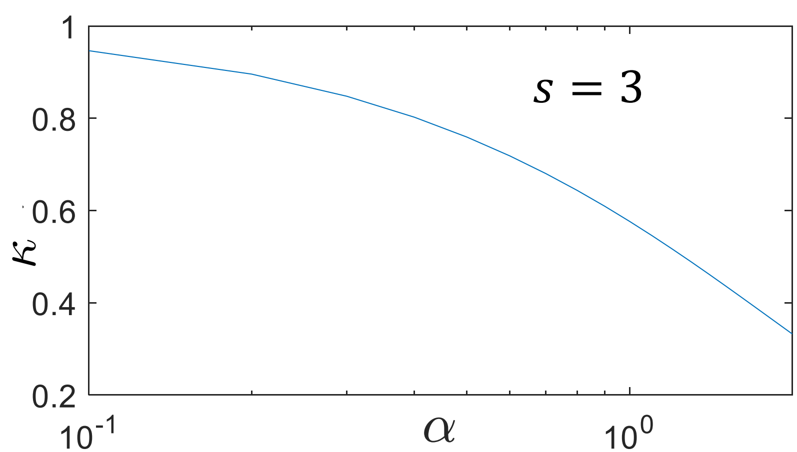
C. Wang, J. Ren and J. Cao, Scientific Reports **5**, 11787 (2015).
DZX, C. Wang, Y. Zhao, and J. S. Cao, New J. Phys. **18**, 023003 (2016).

Some remarks

- ✓ For Ohmic and sub-Ohmic spectral density, $\kappa = 0$, renormalized tunneling is 0. Always giving strong coupling limit result.
- ✓ Super-Ohmic spectral density, e.g. $s = 3$

$$J(\omega) = \pi\alpha\omega^3\omega_c^{-2}e^{-\omega/\omega_c}$$

$$\begin{aligned} Q(\tau) &= \int_0^\infty d\omega \frac{J(\omega)}{\pi\omega^2}\left[(2n(\omega)+1)\cos(\omega\tau) - i\sin\omega\tau\right] \\ &= \alpha\left(\frac{-1+\omega_c^2\tau^2}{(1+\omega_c^2\tau^2)^2} + \frac{2\mathrm{Re}[\psi_1(\frac{1}{\beta\omega_c}+\frac{i\tau}{\beta})]}{(\beta\omega_c)^2} - \frac{2i\omega_c\tau}{(1+\omega_c^2\tau^2)^2}\right) \end{aligned}$$



Tri-gamma function

$$\psi_1(x) = \sum_{n=0}^{\infty}\frac{1}{(n+x)^2}$$

PTRE---weak coupling limit

$\alpha \gg 1$ ➡ $\kappa = \langle \cos B \rangle \approx 1$

$$\cosh\left[Q\left(\tau\right)\right] - 1 \approx 0$$

$$\sinh\left[Q\left(\tau\right)\right] \approx Q\left(\tau\right) \propto \alpha$$

$$\frac{d\rho_S(t)}{dt} = -i[H_S, \rho_S(t)] - \sum_{i,j=\pm} c_i^y c_j^y \Gamma_y\left(\omega_j\right)\left[\tau_i, \tau_j \rho_S(t)\right] + \text{H.c.}$$

➡ Redfield equation in eigen basis

$$\frac{d}{dt}\rho_S^{++} = -\gamma(\Lambda)\left(n\left(\Lambda\right)+1\right)\rho_S^{++} - \gamma(\Lambda) n\left(\Lambda\right)\rho_S^{--}$$

$$\frac{d}{dt}\rho_S^{+-} = -i\Lambda\rho_S^{+-} - \gamma(\Lambda)(n\left(\Lambda\right)+\frac{1}{2})\left(\rho_S^{+-} - \rho_S^{-+}\right)$$

$$\gamma(\Lambda) = \frac{J\left(\Lambda\right)}{2}\sin\theta \propto \alpha$$

PTRE---strong coupling limit

$$\alpha \gg 1 \;\Rightarrow\; \kappa = \langle \cos B \rangle \ll 1,\;\; \theta \approx 0$$

Eigen basis returns to local basis

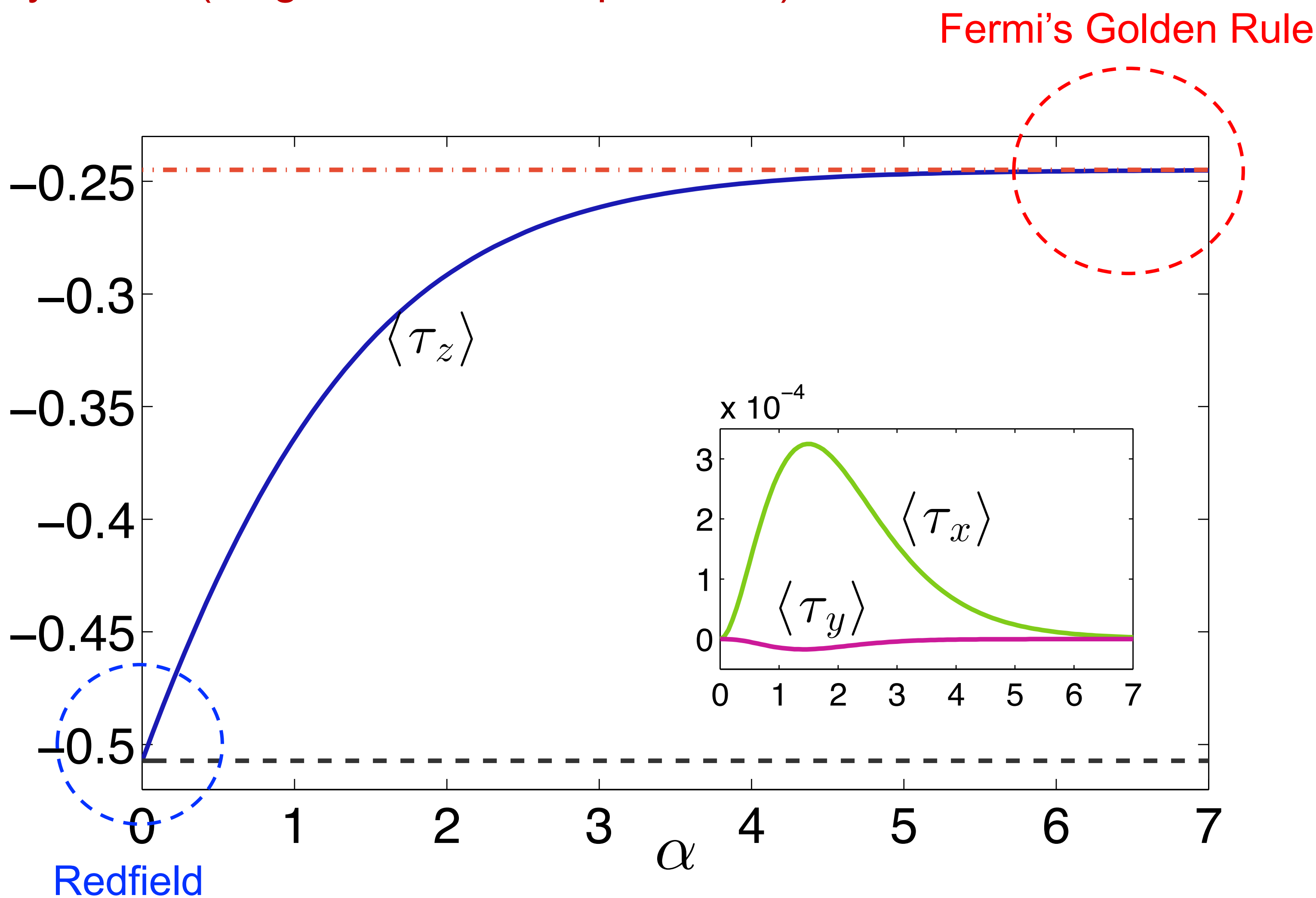
$$\begin{aligned} \left|+\right\rangle &\approx \left|e\right\rangle , \\ \left|-\right\rangle &\approx -\left|g\right\rangle . \end{aligned}$$

⇒ Rate equation in local basis $\quad Q^{*}\left(s\right) = Q\left(-s\right)$

$$\begin{aligned} \frac{d}{dt}\rho_S^{ee} &= -\gamma(\epsilon)\rho_S^{ee} + \gamma(-\epsilon)\rho_S^{gg} \\ \frac{d}{dt}\rho_S^{gg} &= \gamma(\epsilon)\rho_S^{ee} - \gamma(-\epsilon)\rho_S^{gg} \end{aligned}$$

Fermi's Golden Rule rate $\quad \gamma(\epsilon) = \left(\frac{\kappa\Delta}{2}\right)^2 \int_{-\infty}^{\infty} ds e^{i\epsilon s} \left(e^{Q(s)} - 1\right)$

Steady states (long time limit → equilibrium)



$$\langle \tau_z \rangle = \frac{1 - \exp(\beta\sqrt{\epsilon^2 + \kappa^2\Delta^2})}{1 + \exp(\beta\sqrt{\epsilon^2 + \kappa^2\Delta^2})}$$

List of Publications on PTRE

Accuracy of second order perturbation theory in the polaron and variational polaron frames. Lee, Moix, and Cao, J. Chem. Phys. 136, 204120 (2012)

Noncanonical statistics of a spin-boson model: Theory and exact Monte Carlo simulations. .
Lee, Cao, and Gong, Phys. Rev. E 86, 021109 (2012)

Coherent quantum transport in disordered systems: A unified polaron treatment of hopping and band-like transport. Lee, Moix, and Cao, J. Chem. Phys. 142, 164103 (2015)

Nonequilibrium energy transfer at nanoscale: A unified theory from weak to strong coupling.
Wang, Jie, and Cao, Sci. Rep. 5, 11787 (2015)

Polaron effects on the performance of light-harvesting systems: A quantum heat engine perspective. Xu, Wang, Zhao, and Cao, New J. Phys. 18, 023003 (2016)

Non-canonical distribution and non-equilibrium transport beyond weak system-bath coupling regime.
Xu and Cao, Front. Phys. 11, 1 (2016) [review article]

Unifying quantum heat transfer in a nonequilibrium spin-boson model with full counting statistics.
Wang, Ren, and Cao, Phys. Rev. A 95, 023610 (2017)

Frequency-dependent current noise in quantum heat transfer with full counting statistics.
Liu, Hsieh, Wu, and Cao, J. Chem. Phys. 148, 234104 (2018)

Tuning the Aharonov-Bohm effect with dephasing in non-equilibrium transport
G. Engelhardt and J. Cao, Phys. Rev. B 99, 075436 (2019)

A non-equilibrium variational polaron theory to study quantum heat transfer
Hsien, Liu, Duan, and Cao (2019, submitted)

A Unified Description of System-Bath Coupling: Polaron Solution and Its Applications to Non-Equilibrium Transport (II)

Dazhi Xu (徐大智)
School of Physics, Beijing Institute of Technology

CSRC Summer School on Quantum Non-Equilibrium Phenomena: Methods and Applications, 20th June 2019

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1. Back ground
2. Polaron frame method
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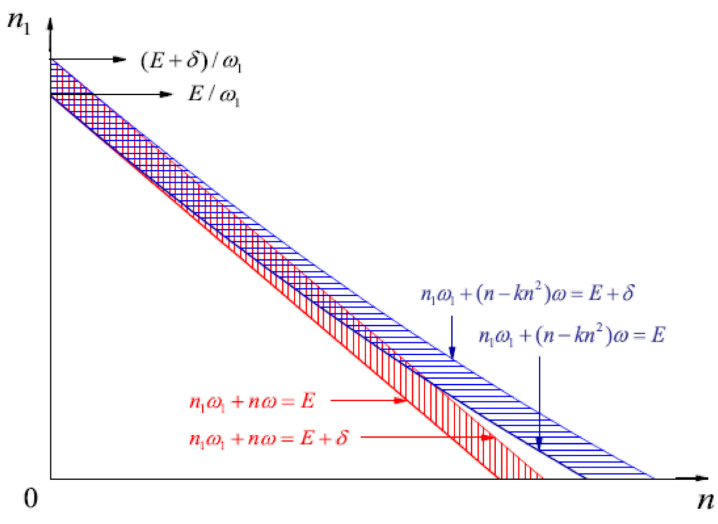
Applications --- 1. Non-canonical Equilibrium State

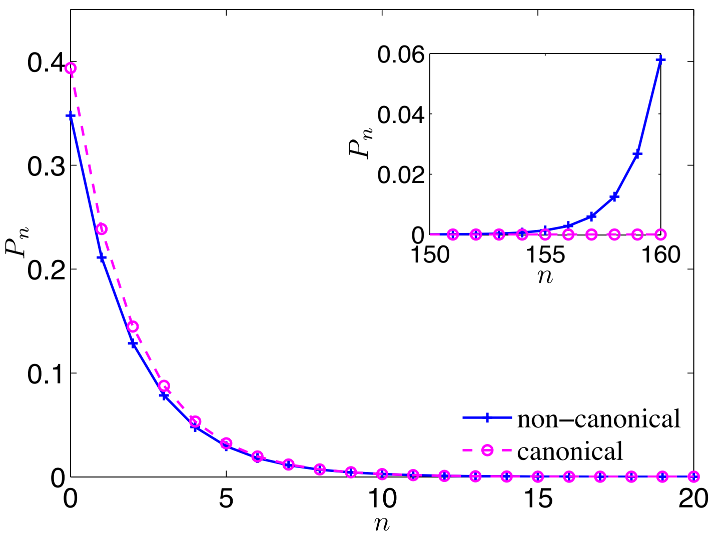
non-canonical equilibrium distribution

Weak system-bath coupling $$\rho_S = \frac{e^{-\beta H_S}}{\mathrm{Tr}\left[e^{-\beta H_S}\right]}$$

Strong system-bath coupling →deformation of energy shell

$$\frac{e^{-\beta n\omega}}{\mathcal{Z}} \longrightarrow \frac{e^{-\beta n\omega+\mathcal{O}(n^2)}}{\mathcal{Z}}$$





H. Dong, S. Yang, X. F. Liu, and C. P. Sun, Phys. Rev. A **76**, 044104 (2007).
DZX, S. W. Li, X. F. Liu, and C. P. Sun, Phys. Rev. E **90**, 062125 (2014).

