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School on New Trends in Quantum Dynamics and Quantum Entanglement

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OUT OF EQUILIBRIUM, DRIVEN OPEN QUANTUM SYSTEMS. TOWARDS QUANTUM EFFECTS IN BIOLOGY.
Part II. Conformational-motion induced quantum effects

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Out of equilibrium, driven open quantum systems

Towards quantum effects in biology

Part II. *Conformational-motion induced quantum effects*

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ICTP, Trieste

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Plan of the lectures

Part I.

A quantum toolbox for biological systems

- *learning simple mechanisms & ingredients*
- *in driven, open quantum systems with spin gases*

Part II.

Conformational-motion induced quantum effects

- *applying the learned concepts to biologically inspired model systems*

Part III.

The avian compass

- *discussing a real world example where quantum dynamics make a difference*

Outline of Part II

- Conformational motion in biology
- Model system 1:
  Entanglement generation driven by a moving molecule
- Model system 2:
  Enhancement of quantum transport due to molecule motion

Motion in biology

Part I:

undirected, random motion of a gas
governed the quantum Hamiltonian

Now:

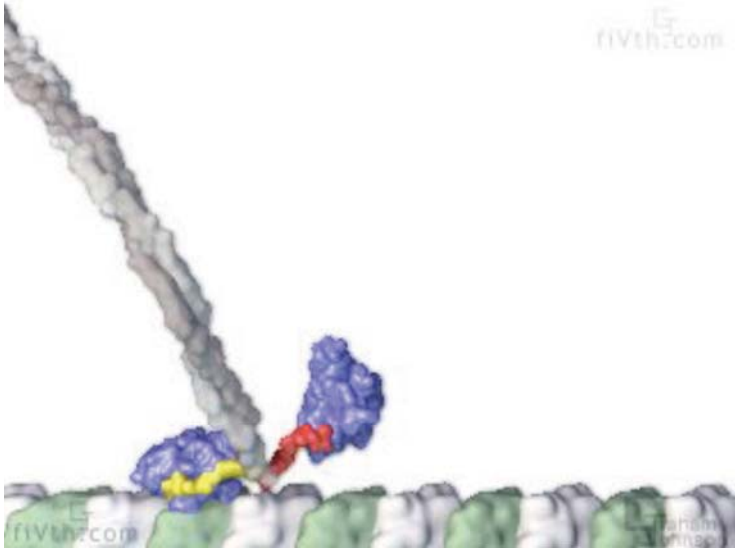
directed, functional motion in biological systems,
e.g. in protein structures

Functional molecular motion
is **ubiquitous** in biology,
most protein function requires motion!

Protein motion is **classical,**
there are plenty of decoherence
sources at T=310K.

Example: Motor proteins & Allosteric processes

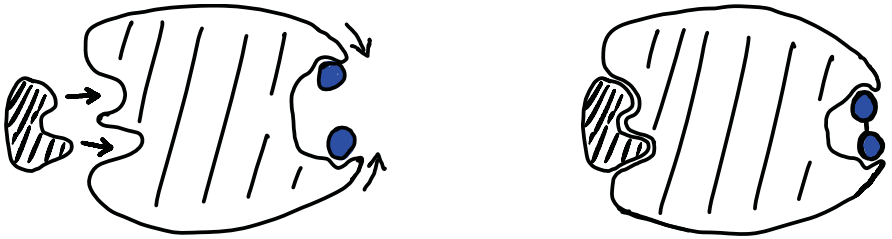
Kinesin motor protein walking on a microtubule:



[see Vale & Milligan, Science **288**, 88 (2000)]

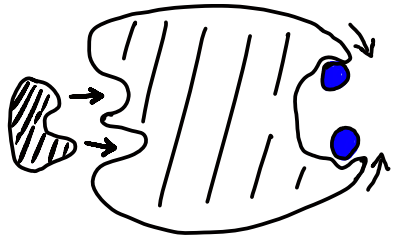
Function: (examples)
=> directed transport in cells
(faster than diffusion)
=> change of cytoskeleton
(e.g. for cell movement,
muscle contraction)

Enzyme regulation by modifying the active site through conformational changes induced by additional chemicals



Quantum degrees of freedom

attached to the classically moving “backbone” structure
are individual quantum degrees of freedom



conceivable are:

- spins of unbound electrons (see Part III)
- perhaps even nuclear spins (usually thermalized, but see Part III)
- localized high energetic vibrational states (e.g. in alpha-helices)
- excitons (e.g. in photosynthesis)

For the moment,
the actual **nature** and possible **functional role**
of the quantum degrees of freedom
is still **to be identified** by the experts… (but see Part III)

Ingredients

Our humble set of assumptions:

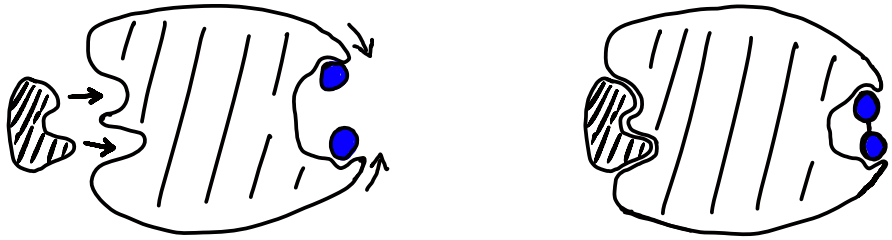
1. classically moving backbone structure
   with (functionally relevant) directed motion

2. existence of localized quantum degrees of freedom,
   which are carried along

Let's look at the possibilities and implications!

Model system 1:

Entanglement generation driven by a moving molecule



Reference:

J. Cai, S. Popescu & H. J. Briegel
"Dynamic entanglement in oscillating molecules and potential biological implications"
Phys. Rev. E **82,** 021921 (2010)

Basic idea

biological systems contain **many decoherence sources** (T=310K)
but they operate **far away from thermal equilibrium**

propose an (abstract) mechanism for a driven open quantum system
with the following properties:

- a **hostile environment** pushes the state of two quantum degrees of freedom to a **separable thermal state**
- quantum system experiences **external driving** (motion of molecular backbone structure)

Can non-trivial entanglement perpetually exist
in such a system?

Trivial versus non-trivial quantum effects

To discuss the meaning and potential role of entanglement/coherence in biological systems, it is useful to distinguish three types:

1. Entanglement of basic constituents ← "static"

2. *Dead* entanglement

3. *Live* entanglement

→ "dynamic"

[Briegel, Popescu, arXiv:0806.4552]

Naturally, the borders are fuzzy...

