Quantum dynamics and thermodynamics at strong reservoir coupling

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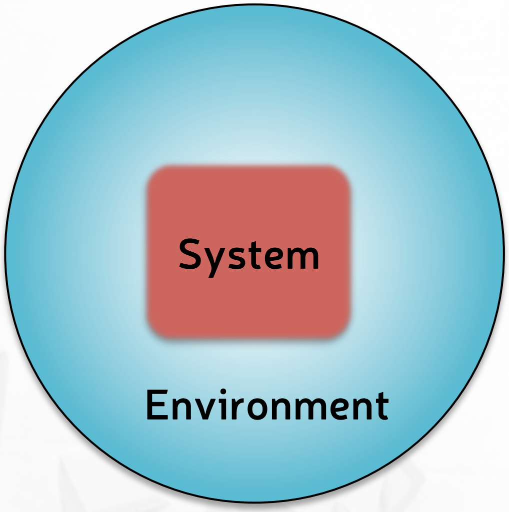
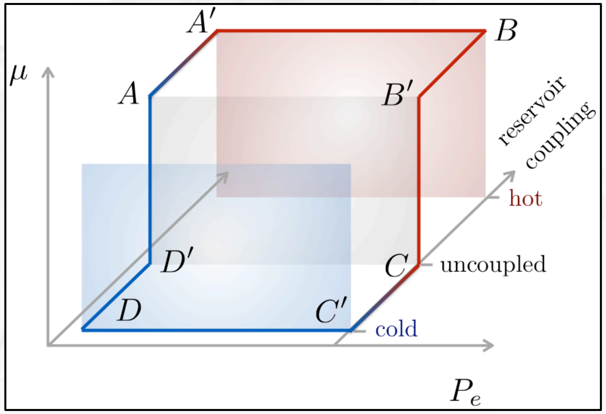


Manchester **N**oisy **Q**uantum **S**ystems Group



Phys. Rev. E 95, 032139 (2017)

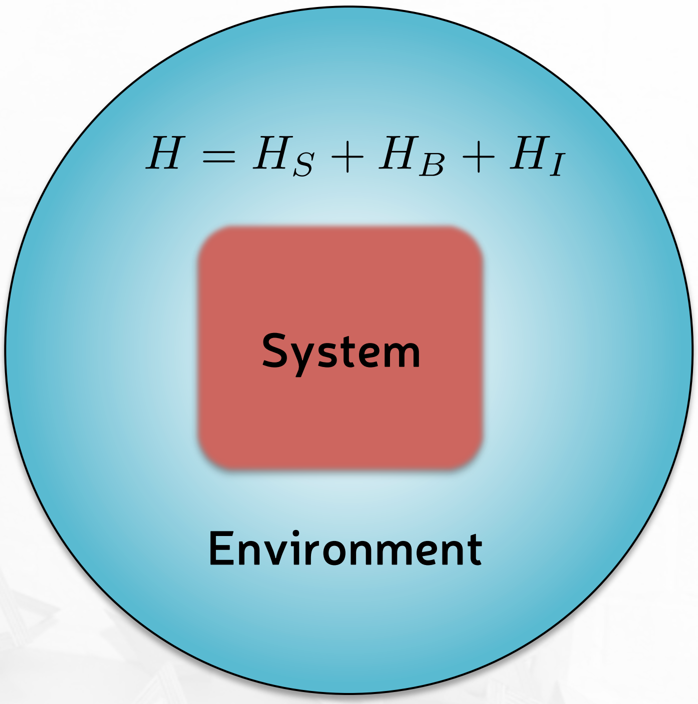
Open Quantum Systems

What is an open quantum system?

- quantum system that is not isolated
- interacts with and evolves under the influence of its surroundings

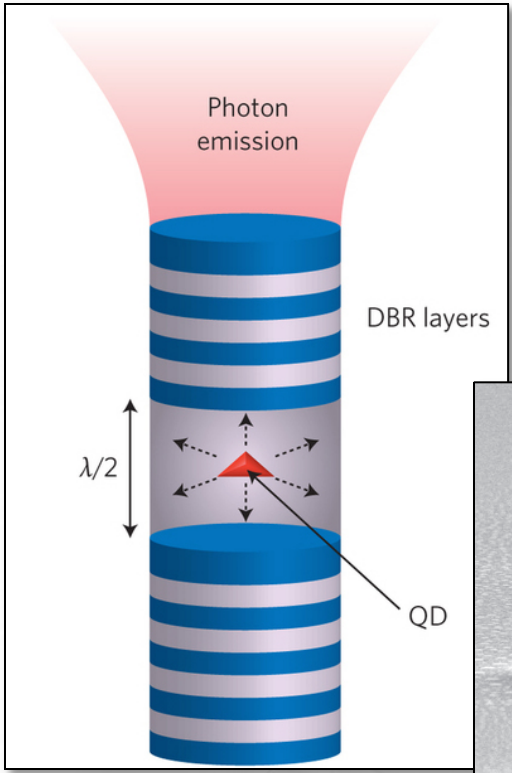
All quantum systems are open

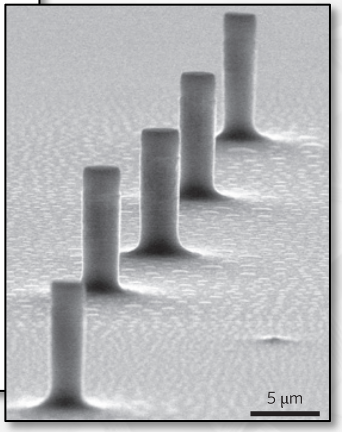
- understanding vital for both applications and fundamentals
- underpins multiple aspects of contemporary physics:
    - interpretation of quantum mechanical laws to feasibility of developing quantum-enhanced technologies
- difficult many-body theoretical problem



Example Open Quantum Systems

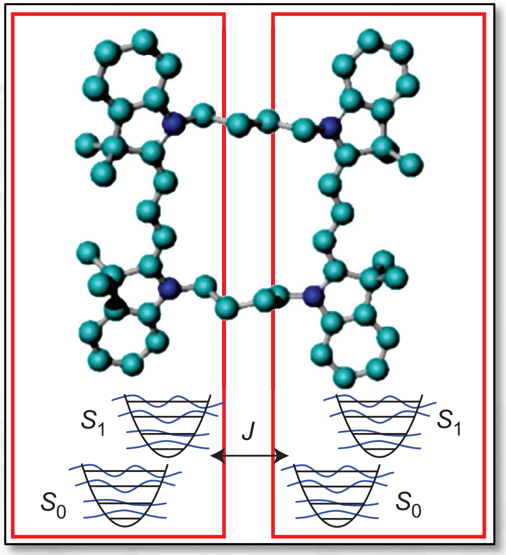
Semiconductor Nanostructures





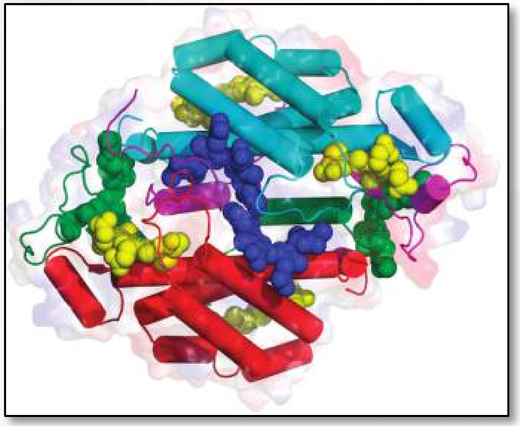
Oulton, Nature Nano. 9, 169 (2014)

Molecular Systems



Synthesised
Halpin et al.,
Nature Chem. 6, 196 (2014)

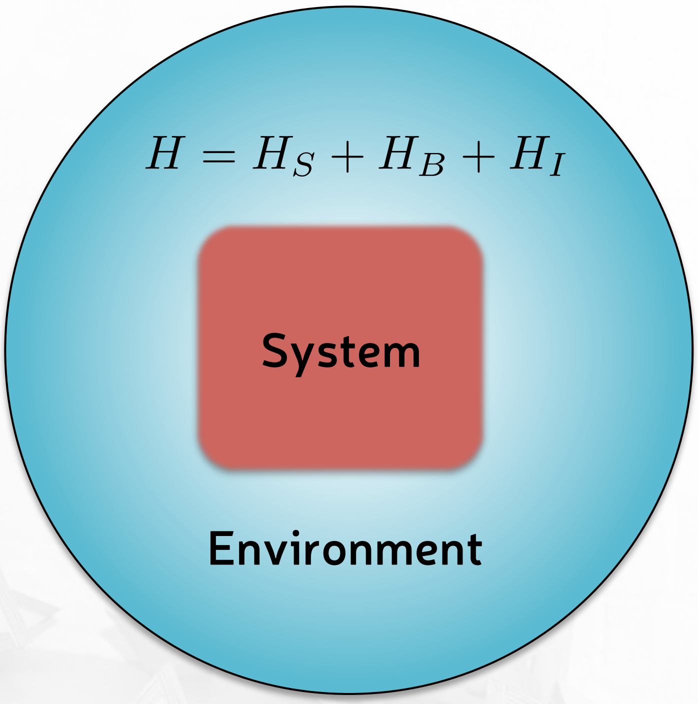
Natural
Novelli, Nazir, et al.,
J. Phys. Chem. Lett. 6, 4573 (2015)



Open Quantum Systems – theoretical description

Master equations

- first order differential equation describing time evolution of the system of interest
- trace out environmental degrees of freedom
  - eliminates all information on environmental state
  - retain (approximately) influence on system
- reduced description only in terms of system states
- intuitive, efficient and straightforward to work with
  - e.g. relate microscopic parameters to experimental observables