Perturbative theory in the polaron frame

Equilibrium state

$$\tilde{\rho}_S = \frac{\mathrm{Tr}_B[e^{-\beta \tilde{H}_{tot}}]}{\mathrm{Tr}_{S+B}[e^{-\beta \tilde{H}_{tot}}]}$$

Kubo identity

$$e^{-\beta \tilde{H}_{tot}} \approx e^{-\beta H_0}\left[1 - \int_0^\beta d\beta' e^{\beta' H_0} H_I e^{-\beta' H_0} + \int_0^\beta \int_0^{\beta'} d\beta' d\beta'' e^{\beta' H_0} \tilde{H}_I e^{-(\beta'-\beta'')H_0} H_I e^{-\beta'' H_0}\right].$$

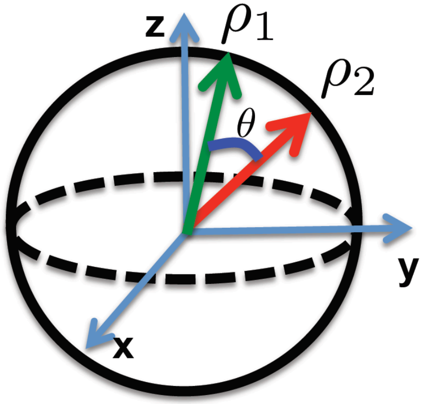
Second order perturbation:

$$\tilde{\rho}_S = \tilde{\rho}_S^{(0)} + \tilde{\rho}_S^{(2)} + \ldots,$$

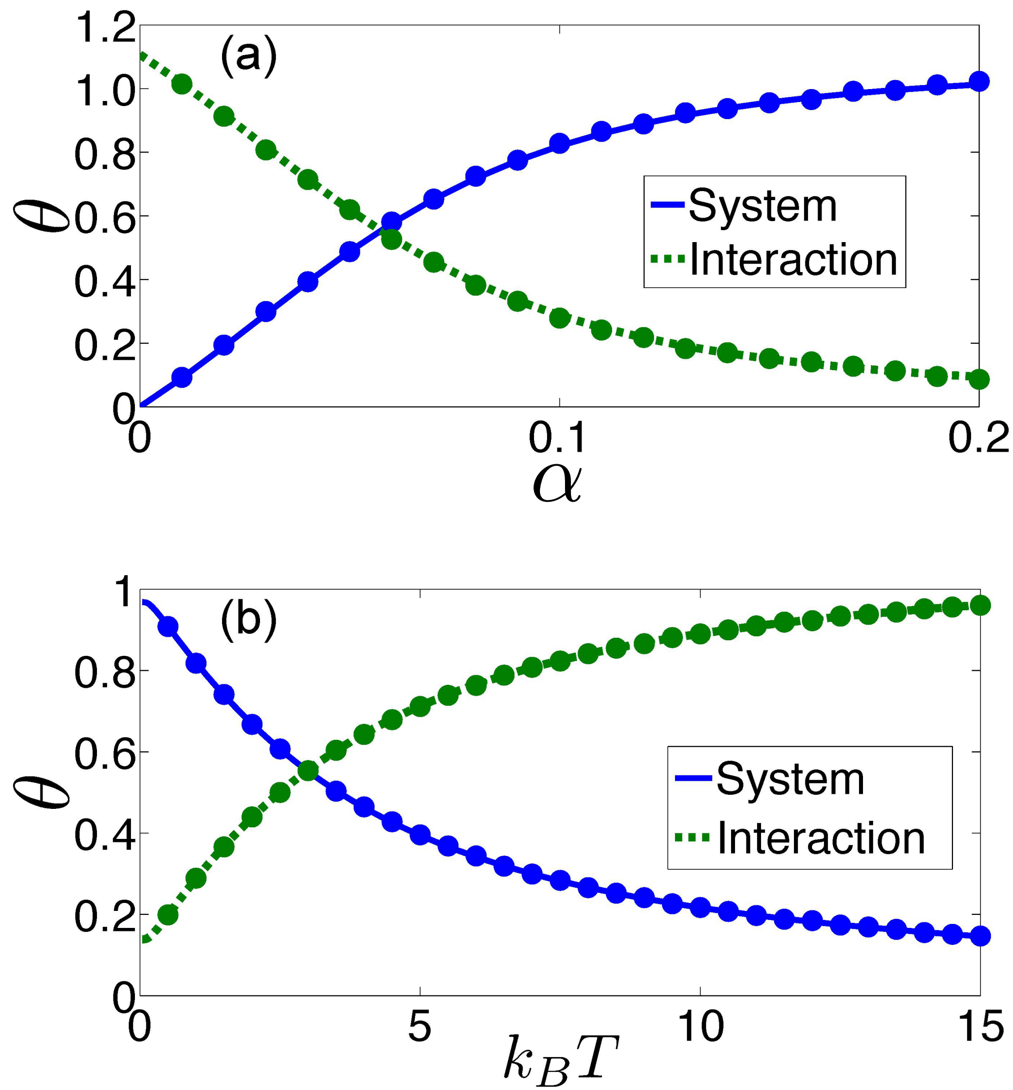
$$\tilde{\rho}_S^{(0)} = \frac{e^{-\beta H_S}}{\mathcal{Z}_S^{(0)}}$$

$$\tilde{\rho}_S^{(2)} = \frac{A}{\mathcal{Z}_S^{(0)}} - \frac{Z_S^{(2)}}{\left[\mathcal{Z}_S^{(0)}\right]^2} e^{-\beta H_S}.$$

C. K. Lee, J.S. Cao, and J. Gong, Phys. Rev. E **86**, 021109 (2012).

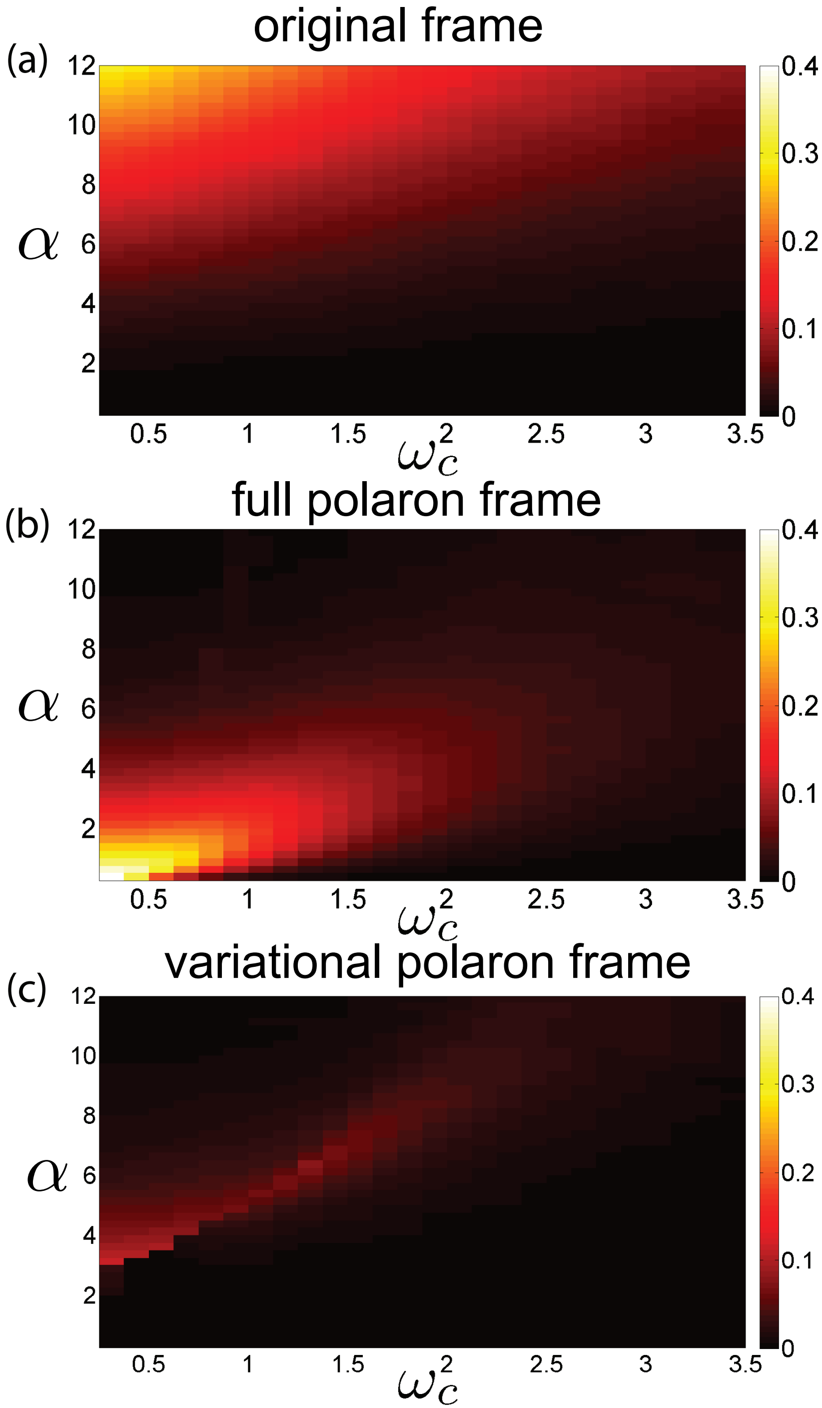


ρ_1: eigen frame
ρ_2: polaron frame



Angle rotated from the diagonal frame of $\tilde{\rho}_S$ to eigen state of H_S or H_I.