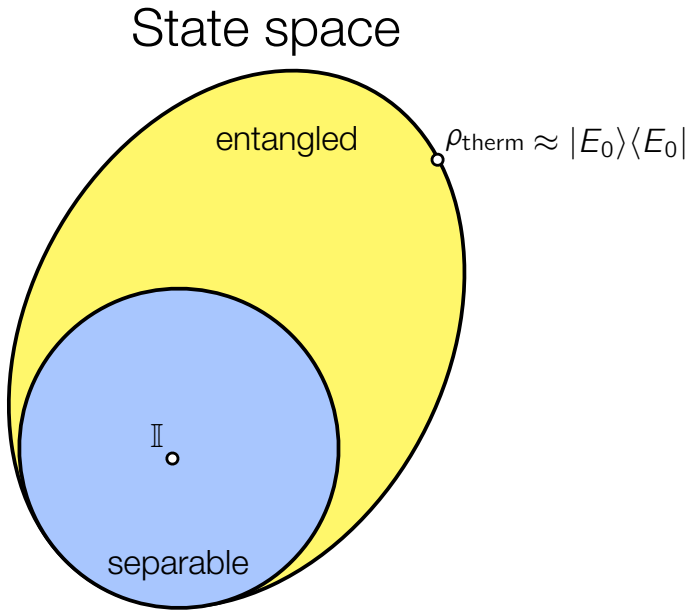
Entanglement in Biology – What can we expect?

1. Entanglement of basic constituents

Clearly, this type of entanglement is omnipresent in biology:

- Quantum mechanics determines the **structure of atoms, molecules, solids**.
- Obviously entanglement in these systems (electrons, nuclei,...).

➡ Molecular substrate/basis on which biological processes are built.



Entangled "thermal" state is usually the **ground state.**

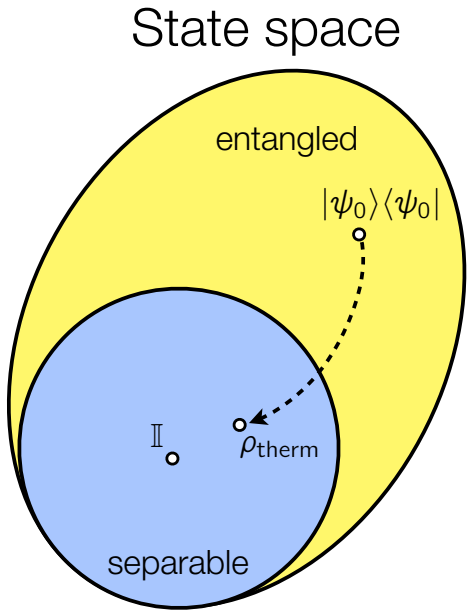
[Briegel, Popescu, arXiv:0806.4552]

Entanglement in Biology – What can we expect?

2. “Dead” entanglement

- Occurs in molecules that have biological origin or occur in biology.
- But, no metabolic process is required for it to function.

➡ Such molecules can, in principle, be taken out of the cell and continue to work.



State **temporarily** taken away from equilibrium where it may be **entangled**, but **quickly relaxes** to thermal state.

[Briegel, Popescu, arXiv:0806.4552]

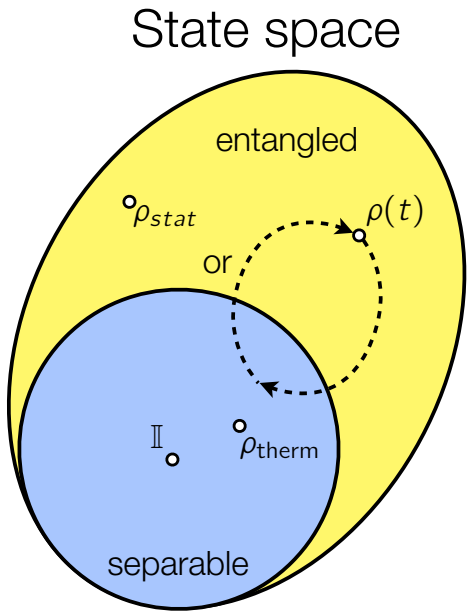
Entanglement in Biology – What can we expect?

3. “Live” entanglement

This type of entanglement *per definition* exists only while **metabolic processes** take place.

➡ Open, driven non-equilibrium quantum system

➡ Presumably requires **molecular motion**



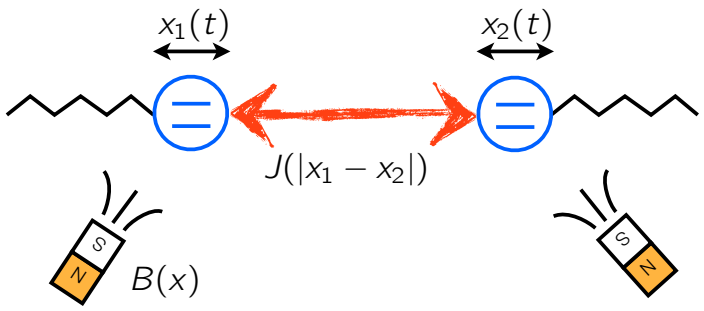
State is **actively maintained far from equilibrium.**

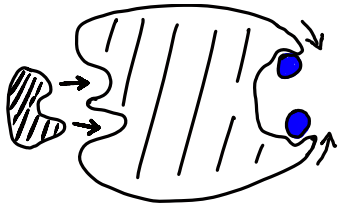
Here we would expect a biological process, whose purpose it is to generate and sustain entanglement!

