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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 I. A quantum toolbox for biological systems

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Out of equilibrium, driven open quantum systems

Towards quantum effects in biology

Part I. *A quantum toolbox for biological systems*

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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 I

- What is a spin gas?
- State structure of spin gases and entanglement dynamics
- Adding decoherence
- Reset mechanism

“Biology”

Here:

synonymous with microbiology/biochemistry

Regarding the lowest structural level on which processes of life appear.

In contrast to

debates about quantum physics and the brain/consciousness.

Quantum effects in biology?

On the fundamental level everything is quantum mechanical, so what?

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Robert Huber
(Nobel Prize Chemistry 1988 for protein structure determination)

"Processes in biology are fully explained by classical physics (apart from tunneling of electrons or protons)."

Biologist's answer:

Biomolecular function (e.g. protein function) is well explained by classical mechanical models.

Quantum physics only provides substrate (molecules) on which biological processes take place.
=> applications in molecular dynamics, protein folding

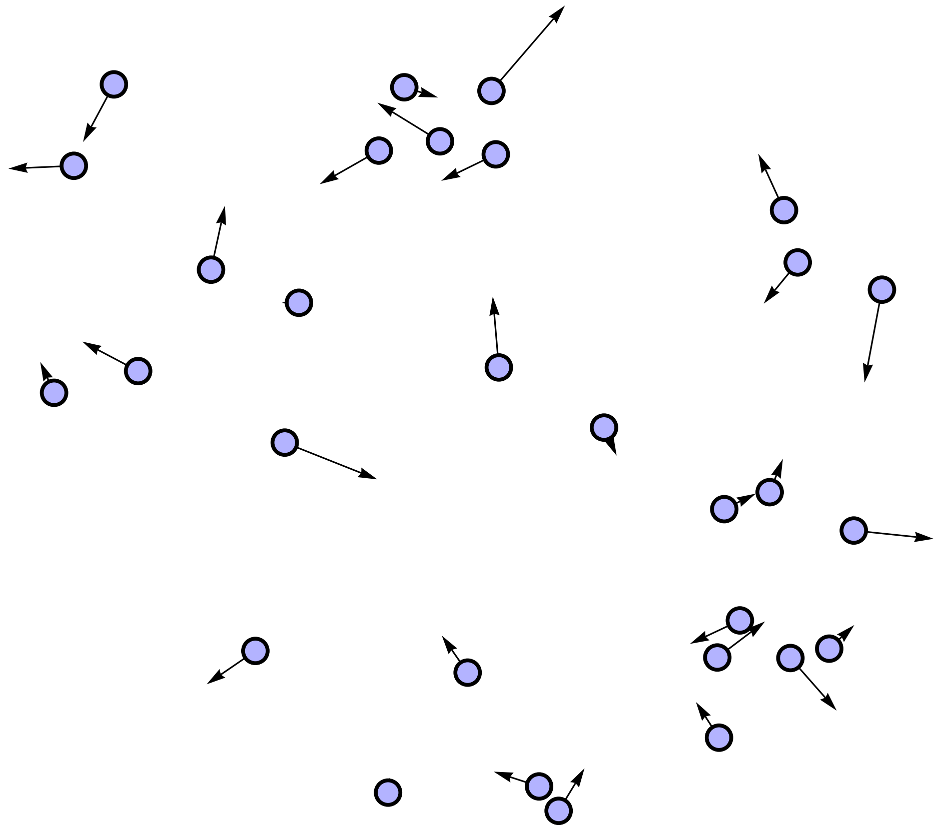
Physicist's answer:

Biological systems are "warm wet, and noisy".
=> plenty of **decoherence!**

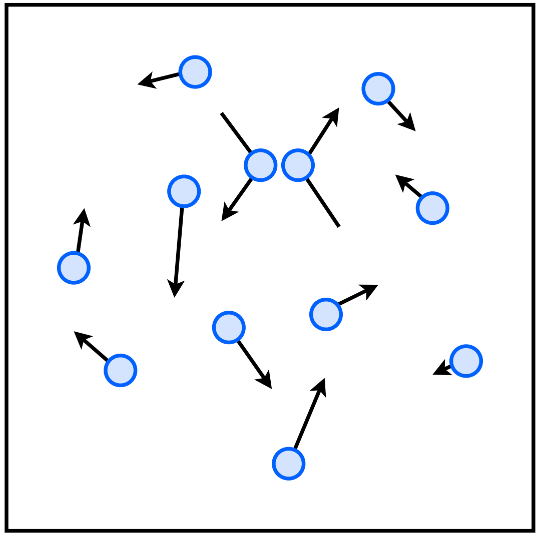
But:

Biological systems are **open quantum systems** that are driven and therefore operate **far away from thermal equilibrium.**