C. K. Lee, J.S. Cao, and J. Gong, Phys. Rev. E **86**, 021109 (2012).



Relative errors

$$\left|\frac{\langle\sigma_z\rangle_{\mathrm{Pert}} - \langle\sigma_z\rangle_{\mathrm{PI}}}{\langle\sigma_z\rangle_{\mathrm{PI}}}\right|$$

Pert: 2nd order perturbative theory in the polaron frame

PI: path integral integral

C. K. Lee, J. Moix, and J. Cao, J. Chem. Phys. **136**, 204120 (2012).

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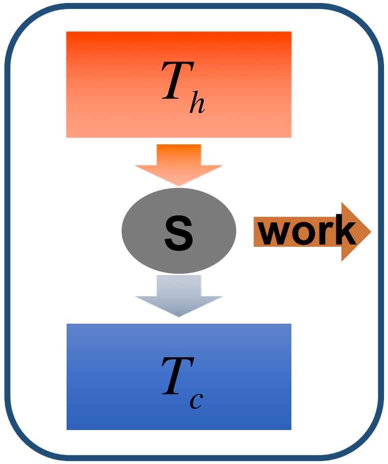
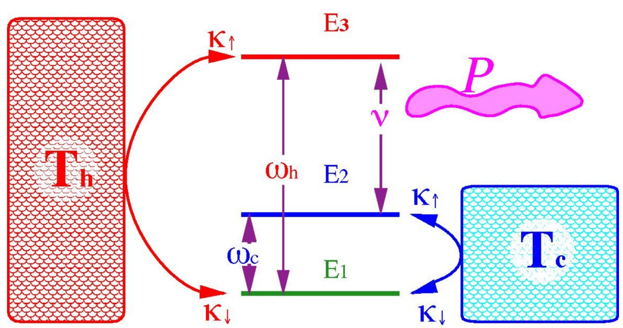
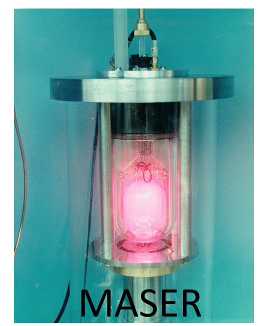
Application --- 2. Three-level heat engine

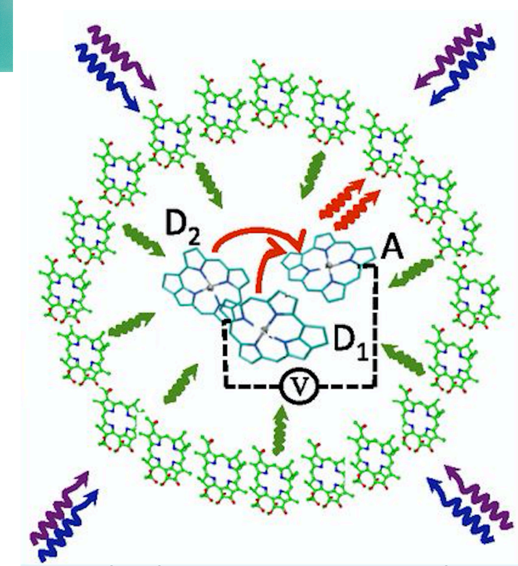


$$\eta_C = 1 - \frac{T_c}{T_h}$$



$$\eta_{SSD} = \frac{\nu}{\omega_h} \leq \eta_C$$

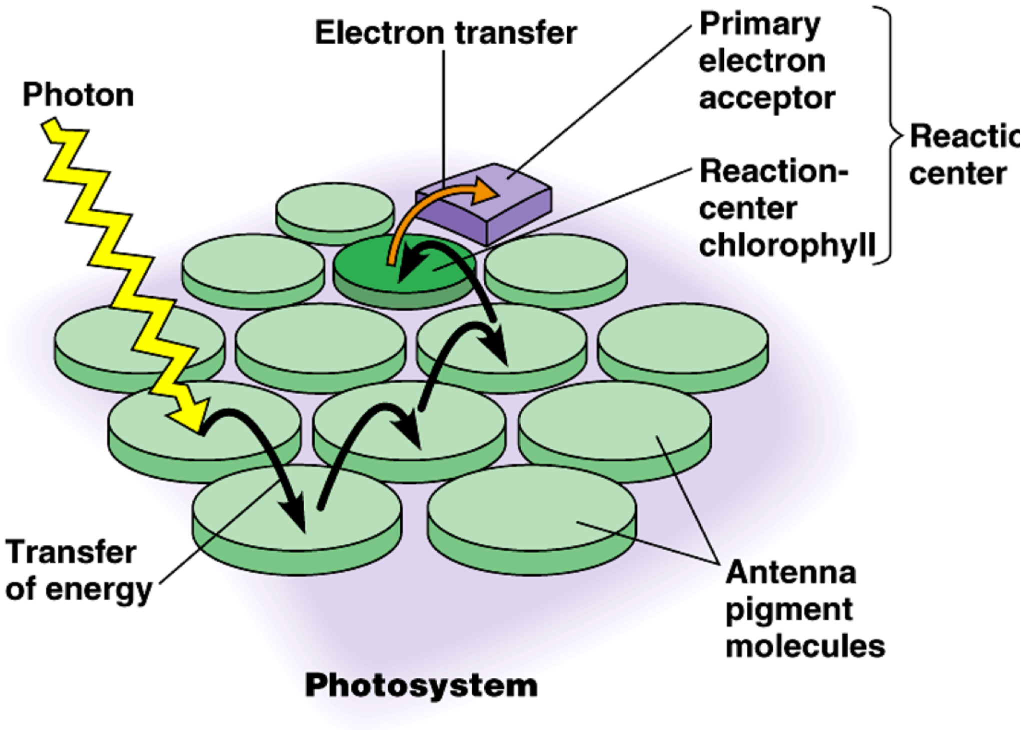


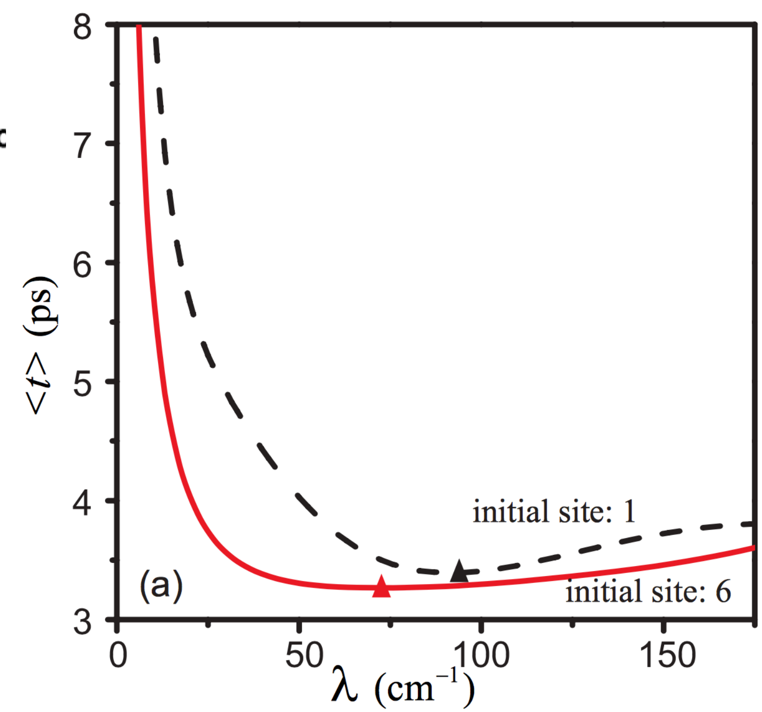


Light-harvesting complex

H. E. D. Scovil and E. O. Schulz-DuBois, PRL **2**, 262 (1959).
E. Geva and R. Kosloff, JCP **104**, 7681 (1996);PRL **108**, 070604 (2012)
E. Boukobza, and D. Tannor, PRA **74**, 063822 (2006).
M. O. Scully, et al., PNAS **108** (37), 15097 (2011).
J. Roßnagel, et al., PRL **112**, 030602 (2014).
H. T. Quan,et al., PRE **76**, 031105 (2007).

Energy transfer in photosystem: beyond weak coupling

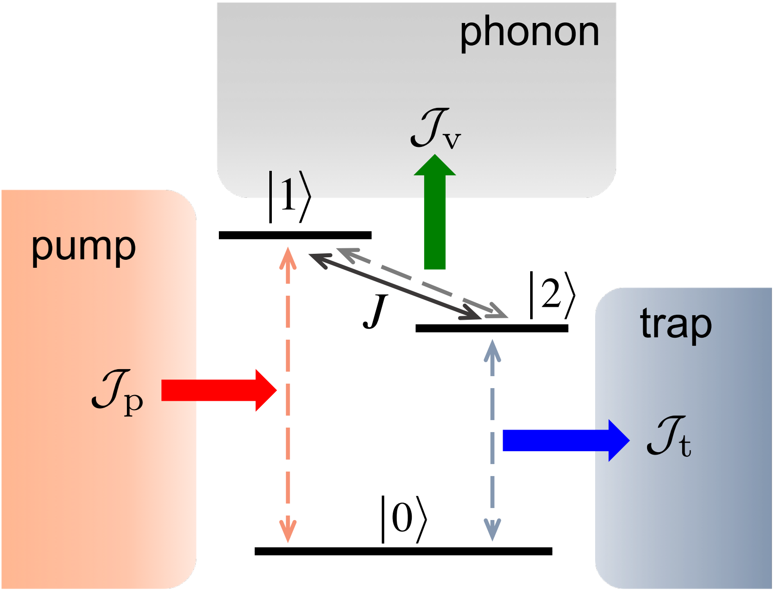




Beyond weak system-bath coupling regime

J. Cao and R. J. Silbey, JPC A, 113, 13825 (2009)
J. Wu, et al., NJP, 12, 105012 (2010)

Three-level light harvesting system based on QHE model



$$H_S = \epsilon_1|1\rangle\langle 1| + \epsilon_2|2\rangle\langle 2| + \frac{\Delta}{2}(|1\rangle\langle 2| + |2\rangle\langle 1|)$$

pump and trap baths (weak)

$$H_{i=\rm p,t} = \sum_k \omega_{ik} a_{ik}^\dagger a_{ik} + \left(g_{ik} a_{ik}^\dagger |0\rangle\langle i| + \rm{H.c.}\right)$$

phonon bath (intermediate or strong)

$$H_{\rm v} = \sum_k \omega_k b_k^\dagger b_k + (|1\rangle\langle 1| - |2\rangle\langle 2|)\sum_k (f_k b_k^\dagger + \rm{H.c.})$$

DZX, C. Wang, Y. Zhao, and J. S. Cao, New J. Phys. **18**, 023003 (2016).

Time evolution and steady state efficiency

Master equation

$$\frac{d\rho_s(t)}{dt} = -i\left[H_0, \rho_s(t)\right] + \mathcal{L}_{\rm p}[\rho_s(t)] + \mathcal{L}_{\rm t}[\rho_s(t)] + \mathcal{L}_{\rm v}[\rho_s(t)]$$

$+\mathcal{L}_{\rm p}[\rho_s(t)] + \mathcal{L}_{\rm t}[\rho_s(t)]$ → weak coupling, Lindblad operator

$+\mathcal{L}_{\rm v}[\rho_s(t)]$ → strong coupling, polaron approach

Steady state energy flux

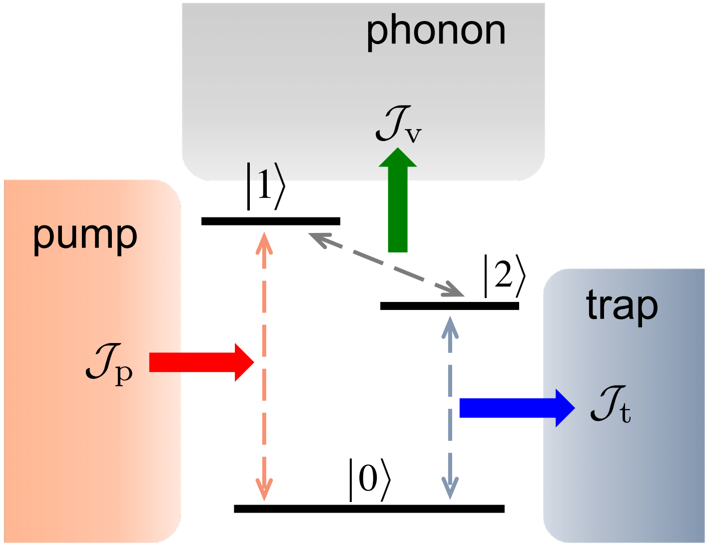
$$\mathcal{J}_{\rm p} = {\rm Tr}_s[H_0 \mathcal{L}_{\rm p}[\rho_s(\infty)]]$$

$$\mathcal{J}_{\rm t} = {\rm Tr}_s[H_0 \mathcal{L}_{\rm t}[\rho_s(\infty)]]$$

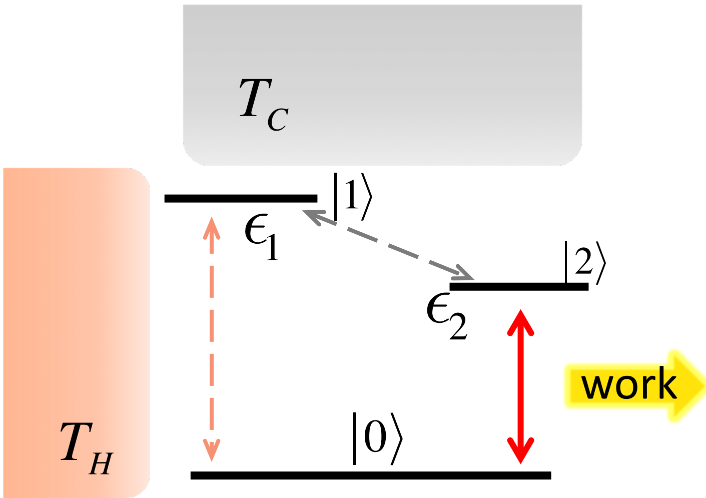
$$\mathcal{J}_{\rm v} = {\rm Tr}_s[H_0 \mathcal{L}_{\rm v}[\rho_s(\infty)]]$$

