Entanglement and (de-)coherence in biology

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Plan of talk

- General & introductory remarks
  - Preliminaries & Motivation
  - Types of biological entanglement
- Persistent entanglement in a hot and noisy environment
  - Molecular motion as a non-equilibrium dynamics
- Chemical compass & Bird navigation
  - Do birds use entanglement during migration?
  - Spin chemistry experiments
  - Avian chemical compass
- Summary & Outlook

Quantum entanglement in biological systems?

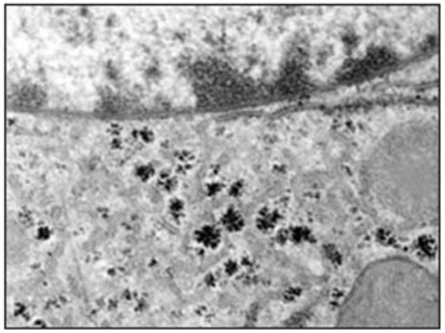
→ QuEBS 2009, Lisbon

- Do quantum coherence & **entanglement** play any role in biology?

- Biological systems are not only complex,
  but also „warm, wet, & noisy."

  → Plenty of decoherence sources!

T=37°C



- How can we expect fragile phenomena like entanglement to play any role?

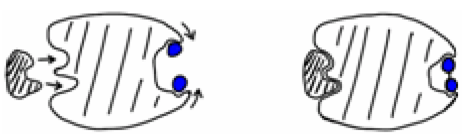
Quantum entanglement in biological systems?

- Biological systems are not only warm, wet and noisy, but they are open systems, operating far away from thermal equilibrium.

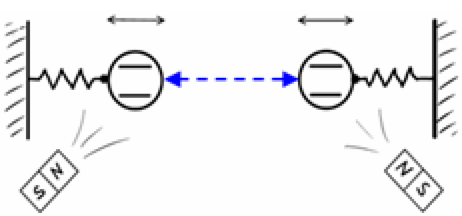
→ Quantum non-equilibrium systems

→ Non-trivial quantum effects due to ***motion***

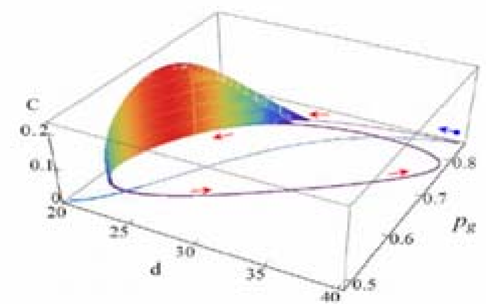
→ Static versus dynamic entanglement



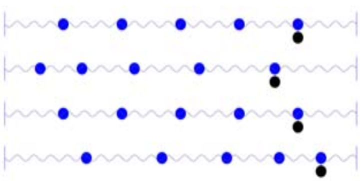
- Briegel, Popescu, arXiv:0806.4552.
  Programmatic paper & perspectives. Entanglement categories.



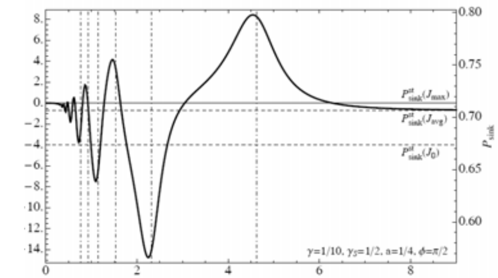
- Cai, Popescu, Briegel, arXiv:0809.4906.
  "Entanglement in oscillating molecules & potential biological implications".

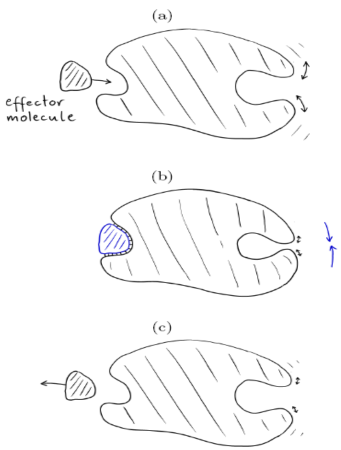


Some recent papers

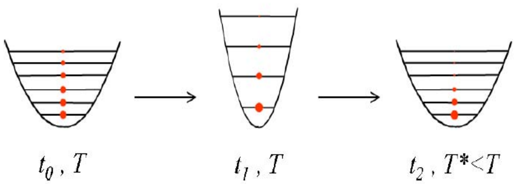


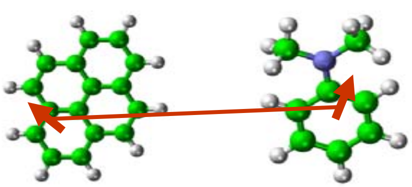
- Asadian, Tiersch, *et al.* arXiv:1002.xxxx
  "Motional effects on the efficiency of excitation transfer"