Spin gases



Boltzmann gas



- dilute gas of **classical particles**
  (mean free path ~ dimensions of container)

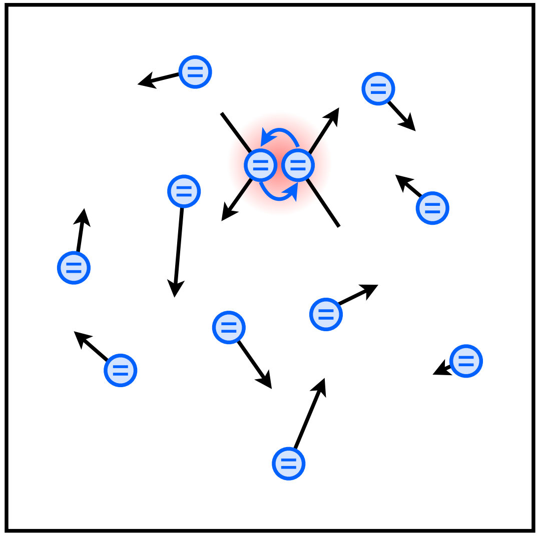
- **thermal equilibrium**
  (gas completely described by density, volume, temperature)

- molecular chaos
  ➡uncorrelated spacial distribution (uniform density)
  ➡uncorrelated velocities (Maxwell-Boltzmann distribution)
  only parameter: $\sigma = \sqrt{k_B T / m}$

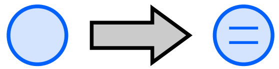
▸ distinguishable particles move on classical, deterministic trajectories $\vec{r}_k(t)$

▸ temperature T determines the collision rate r

Spin gas = Boltzmann gas + Spins



each gas particle carries an internal **quantum** degree of freedom, e.g. here a spin-1/2 or qubit



=> *semi-quantal* Boltzmann gas

[Calsamiglia, PRL (2005)]

collision-type **interactions** between spins

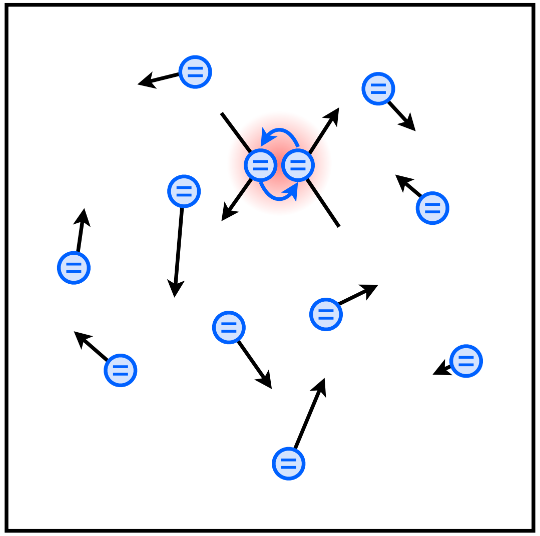
$$H_{int}(t) = \sum_{k<l} g\left[\vec{r}_k(t), \vec{r}_l(t)\right] H_{kl}$$

couplings: **stochastic functions** of time

Driving =
external time dependence
in the system Hamiltonian

Here: classical dynamics (gas)
drive the quantum dynamics (spins)

State evolution in a spin gas



simplest case: $[H_{kl}, H_{k'l'}] = 0$ of Ising-type

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle = \prod_{k<l} e^{-i\phi_{kl}(t)H_{kl}}|\psi(0)\rangle$$

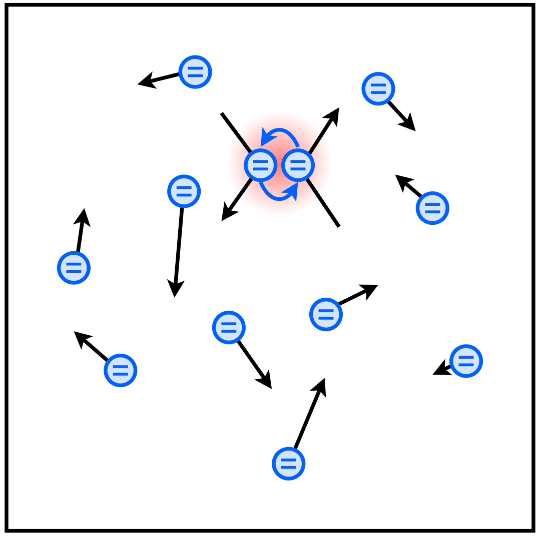
at time t all the interaction phases suffice to describe the state completely (including the entire interaction history)

$$\phi_{kl}(t) = \int_0^t g\left[\vec{r}_k(\tau), \vec{r}_l(\tau)\right] d\tau$$

collision model:

hard spheres of diameter *d,*
acquired phases ~1/(relative speed),
e.g. large interaction constant or low *T* (non-perturbative!)
=> random phase $\phi \in [0, 2\pi]$