Open Quantum Systems – The Challenge

A tractable master equation nearly always requires some kind of approximation

- often valid only for rather restrictive parameter regimes

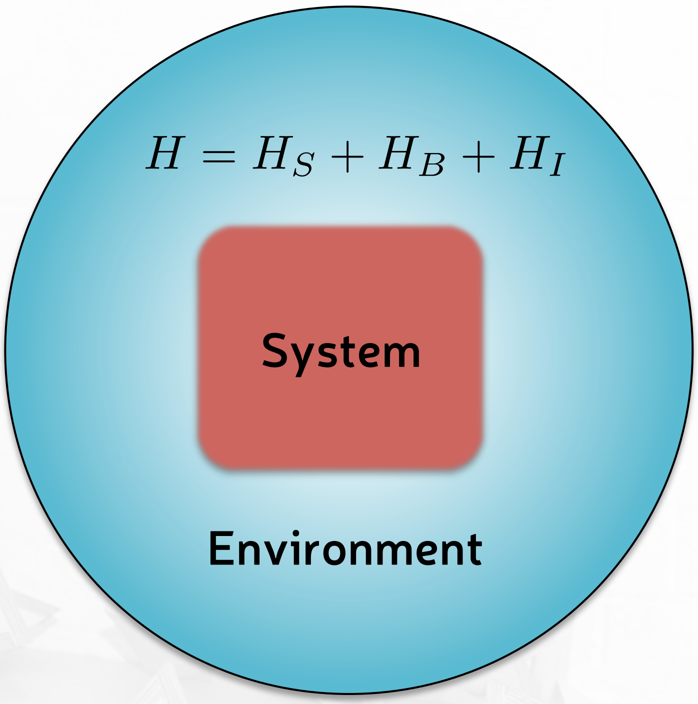
Existing methods

- commonly treat environment as static
- system-environment correlations ignored

⇨ vanishingly weak coupling

Rapid experimental progress in probing larger and more complex quantum systems

- existing methods no longer work, approximations too severe



An alternative approach is required

Weak coupling limit

- System-environment boundary well defined, density operator separable

$$\rho_{SE} \approx \rho_S \otimes \rho_E$$

- Interaction energy ignored in cycle analysis

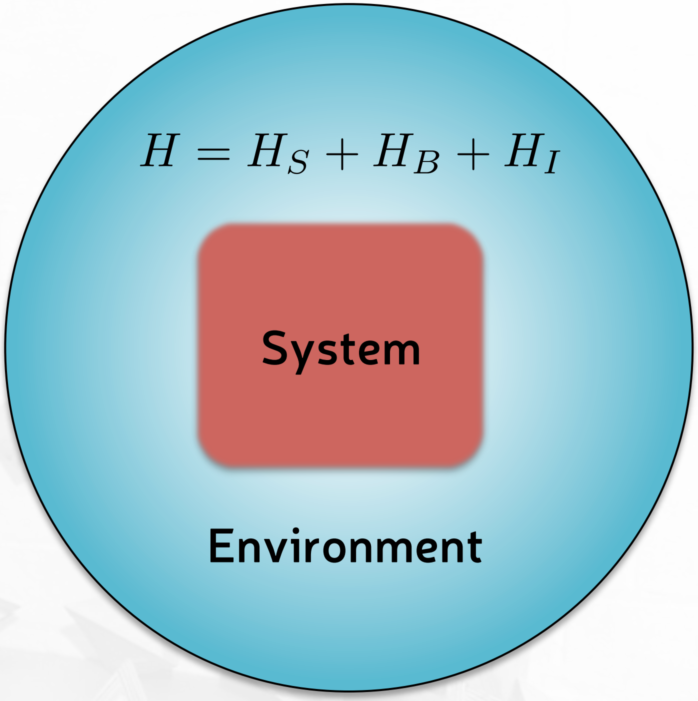
$$U_{S+E} = U_S + U_E + U_{SE} \approx U_S + U_E$$

$$U_S = \mathrm{tr}_S\{H_S \rho_S\}$$

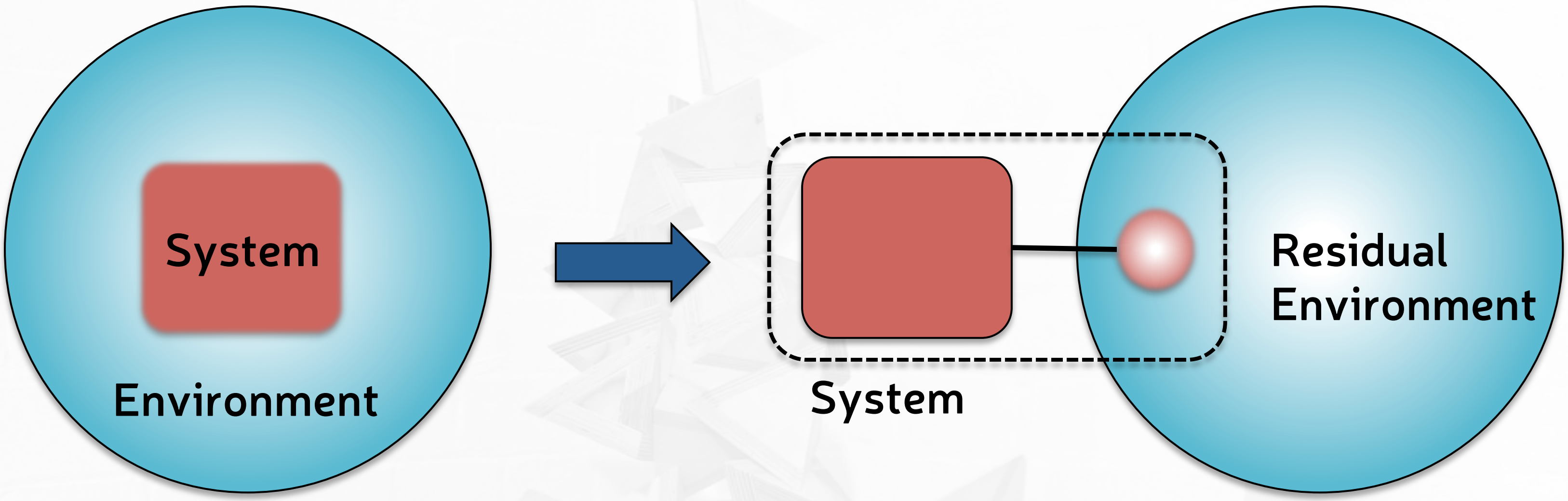
- Environment static. System reaches a canonical thermal state with respect to its internal Hamiltonian in long time limit

$$\rho_S(\infty) = e^{-\beta_E H_S}/Z_S$$

- Can we overcome these limitations but retain a similar description?



Theme – Redrawing the Boundaries



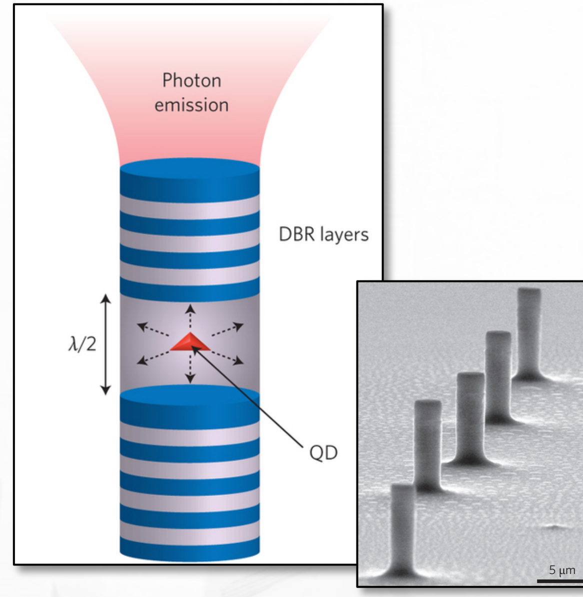
Redefine the system-environment boundary to allow:

- **Environmental dynamics and accumulation of correlations**
- Study of larger and more complex systems
- New physical insight
- New principles for experimentally controlling real quantum systems

Solid-state quantum optics

How do we modify standard quantum optics to model solid-state photonic devices?

- e.g. what effect do lattice vibrations (phonons) have on emitted photon properties?