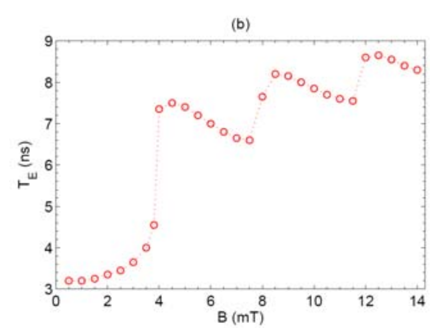


- Briegel, Popescu, arXiv:0912.2365
  "Intra-molecular refrigeration in enzymes"





- Cai, Guerreschi, Briegel, arXiv:0906.2383
  "Quantum control and entanglement in a chemical compass"



(*Phys. Rev. Lett.*, in press)

Trivial versus non-trivial quantum effects

To discuss the meaning and potential role of entanglement/coherence in biological systems, we distinguish three different types:

1. Entanglement of basic constitutents ⟵ „static“

2. Dead entanglement } ⟵ „dynamic“

3. Live entanglement

HJB, Popescu, arXiv: 0806.4552.

N.B.: - Naturally fuzzy borders

Basic entanglement

1. Entanglement of basic constitutents

Clearly, this type of entanglement is omnipresent in biology:

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

→ Molecular substrate/basis on which biological processes build.

However, this entanglement is ***trivial*** in ***present context***.
It is ***not*** what we are concerned with.

N.B.: Interesting boundary cases may exist:
e.g. Coherence/entanglement within orbitals that extend over large molecules.

Dead entanglement

2. „Dead“ entanglement

- Occurs in molecules that have biological origin or occur in biological cells.
- However, occurence of this kind of entanglement does not require metabolic processes to be sustained and function.
- Such molecules can, in principle, be taken out of the cell, and continue to work.

Systems generally in thermal equilbrium. External perurbation will take them temporarily out of equilibrium, coherent phenomenon may be generated, which quickly dies out.

Paradigmatic example: ***Optical fibre***.

Properties associated w/ such type of entanglement

- Incidental | Side effect | Short time | May have biological functionality

Live entanglement

3. „Live“ entanglement

This type of entanglement *per definition* exists only while metabolic processes take place.
System needs to be actively maintained far from thermal equilibrium.

⟶ Open, driven non-equilibrium quantum system

Properties associated with such type of entanglement

- Persistent | Dynamically controllable | Biological functionality | Evolutionary selected

⟶ Presumably requires ***molecular motion***

> Here we would expect a biological process, whose very purpose is to generate and sustain entanglement!
>
> N.B.: There is no existing example, yet, of such type of process!

Current candidate systems in biology

Photosynthesis:
• Exciton propagation in the light harvesting complex.

Does Nature exploit quantum entanglement/coherence to enhance light harvesting effiiency in photosynthesis?

Radical-pair mechanism:
• Spin chemistry experiments.
• Avian magnetic compass.

Does entanglement play a crucial/non-incidental role in the RPM?

Do *birds* use entanglement in the magnetic compass?

Can we fruitfully apply concepts and tools from quantum information to study the RPM and possibly propose *new experiments*?

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Entanglement through molecular motion?

Molecular motion is omnipresent in biology: e.g. Molecular motors & machines

How to describe this motion? → Depends on degrees of freedom you want to follow

Example: „Protein folders“ describe folding process essentially classically?
Why do they not care about, say, entanglement?

Good reason: Noise @ T=300K! → treat interactions classically

More refined description

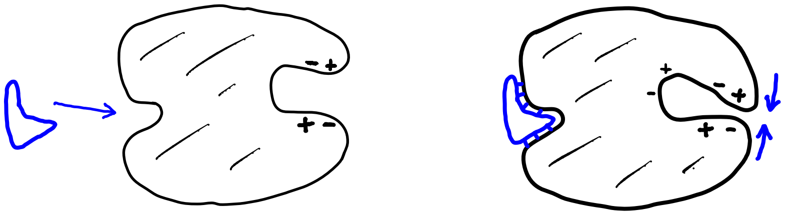
Take conformation/shape of the molecule as a ***classical backbone*** structure, which carries ***q.m. degrees of freedom*** at specific sites.

Semi-quantal model
arXiv:0809.4906

→ Time-dependent Hamiltonians (+ Noise!)