Energy transfer efficiency

$$\eta = \left|\frac{\mathcal{J}_{\rm t}}{\mathcal{J}_{\rm p}}\right|$$



Maser as Three-level heat engine

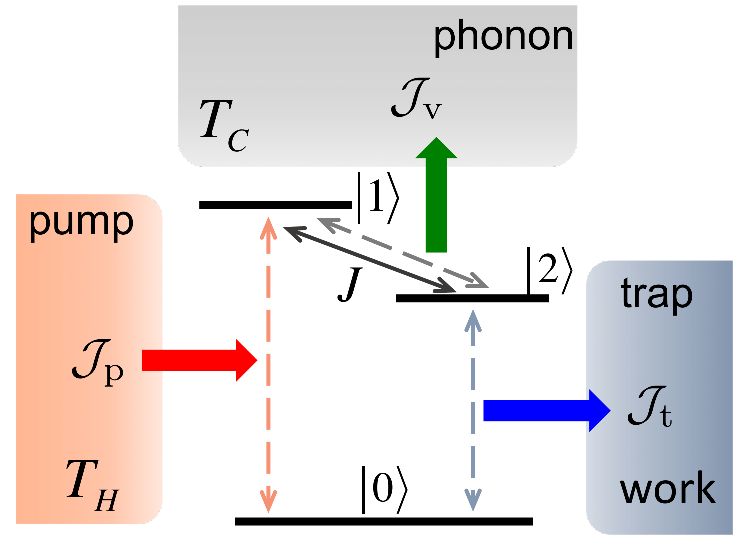


$$\frac{P_1}{P_0} = e^{-\beta_h \epsilon_1}, \frac{P_1}{P_2} = e^{-\beta_c(\epsilon_1 - \epsilon_2)}$$

$$P_2 > P_0 \quad \Rightarrow \quad \eta_{\mathrm{SSD}} = \frac{\epsilon_2}{\epsilon_1} \leq 1 - \frac{T_c}{T_h}$$

H. E. D. Scovil and E. O. Schulz-DuBois, PRL **2**, 262 (1959).

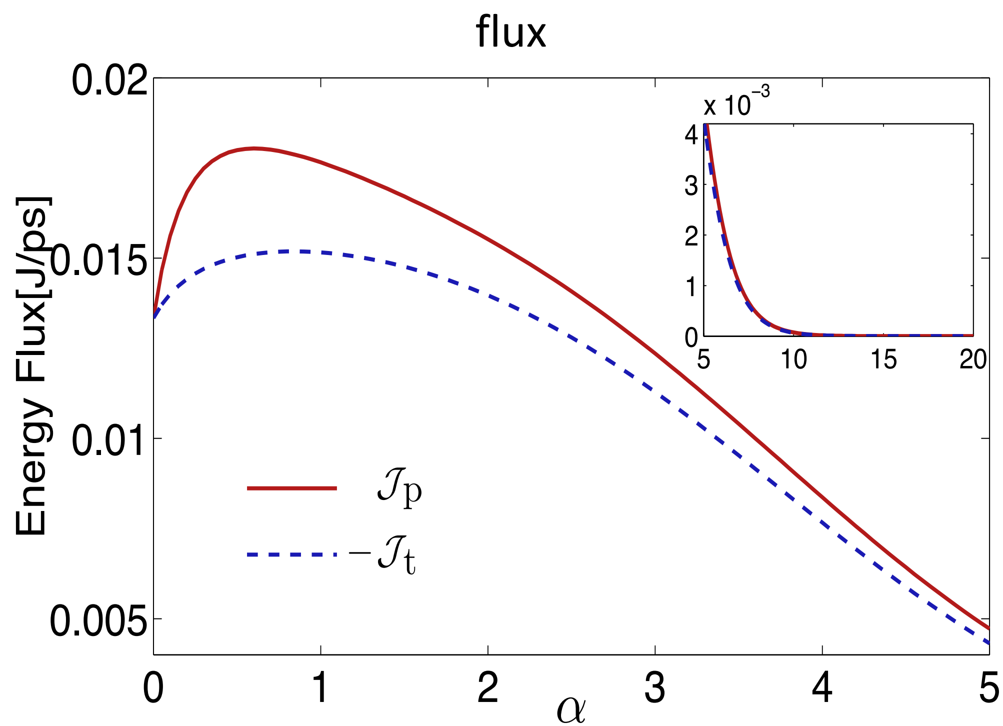
Energy transfer in LH system



$$\eta = \left|\frac{\mathcal{J}_{\mathrm{t}}}{\mathcal{J}_{\mathrm{p}}}\right| \leq \left(1 - \frac{T_{\mathrm{c}}}{T_{\mathrm{h}}}\right)\frac{T_{\mathrm{t}}}{T_{\mathrm{t}} - T_{\mathrm{c}}}$$

Heat pump efficiency

Steady state flux and efficiency



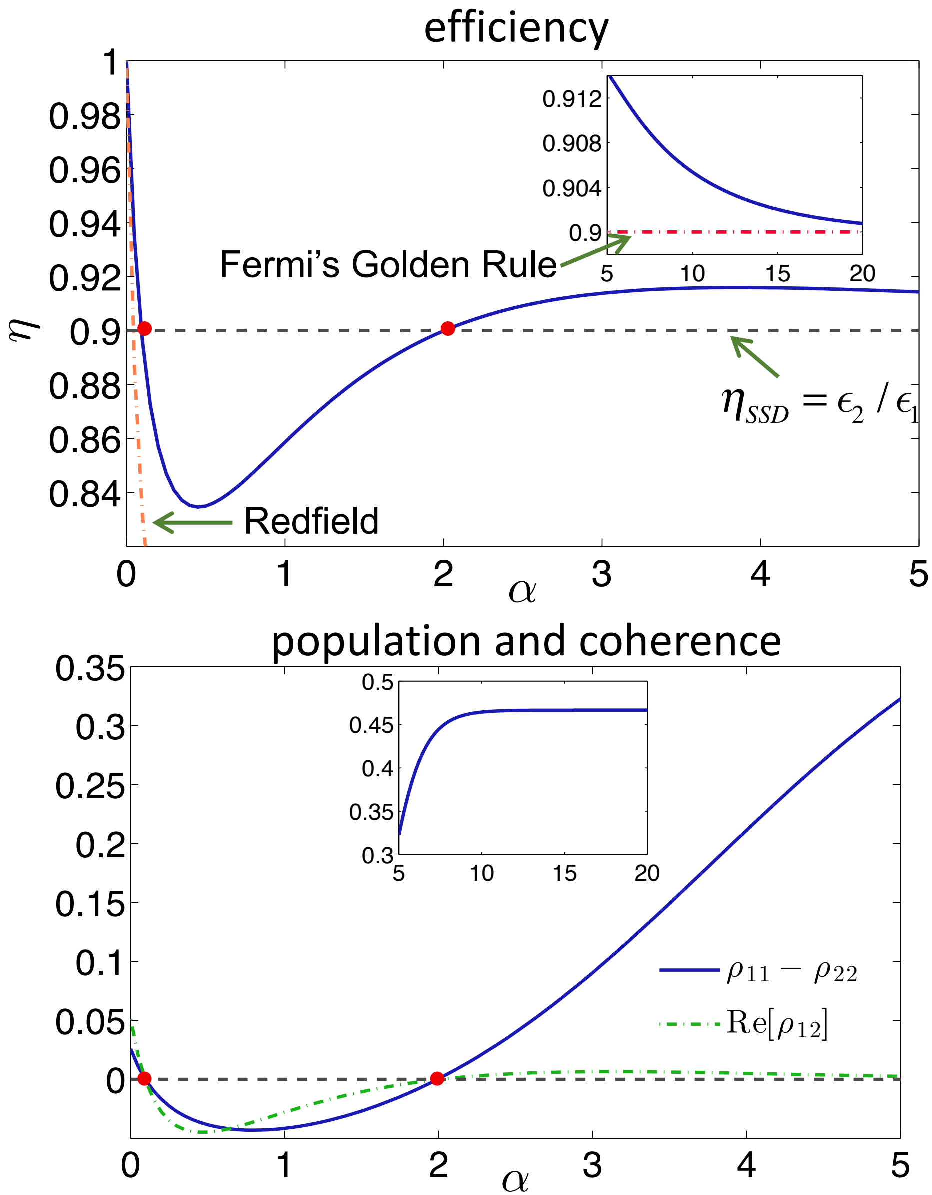
$$\mathcal{J}_\mathrm{p} = \epsilon_1 \gamma_\mathrm{p}[n_\mathrm{p}\rho_{00} - (n_\mathrm{p}+1)\rho_{11}] - \frac{J\gamma_\mathrm{p}}{2}(n_\mathrm{p}+1)\Re[\rho_{12}]$$

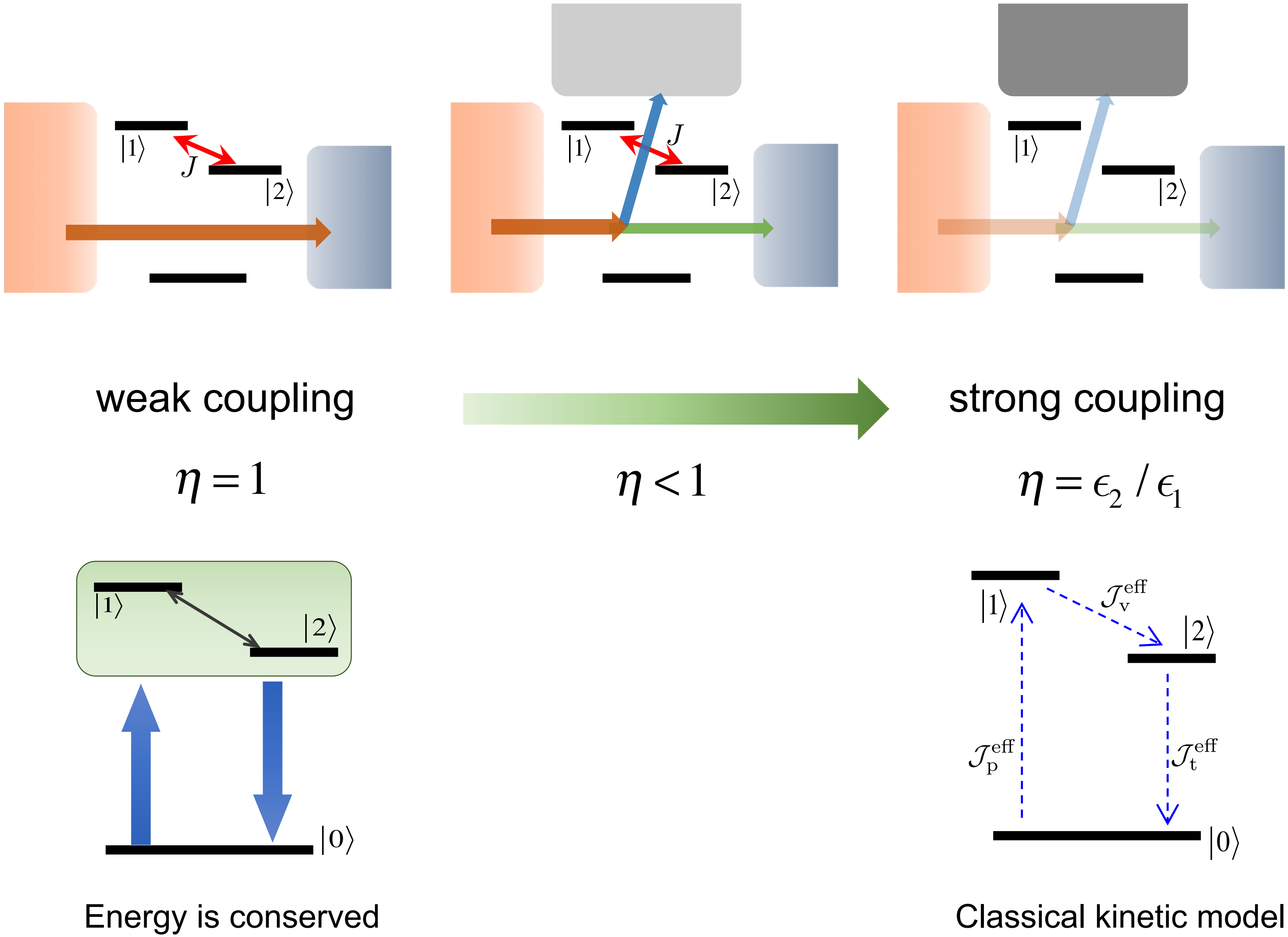
$$\mathcal{J}_\mathrm{t} = \epsilon_2 \gamma_\mathrm{t}[n_\mathrm{t}\rho_{00} - (n_\mathrm{t}+1)\rho_{22}] - \frac{J\gamma_\mathrm{t}}{2}(n_\mathrm{t}+1)\Re[\rho_{12}]$$