Concrete dynamics



For concreteness (and illustration) we use an Ising-type interaction (controlled phase-gate):

$$H_{kl} = \frac{(\mathbb{I} - \sigma_z^{(k)})}{2} \otimes \frac{(\mathbb{I} - \sigma_z^{(l)})}{2} = |11\rangle_{kl}\langle 11|$$

Initial state (not entangled):

$$|\psi(0)\rangle = |+\rangle^{\otimes N} \qquad |+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

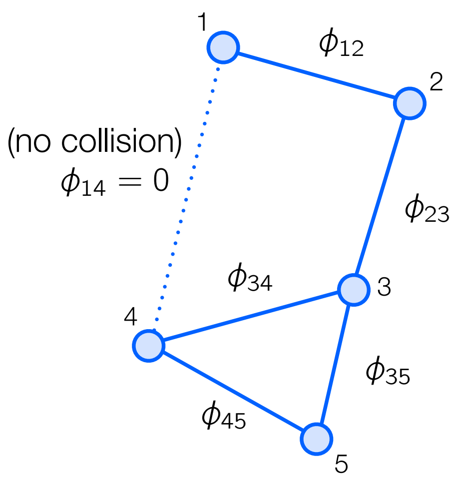
Collisional history completely contained in:

$$\Gamma(t) = \begin{pmatrix} 0 & \phi_{12} & \cdots & \phi_{1N} \\ \phi_{21} & 0 & & \vdots \\ \vdots & & \ddots & \phi_{N-1,N} \\ \phi_{N1} & \cdots & \phi_{N,N-1} & 0 \end{pmatrix}$$

Internal state of gas at time t:

$$|\psi(t)\rangle = U(t)|+\rangle^{\otimes N}$$
$$= \frac{1}{2^{N/2}} \sum_{\vec{s}} e^{i\vec{s}\cdot\Gamma(t)\cdot\vec{s}/2}|\vec{s}\rangle$$

Quantum states as weighted graphs



$$|\psi(t)\rangle = \frac{1}{2^{N/2}} \sum_{\vec{s}} e^{i\vec{s}\cdot\Gamma(t)\cdot\vec{s}/2} |\vec{s}\rangle$$

vector of N bits

exponentially many terms (in N)

N(*N*-1)/2 interaction phases

⇩

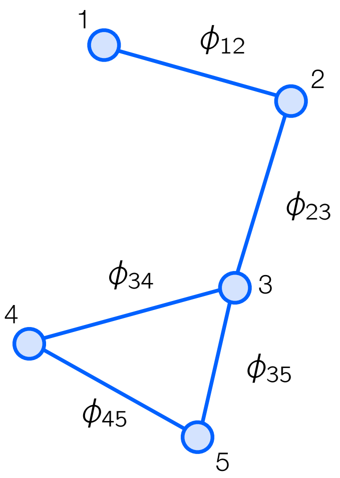
adjacency matrix of a **weighted** graph

$$\Gamma(t) = \begin{pmatrix} 0 & \phi_{12} & \cdots & \phi_{1N} \\ \phi_{21} & 0 & & \vdots \\ \vdots & & \ddots & \phi_{N-1,N} \\ \phi_{N1} & \cdots & \phi_{N,N-1} & 0 \end{pmatrix}$$

Here, in spin gases:
states are **random graphs**
(random edges & weights)

state properties can be conveniently and efficiently(!) discussed by means of its graph

Entanglement properties



entanglement of two collided particles
depends on the collisional phase (weight of edges)

separable: $\phi = 0$ maximally entangled: $\phi = \pi$

$\forall\ \phi_{kl} \in \{0, \pi\}$

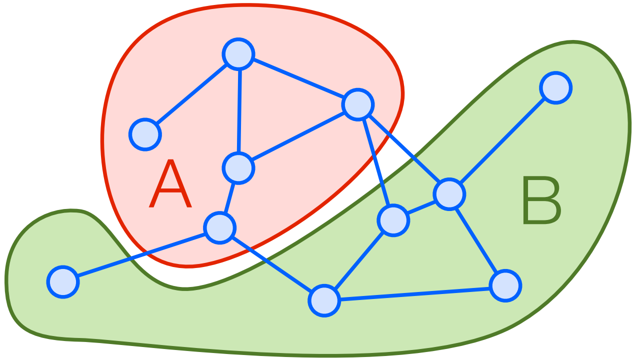
=> subset: graph states,
incl. 2D cluster states
(known as resource states
for measurement-based
quantum computation)

In fact, any two particles that are connected
by a path are (localizable) entangled!