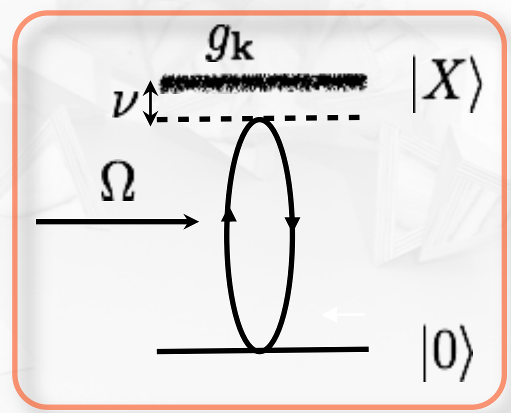


Many applications

- efficient, on-demand single photon sources, lasers, optical switches, quantum networks…
- potential for scalability and integration with current technologies

Model

- two-level system
- coherent manipulations through external laser addressing
- excitation of single electron from valence to conduction band
- oscillations damped by phonon interactions

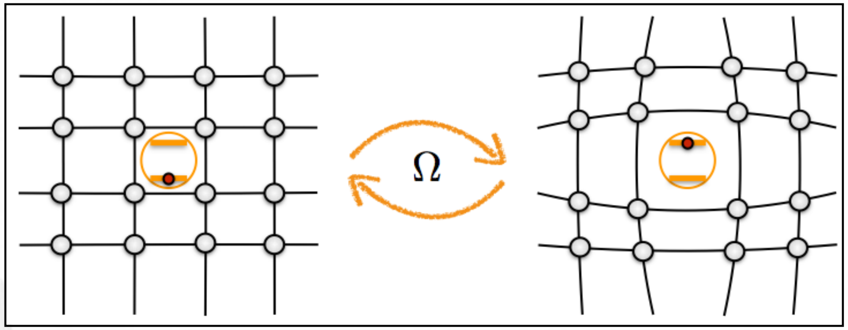


Phonon interactions

Lattice displaces in response to changes in charge configuration

- polaron formation – new boundary
- we incorporate this physics into our master equation via a unitary transformation
- allows strong electron-phonon interactions
- direct expt-theory comparisons

$$H_P = e^S H e^{-S}$$



Topical Review: AN and D. P. S. McCutcheon, JPCM 28, 103002 (2016)

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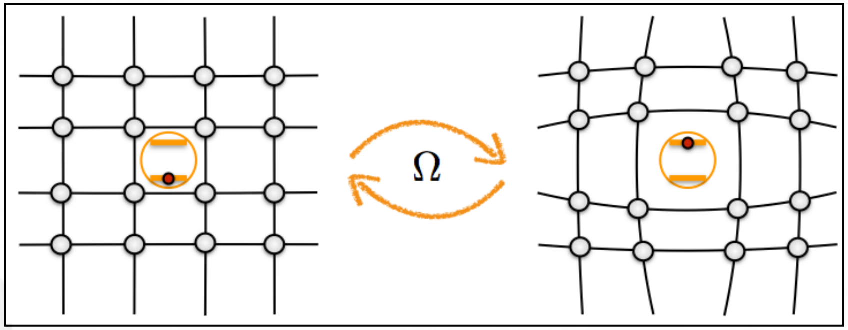
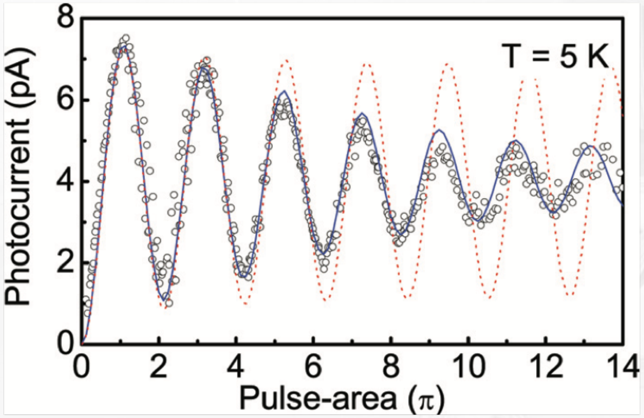


Topical Review: AN and D. P. S. McCutcheon, JPCM 28, 103002 (2016)

Damping of coherent oscillations



A. J. Ramsay et al. PRL 105, 177402 (2010)

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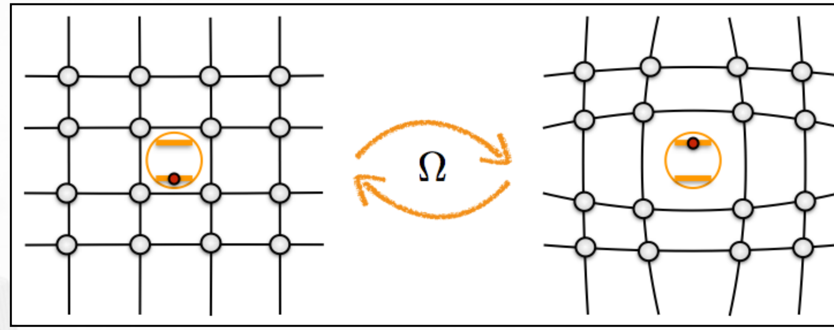

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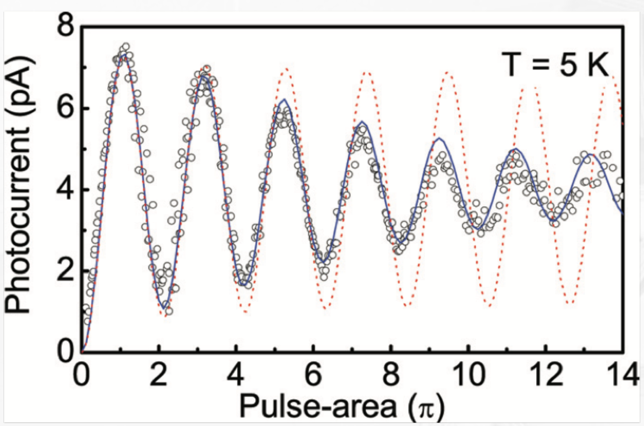
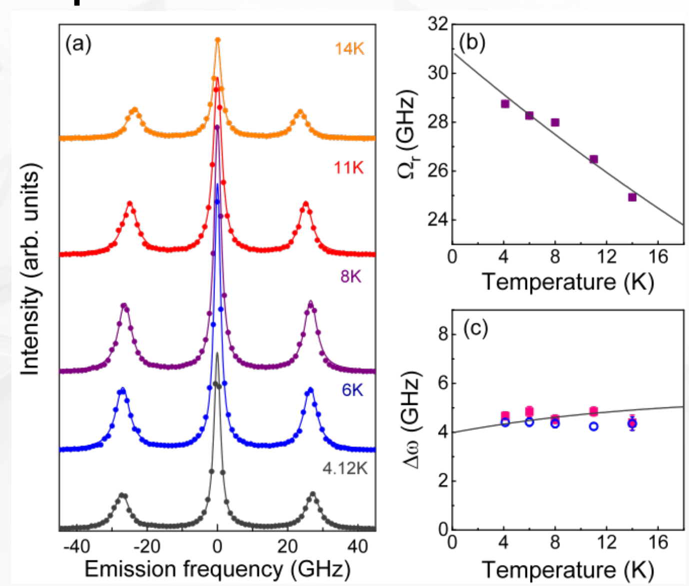


A. J. Ramsay et al. PRL 105, 177402 (2010)

Temp. dependence in resonance fluorescence

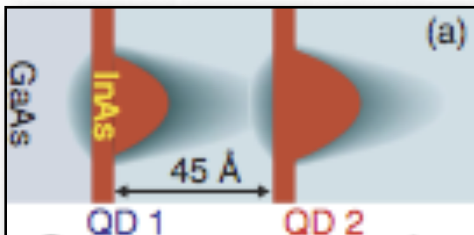


Y. Wei et al., PRL 113, 097401 (2014)
D. P. S. McCutcheon and AN, PRL 110, 217401 (2013)

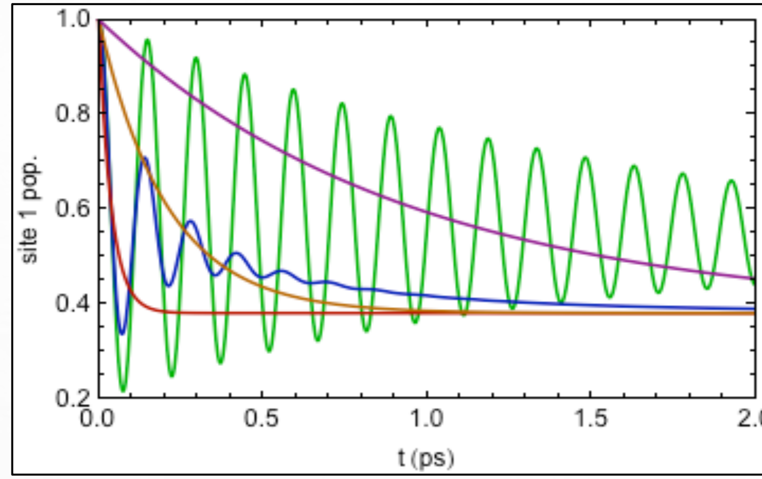
Coherent vs incoherent energy transfer

Closely space pair of quantum dots

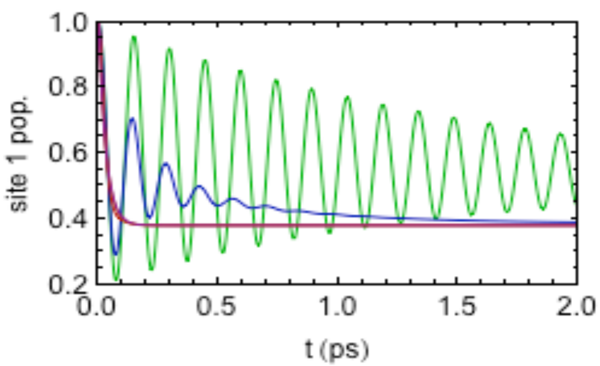
- exchange of excitation under influence of vibrational environment
- coherent or incoherent?
- need a consistent theory



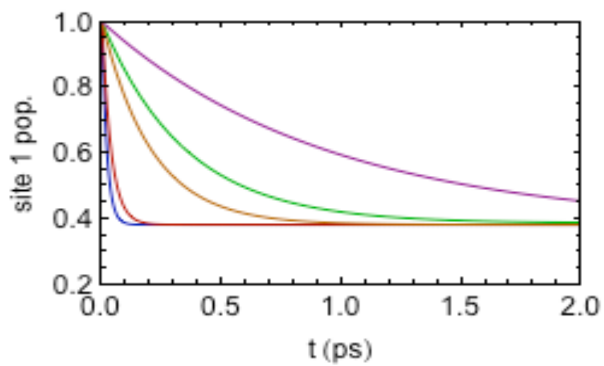
B. D. Gerardot et al., PRL 95, 137403 (2005)