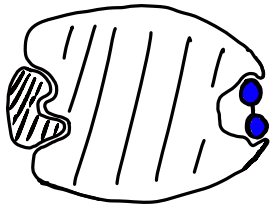
[Briegel, Popescu, arXiv:0806.4552]

Oscillating molecule model

[Cai, Popescu, Briegel, *PRE* **82,** 021921 (2010)]







e.g.

$$B(t) = B_0 - B_1 e^{-x^2(t)/2\sigma}$$

$$J(t) = \frac{J_0}{|x_1(t) - x_2(t)|^3}$$

Similar to spin gases, molecular motion determines the parameters in the Hamiltonian:

$$H(t) = J(t)\sigma_x^{(1)}\sigma_x^{(2)} + B(t)\left(\sigma_z^{(1)} + \sigma_z^{(2)}\right)$$

coupling
(distance dependent,
dominant for close spins)

local fields
dominant for distant spins

Open system dynamics in a hot environment

Lindblad master equation with thermalization

$$\dot{\rho}(t) = -i[H_{int}(t), \rho(t)] + \mathcal{L}_{therm}(t)\rho(t)$$

Worst case assumption:

Instantaneous equilibrium state $\rho_{eq,t}$ $\quad -i[H_{int}(t), \rho_{eq,t}] + \mathcal{L}_{therm}(t)\rho_{eq,t} = 0$

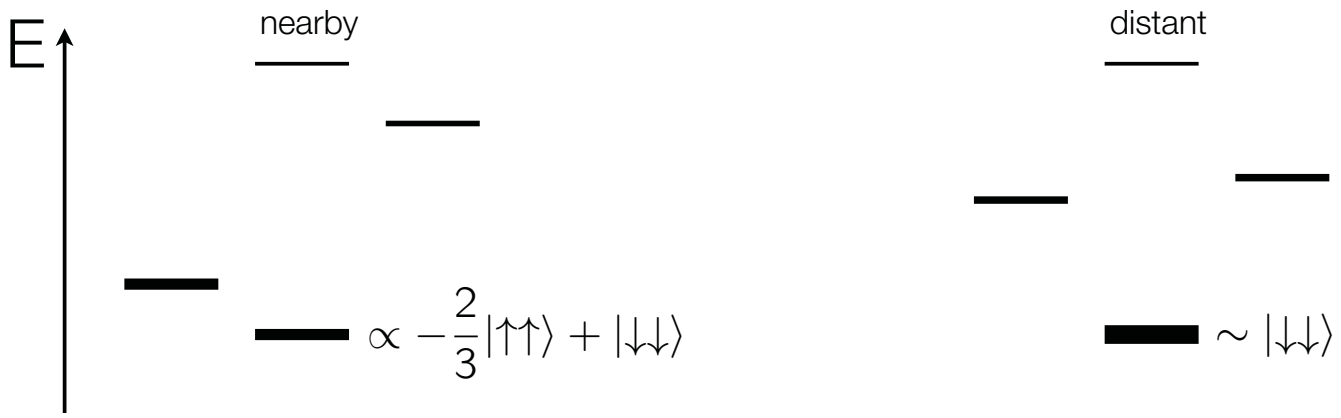
separable for all configurations/times!

Initial state: thermal state at time t=0

$$\rho(0) = \rho_{eq,t=0}$$

=> Thermalization rates must not be the fastest time-scale of the system!

Eigenstates of the closed system (time-dependent!)



motional time-scale vs. gaps in the spectrum:

diabatic evolution
(much faster than typical time scale given by energy gap, quasi-instantly)

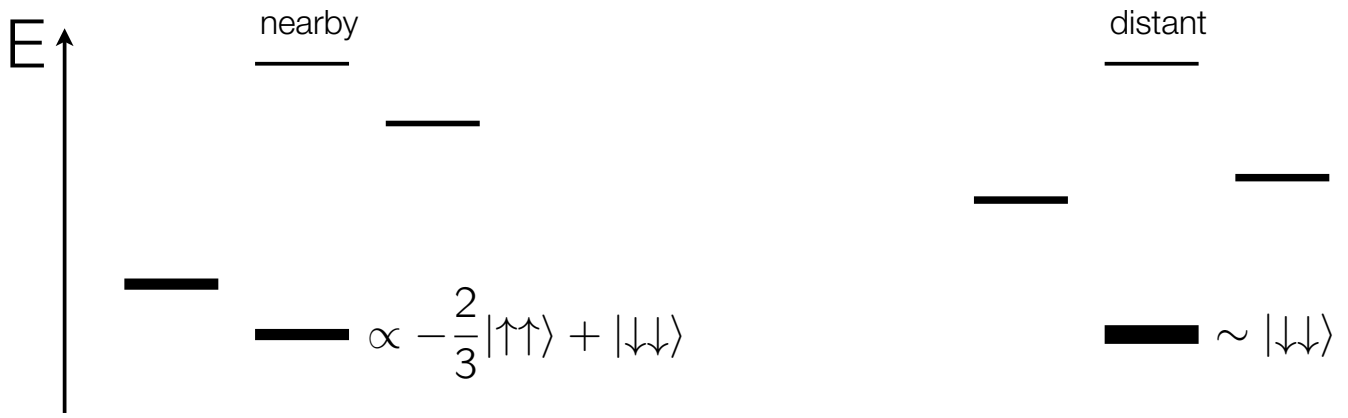
system will thermalize with populations for the avg. Hamiltonian

$$|\psi_0\rangle \to |\psi(t)\rangle = \sum_n \langle E_n(t)|\psi_0\rangle |E_n(t)\rangle = |\psi_0\rangle$$

adiabatic evolution
(much slower than time scale given by the gap, quasi-stationary)

$$|\psi_0\rangle \to |\psi(t)\rangle = \sum_n \langle E_n(0)|\psi_0\rangle |E_n(t)\rangle \neq |\psi_0\rangle$$

State evolution (very slow thermalization)