Procedure from one-way quantum computation:
(1) measure all but the connecting particles along z
(2) measure connecting particles along x

Weighted graph states are
an interesting and useful
class of quantum states!

Entanglement properties II



Entanglement between subsets A and B is given by the entropy of one subsystem for a pure state of A and B.

$$E_{A|B} = S(\rho_A) = -\,\mathrm{Tr}(\rho_A \log_2 \rho_A)$$

$$\rho_A = \mathrm{Tr}_B |\psi(t)\rangle\langle\psi(t)|$$

$$\rho_A = \frac{1}{2^N}\,\mathrm{Tr}_B \sum_{s,s'} e^{i(s\cdot\Gamma\cdot s - s'\cdot\Gamma\cdot s')/2} |s\rangle\langle s'|$$

$$\cong \frac{1}{2^{N_A}} \sum_{s_A,s'_A} \left(\frac{1}{2^{N_B}} \sum_{s_B} e^{i(s_A - s'_A)\cdot\Gamma_{AB}\cdot s_B} \right) |s_A\rangle\langle s'_A|$$

coherences (off-diagonal elements) of are damped by every interaction with a particle of B
=> stronger entanglement of A & B

$$e^{\frac{i}{2}\sum_k (s_A - s'_A)\cdot\Gamma_k} \prod_{k=1}^{N_B} \cos[(s_A - s'_A)\cdot\Gamma_k/2] = C_{s_A,s'_A}(t)$$

$$\rho_{s_A,s'_A}(t) = C_{s_A,s'_A}(t)\,\rho_{s_A,s'_A}(0)$$

Entanglement dynamics

initial state: separable

early times: $rt < 1$ $$\langle S_A \rangle \approx \frac{N_A N_B}{N-1} rt \langle S \rangle_{\phi}^{pair}$$

long-time limit: **equilibrium state** = fully connected graph with random phases (independent, uniform in $[0, 2\pi]$)

$rt \to \infty$

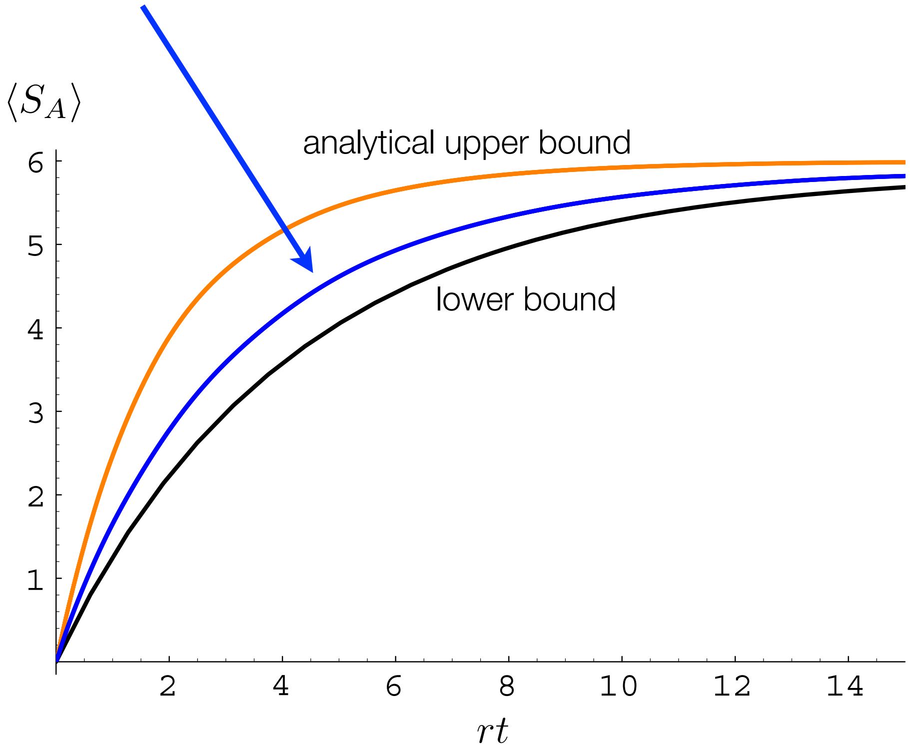
almost maximally entangled with respect to all possible bipartitions $N_A \geq \langle S_A \rangle \geq N_A - 1$

Example: any two pair of spins is connected by a third one with $\phi_{13} \approx \phi_{23} \approx \pi$