coherence

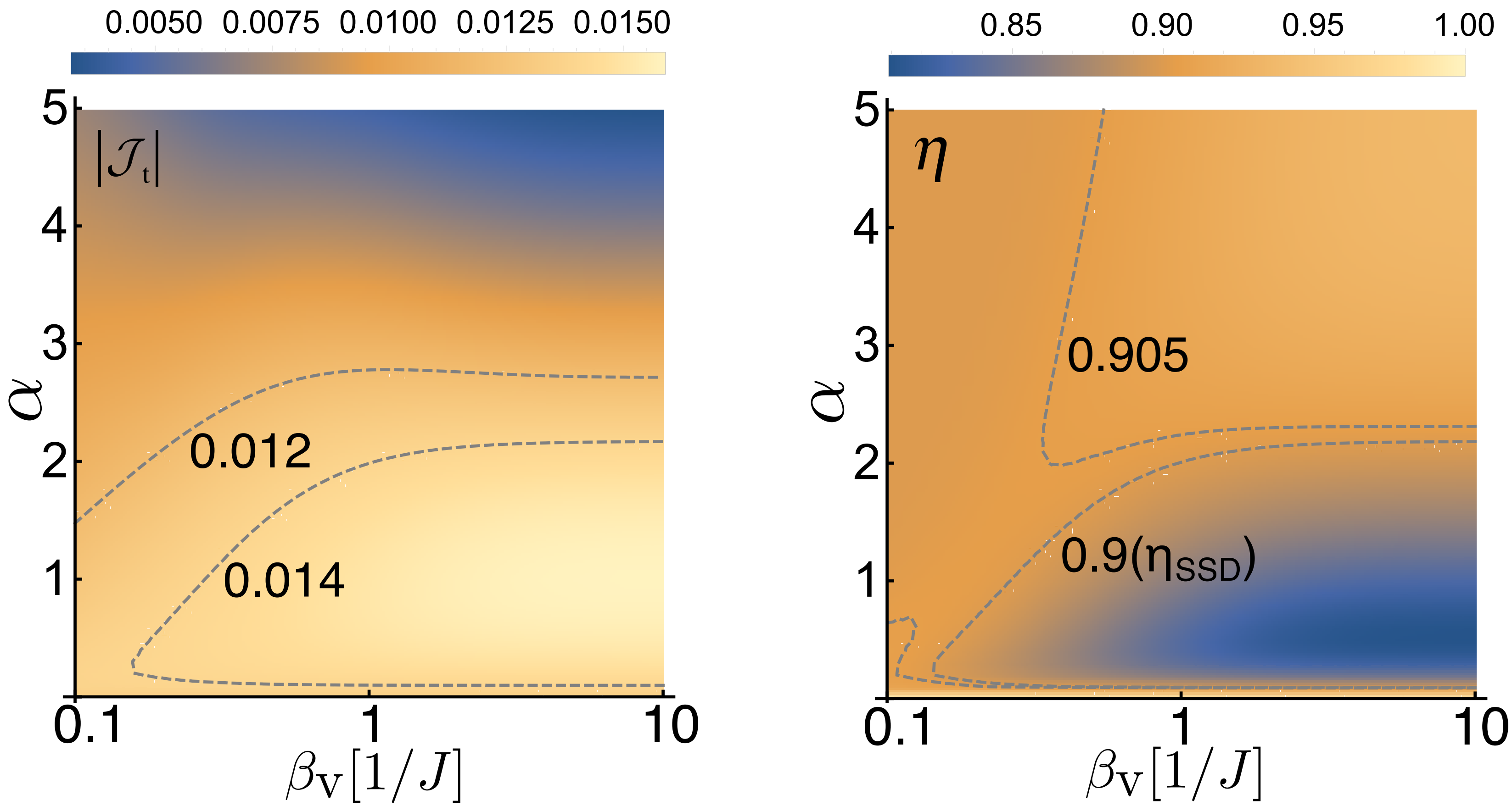
DZX, C. Wang, Y. Zhao, and J. S. Cao, New J. Phys. **18**, 023003 (2016).

Steady state flux and efficiency



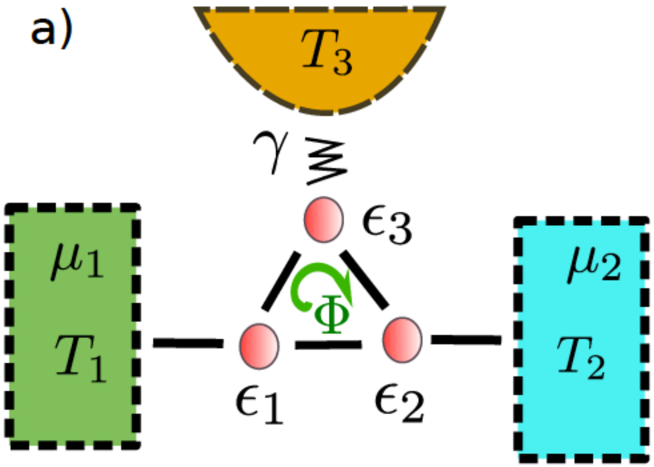

|1⟩
|2⟩
J
weak coupling
strong coupling
$\eta = 1$
$\eta < 1$
$\eta = \epsilon_2 / \epsilon_1$
|0⟩
$\mathcal{J}_{v}^{eff}$
$\mathcal{J}_{p}^{eff}$
$\mathcal{J}_{t}^{eff}$
Energy is conserved
Classical kinetic model

Temperature and coupling strength dependence



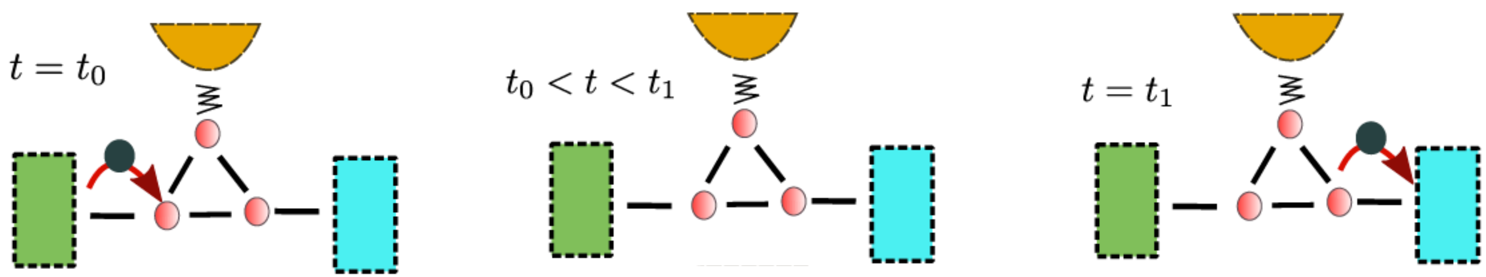
Output flux (power) and efficiency compete with each other.
To avoid their minimums, the optimal regime is intermediate coupling and temperature

Aharonov-Bohm effect with dephasing in nonequilibrium transport

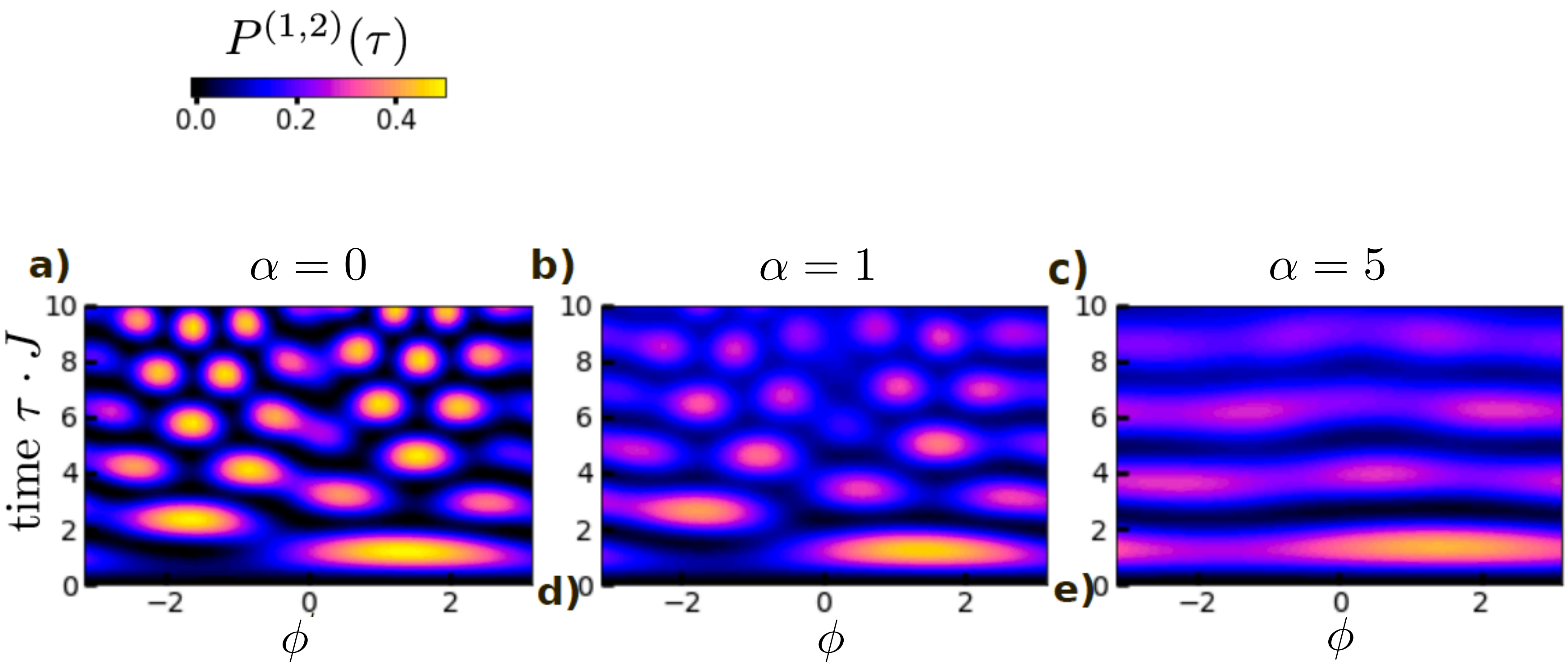


Gauge invariant phase $\phi = \phi_{2\to1} + \phi_{3\to2} + \phi_{1\to3} \mod 2$

Waiting time probability $P^{(1,2)}(t)$



G. Engelhardt and J.S. Cao, Phys. Rev. B **99**, 075436 (2019)


$P^{(1,2)}(\tau)$
0.0
0.2
0.4
a)
$\alpha = 0$
b)
$\alpha = 1$
c)
$\alpha = 5$
time $\tau \cdot J$
10
8
6
4
2
0
−2
0
2
ϕ
d)
e)

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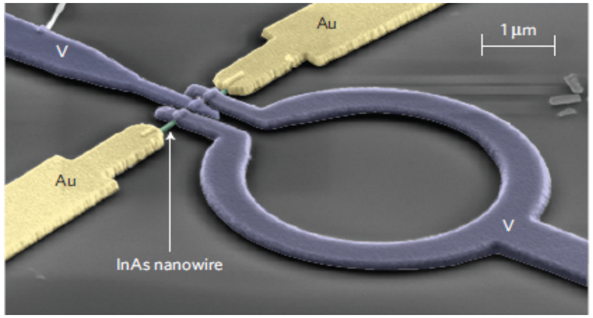
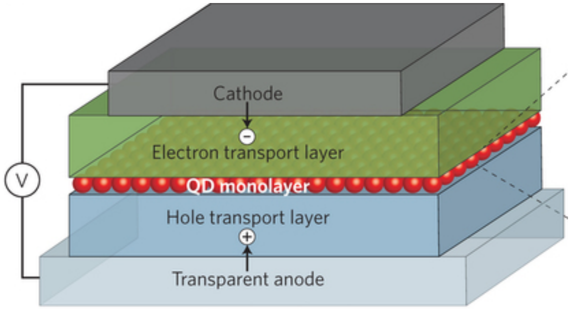
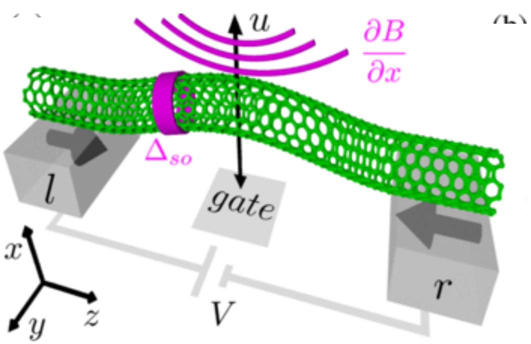
Applications --- 3. Non Equilibrium Heat Transport



