A quantum limit to non-equilibrium heat engine performance imposed by strong system-reservoir coupling

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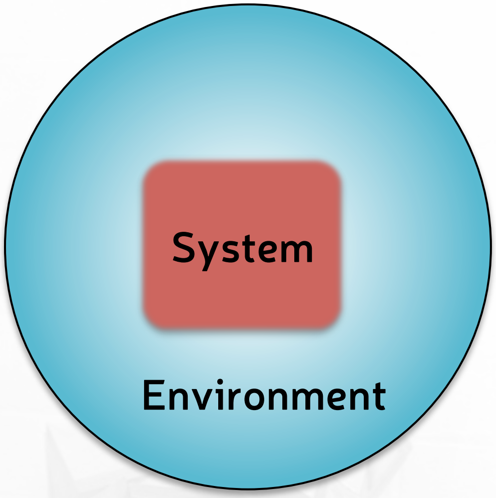
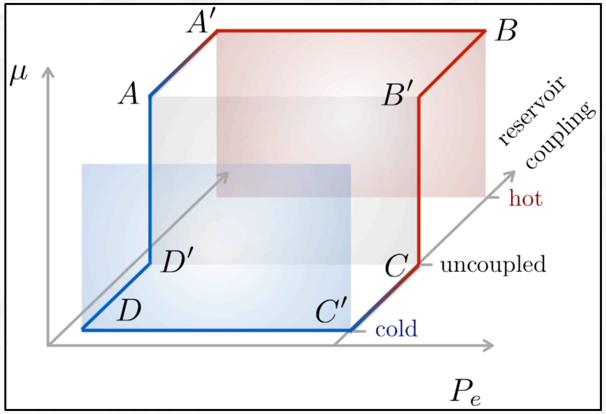


arXiv:1906.09167

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



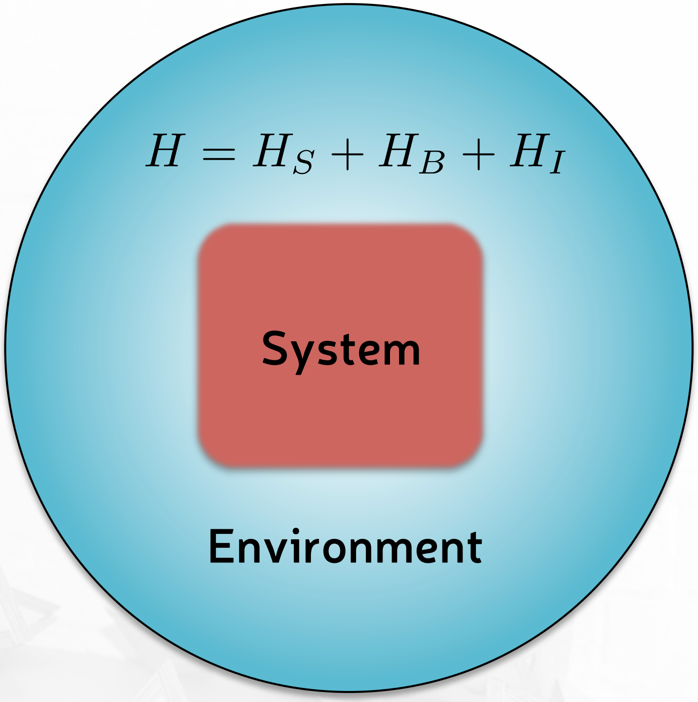
Open Quantum Systems

What is an open quantum system?

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

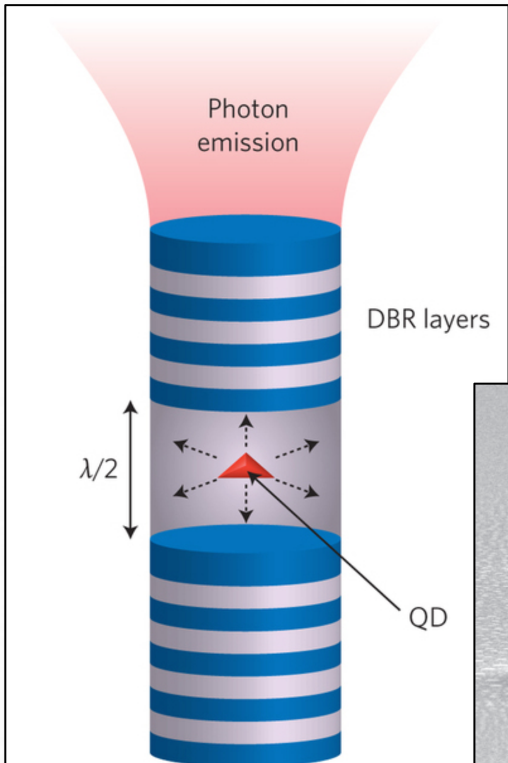
All quantum systems are open

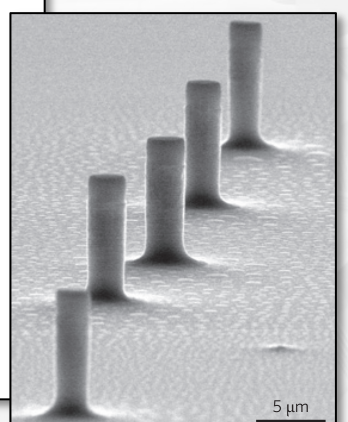
- understanding vital for both applications and fundamentals (e.g. in thermodynamics)
- underpins multiple aspects of contemporary physics:
    - interpretation of quantum mechanical laws to feasibility of developing quantum-enhanced technologies
- difficult many-body theoretical problem