=> Localize maximal entanglement between 1 & 2

Entanglement dynamics: Example

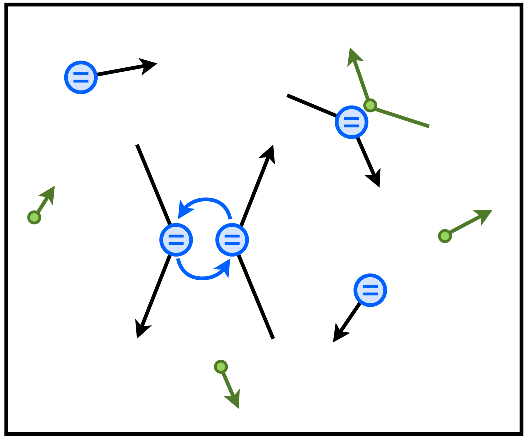
Entropy of state of 6 particles
of a 100 particle gas



average over
100 simulation runs

[Hartmann, J. Phys. B. (2007)]

Adding decoherence



Second gas species (background gas) plays the role of an **environment**

=> strongly interacting,
non-Markovian (for small particle number or spacial restrictions, e.g. in a lattice gas)

Ising-type interaction effectively leads to a **dephasing environment**

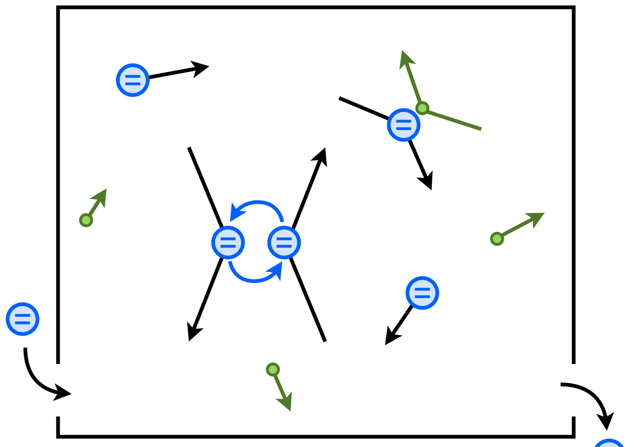
Lindblad master equation using the Markov-approximation
(large collisional phases, many background gas particles)

$$\dot{\rho} = -i[H_{int}, \rho] + \mathcal{L}_{deph}\rho$$

$$\mathcal{L}_{deph}\rho = \gamma \sum_{k=1}^{N} \left[\sigma_z^{(k)} \rho \sigma_z^{(k)} - \rho\right]$$

Note, exact results via
$\rho_{s_A,s'_A}(t) = C_{s_A,s'_A}(t)\rho_{s_A,s'_A}(0)$

The reset mechanism



$\rho_{reset} = |\chi\rangle\langle\chi|$ $\rho_k \propto \mathbb{I}$

Problem: entanglement is first built up but also quickly destroyed due to the environment

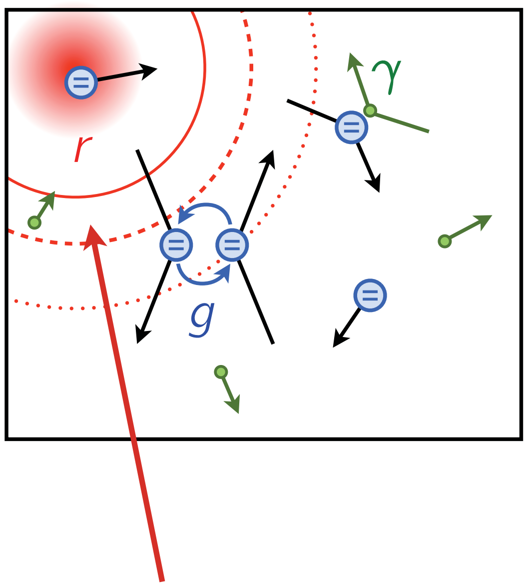
Solution: reset phases (and kill entanglement) between system and environment

Reset the state of particles in a certain region back to initial state
(local operation on particles, does not introduce entanglement)

or **replace particles** with fresh one (e.g. just as in a cell), i.e. **get rid of entropy**.

Result: All existing entanglement is destroyed environment,
both **between system particles** and **between system and environment**
=> fresh entanglement between system particles is created

The reset mechanism



Particle k is reset: $\rho_k \to \rho_{reset} = |\chi\rangle\langle\chi|$

$$\rho \to |\chi\rangle\langle\chi|_k \otimes \mathrm{Tr}_k\, \rho$$

Reset term in the Lindblad master equation:

$$\mathcal{L}_{reset}\rho = \sum_{k=1}^{N} \underbrace{r}_{\text{reset rate}} \left(|\chi_k\rangle\langle\chi_k|\, \mathrm{Tr}_k\, \rho - \rho\right)$$

Regions of persistent entanglement around the reset area
=> non-equilibrium structure