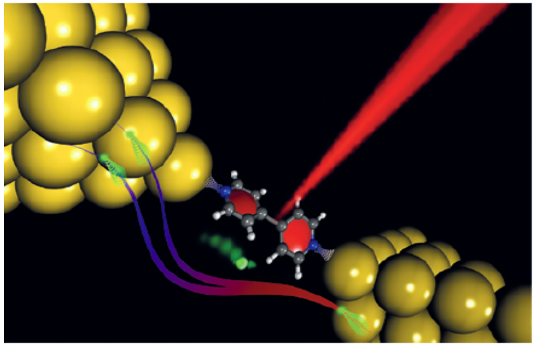
Nature Phys. 7, 857 (2011)



Nature Photonics 7, 13 (2013)

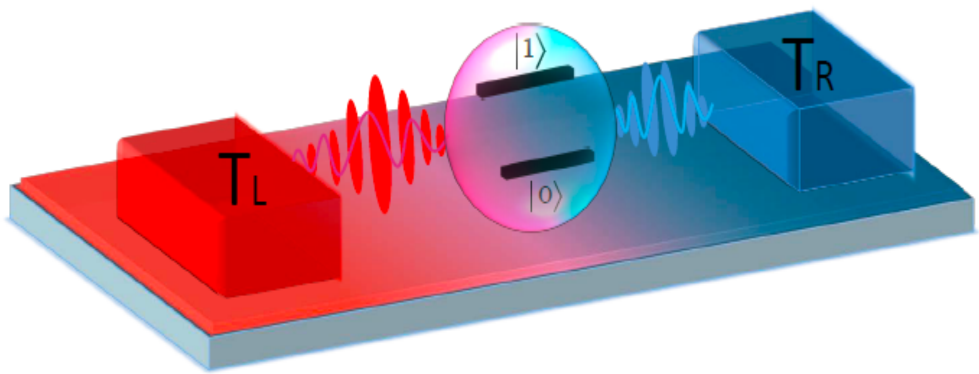


PRL 113, 047201 (2014)



Nature Nanotech 8, 377 (2013)

Heat transfer: non-equilibrium spin-boson model



Weak coupling: Redfield

$$H = \frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sigma_z \sum_{v=L,R} \sum_{k} (g_{k,v} b_{k,v}^{\dagger} + g_{k,v}^{*} b_{k,v}) + H_B$$

D. Segal, et al. PRL **94**, 034301 (2005)
J. Ren, et al. PRL **104**,170601(2010)

Strong coupling: NIBA (non-interacting blip approximation)

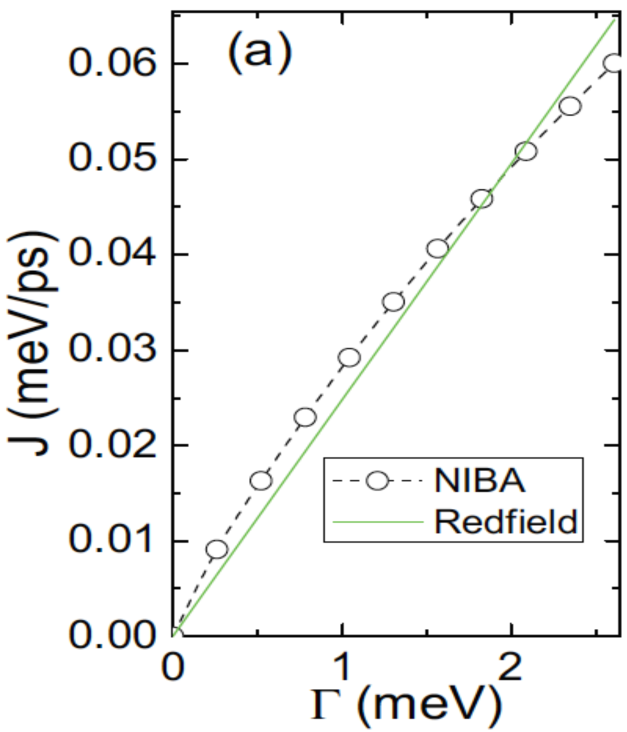
$$\tilde{H} = U^{\dagger} H U = \frac{\epsilon}{2}\sigma_z + (\cos B\sigma_x + \sin B\sigma_y) + H_B$$

$$B = 2i \sum_{v=L,R} \sum_{k} (\frac{g_{k,v}}{\omega_{k,v}} b_{k,v}^{\dagger} - \frac{g_{k,v}^{*}}{\omega_{k,v}} b_{k,v})$$

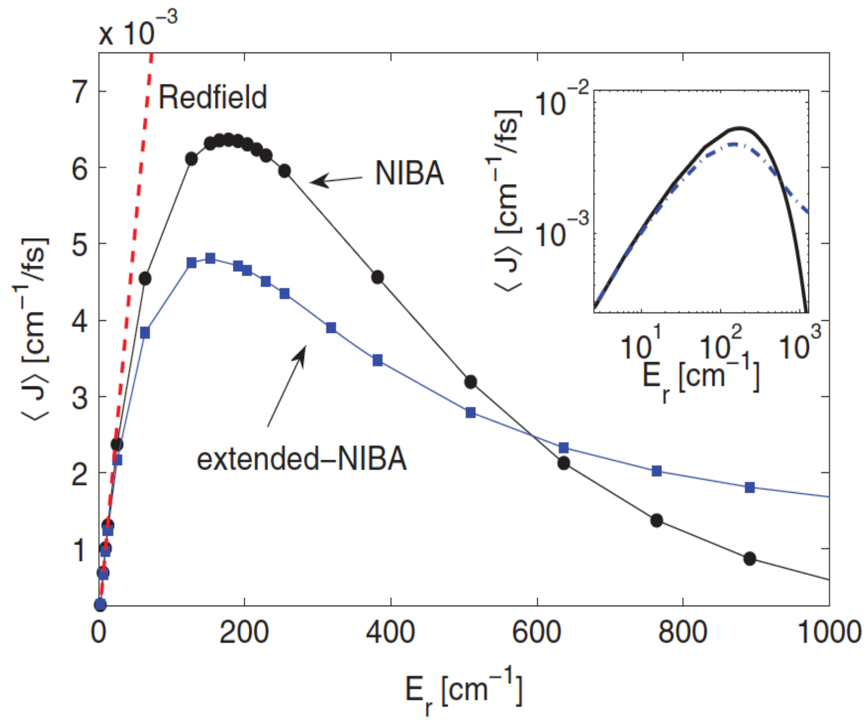
D. Segal, et al. PRB **73**, 205415 (2006)
T. Chen, et al. PRB **87**, 144303 (2013)

Weak coupling: NIBA and Redfield are not coincident

Strong coupling: turnover of flux



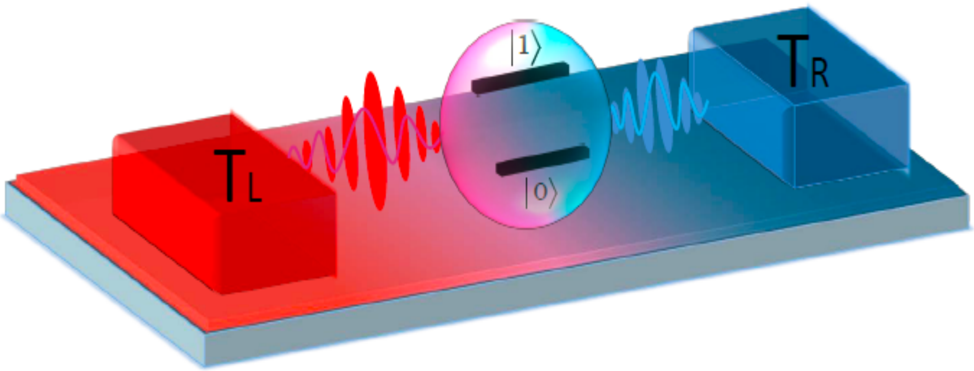
T. Chen, et al. PRB **87**, 144303 (2013)



L. Nicolin, et al. JCP **135**, 164106 (2011)

Unified approach: Non-equilibrium PTRE

$$H = \frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sigma_z \sum_{v=L,R} \sum_k (g_{k,v} b_{k,v}^\dagger + g_{k,v}^* b_{k,v}) + H_B$$



Polaron transformation

$$\tilde{H} = U^\dagger H U = \frac{\epsilon}{2}\sigma_z + \frac{\kappa\Delta}{2}\sigma_x + (\cos B - \kappa)\sigma_x + \sin B\sigma_y + H_B$$

$$B = 2i \sum_{v=L,R} \sum_k \left(\frac{g_{k,v}}{\omega_{k,v}} b_{k,v}^\dagger - \frac{g_{k,v}^*}{\omega_{k,v}} b_{k,v}\right)$$

$$\kappa = \exp\left[-\sum_{v=L,R} \int_0^\infty \frac{d\omega}{2\pi} \frac{J_v(\omega)}{\omega^2} \coth\left(\frac{\beta_v \omega}{2}\right)\right]$$

C. Wang, J. Ren and J. Cao, Scientific Reports **5**, 11787 (2015).

Unified approach: Non-equilibrium PTRE

$$\frac{\partial}{\partial t}\hat{\rho}_S = -i[\hat{H}_S, \hat{\rho}_S] + \sum_{l=x,y} \sum_{\omega,\omega'=0,\pm\Lambda} \Gamma_l(\omega)[\hat{P}_l(\omega)\hat{\rho}_S, \hat{P}_l(\omega')] + \mathrm{H.c.}$$

$\hat{P}_l(\omega)$ are the projection operators in the eigen basis

$$\hat{\sigma}_{x(y)}(-s) = \sum_{\omega=0,\pm\Lambda} \hat{P}_{x(y)}(\omega) e^{i\omega s}$$

Transition rates

$$\begin{aligned}
\Gamma_x(\omega) &= (\frac{\kappa\Delta}{2})^2 \int_0^\infty ds e^{i\omega s}(\cosh[Q(s)] - 1) \\
\Gamma_y(\omega) &= (\frac{\kappa\Delta}{2})^2 \int_0^\infty ds e^{i\omega s} \sinh[Q(s)]
\end{aligned}$$

$$Q(s) = Q_L(s) + Q_R(s)$$

Heat currents: Full Counting Statistics

Current is defined by the rate of energy (particles, etc) change of the corresponding heat bath.

$$\mathcal{J}_v(t) = -\langle \frac{dH_v(t)}{dt} \rangle$$

$$Q_v(t,0) = \int_0^t J_v(t')dt' = H_v(0) - H_v(t)$$

Characteristic function: $\chi = \{\chi_\mu\}$ are the auxiliary counting fields

$$\begin{aligned}
\mathcal{Z}(\chi = \{\chi_\mu\}, t) &\equiv \mathrm{Tr}[e^{i\sum_\mu \chi_\mu H_\mu(0)} e^{-i\sum_\mu \chi_\mu H_\mu(t)} \rho(0)] \\
&= \mathrm{Tr}[e^{i\sum_\mu \chi_\mu H_\mu(0)} U^\dagger e^{-i\sum_\mu \chi_\mu H_\mu(0)} U \rho(0)] \\
&= \mathrm{Tr}[U^{-\chi}(t)\rho(0)U^{\chi\dagger}(t)] \\
&= \mathrm{Tr}[\rho^\chi(t)].
\end{aligned}$$

$$U^\chi(t) = e^{i\sum \chi_\mu H_\mu/2} U(t) e^{-i\sum \chi_\mu H_\mu/2}$$

M. Esposito, U. Harbola, and S. Mukamel, Rev. Mod. Phys. **81**, 1665 (2009).

Steady state current $$\mathcal{J}_v(\infty) = \lim_{t\to\infty} \frac{H_v(0) - H_v(t)}{t}$$

Cumulant generating function $$G(\chi) \equiv \lim_{t\to\infty} \frac{1}{t} \ln \mathcal{Z}(\chi)$$

$$\rightarrow \quad \boxed{\mathcal{J}_v(\infty) = \frac{\partial}{\partial(i\chi_v)} G(\chi)|_{\chi=0}}$$