Population dynamics (polaron approach) $H_P = e^S H e^{-S}$



Redfield:
Perturbation in coupling H_I



Foerster:
Perturbation in system H_S

AN, PRL 103, 146404 (2009)

D. P. S. McCutcheon and AN, PRB 83, 165101 (2011)

D. P. S. McCutcheon and AN, JCP 135, 114501 (2011)

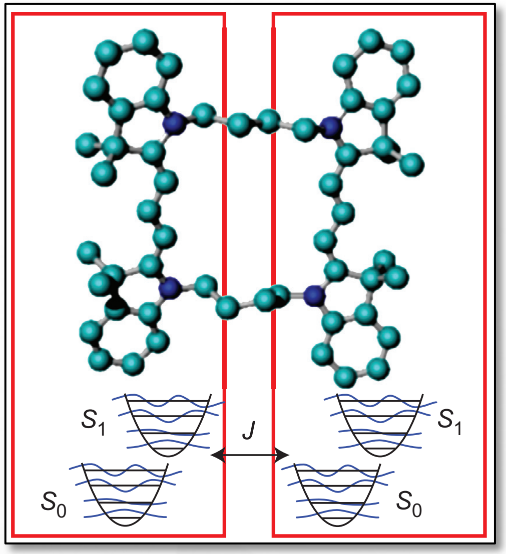
Molecular energy transfer

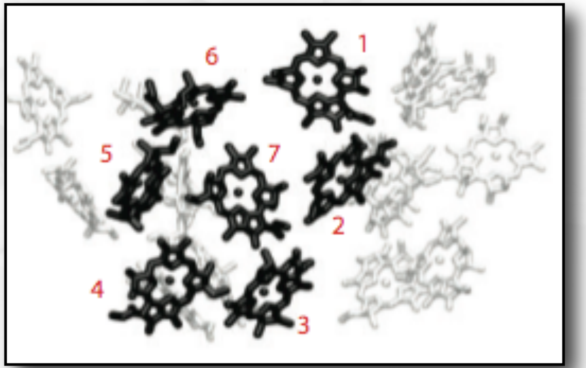
Charge and energy transfer in molecular dimers

- low energy vibrations
- long-lived system-environment correlations
- strong coupling and high temperatures
- polaron representation no longer optimal

Larger molecular complexes

- coherence observed at room temperature in some light harvesting complexes
- functional role, e.g. in efficiency or robustness?
- can lessons be learnt for artificial light harvesting?
- again, strong coupling to low energy vibrations and high temperatures



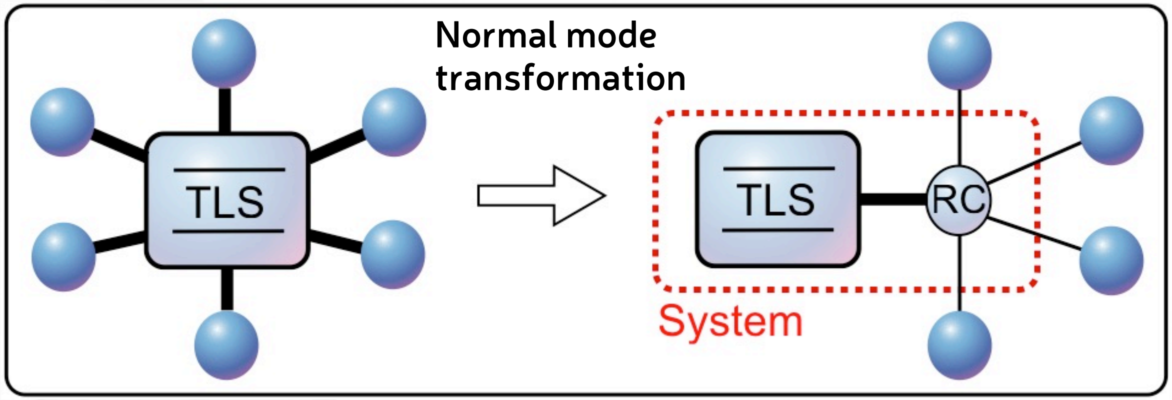


FMO: Y. C. Cheng and G. R. Fleming, Annu. Rev. Phys. Chem. 60, 241 (2009)

Collective coordinate mapping

Normal mode transformation

- "system" now enlarged
- original system plus mode treated exactly
- residual environment traced out in usual manner



$$\hat{s} \otimes \sum_k g_k (b_k^\dagger + b_k) \rightarrow \lambda \hat{s} \otimes (a^\dagger + a)$$

Spin-boson model

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

$$\sum_q \nu_q r_q^\dagger r_q + (a + a^\dagger) \sum_q f_q (r_q^\dagger + r_q)$$

$$\boxed{\sum_k g_k (b_k^\dagger + b_k) = \lambda (a^\dagger + a)}$$

Iles-Smith et al., PRA 90, 032114 (2014); JCP 144, 044110 (2016)

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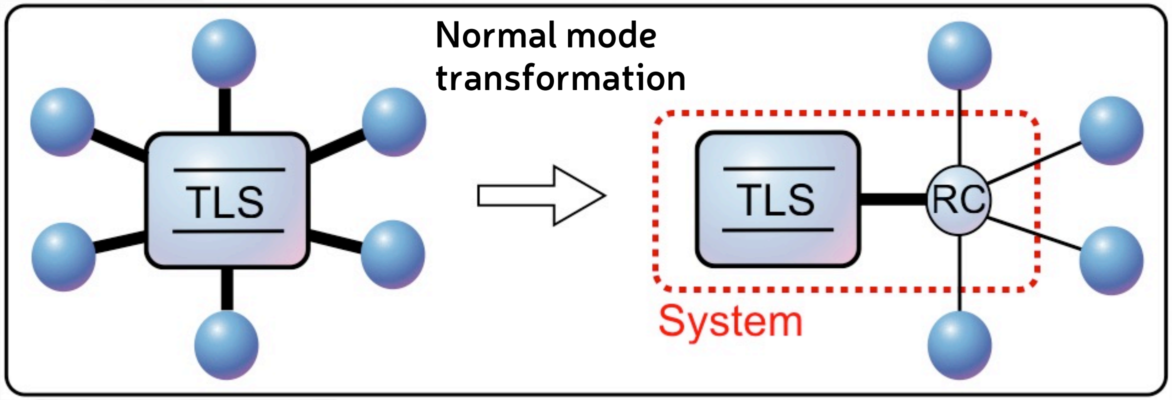
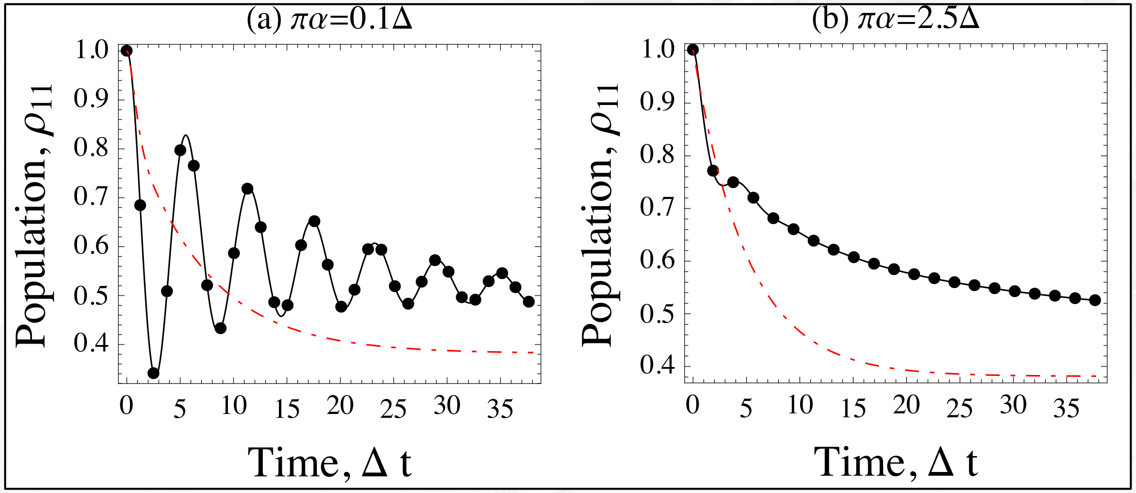


$$\hat{s} \otimes \sum_k g_k (b_k^\dagger + b_k) \rightarrow \lambda \hat{s} \otimes (a^\dagger + a)$$

Benchmarking

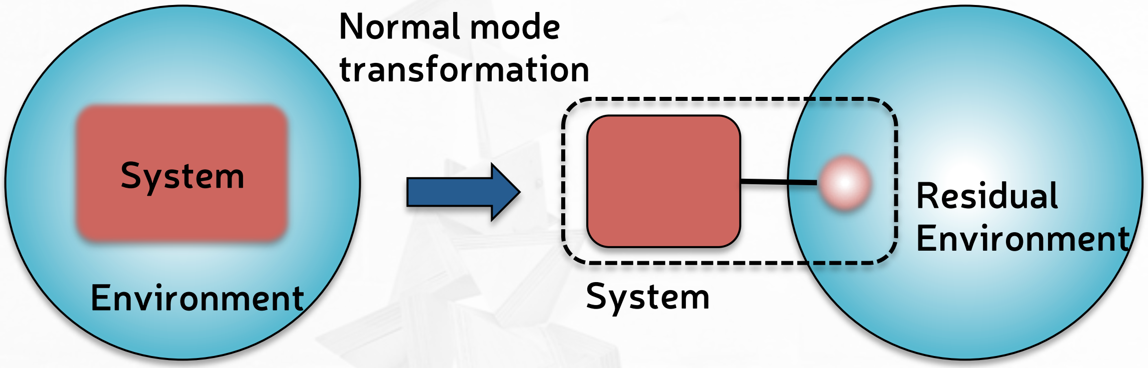
- weak coupling fails
- all important system-bath correlations captured through mapping