(2) large ground state population (entangled) of the non-equilibrium state

adiabatic transfer

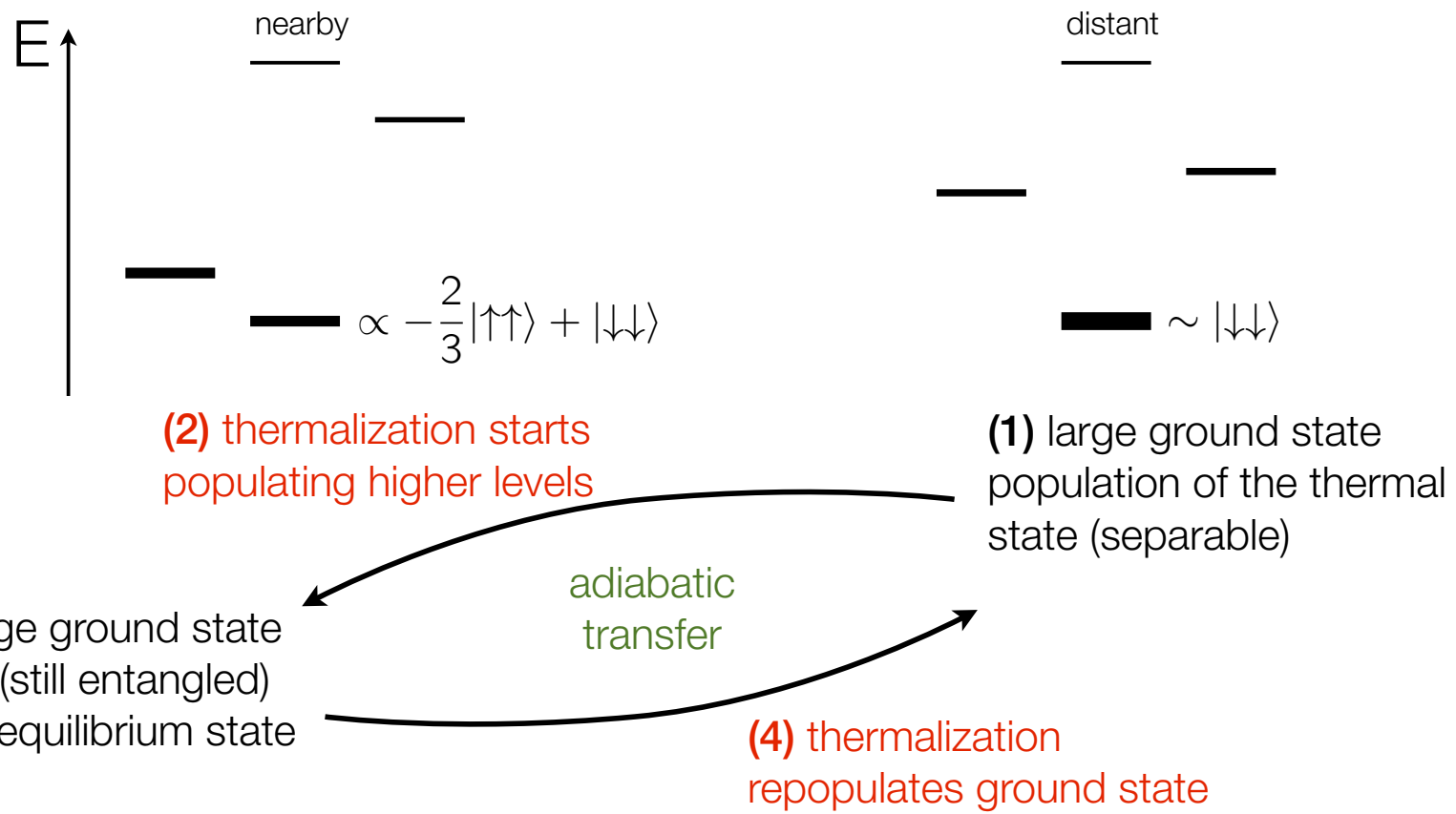
(1) large ground state population of the thermal state (separable)

Entanglement occurs periodically...

But: Thermalization process slowly
destroys purity of the distant ground state
=> drives state towards the separable equilibrium state of the time-averaged Hamiltonian.

Only transient entanglement!

State evolution (moderately fast thermalization)



Entanglement occurs persistently, freshly generated in every cycle!

Entropy is reduced!
Reset mechanism!

Summarizing the time-scales

thermalization rate

$\approx$

mechanical motion

$\vee$

energy gap

$\lll$

bath correlations time

thermalization and driving can effectively **interact**

non-adiabatic motion with respect to the open system dynamics

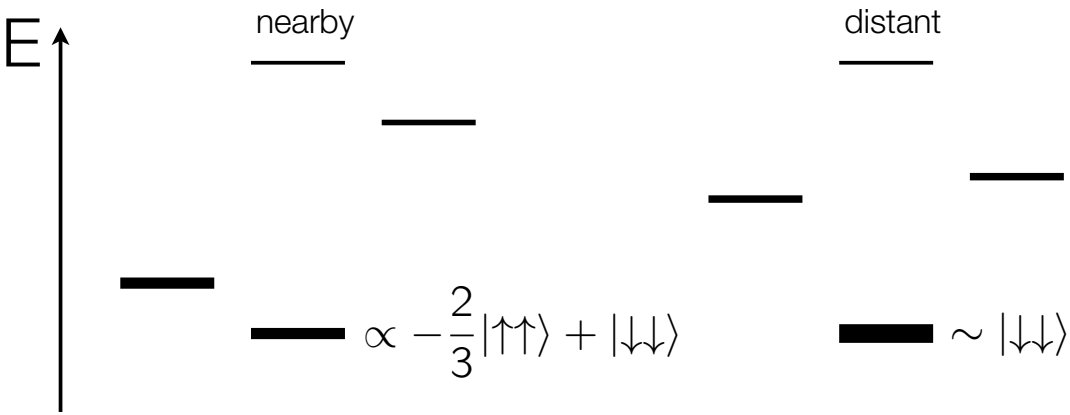
molecule motion on picoseconds

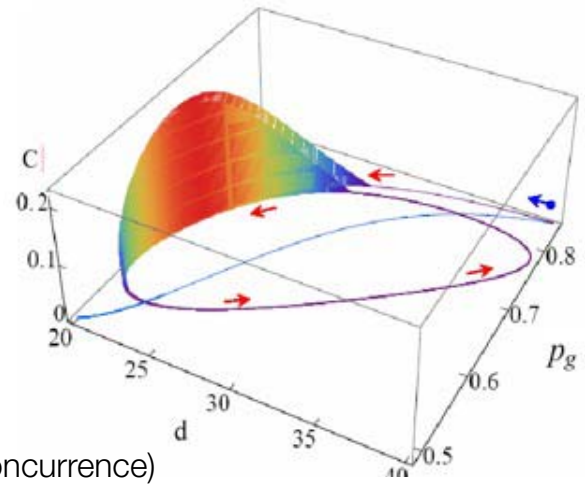
driving does not change level populations (adiabatic evolution)