Total density matrix with counting field satisfies the Liouville equation:

$$\frac{d}{dt}\rho^{\chi}(t) = i\rho^{\chi}(t)H_I^{\chi}(t) - iH_I^{-\chi}(t)\rho^{\chi}(t)$$

$$H_I^{\chi}(t) = e^{i\sum_{\mu}\chi_{\mu}H_{\mu}/2} H_I(t) e^{-i\sum_{\mu}\chi_{\mu}H_{\mu}/2}$$

A phase factor containing χ is added to the bath operator:

$$B \to B_{\chi} = 2i \sum_{v=L,R} \sum_{k} \left(\frac{g_{k,v}}{\omega_{k,v}} e^{i\delta_{v,R}\chi\omega_{k,v}/2} b_{k,v}^{\dagger} - \frac{g_{k,v}^{*}}{\omega_{k,v}} b_{k,v}\right)$$

Non-equilibrium PTRE with counting field

$$\frac{\partial}{\partial t}\hat{\rho}_S^{\chi} = -i[\hat{H}_S, \hat{\rho}_S^{\chi}] + \sum_{l=x,y} \sum_{\omega,\omega'=0,\pm\Lambda} \{[\Gamma^{\chi}_{l,-}(\omega) + \Gamma^{\chi}_{l,+}(\omega')]\hat{P}_l(\omega')\hat{\rho}_S^{\chi}\hat{P}_l(\omega) - [\Gamma^{\chi}_{l,+}(\omega)\hat{P}_l(\omega')\hat{P}_l(\omega)\hat{\rho}_S + \mathrm{H.c.}]\}$$

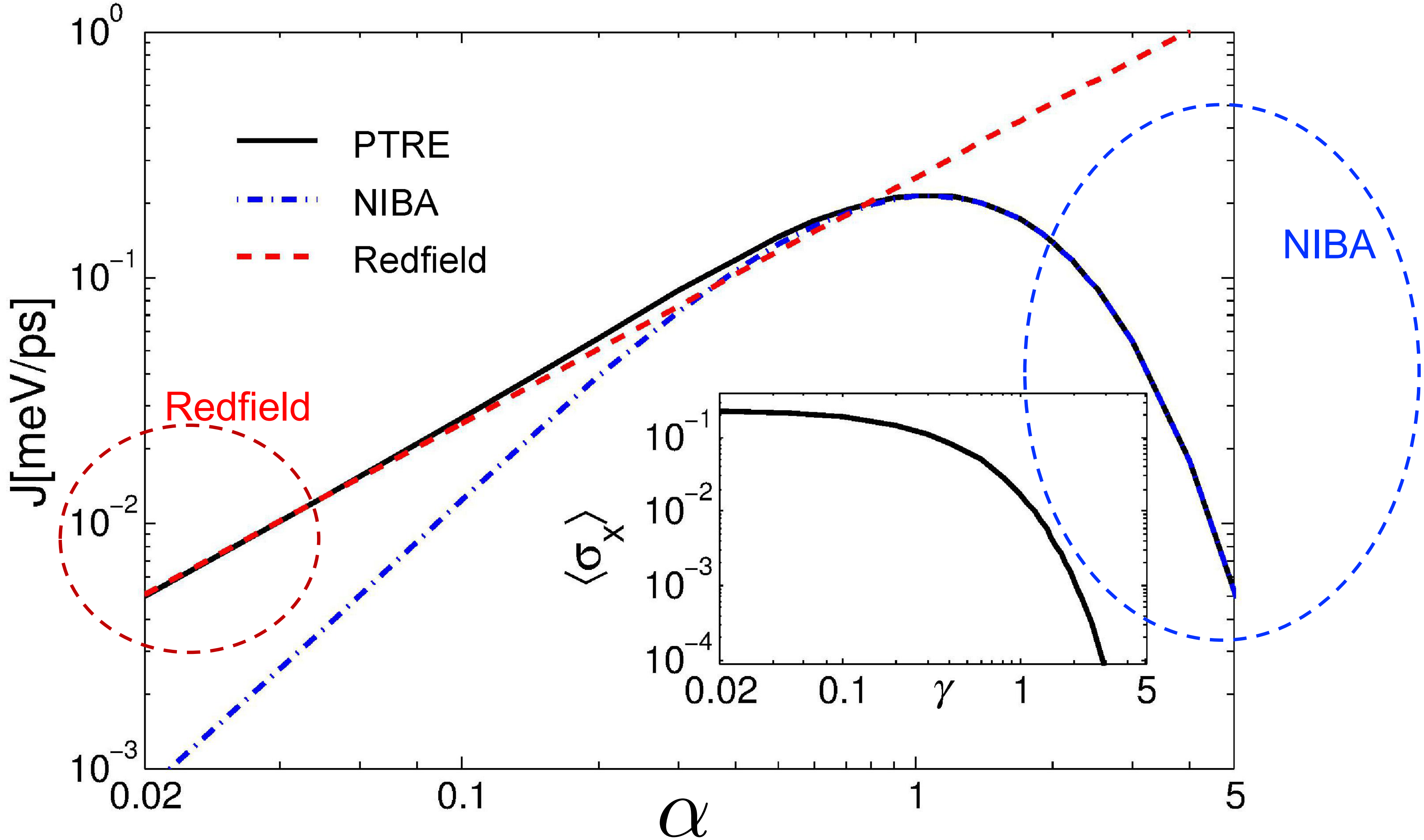
Transition rates

$$\Gamma^{\chi}_{x,\sigma}(\omega) = (\frac{\kappa\Delta}{2})^2 \int_0^{\infty} ds e^{i\omega s}(\cosh[Q(\sigma s - \chi)] - 1)$$

$$\Gamma^{\chi}_{y,\sigma}(\omega) = (\frac{\kappa\Delta}{2})^2 \int_0^{\infty} ds e^{i\omega s}\sinh[Q(\sigma s - \chi)]$$

$$Q(s-\chi) = Q_L(s) + Q_R(s-\chi)$$

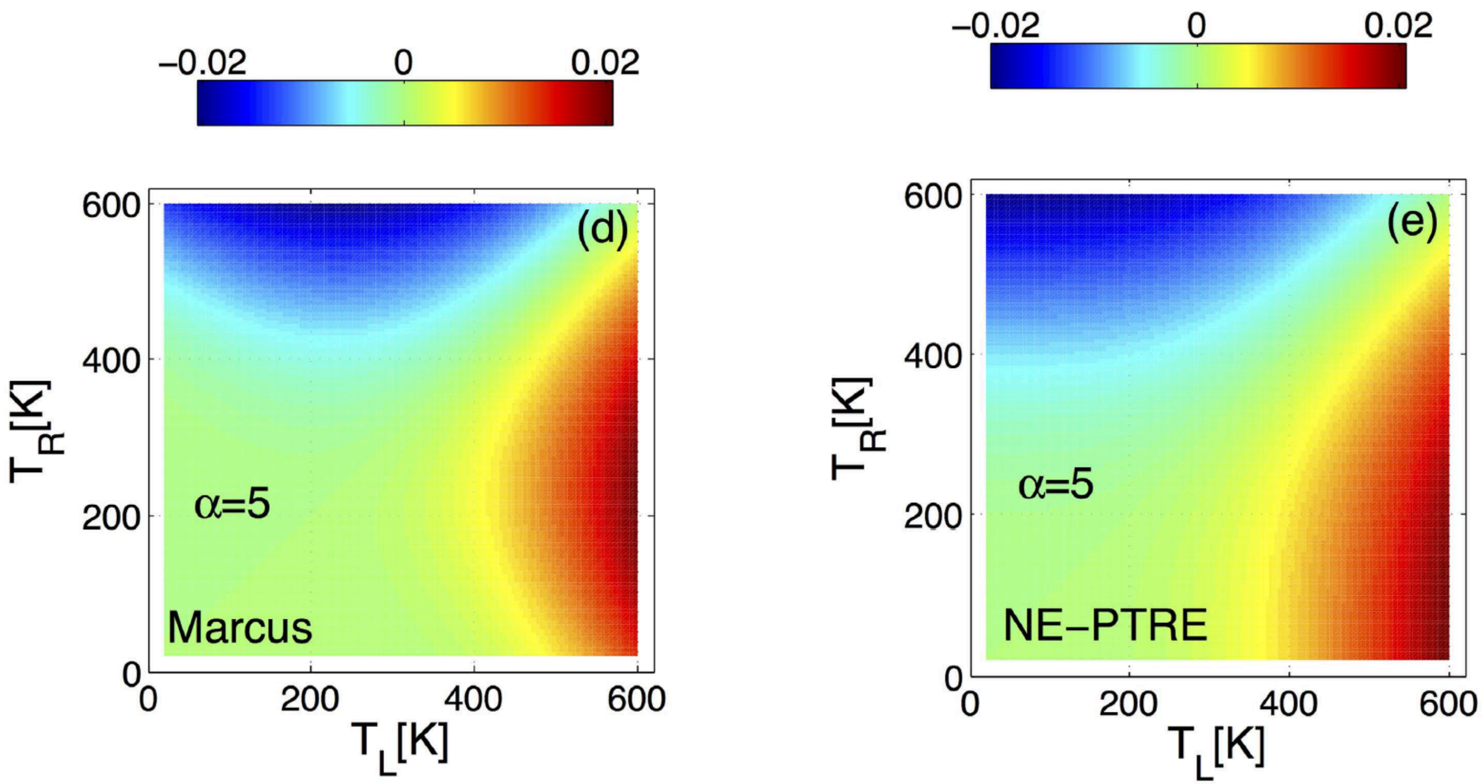
Steady state heat flux



$$\mathcal{J} = \frac{\kappa^2\Delta^2}{8\pi}\int_{-\infty}^{\infty} d\omega\omega \left[\frac{\phi_x(\kappa\Delta)C_x(-\kappa\Delta,\omega)+\phi_x(-\kappa\Delta)C_x(\kappa\Delta,\omega)}{\phi_x(\kappa\Delta)+\phi_y(-\kappa\Delta)} + C_y(0,\omega)\right]$$

Negative differential thermal conductance (NDTC)

$$\mathrm{NDTC} \equiv \frac{\partial \mathcal{J}}{\partial \Delta T}$$



Marcus approximation:
High T, strong coupling,
short time

C. Wang, J. Ren and J. Cao, Scientific Reports **5**, 11787 (2015)

Variational non-equilibrium PTRE

Variational equilibrium polaron transformation $F \leq F_0 + \langle H_I \rangle_{H_0} \equiv A_B$

$$F_0 = -\frac{1}{\beta} \ln \mathrm{Tr}\left[e^{-\beta H_0}\right]$$

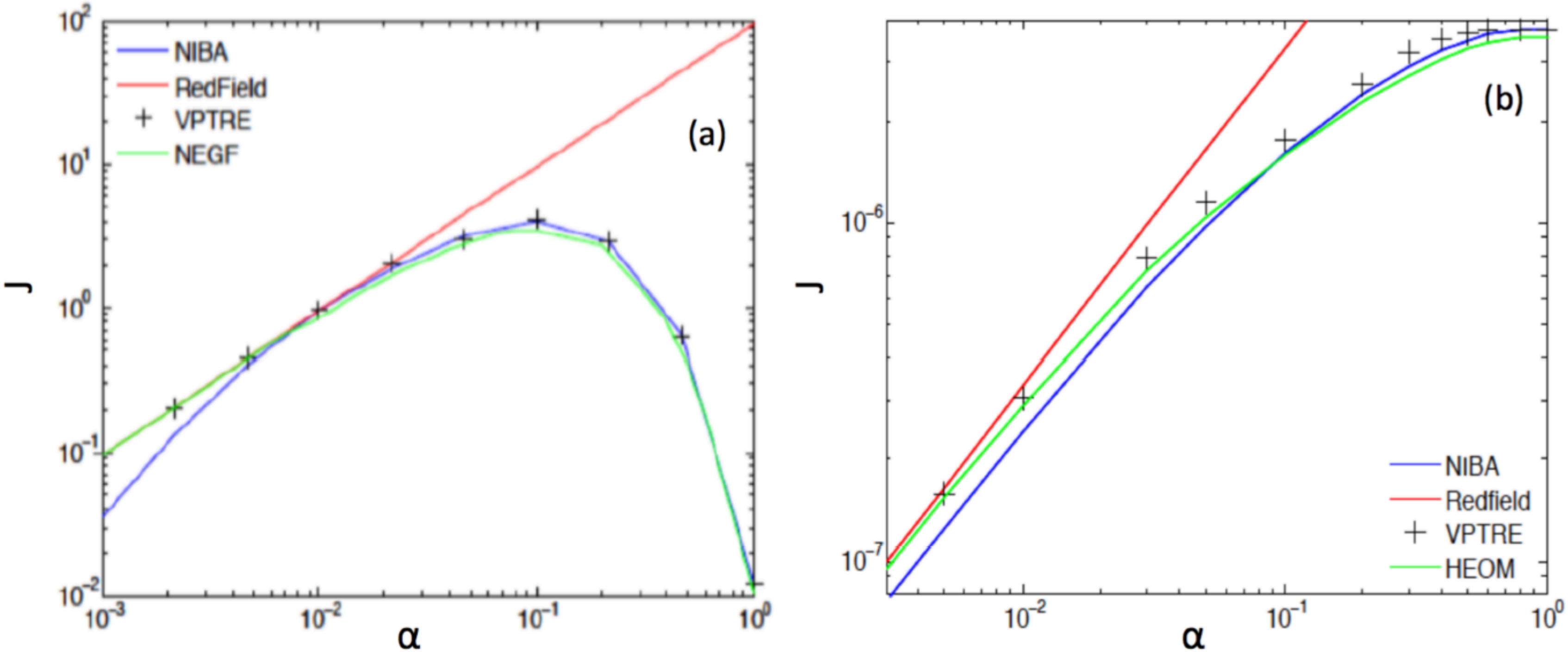
➡ $$f_k = g_k \xi(\omega_k), \qquad \xi(\omega_k) = \left[1 + \frac{\kappa^2 \Delta^2}{\omega_k \Lambda} \coth\left(\frac{\beta \omega_k}{2}\right) \tanh\left(\frac{\beta \Lambda}{2}\right)\right]^{-1}$$