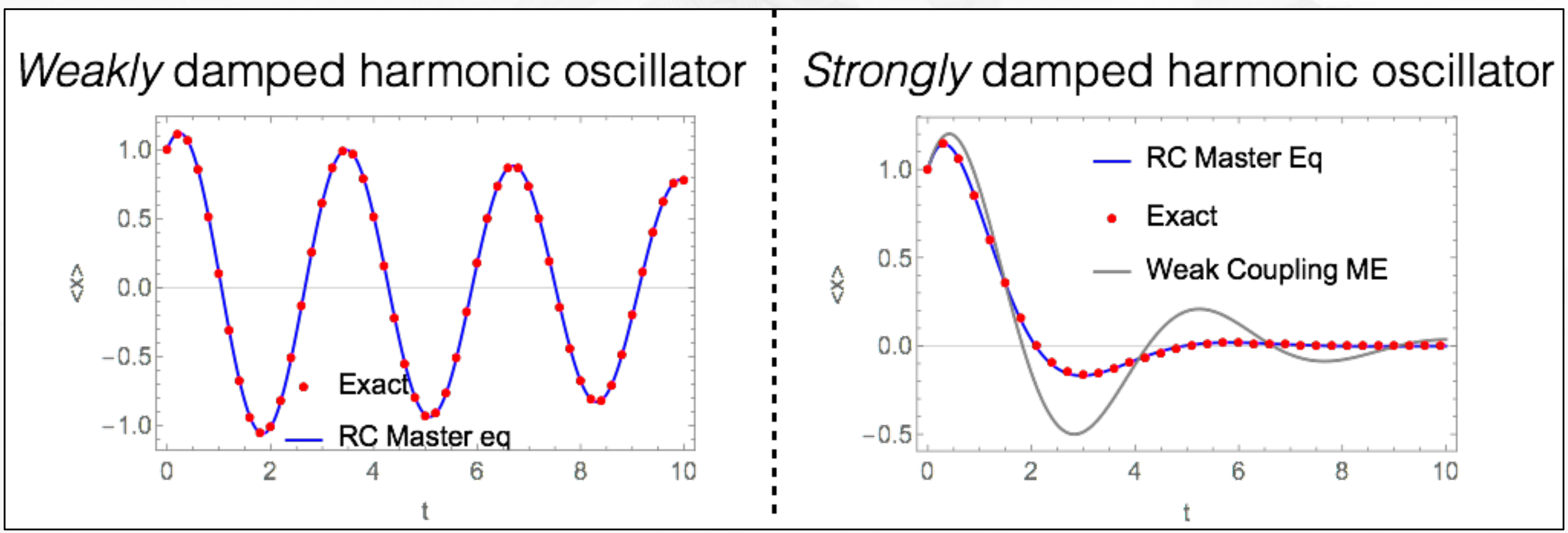
- CC master equation
- Numerical benchmark
- Weak-coupling

Iles-Smith et al., PRA 90, 032114 (2014); JCP 144, 044110 (2016)

Aside: Harmonic oscillator



$$H = \omega_0 a^\dagger a + \sum_k \omega_k b_k^\dagger b_k + (a + a^\dagger) \sum_k g_k (b_k^\dagger + b_k)$$

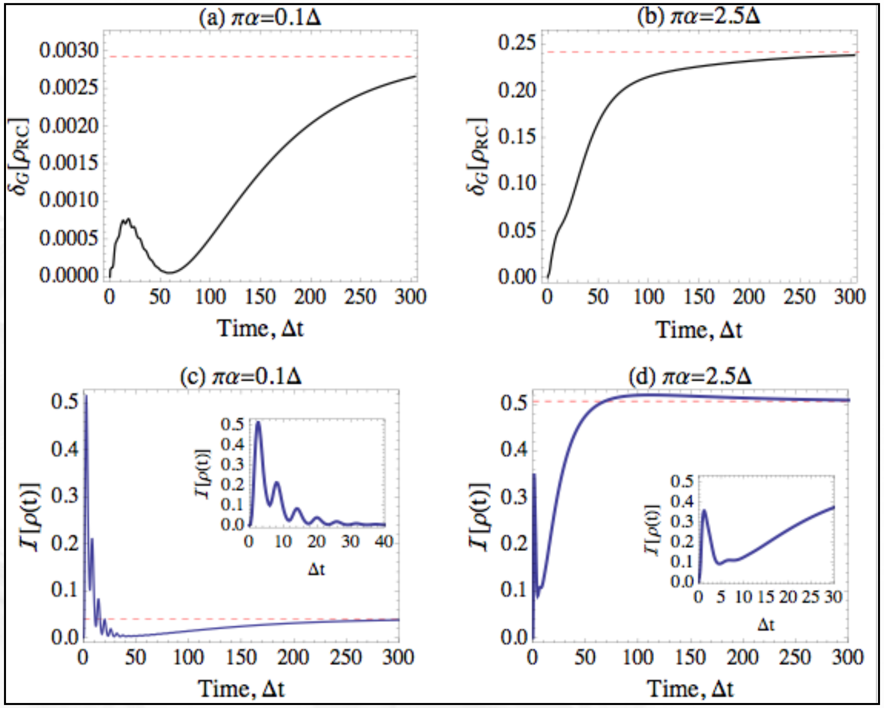


Environmental dynamics and correlations

Also allows environmental dynamics and correlations to be probed

- lower bounds on original bath non-Gaussianity and system-bath correlations (mutual information)
- Explore dynamic generation of correlations and deviations from initial (Gaussian) thermal state - **two timescales**

$$\mathcal{I} = S(\rho_S) + S(\rho_{CC}) - S(\rho_{S+CC})$$



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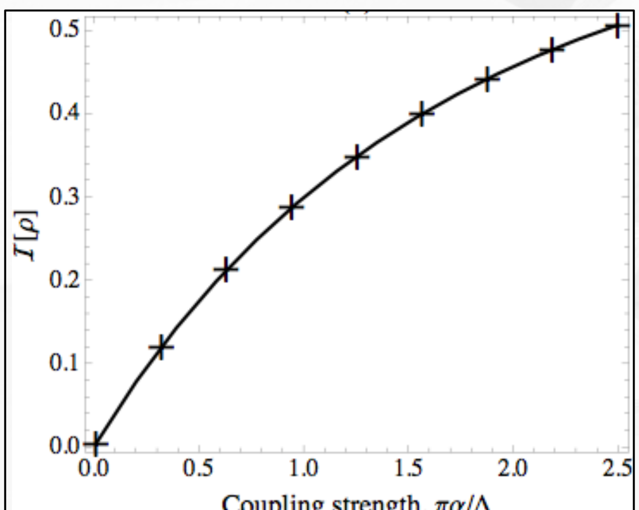

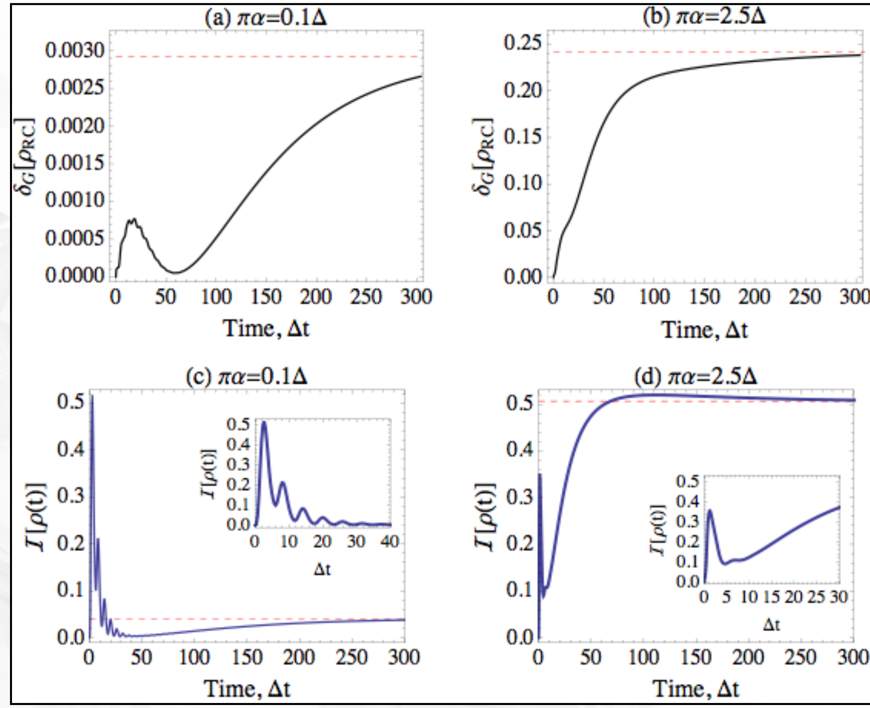

System-bath correlations persist into steady state

- system state no longer a thermal distribution over its (isolated) eigenstates – non-canonical statistics
- instead, we have a thermal state of mapped Hamiltonian