electronic energies on femtoseconds

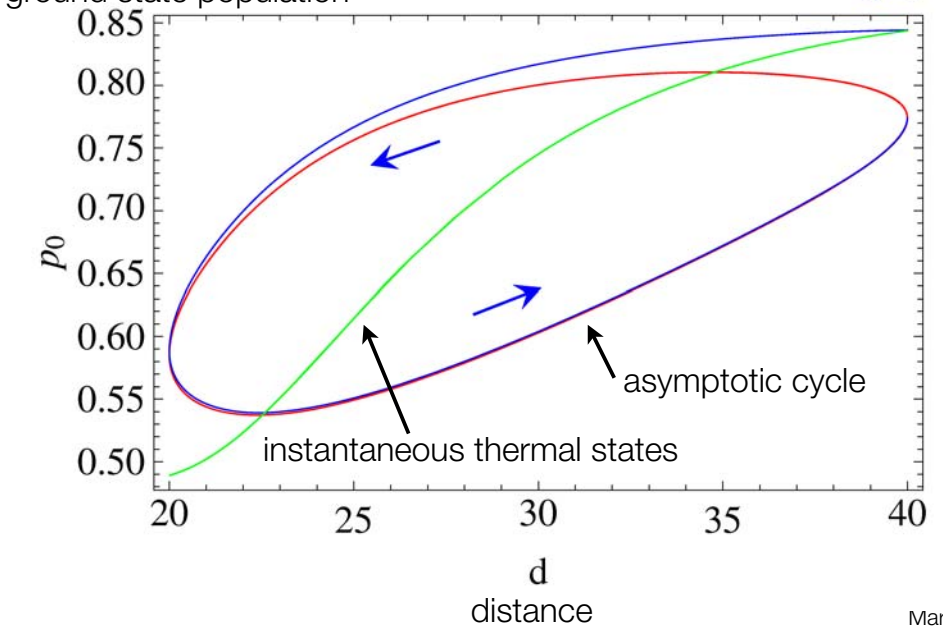
technical requirement for using master equations of Lindblad type (Markov approximation)

Entanglement dynamics

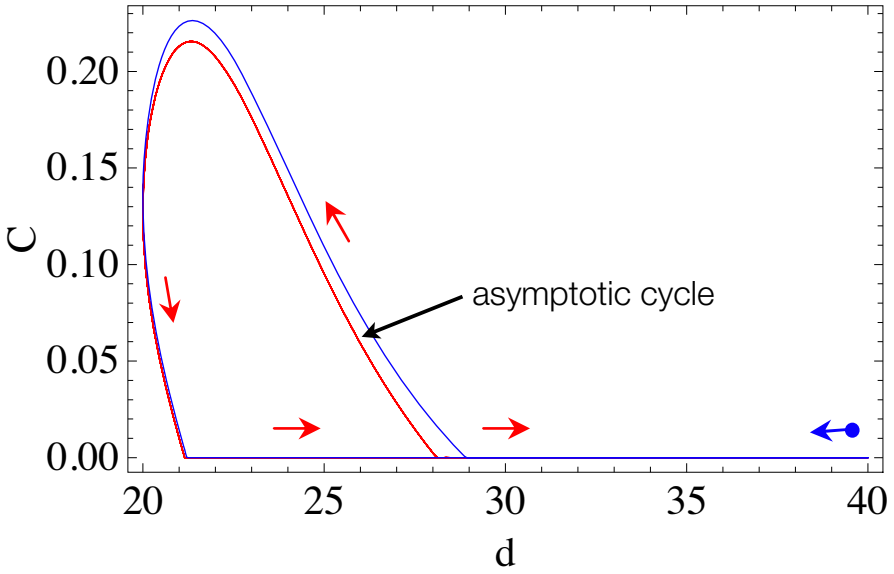




ground state population

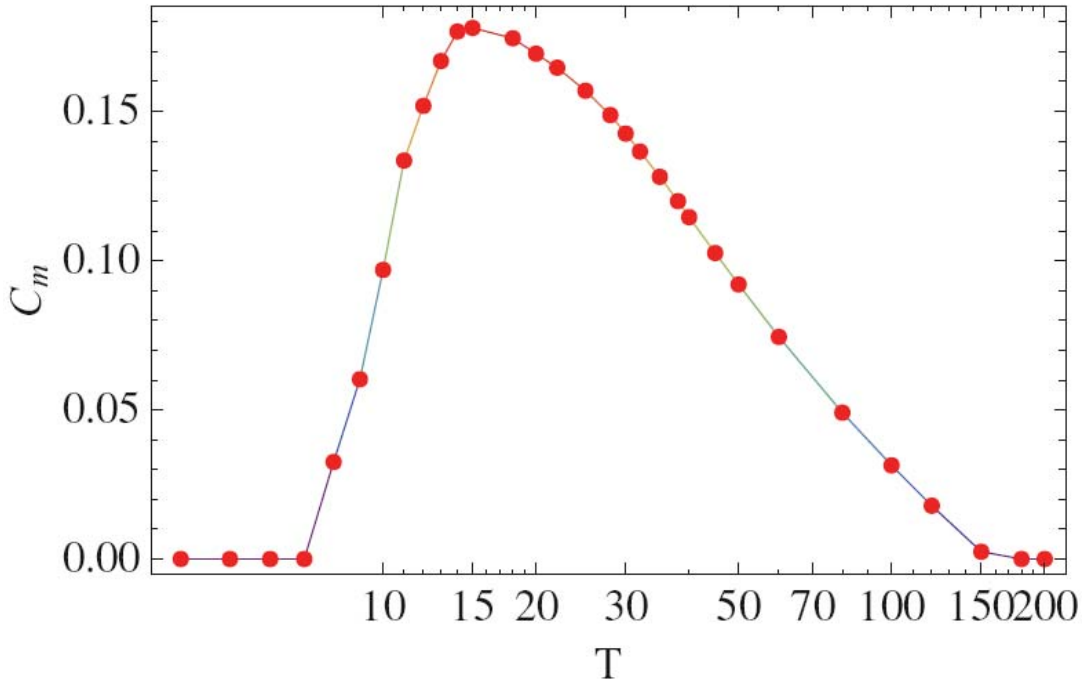


Entanglement (concurrence)



Parameter region for entanglement generation

Max. entanglement during cycle



Oscillation period

=> Entanglement is only generated in a finite parameter region

=> Existence of entanglement is non-trivial!