Example Open Quantum Systems

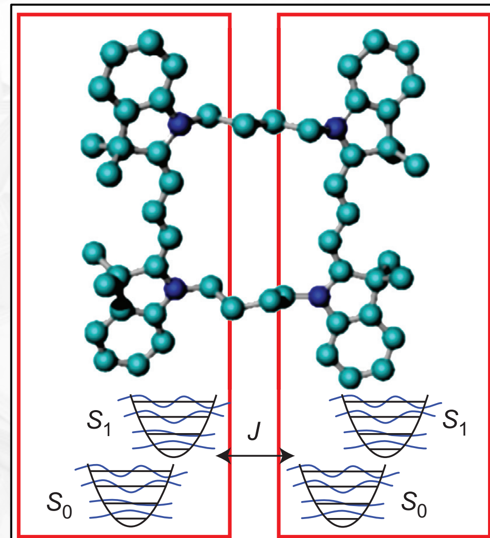
Semiconductor Nanostructures





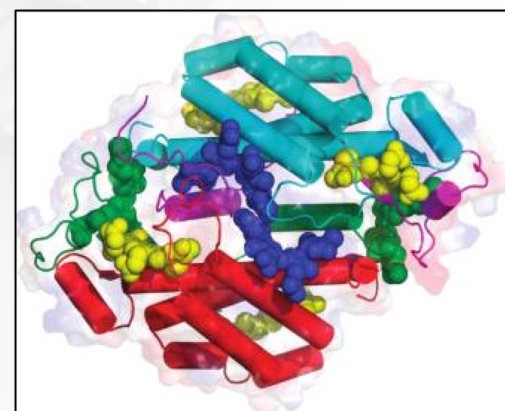
Oulton, Nature Nano. 9, 169 (2014)

Molecular Systems



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

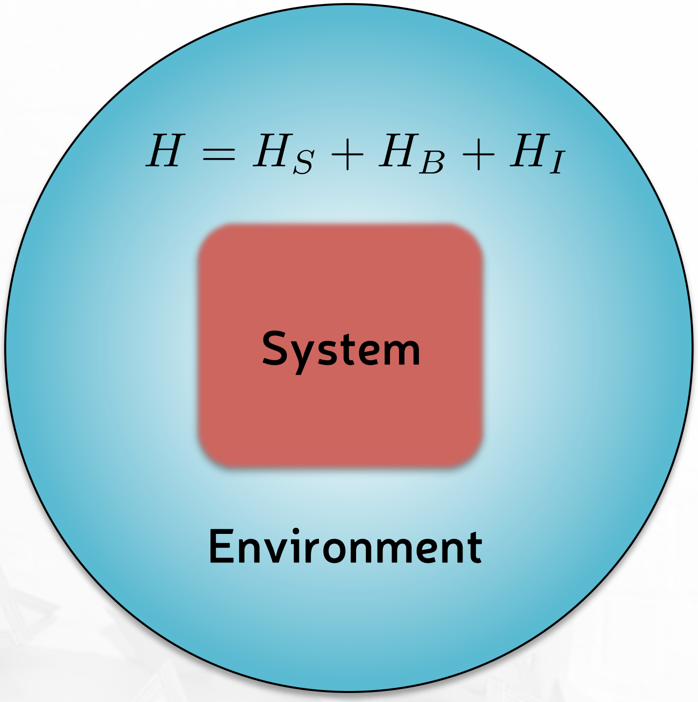
Natural
Novelli, Nazir, et al.,
J. Phys. Chem. Lett. 6, 4573 (2015)