Molecular motion

Consider e.g. allosteric transitions

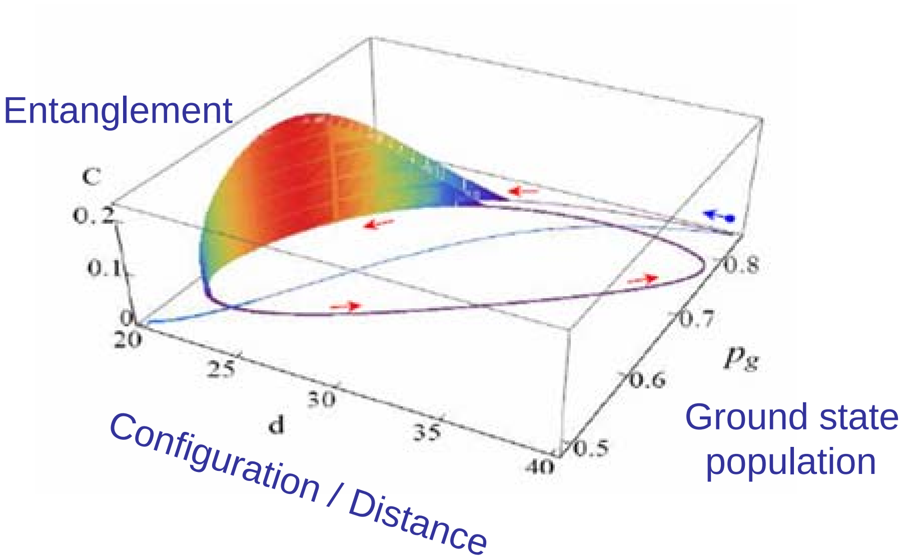


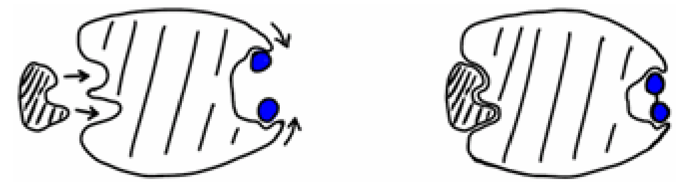
Assumption: thermal equilibrium state (@ T=300K), **completely separable for every (static) molecular configuration.**

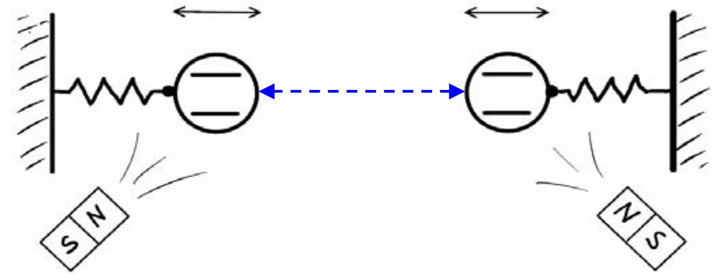
Q: What happens during motion?
Can quantum degrees of freedom become entangled?

A: Yes they can. (Non-equilibrium effect)

Entanglement generation on limiting cycle



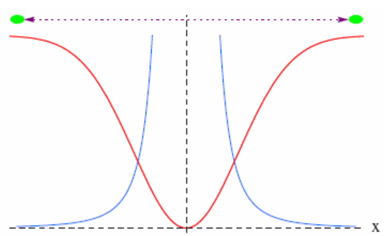




Example: $H_M(t) = J(t)\sigma_X^{(1)}\sigma_X^{(2)} + B(t)\left(\sigma_Z^{(1)} + \sigma_Z^{(2)}\right)$

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

$$J(t) = J_0 \left| x_l(t) - x_r(t) \right|^{-3} = J_0 / d^3(t)$$



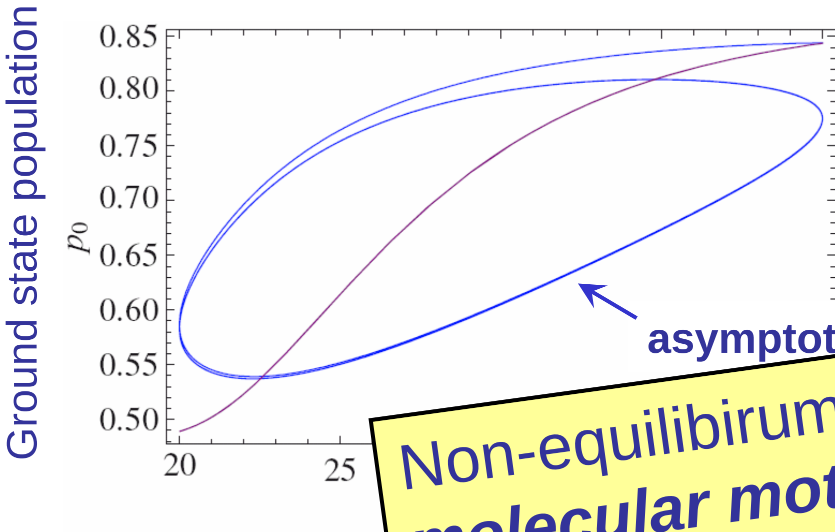
Master equation:

"hot & noisy"

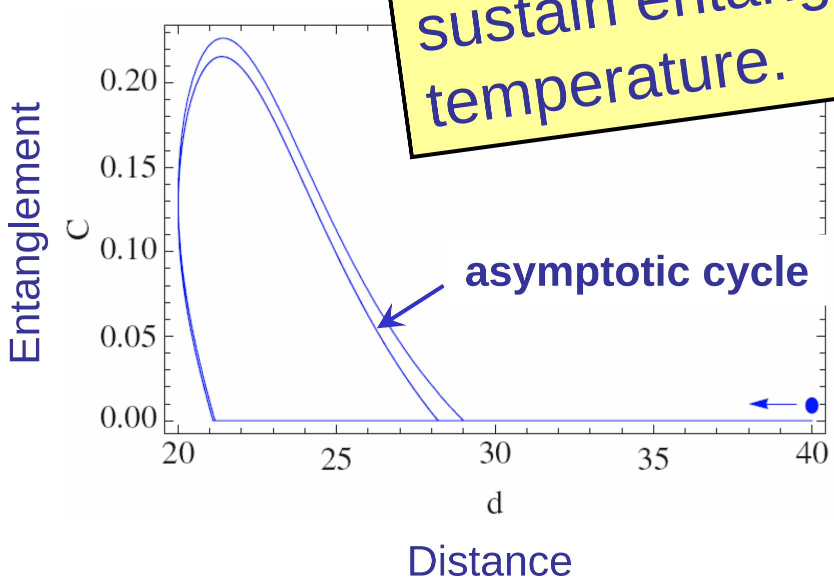
$$\frac{\partial}{\partial t}\rho(t) = -i\left[H_M(t), \rho(t)\right] + L(t)\rho(t)$$

→ arXiv: 0809.4906.

Entanglement during periodic motion



Non-equilibirum processes due to ***molecular motion*** can, in principle, sustain entanglement at room temperature.



p_0:= population of ground state

C: = concurrence

... t measure

$$\ldots _2 - \lambda_3 - \lambda_4\}$$

$$\ldots ^*(\sigma_y \otimes \sigma_y)$$

Parameters:

T= 100
$\gamma = 0.01$
$\beta = 1/k_B T = 1$
B ~ 1.2 .. 0.2
J ~ 0.2 .. 1.2

Cai, Popescu, HJB; arXiv: 0809.4906

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  - Types of biological entanglement
  - Recent work
- Persistent entanglement in a hot and noisy environment
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Avian magneto-reception

- Birds use Earth‘s magnetic field for naviagation (migration).
  → Inclination compass

Wiltschko & Wiltschko, Science 1972
ibid., J. Exp. Biol. 1996
ibid., Bioessays 2006

- Effect also established for many other species (e.g. insects)

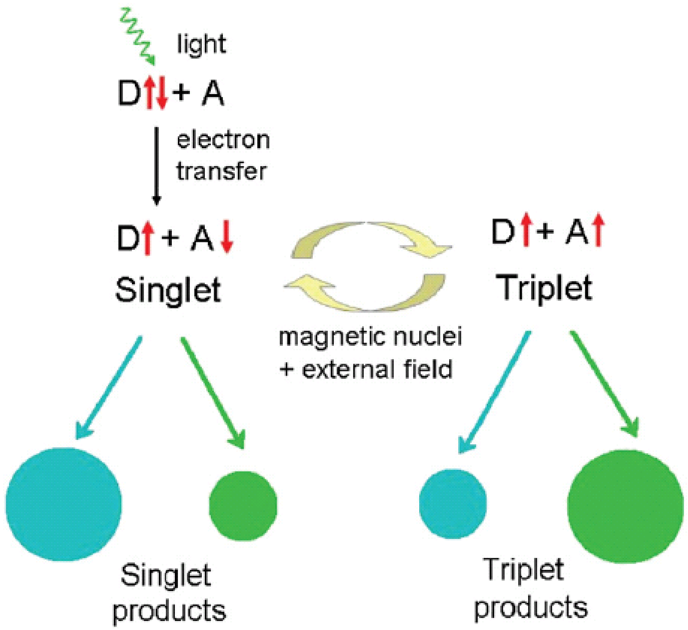
Wiltschko & Wiltschko, Bioessays 2006
Gegear *et al.* Nature 2008
Burda *et al.* PNAS 2009
…

- Two main hypotheses for underlying mechanism
    - Magnetite-based mechanism
    - Radical pair chemical reaction mechanism (RPM)

Schulten *et al.* Z. Phys. Chem. **1978**

Chemical compass model

In pioneering work by Schulten et al., the radical pair mechanism (RPM) was proposed to be responsible for bird navigation. Such a „chemical compass model“ has since been widely studied.