Environmental dynamics and correlations

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- lower bounds on original bath non-Gaussianity and system-bath correlations (mutual information)
- Explore dynamic generation of correlations and deviations from initial (Gaussian) thermal state - **two timescales**

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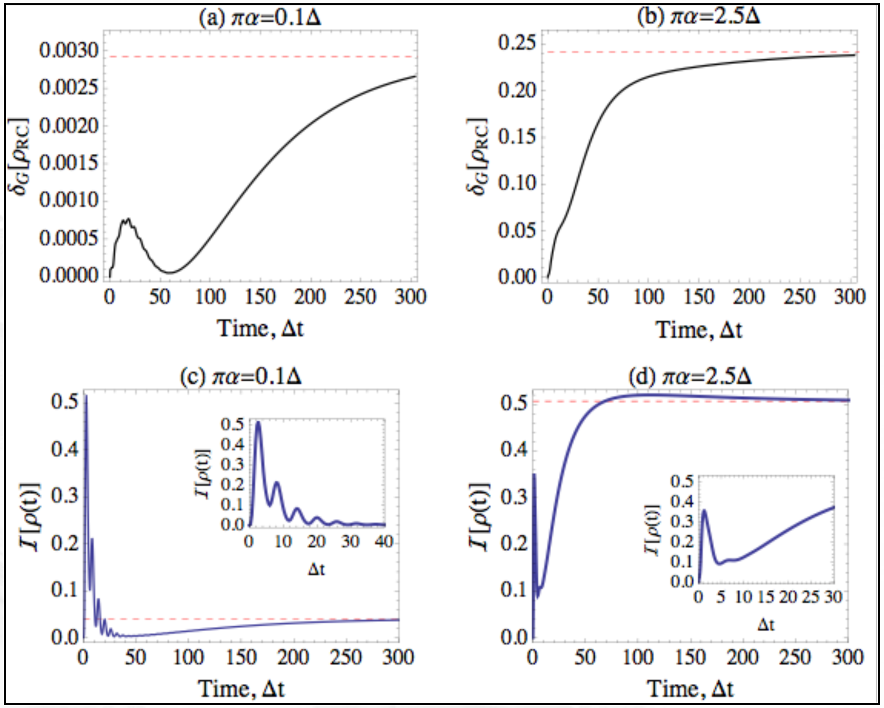
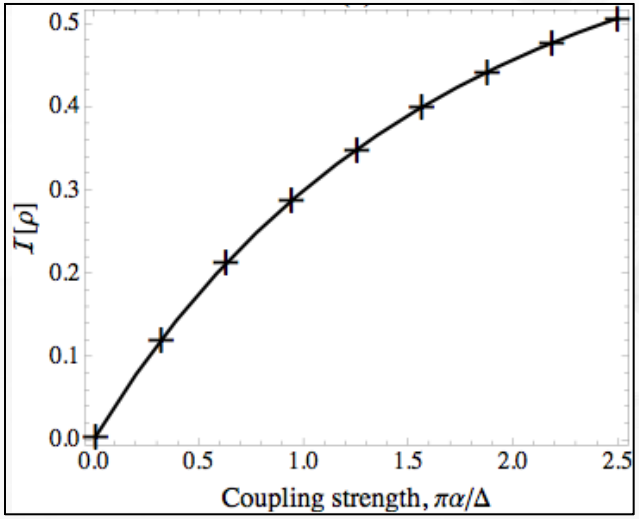
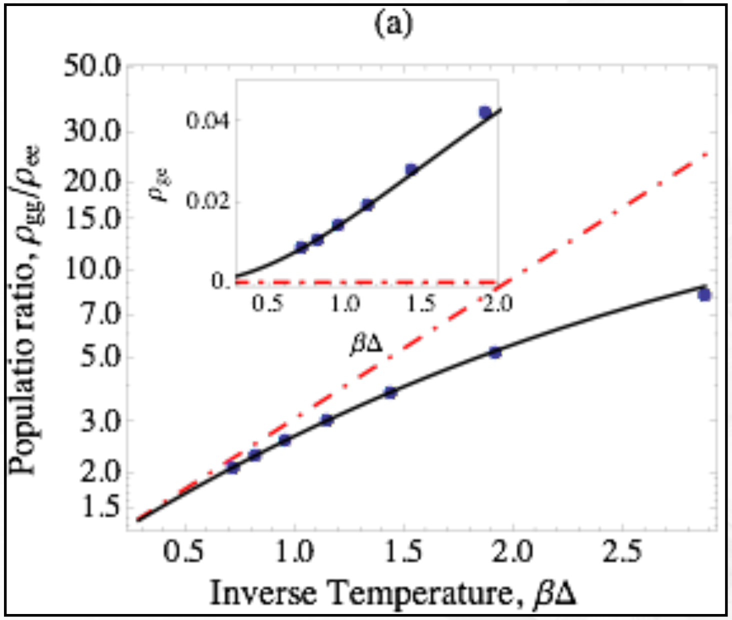


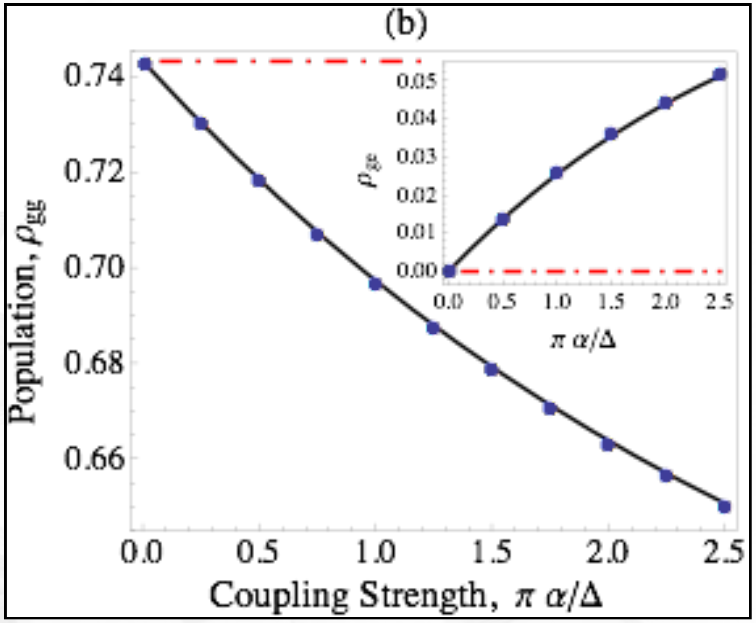


System-bath correlations persist into steady state

$$\rho_{S+CC}(\infty) = e^{-\beta_{E'} H_{S+CC}} / Z_{S+CC}$$

System steady-state





- CC master equation
- Numerical benchmark
- Weak-coupling

$$\rho_{SS} = \frac{1}{Z}\mathrm{tr}_{CC}\left\{e^{-\beta[H_S+\Omega a^\dagger a+\lambda\hat{s}(a^\dagger+a)]}\right\}$$

Departures from weak-coupling

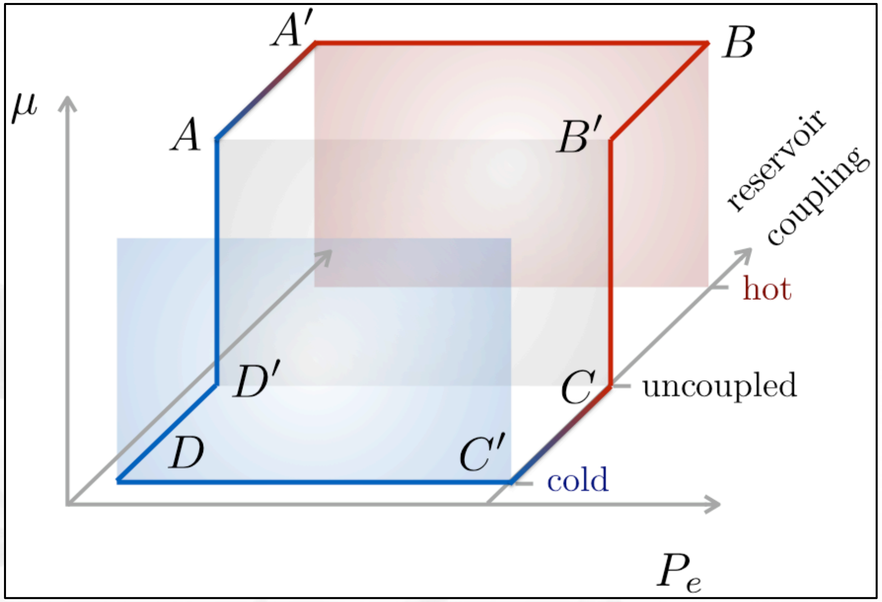
- Log of (eigenstate) population ratio no longer linear with inverse temperature
- populations now vary with system-bath coupling strength
- coherences present in system eigenbasis

Iles-Smith et al., PRA 90, 032114 (2014); JCP 144, 044110 (2016)

Heat engines at finite coupling

Thermodynamics at finite coupling

- mapping incorporates system-reservoir correlations into a consistent thermodynamic analysis
- i.e. retain description in terms of thermal states
- circumvents the usual restriction to weak coupling and vanishing correlations between the two



$$\begin{aligned}\langle H \rangle &= \mathrm{tr}\{H \rho_{SE}\} \\ &\approx \mathrm{tr}_{S+CC}\{H_{S+CC}\rho_{S+CC}\} + U_{E'}\end{aligned}$$