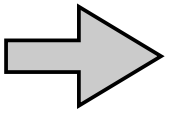
Thermalization parameters

rate $\gamma = 0.1$

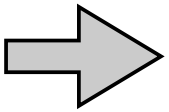
inversion s=0.2 i.e. $k_B T \approx 0.72\hbar\bar{\omega}$

Entanglement for $T \approx 1 \ldots 10\gamma^{-1}$

Conclusions



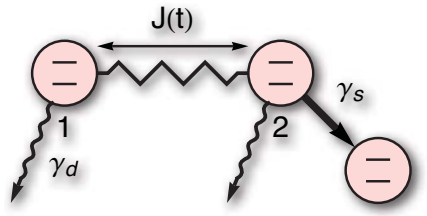
proof of principle that non-trivial (dynamical, perpetually existent)
entanglement may exist in biological systems



only classical motion and thermalization are needed
to establish a reset mechanism in suitable parameter regimes
(when acting on a comparable time-scale)

Model system 2:

Enhancement of quantum transport due to molecule motion



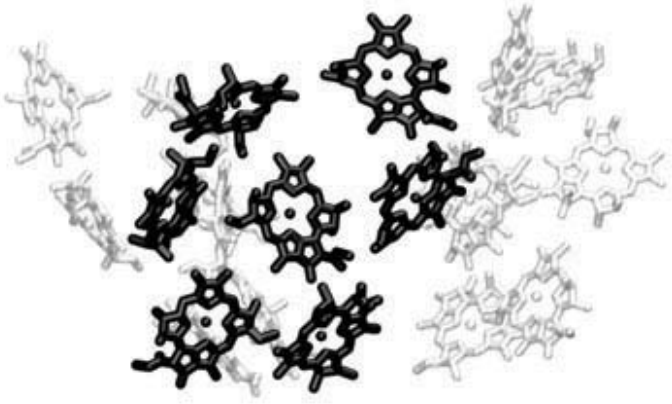
Reference:

A. Asadian, M. Tiersch, G. G. Guerreschi, J. Cai, S. Popescu & H. J. Briegel
"Motional effects on the efficiency of excitation transfer"
New J. Phys. **12,** 075019 (2010)

Basic idea

quantum coherence in light-harvesting proteins has been suggested to **improve excitation-transport efficiency**

but quantum and classical transport may yield a similar throughput

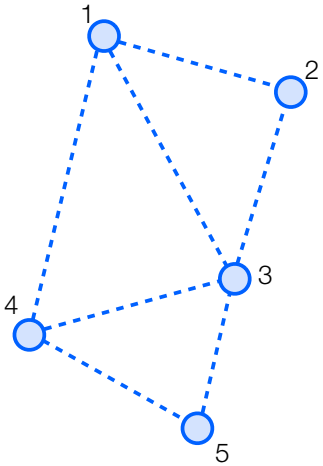


propose an abstract model that **captures the quantum advantage** in a transport scenario and establish **well-defined classical and quantum scenarios** which are to be compared

How does external driving influence the transport?

Classical transport

Network where N coupled sites exchange particles/energy/excitations probabilistically at a given rate.



Rate equation

$$\frac{dP_n(t)}{dt} = \sum_m \left(M_{nm}(t) P_m(t) - M_{mn}(t) P_n(t) \right)$$

transfer rate from site m to n

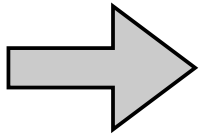
population at site m

Here: Only a **single** particle/excitation is being transported.

$$P_m \to 1/N$$

Detailed balance

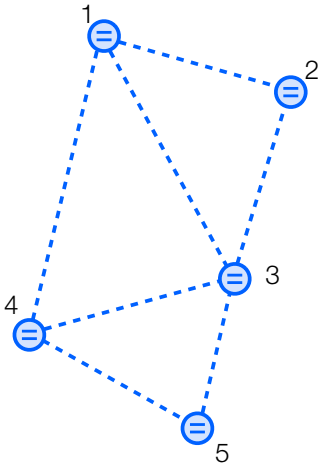
$$M_{nm} = M_{mn}$$



diffusive evolution until equilibrium is reached

Quantum transport

Network where N coupled sites exchange a single excitation under a given inter-site coupling.

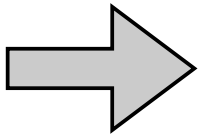


System Hamiltonian

$$\mathcal{H}(t) = \sum_n E_n(t)|n\rangle\langle n| + \sum_{m,n} J_{mn}(t)\Big(|n\rangle\langle m| + |m\rangle\langle n|\Big)$$

=> Solve Schrödinger equation

- Interference effects
- Localization effects due to disorder in couplings or on-site energies
- no asymptotic state

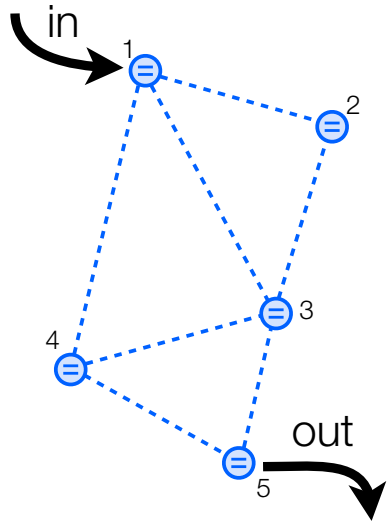


wave-like evolution

How to measure transport efficiency?

steady state scenario:

transport **through** the network (requires leads)
=> measure **conductance**

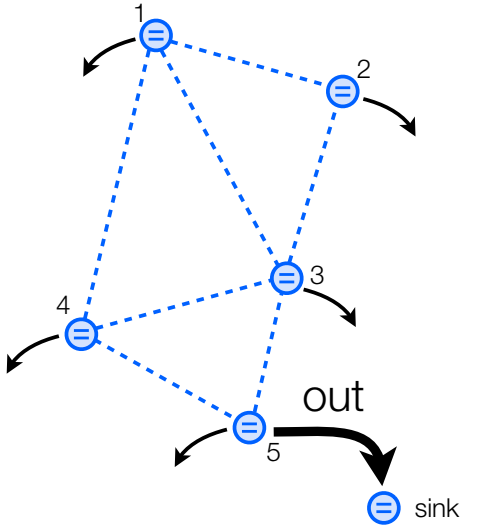


here: transient “one-shot” scenario

e.g. only one excitation starts at site 1, exits at site 5 to the sink

amount of excitation in the sink only measures
localization in the network

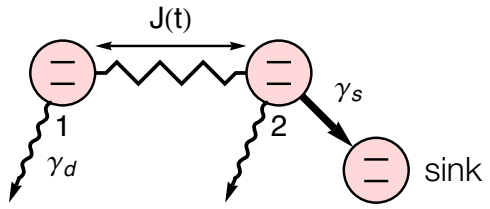
=> measure speed by adding a **competing mechanism**
e.g. excitation leaks out from every site into environment