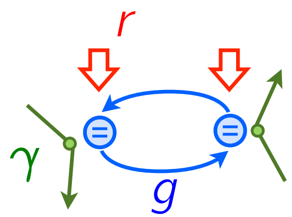
Reset mechanism drives the quantum system out of the equilibrium state

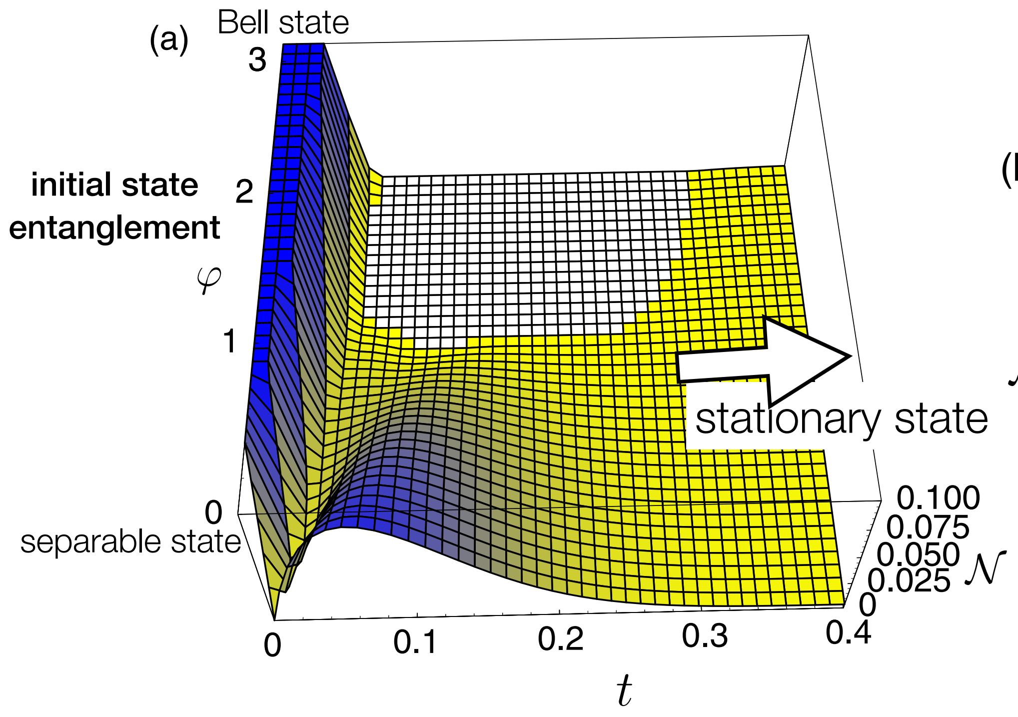
Entanglement dynamics of two particles

Ising interaction

$$\dot{\rho} = -i[H_{int}, \rho] + \mathcal{L}_{deph}\rho + \mathcal{L}_{reset}\rho$$

$\downarrow g \qquad \downarrow \gamma \qquad \downarrow r$

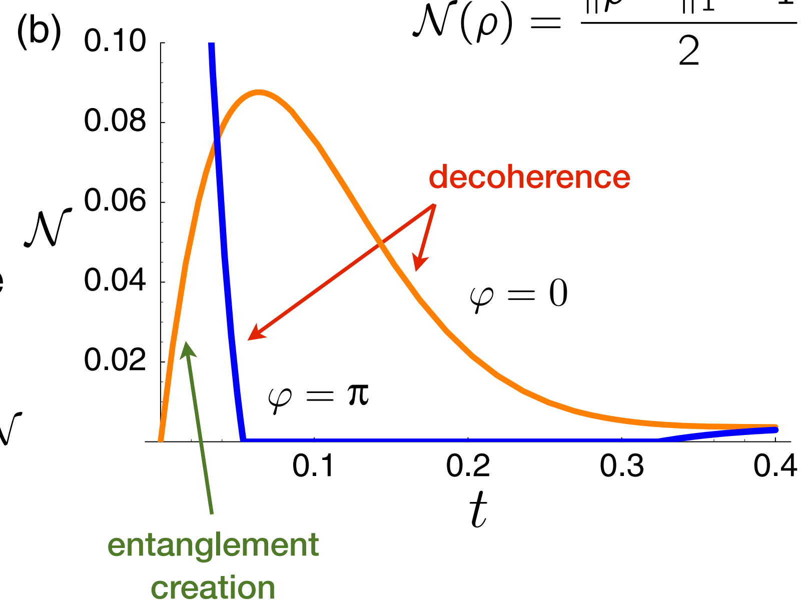




$r = 10\gamma, \quad g = 5\gamma$

Entanglement quantified by negativity:

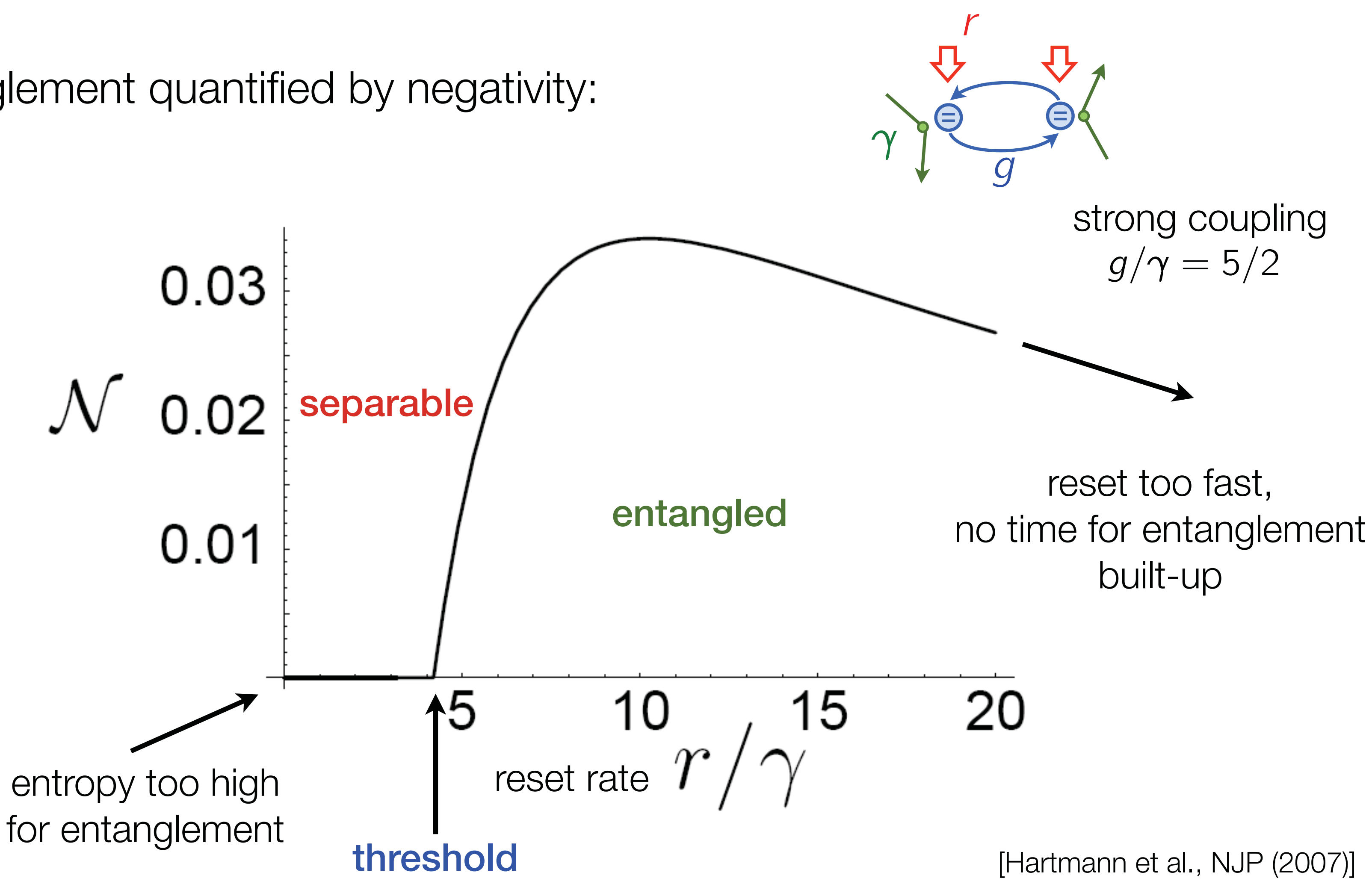
$$\mathcal{N}(\rho) = \frac{\|\rho^{PT}\|_1 - 1}{2}$$



[Hartmann et al., NJP (2007)]

Steady-state entanglement

Entanglement quantified by negativity:



[Hartmann et al., NJP (2007)]

Generalizations

[Hartmann et al., PRA (2006)]