- Long-time limit

$$\rho_{S+CC}(\infty) = e^{-\beta_{E'} H_{S+CC}}/Z_{S+CC}$$

Otto cycle at finite coupling

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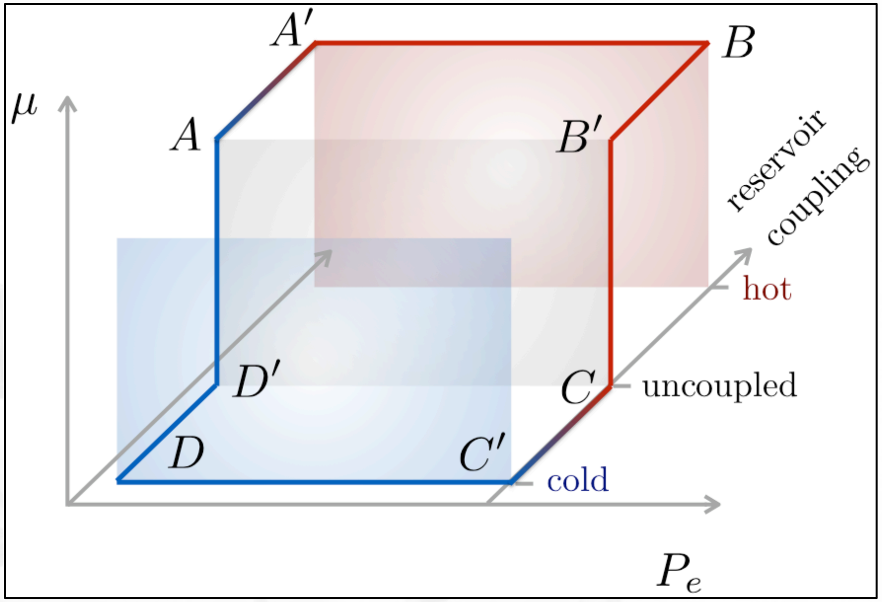
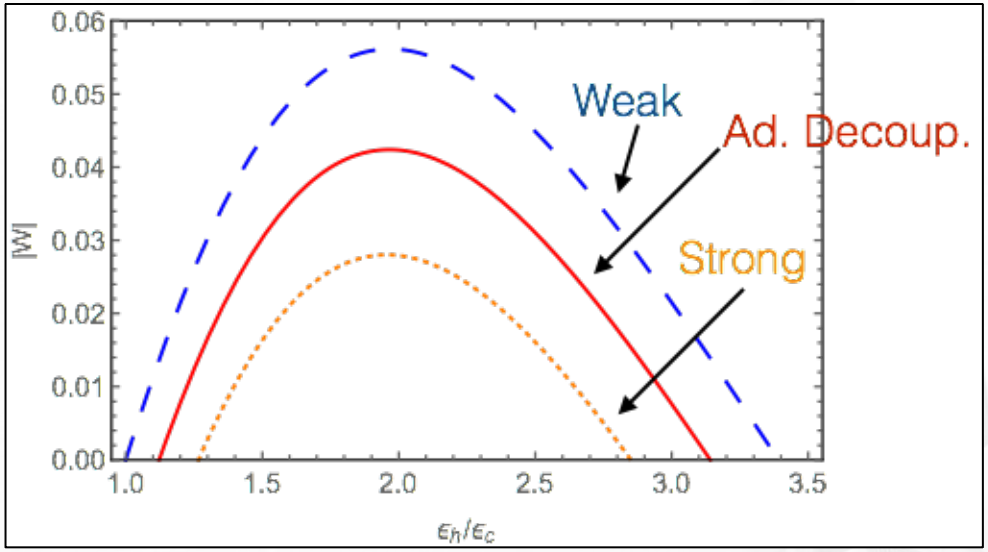


Quantum Otto cycle – standardly a 4 stroke heat engine, separates heat and work

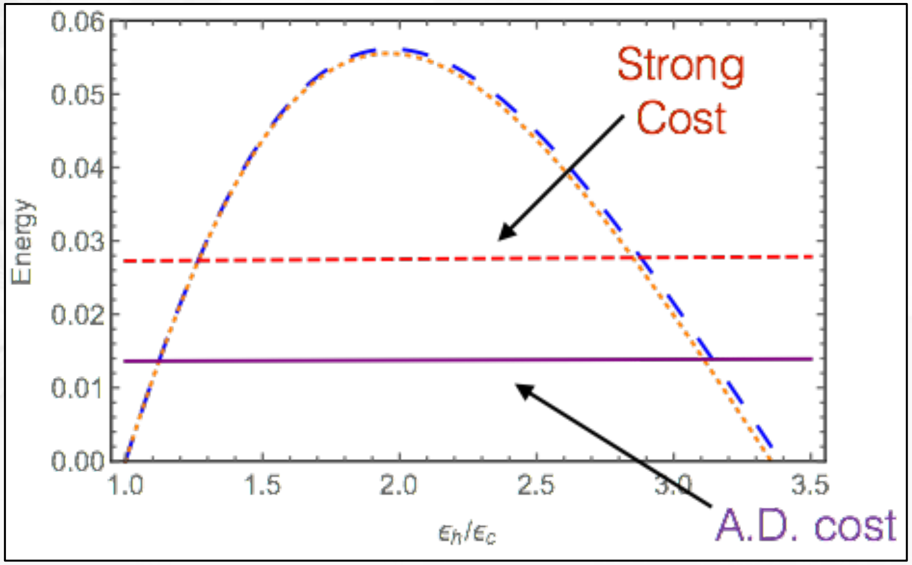
- A'-B: hot isochore (infinite time)
- B'-C: isentropic expansion (adiabatic or sudden)
- C'-D: cold isochore (infinite time)
- D'-A: isentropic compression (adiabatic or sudden)
- We also explicitly include coupling/decoupling steps

Work output and decoupling energy cost

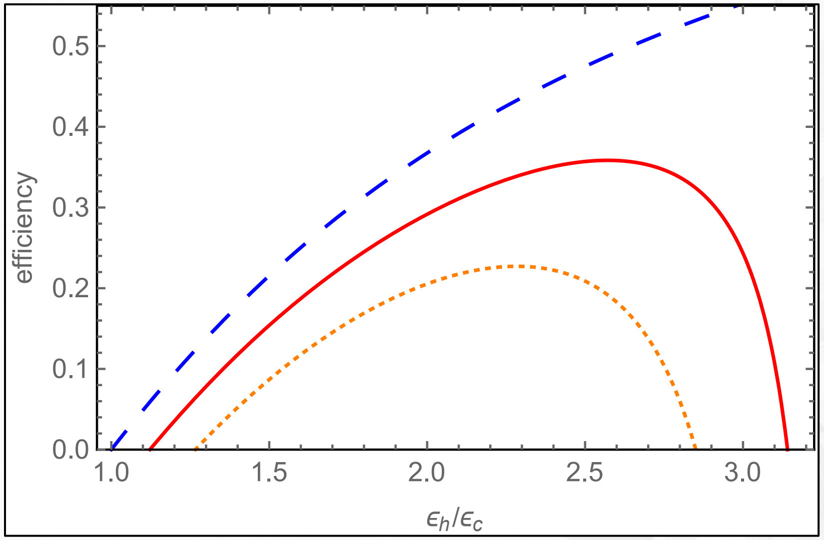


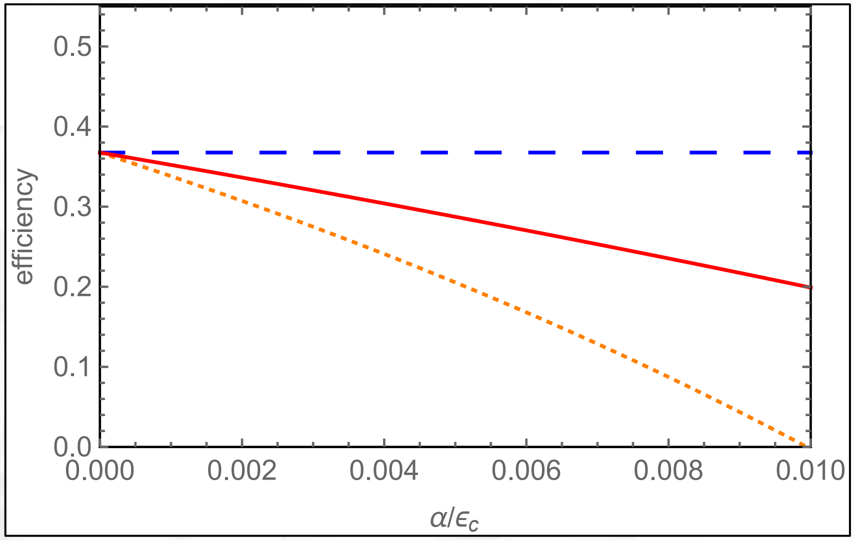
- Work output is reduced in the strong coupling limit
- Reduction occurs due to decoupling costs

- Costs can be mitigated by an adiabatic decoupling procedure
- Sometimes possible to extract more work along isentropes for strong coupling, though always counteracted by decoupling costs