Non-equilibrium state: what is β of the system?

canonical state ansatz $$\rho_{\mathrm{NESS}} = \frac{\exp(-\beta_L H_L - \beta_R H_R - \bar{\beta} H_I)}{\mathrm{Tr}\left[\exp(-\beta_L H_L - \beta_R H_R - \bar{\beta} H_I)\right]}$$

Effective temperature $$\bar{\beta} = \frac{\alpha_L + \alpha_R}{\alpha_L T_L + \alpha_R T_R}$$

$$\xi_{v=L,R}(\omega_k) = \left[1 + \frac{\kappa^2 \Delta^2}{\omega_k \Lambda} \coth\left(\frac{\beta_v \omega_k}{2}\right) \tanh\left(\frac{\bar{\beta} \Lambda}{2}\right)\right]^{-1}$$

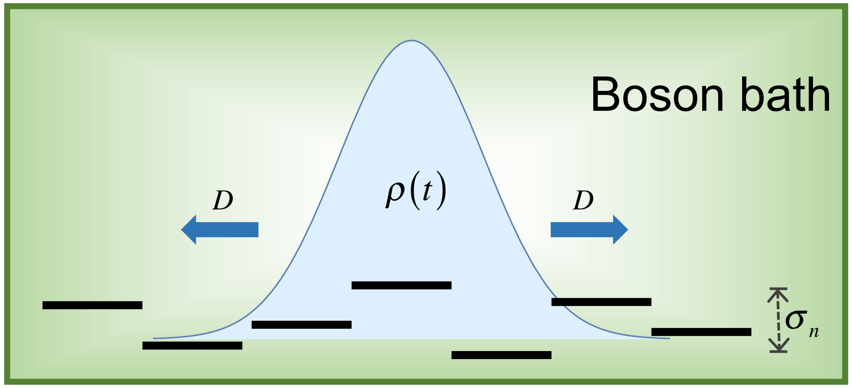


C. Y. Hsieh, J. J. Liu, C. R Duan, and J. Cao, to be published

Outline

1. Back ground
2. Polaron frame method
    - Polaron transformation
    - Polaron Transformed Redfield Equation (PTRE)
3. Applications of polaron frame
    - Non-canonical distribution
    - Quantum heat engine
    - Heat transfer
    - Quantum coherent transport in disordered systems
4. Summary

Application --- 4. One dimensional diffusion



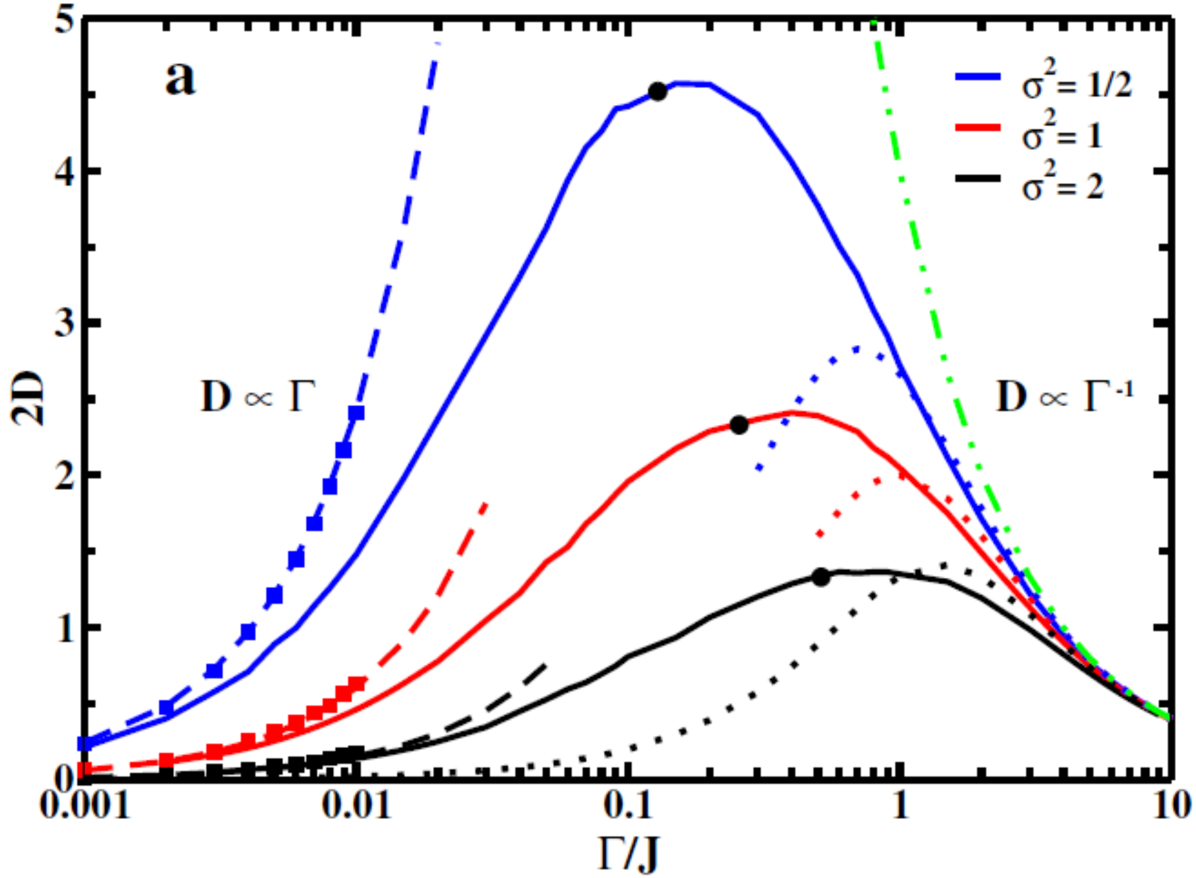
$$H_S = \sum_n \epsilon_n |n\rangle\langle n| + \sum_{m\neq n} J_{mn}|m\rangle\langle n|$$

$$H_I = \sum_{k,n} g_{k,n}|n\rangle\langle n|(b_{nk}^\dagger + b_{nk})$$

Diffusion constant *D*

$$D \equiv \lim_{t\to\infty} \frac{1}{2t}\overline{\langle R^2(t)\rangle} = \lim_{t\to\infty}\frac{1}{2t}\overline{\sum_n n^2 \rho_{nn}(t)}$$

1D Diffusion: Haken-Strobl-Reneiker model



Γ is the strength of the local markovian noise

coherent band-like transport (Redfield rate)

$$D_{coh} = 2\Gamma L^2$$

incoherent hopping (FGR rate)

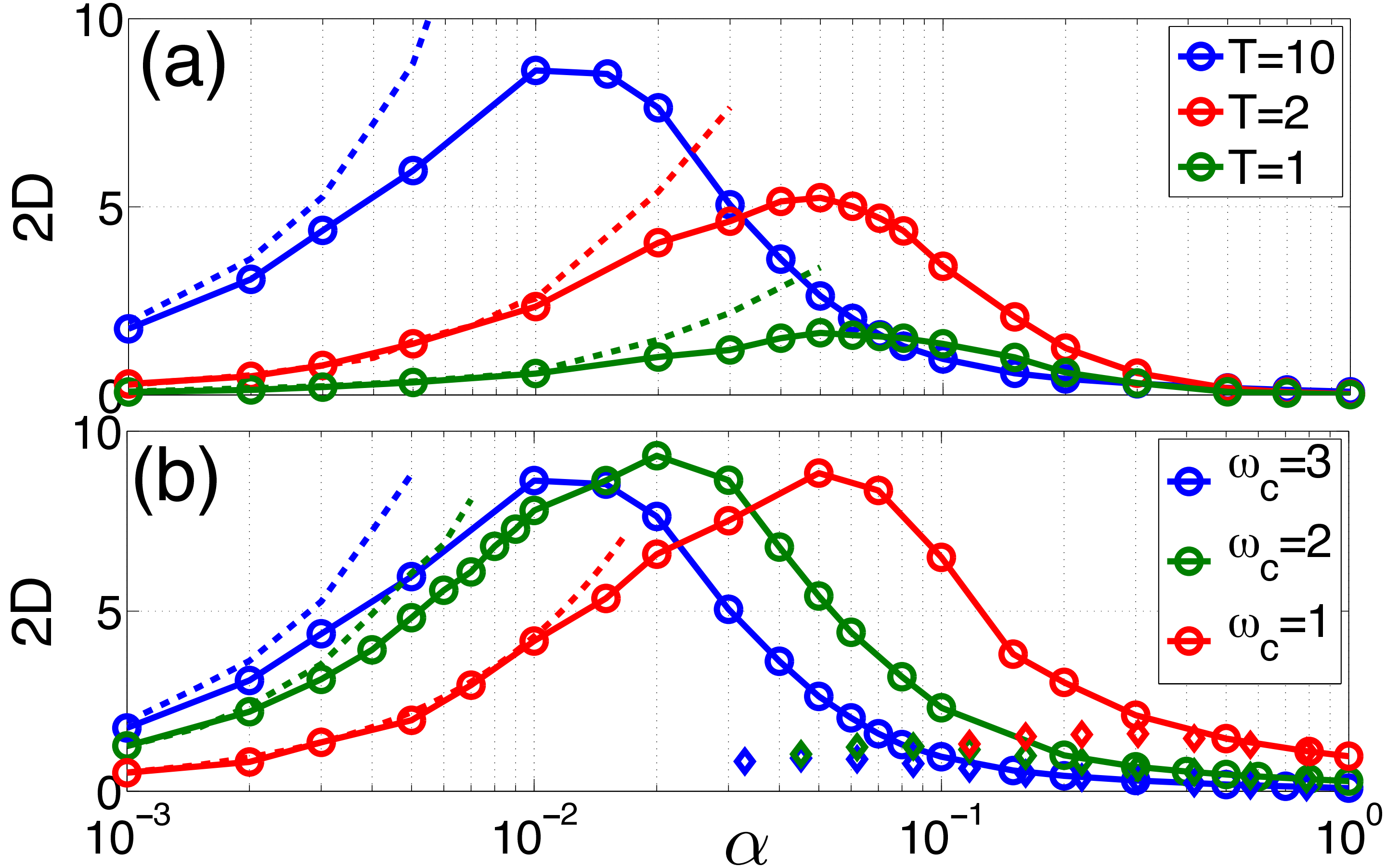
$$D_{incoh} = 2k_{ET} \propto 1/\Gamma$$

Moix, Khasin, and Cao, *New J. Phys.* 15, 085010 (2013)

PTRE with secular approximation

$$\frac{d\tilde{\rho}_{\nu\nu}(t)}{dt} = \sum_{\nu'} R_{\nu\nu,\nu'\nu'}\tilde{\rho}_{\nu'\nu'}(t),$$

$$\frac{d\tilde{\rho}_{\mu\nu}(t)}{dt} = (-i\omega_{\nu\mu} + R_{\mu\nu,\mu\nu})\tilde{\rho}_{\mu\nu}(t),\ \nu \neq \mu.$$



C. K. Lee, J. M. Moix, and J. Cao, JCP **142**, 164103 (2015)

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Summary

- Unified theory valid from weak to strong system-bath coupling
- consistent with numerically exact methods
- Applicable for both static and dynamic, equilibrium and non-equilibrium systems