$H_{Ising} \to H_{xyz}$

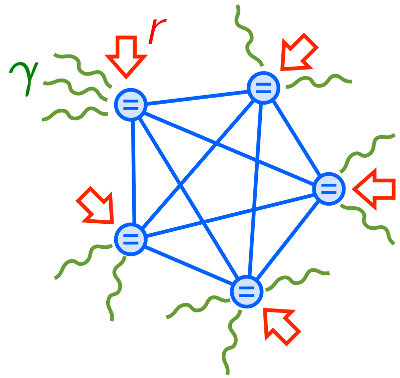
$N = 2 \longrightarrow$ larger N

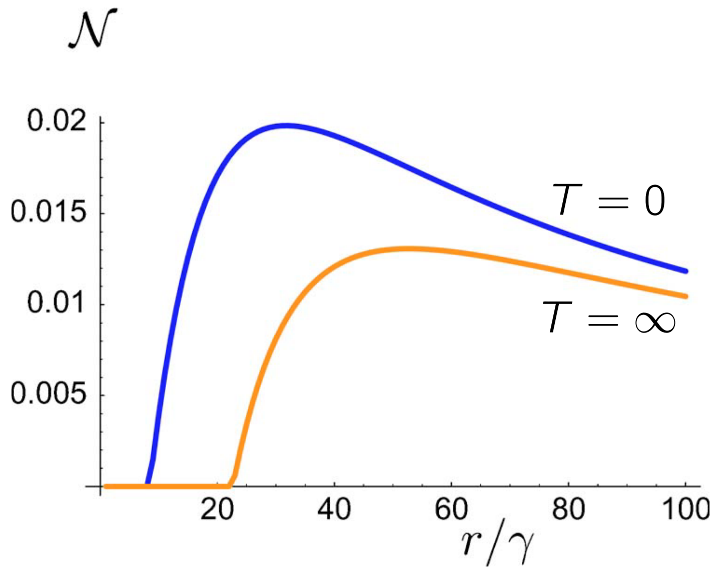
Dephasing $\longrightarrow$ Depolarizing

fixed $N \longrightarrow \bar{N} \pm \delta N$ fluctuating

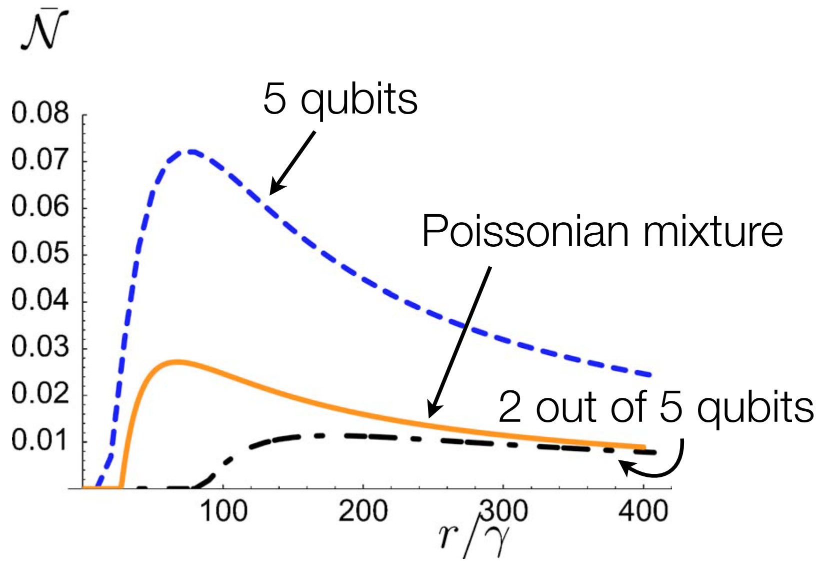
Details change

Main features robust!





$H = H_{xyz} \qquad 0 \leq T \leq \infty$



5 qubits, average negativities

Summarizing the toolbox ingredients

- Quantum systems driven by classical dynamics
  (mixed quantum/classical, i.e. semi-quantal model)
- Entangling interaction (accessible Hilbert space large enough)
- Strong decoherence mechanism
- Few/no symmetries
- Simple **reset mechanism**
  (external field or any dissipative structure to reduce entropy)
- Reset process **drives/maintains** system away from equilibrium
  => Only then entanglement exists
  Be aware: classical probabilistic rate equations might fail!

⇨ Ingredients simple enough to exist in biology

Some references...

Spin gases

Calsamiglia et al., PRL **95**, 180502 (2005)
Calsamiglia et al., Int. J. Quant. Inf. **5**, 509 (2007)

non-Markovian aspects:

Hartmann et al., PRA **72**, 052107 (2005)

proposal for ultra-cold atoms:

Jaksch et al., PRL **82,** 1975 (1999)
and experimental work based thereon

Reset mechanism and non-equil. aspects:

Hartmann et al., PRA **74**, 052304 (2006)
Hartmann et al., N. J. Phys. **9**, 230 (2007)

Weighted graph states and applications to spin systems

Hartmann et al., J. Phys. B. **40**, S1 (2007)
Dür et al., PRL **94,** 0907203 (2005)

Lecture notes:

Hein et al., arXiv/quant-ph/0602096 (2006)