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

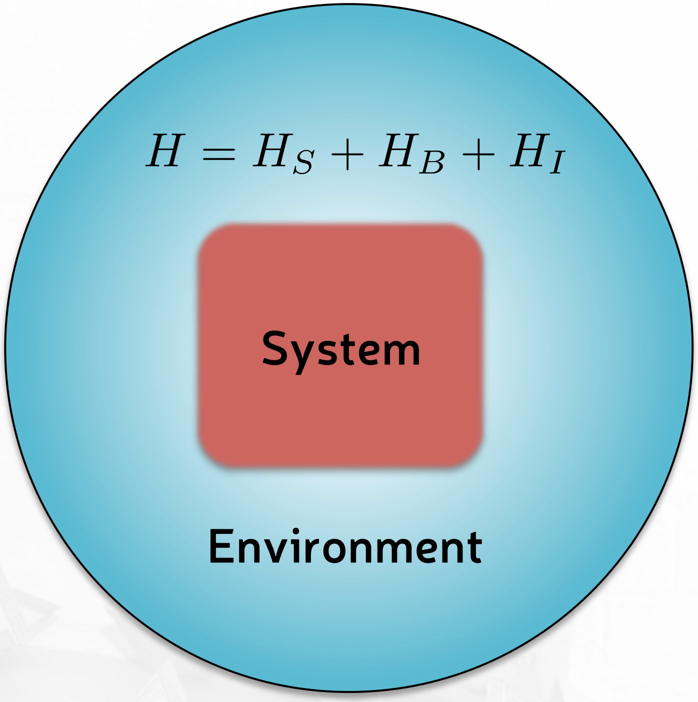
Existing methods

- 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

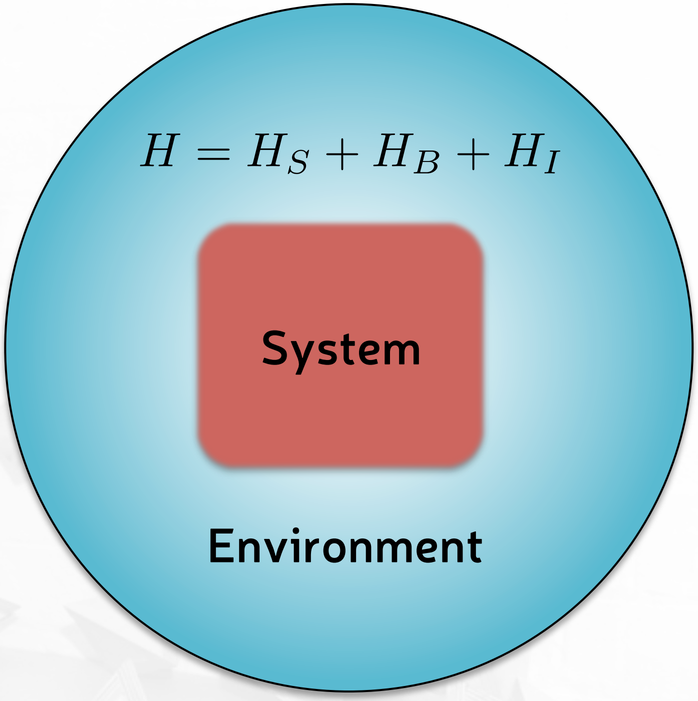
$$U_{S+E} = U_S + U_E + U_{SE} \approx U_S + U_E$$

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

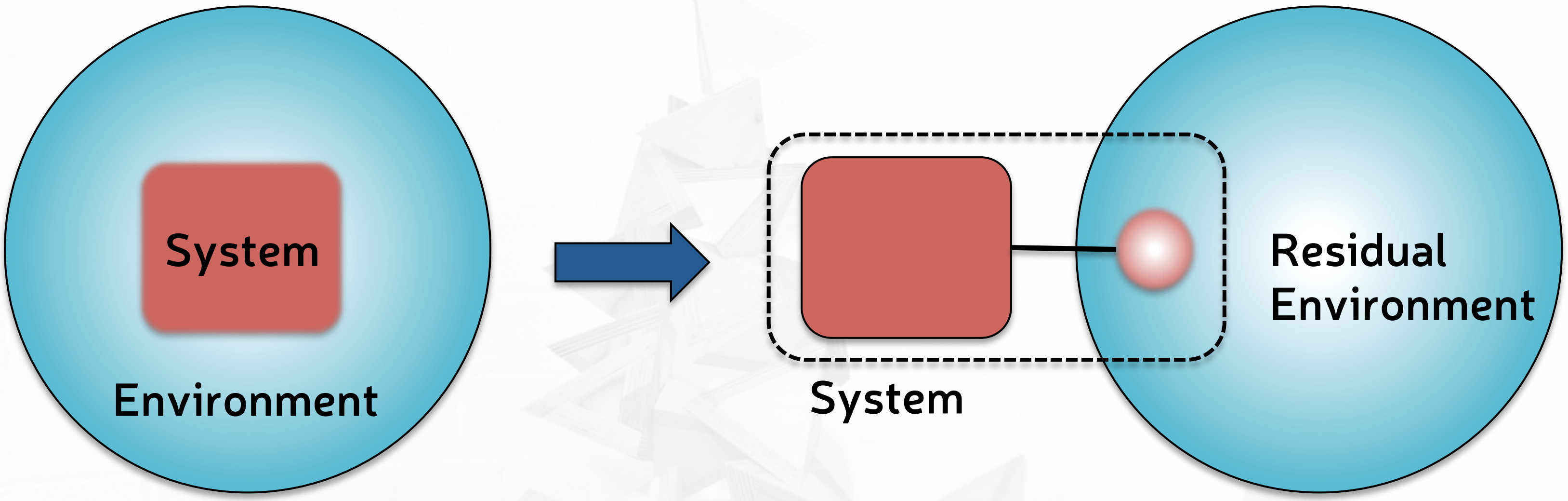
- Environment static. Assume system reaches a canonical thermal state with respect to its internal Hamiltonian in long time limit

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

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



Theme – Redrawing the Boundaries

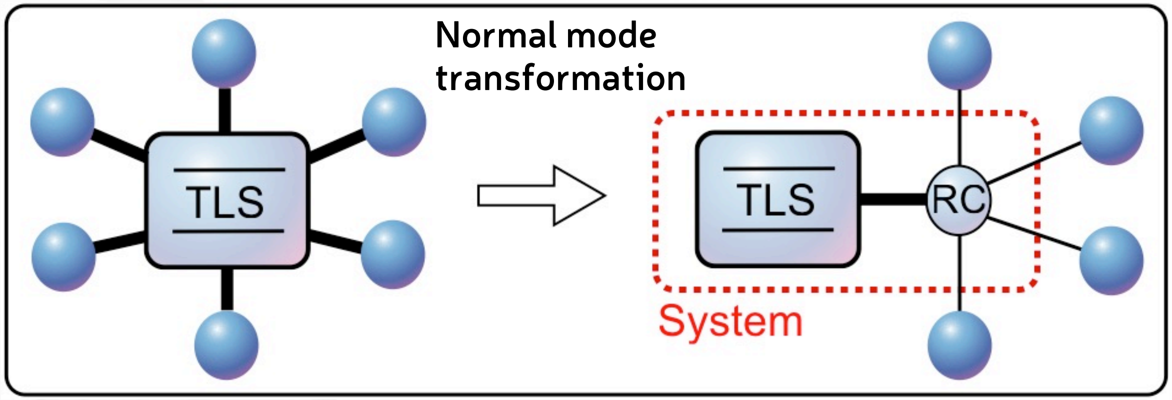


Redefine the system-environment boundary to allow us to track environmental dynamics and accumulation of correlations