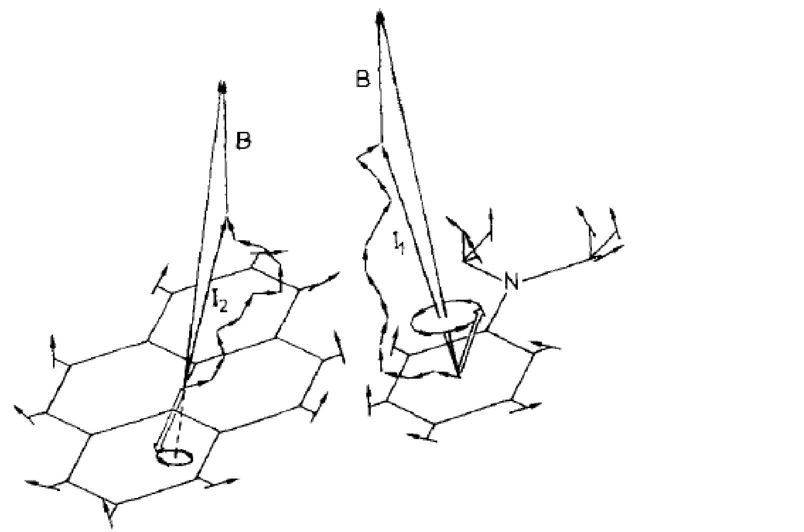


FIG. 1. Schematic illustration of the electron spin precession in the pyrene–dimethylaniline ($^2Py^- + ^2DMA^+$) radical pair.

Ritz *et al. Biophys. J.* 96 (2009).

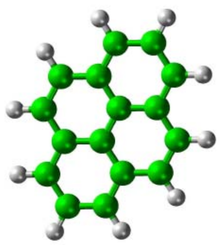
Schulten *et al.* J. Chem. Phys. 68 (1978).

Steiner & Ulrich, Chem. Rev. 89, 51 (1989).

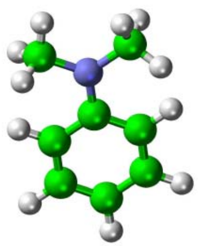
Specific examples of radical pairs

I

Pyrene



Dimethylaniline



$$\mathrm{Py}-h_{10}^{\bullet -} \quad \mathrm{DMA}-h_{11}^{\bullet +}$$

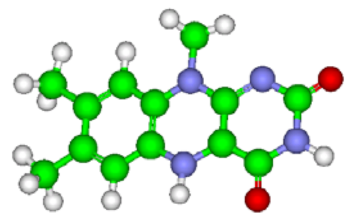
- Well-studied in **spin chemistry experiments**

  Rodgers *et al., J. Am. Chem. Soc.* 129 (2007)
  Schulten et al. *J. Chem. Phys*. 67, 664 (1977)

- Isotropic hyperfine coupling
- Radical pair lifetime is **short** ~ 10ns

II

Flavin adenin di-nucleotide in cryptochrome



$$FADH^{\bullet}-O_2^{\bullet -}$$

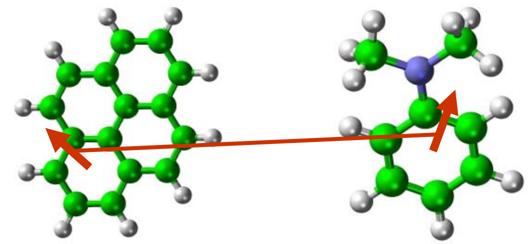
- Current molecular candidate for **avian compass**

  Ritz *et al. Biophys. J.* 96 (2009).
  Cintolesi *et al. Chem. Phys*. 294, 385 (2003)

- Non-isotropic hypefine coupling
- Radical pair lifetime is **long** ~ μs

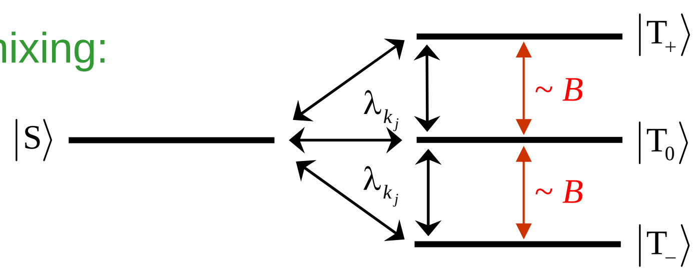
Radical pair mechanism (isotropic HF interactions)

$$H = \sum_{k=1,2} H_c^{(k)} = -\gamma_e B \sum_k S_z^{(k)} + \sum_{k,j} \lambda_{k_j} \vec{S}^{(k)} \cdot \vec{I}^{(k_j)}$$