[Plenio & Huelga, New J. Phys. 2008]

Transport model

single excitation propagating in a chain of coupled two-level sites



single excitation subspace

$$|1\rangle = |e\rangle|g\rangle$$
$$|2\rangle = |g\rangle|e\rangle$$

$$\mathcal{H} = \sum_{n=1}^{2} \epsilon |n\rangle\langle n| + J(t)\big(|1\rangle\langle 2| + |2\rangle\langle 1|\big)$$

open system dynamics

$$\frac{d\rho}{dt} = i[\rho, \mathcal{H}] + L_{\text{diss}}\rho + L_{\text{sink}}\rho \qquad \rho(0) = |1\rangle\langle 1|$$

dissipation

$$L_{\text{diss}}\rho = \sum_{n=1}^{2} \gamma_d \big(2\sigma_n^- \rho \sigma_n^+ - \{\sigma_n^+ \sigma_n^-, \rho\}\big)$$

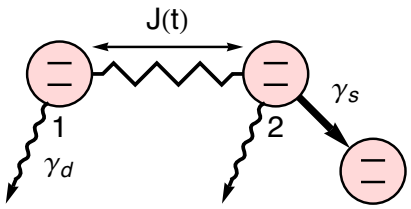
transfer efficiency measured by sink population

Plenio & Huelga, New J. Phys. 2008

$$L_{\text{sink}}\rho = \gamma_s \big(2|S\rangle\langle 2|\rho|2\rangle\langle S| - \{|2\rangle\langle 2|, \rho\}\big)$$

$$P_{sink}(t) = \int_0^t 2\gamma_s P_2(\tau) d\tau$$

Two-site toy model



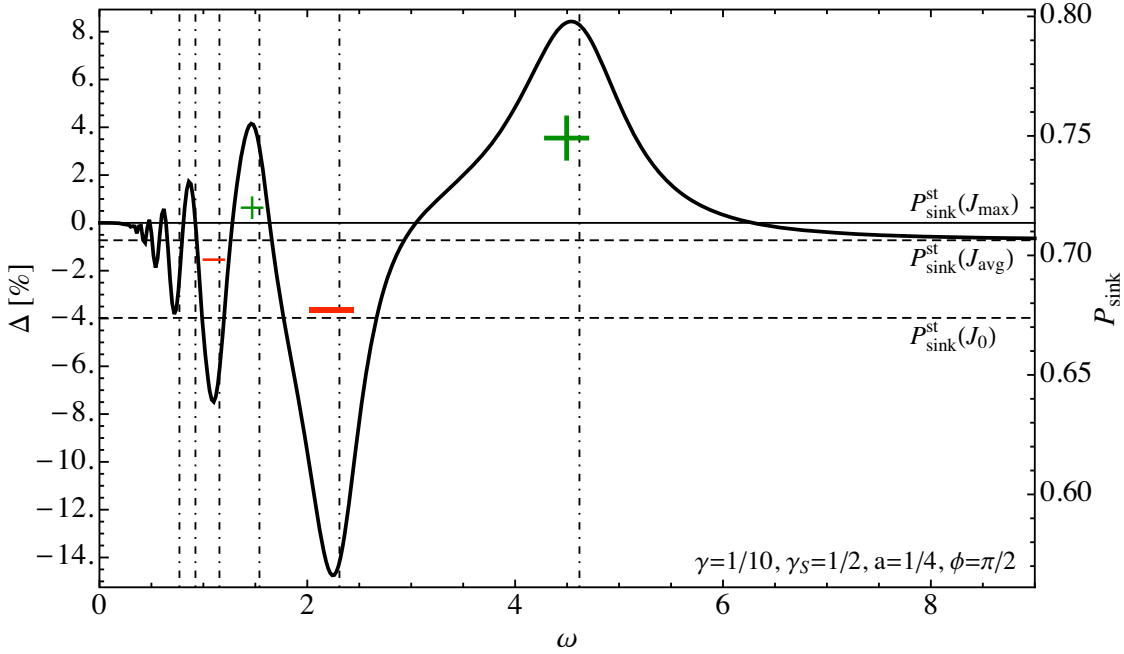
$$J(t) = \frac{\tilde{J}_0}{[d(t)]^3} = \frac{J_0}{[1 - 2a\sin(\omega t + \phi)]^3}$$

molecule oscillation modulates coupling strength

$$J_{\max} = \frac{J_0}{[d_{\min}]^3}$$

transport **efficiency enhancement** over best static configuration

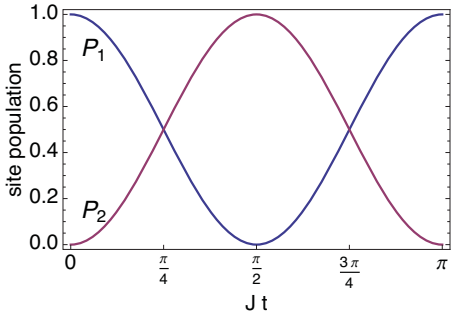
$$\Delta(\omega) \equiv P_{\text{sink}}(\omega) - P_{\text{sink}}^{\text{static}}(J_{\max})$$