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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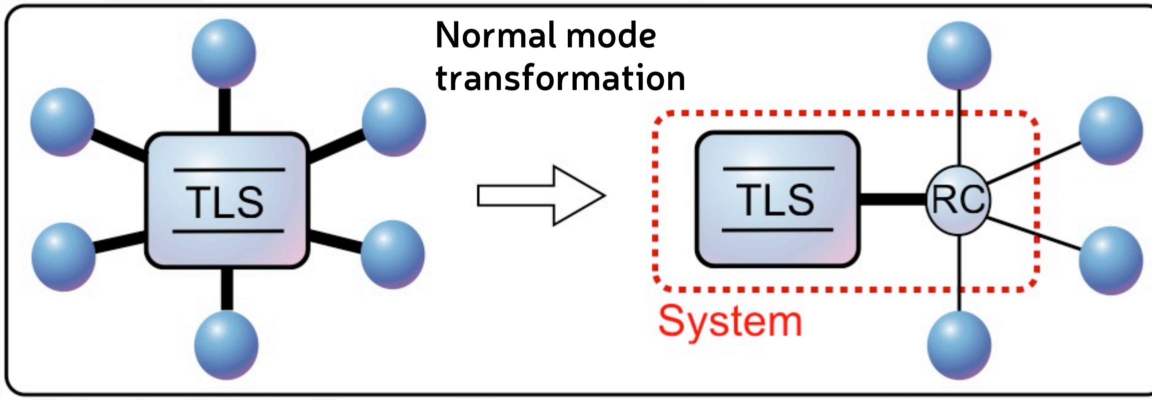
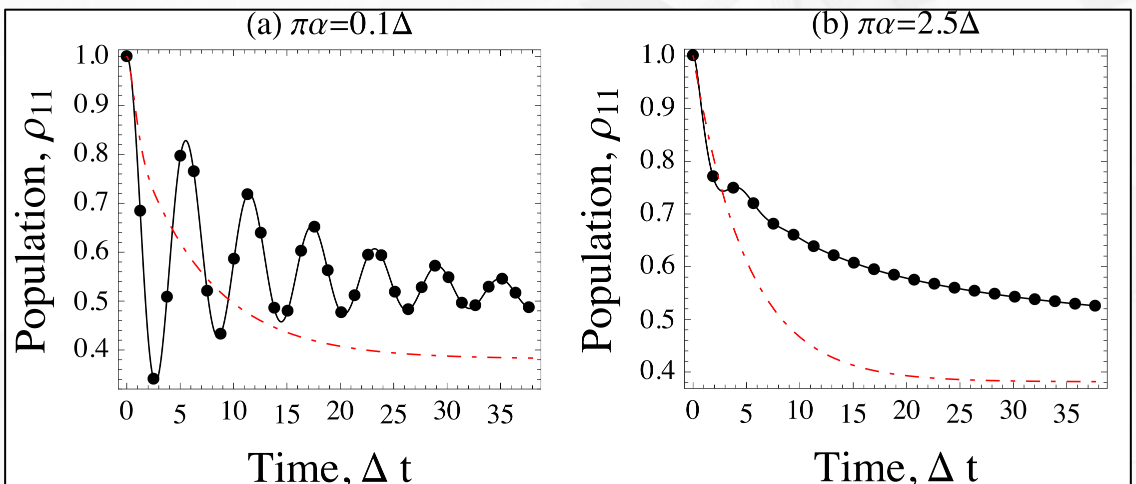


$$\hat{s} \otimes \sum_k g_k (b_k^\dagger + b_k) \rightarrow \lambda \hat{s} \otimes (a^\dagger + a)$$

Benchmarking

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



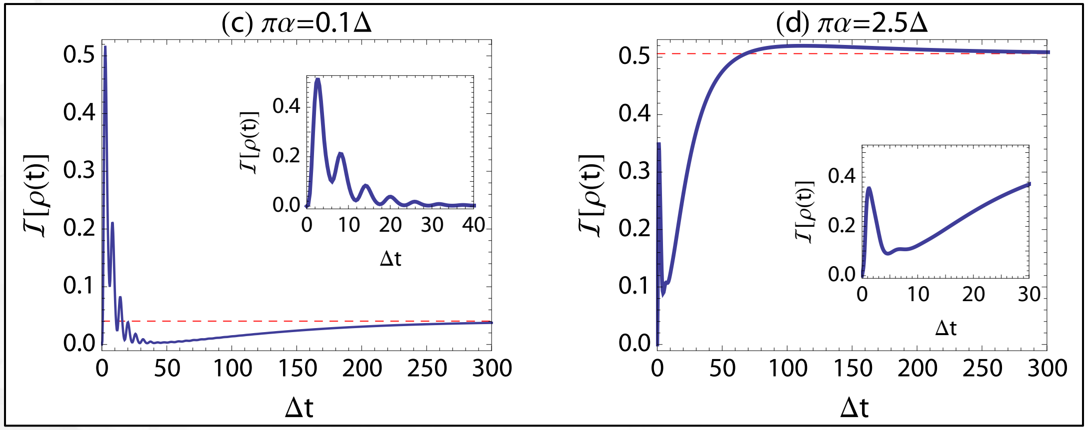
- CC master equation
- Numerical benchmark
- Weak-coupling