$[\text{Py-}h_{10}^{\cdot -}\ \text{DMA-}h_{11}^{\cdot +}]$

Singlet-triplet mixing:

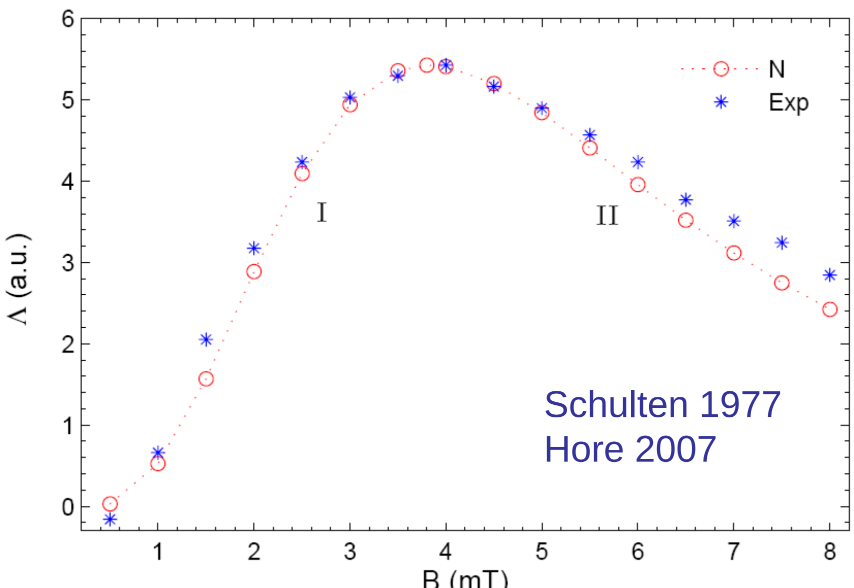


$$|S\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

$$|T_0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$$

$$|T_+\rangle = |\uparrow\uparrow\rangle$$

$$|T_-\rangle = |\downarrow\downarrow\rangle$$



Magnetic field effect:

$$\Lambda(B) = \frac{\partial \Phi_s}{\partial B}$$

Discussion

Q: Isn‘t this a quantum effect par excellence?

→ But: Are the electrons ***entangled***?

→ Does the entanglement make a difference?

N.B.: Here the electrons ***are*** biologically relevant degrees of freedom!

Extreme case: Consider ***classically correlated state***, resulting e.g. from complete de-phasing

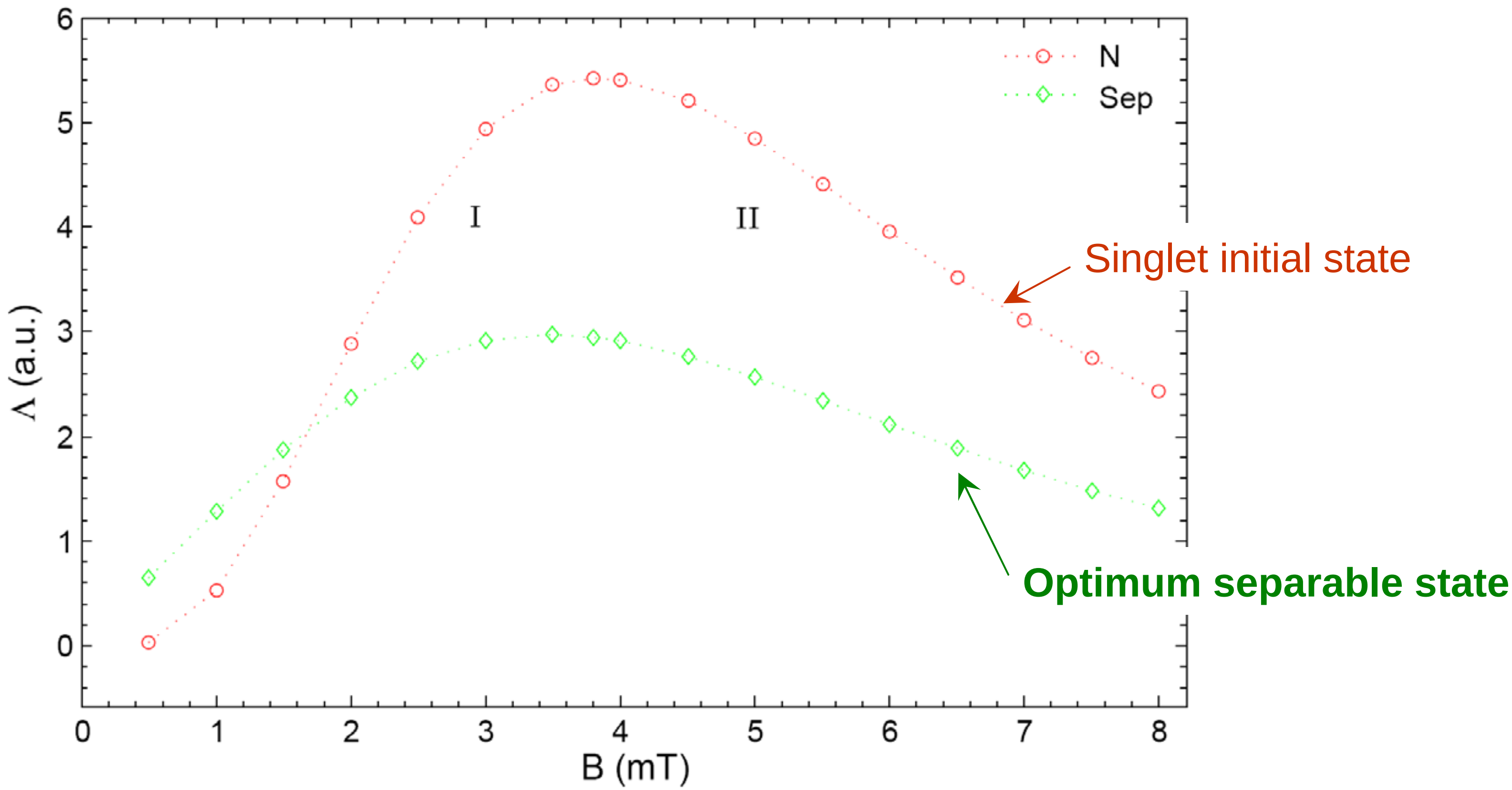
$$\rho_s(0) = \frac{1}{2}\left(|S\rangle\langle S| + |T_0\rangle\langle T_0|\right)$$