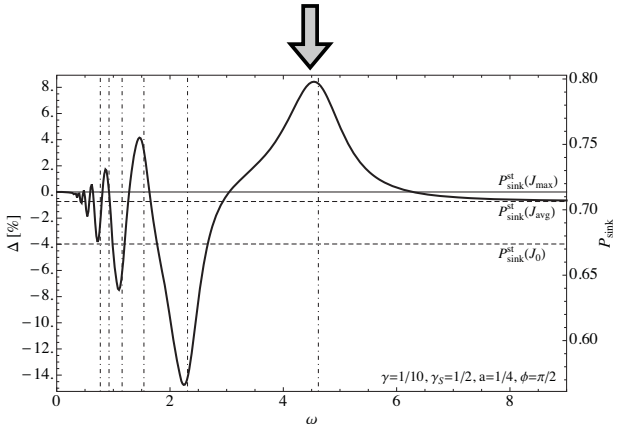


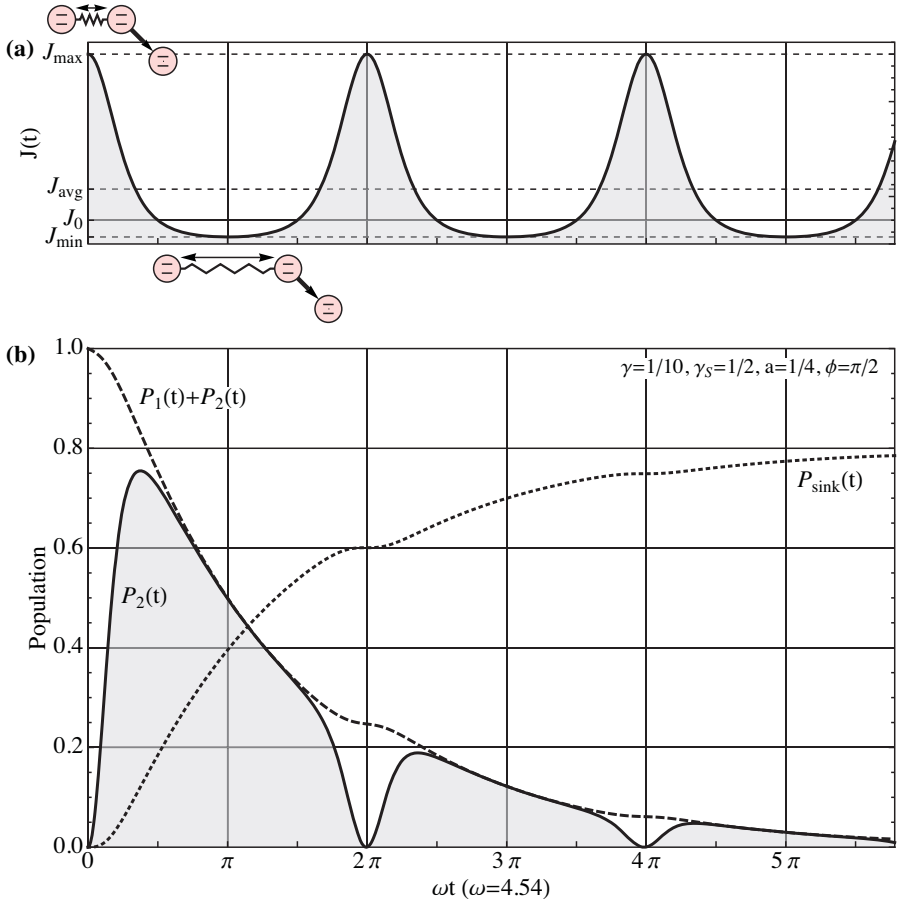
[Asadian et al., NJP (2010)]

Closer look at transfer dynamics

Rabi oscillation
for constant J



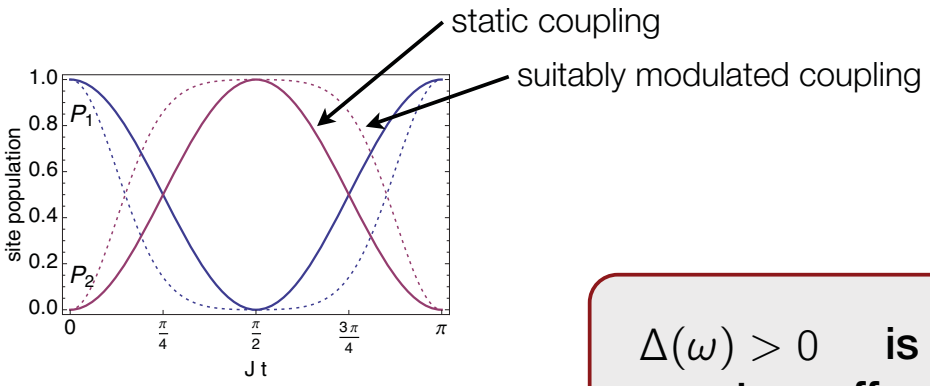




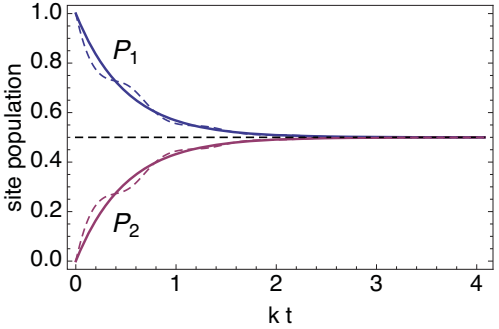
quick-transfer-and-locking scheme [Asadian et al., NJP (2010)]

Quantum to classical comparison

quantum transport



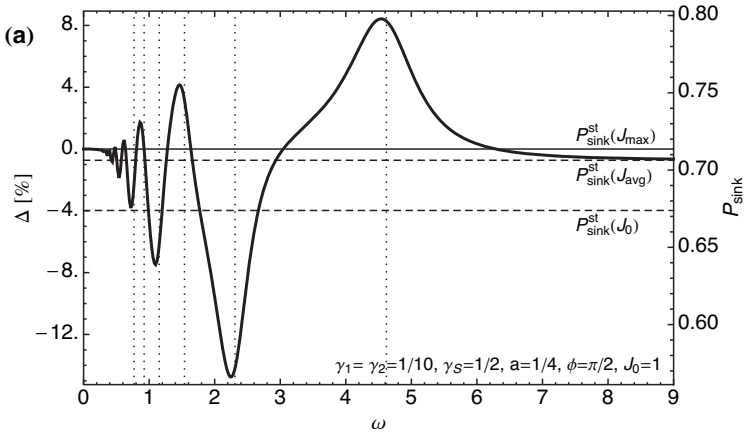
diffusive transport
(classical hopping)



$\Delta(\omega) > 0$ **is a quantum effect!**

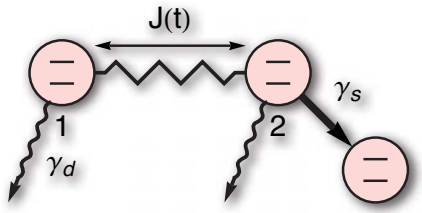
Optimal population at site 2:

$P_{2,opt} = 1$

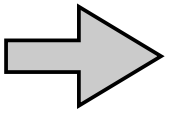


Optimal population at site 2:

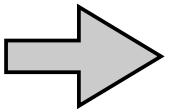
$P_{2,opt} = 1/2$



Conclusions



quantum transport may exhibit
an **increased motion-induced efficiency gain**
which cannot be explained by classical transport



coordinated molecular motion can virtually pump (drive)
an excitation through a transport network