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

System-reservoir correlations

Also allows system-reservoir correlations to be probed

- lower bound on original system-bath correlations (mutual information)
- Explore dynamic generation of correlations - **two timescales**



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

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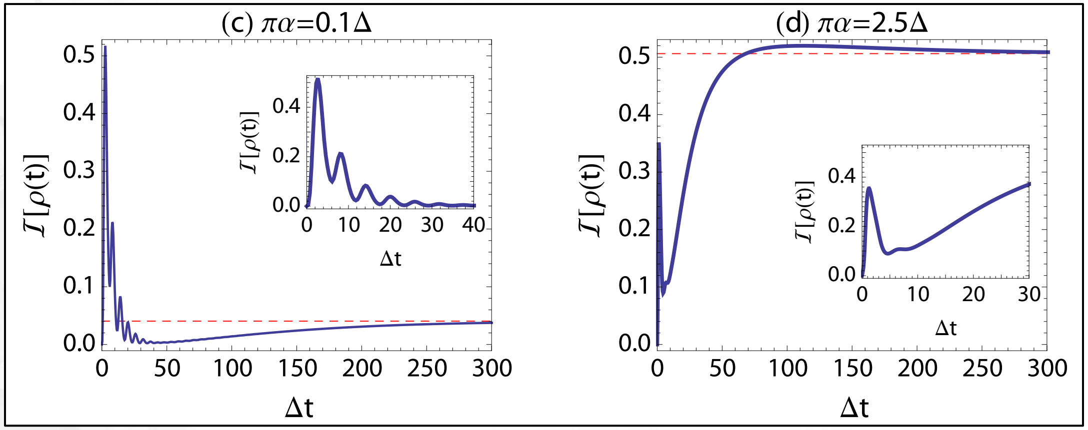

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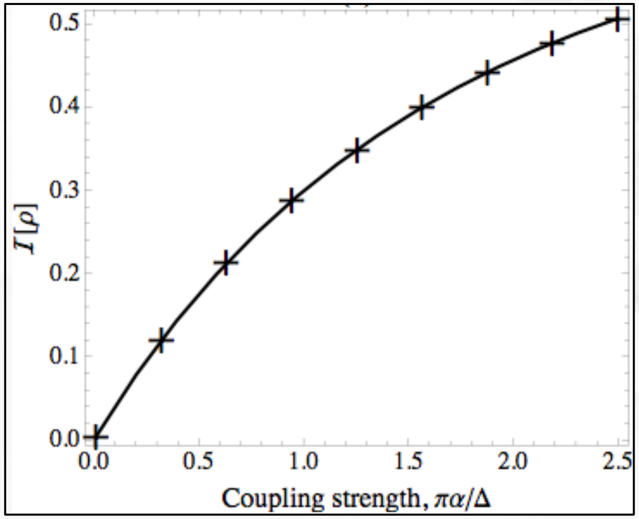

System-bath correlations persist into steady state

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

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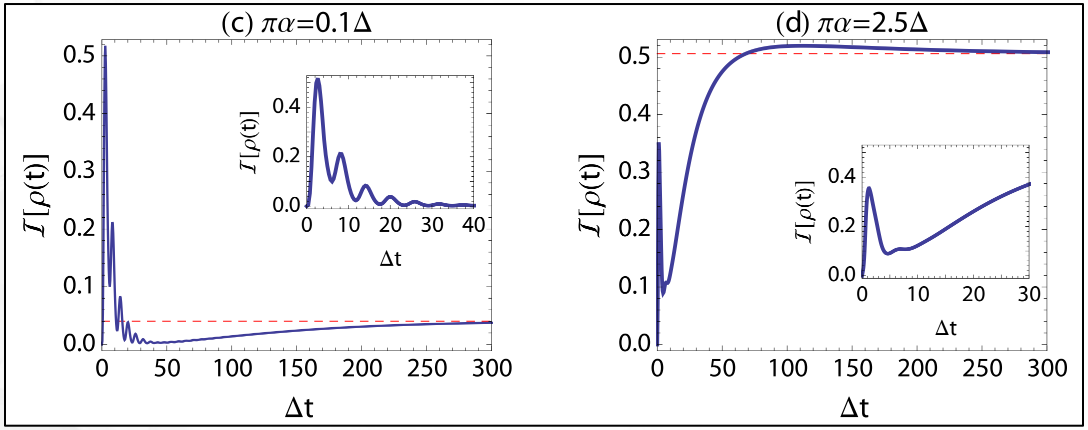