Efficiency

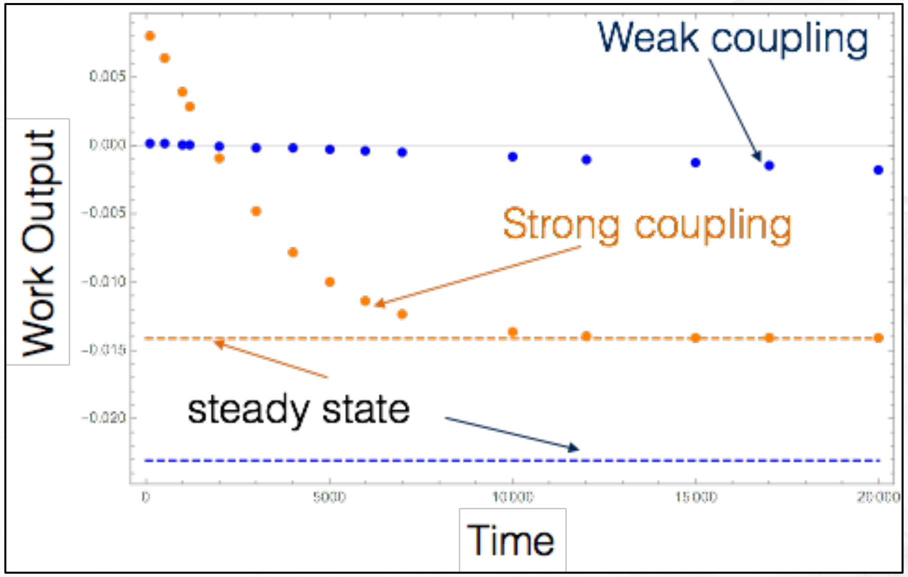




- Efficiency also reduced in the strong coupling limit
- Decreases monotonically with coupling strength

Performance of a quantum heat engine at strong reservoir coupling, D. Newman, F. Mintert and AN, Phys. Rev. E 95, 032139 (2017)

Otto cycle in finite time - adiabatic

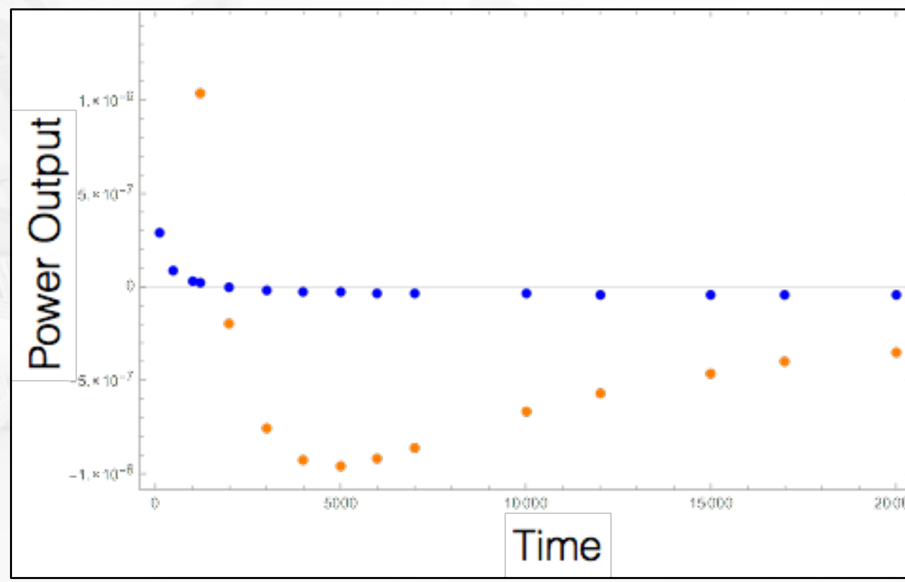


Adiabatic (slow) limit - work

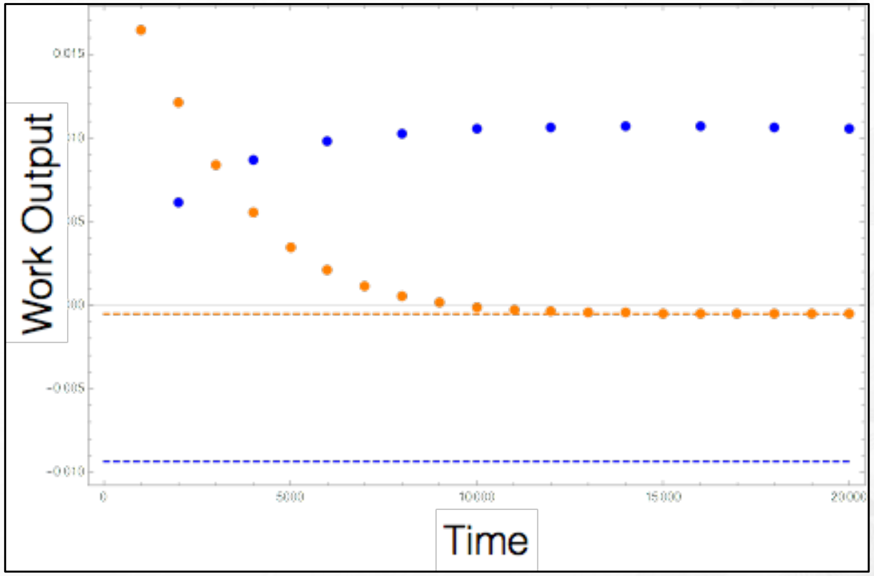
- Can generate greater work output at finite times for finite coupling.
- Long time limit (max. work) is greater in the weak coupling case, as before.

Adiabatic (slow) limit - power

- Max. power output at finite coupling beats the weak coupling counterpart.

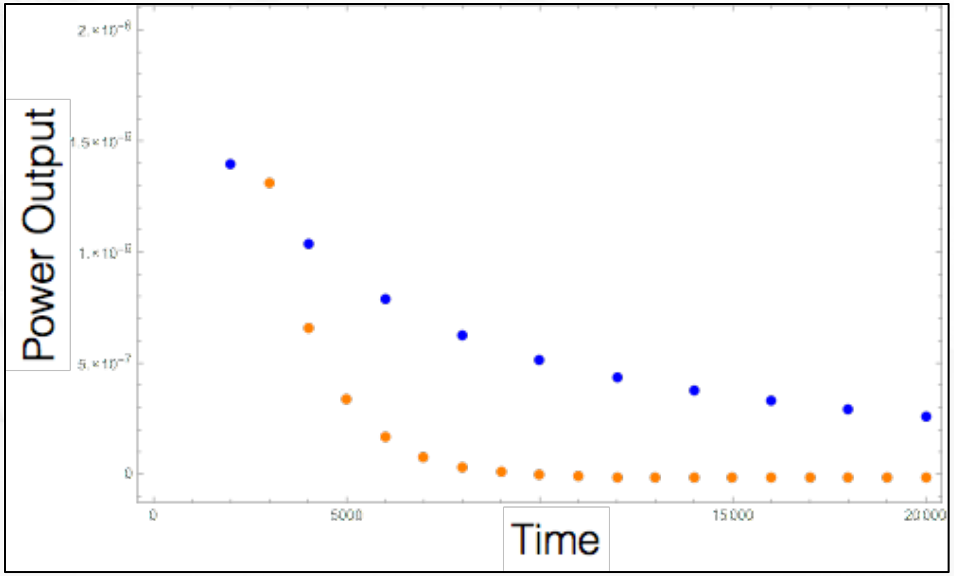


Otto cycle in finite time - sudden



Sudden limit - work

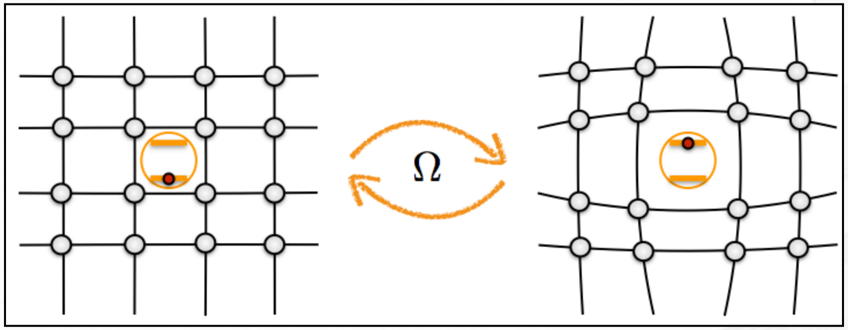
- Can generate work output at finite times for finite coupling, even when weak coupling engine produces no output.
- Long time limit (max. work) is greater in the weak coupling case, as before.



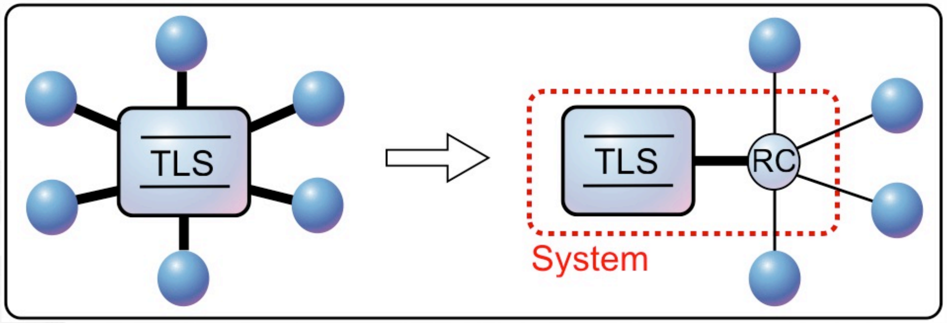
Sudden limit - power

- We can generate power output at finite coupling at times where the weak coupling engine produces no output.

Summary and future work



High frequency modes



Low frequency/memory effects

Ongoing

- Hybrid theory
- Finite time/continuously coupled heat engines and non-equilibrium steady-states
- Fermionic environments
- Many-body systems and lattice models
- Quantum phase transitions
- Artificial light-harvesting

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Thank You