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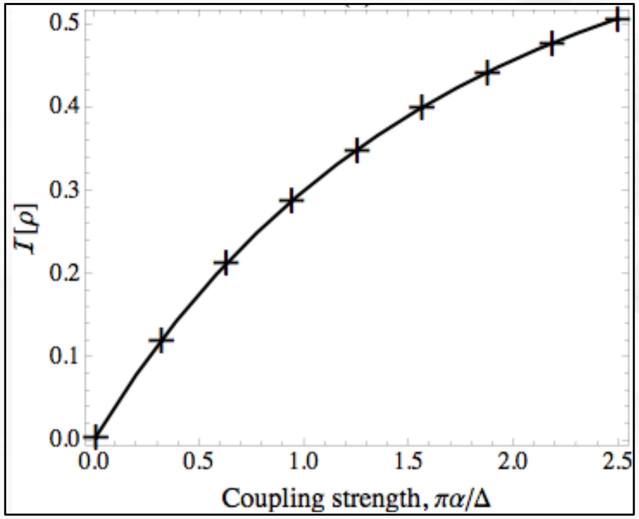
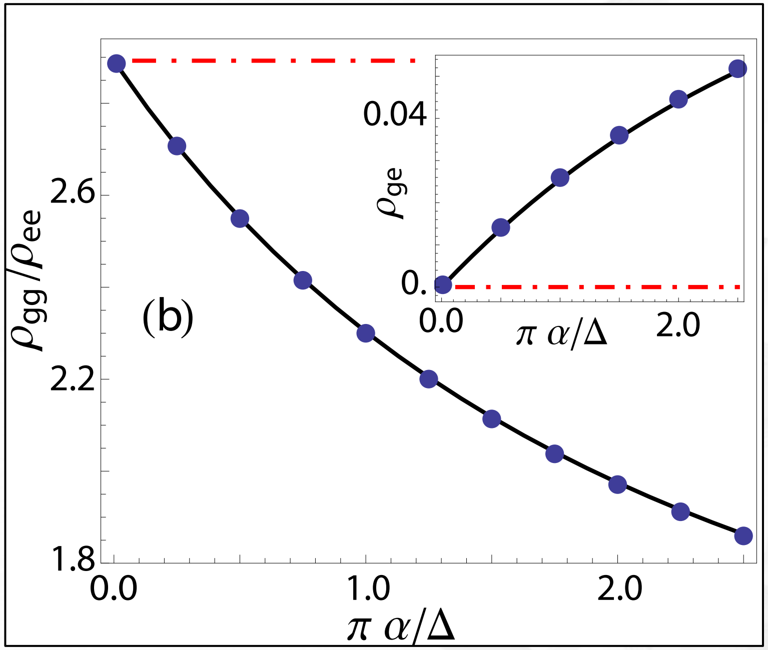


System-bath correlations persist into steady state

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

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

System steady-state



- CC master equation
- Numerical benchmark
- Weak-coupling

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

Departures from weak-coupling canonical statistics

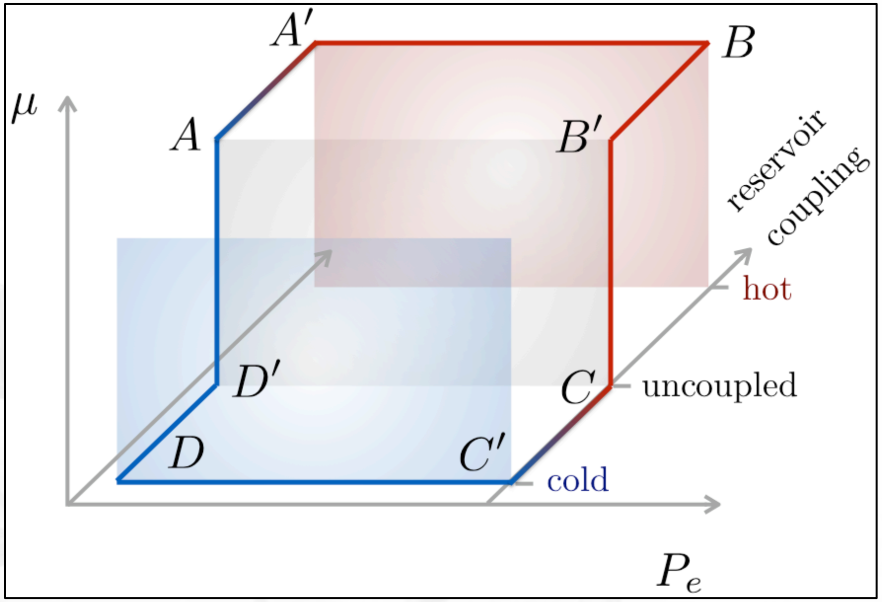
- population ratio in system eigenbasis now varies with system-reservoir coupling strength
- **coherences** present in system eigenbasis in the long time limit
- dynamically generated via strong system-reservoir interactions

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
- e.g. retain description in terms of thermal states in long time limit
- circumvents the usual restriction to weak coupling and vanishing correlations between the two



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

- 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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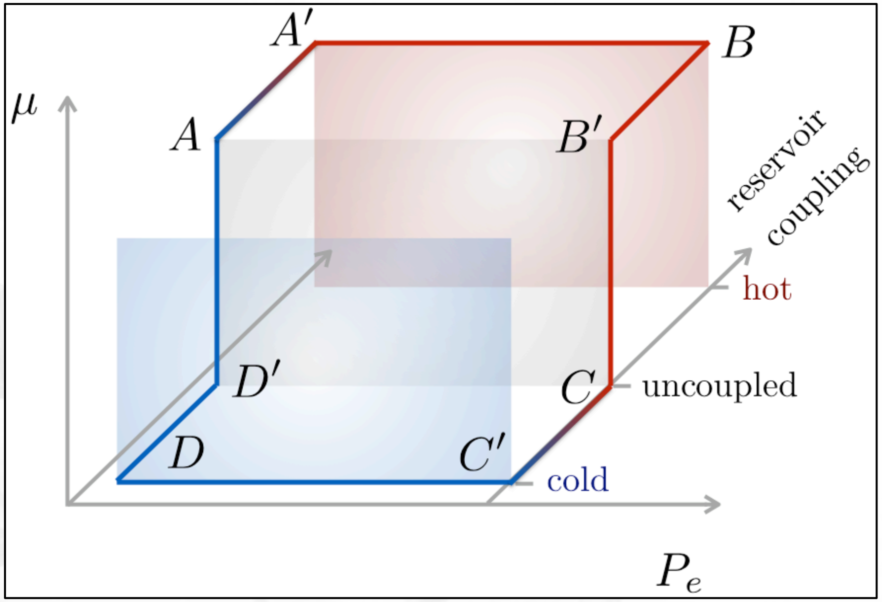
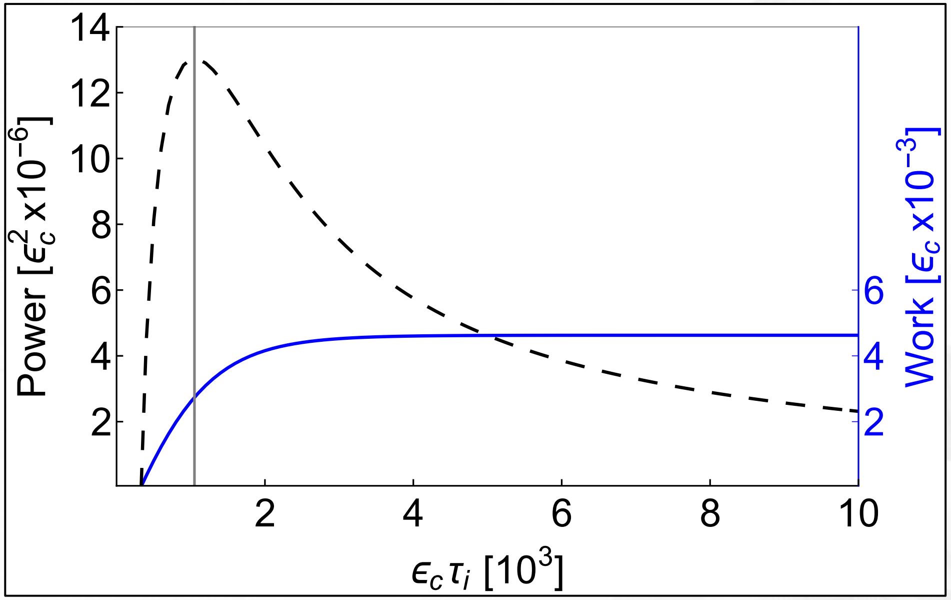


Quantum Otto cycle – standardly a 4 stroke heat engine, separates heat and work

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

Otto cycle in finite time

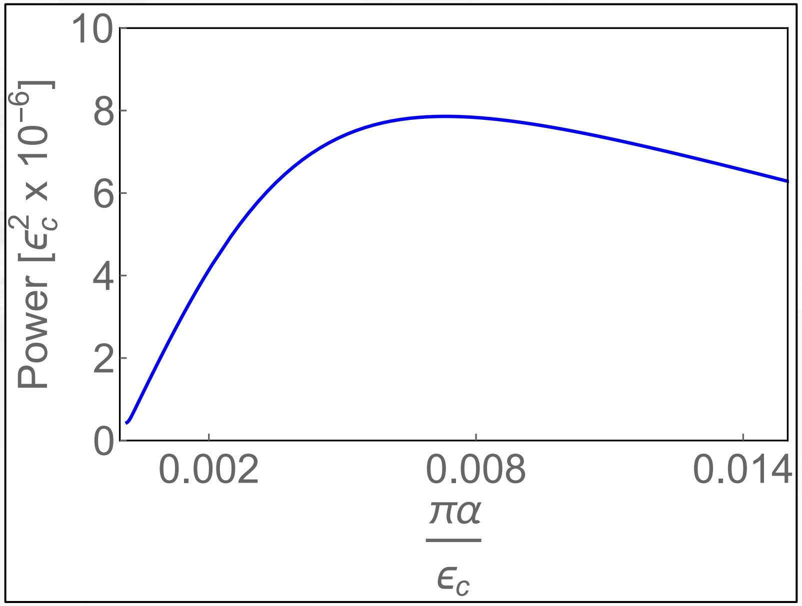


Frictionless isentropic strokes

- Hamiltonian commutes at all times.
- Power and work plotted as function of isochore time.
- Power maximised in non-equilibrium regime, before work plateaus.

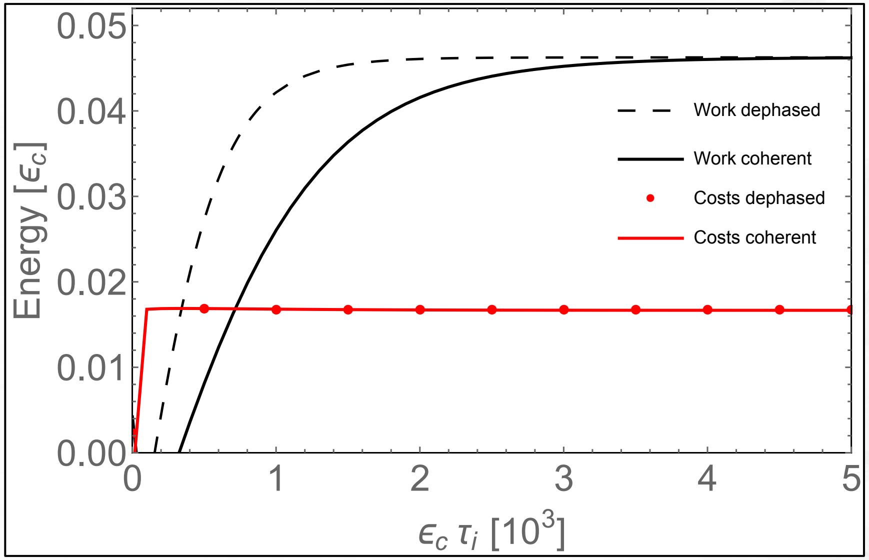
Power vs coupling strength

- Max. power output at finite coupling.
- Power increases with coupling initially due to quicker approach to equilibrium.
- Turnover due to decoupling costs.



M. Perarnau-Llobet et al., PRL 120, 120602 (2018)

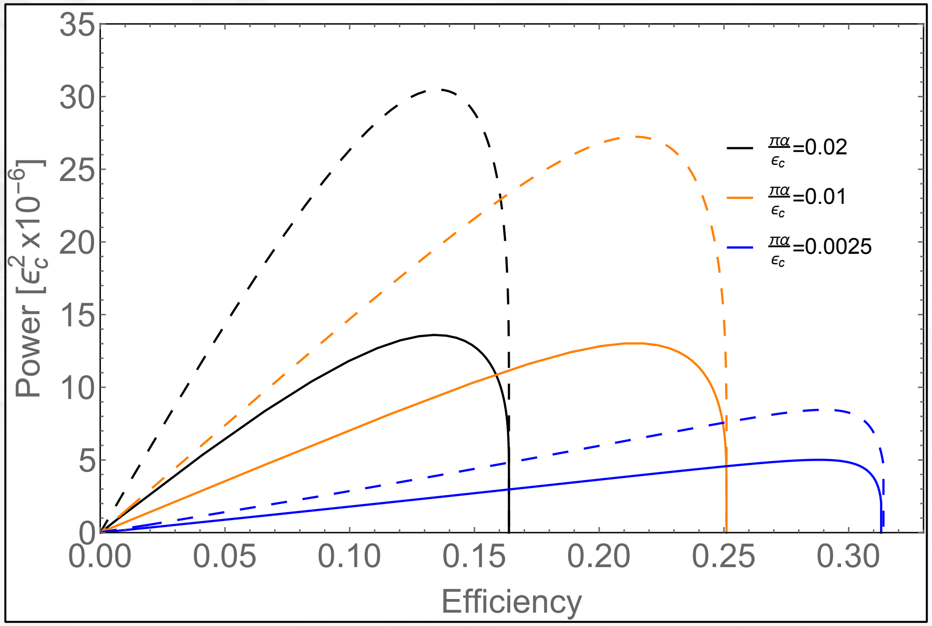
Fully quantum vs dephased engines



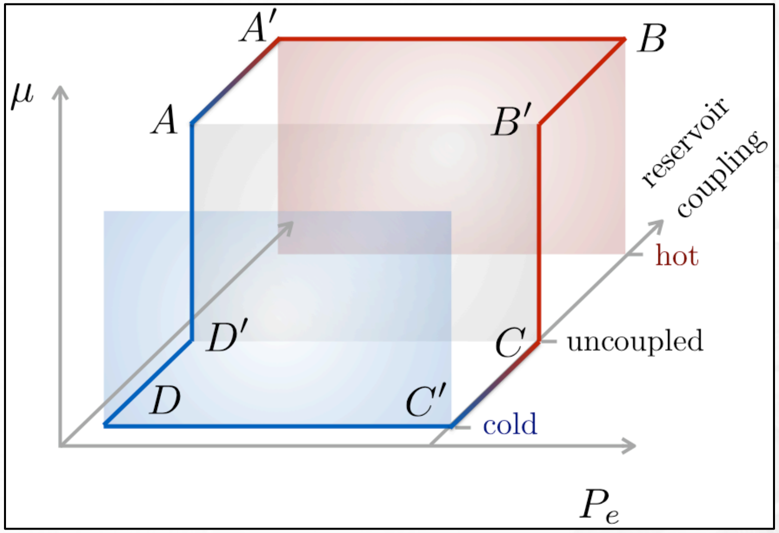
- **Work against isochore time**
- Implement pure dephasing in enlarged system plus collective mode eigenbasis.
- Ensures no energetic contribution.
- However – dephased engine outperforms a fully quantum one.
- Decoupling costs remain comparable.

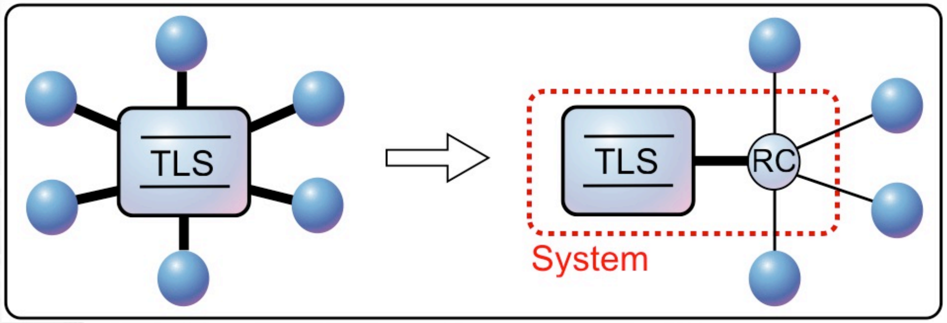
Parametric plot: power vs efficiency

- Dashed – dephased
- Solid – fully quantum
- Varying isochore time shows improvement in power output at a given efficiency for dephased engine.



Summary and ongoing work





A quantum limit to non-equilibrium heat engine performance imposed by strong system-reservoir coupling
D. Newman, F. Mintert, AN
arXiv:1906.09167

Ongoing

- Finite time/continuously coupled heat engines
- Non-equilibrium steady states
- Fermionic environments
- Artificial light-harvesting

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Thank You