$$\rho_s(0) = \frac{1}{2}\left(|\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow|\right)$$

Is entanglement relevant?

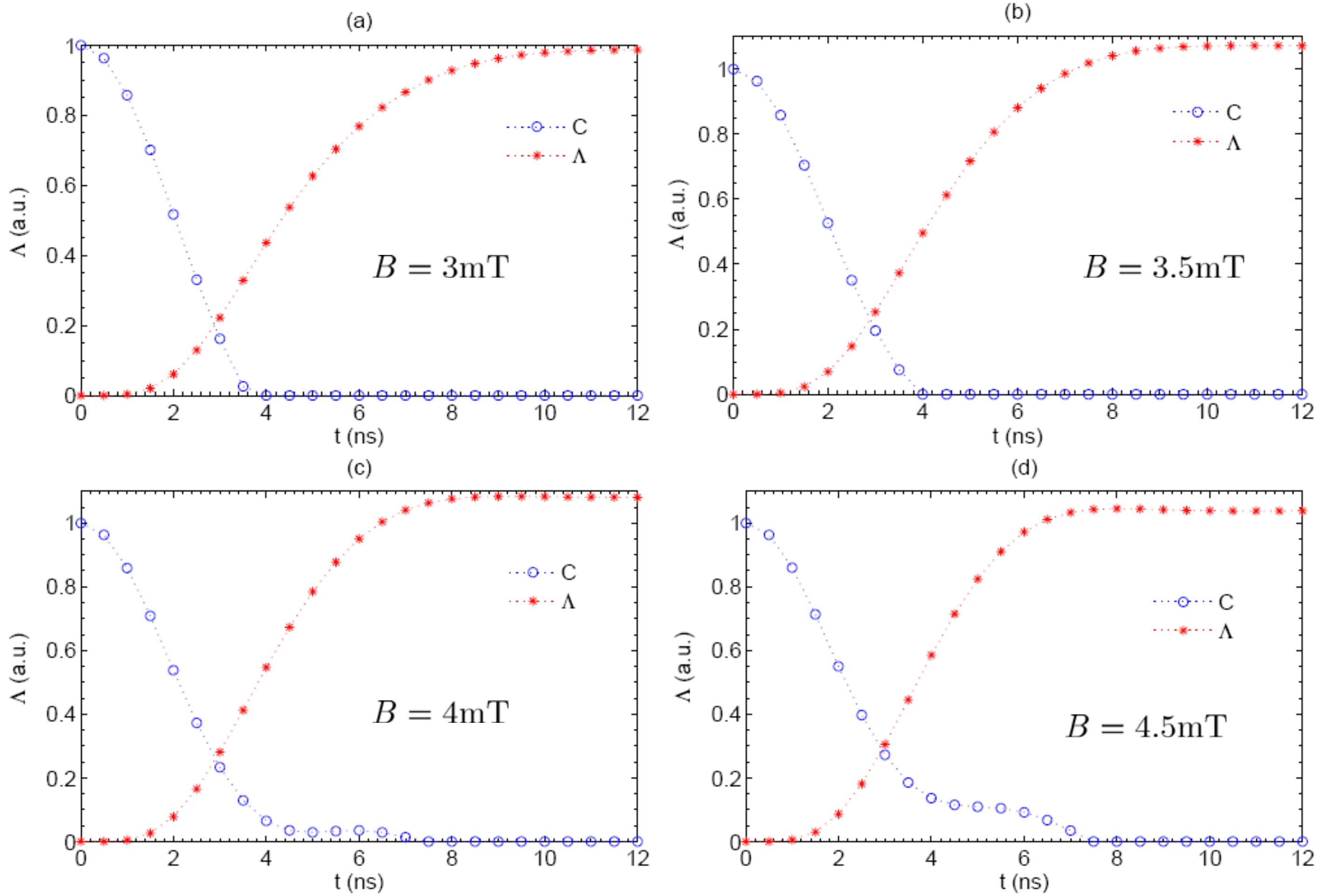
Optimum sensitivity for **separable initial states**:

Cai et al. arXiv:0906.2383



➢ *Entanglement really makes a difference: It is **necessary** for high B-field sensitivity*

Time evolution of entanglement (initial singlet)



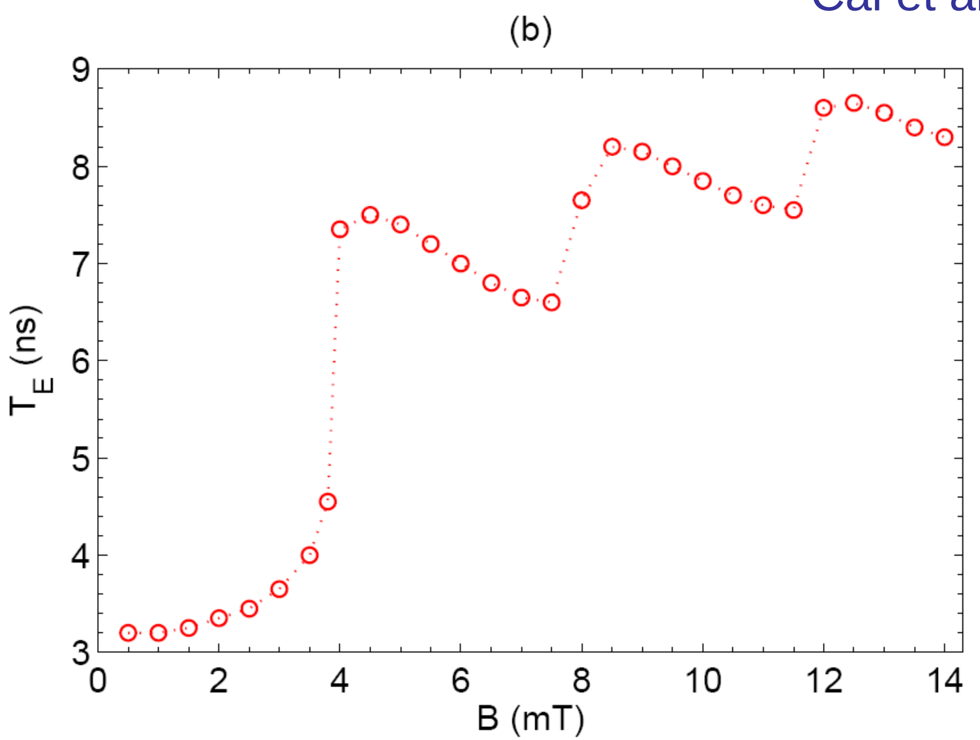
Def.: Entanglement lifetime

$$T_E = \max\{t|E(t) > 0\}$$

Lifetime of entanglement $\sim$ Reaction time

Lifetime of entanglement as signature

Cai et al. arXiv:0906.2383



Discontinuity in the lifetime T_E of entanglement as a function of B

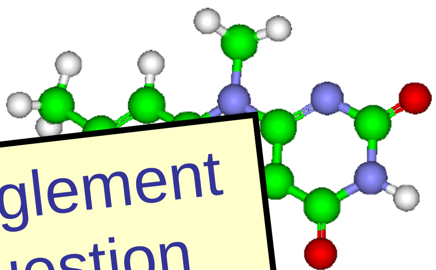
Steps: ←→ Finite size nuclear spin environment
Overall increase: Reshaping of mixed state towards binary mixture

- *Entanglement is a different, and generally more sensitive, signature of RPM*

Molecular candidate for radical pair in Europe robins

Ritz *et al*. Biophys. J. 96, 3451 (2009)

$\mathrm{FADH}^{\bullet} - \mathrm{O}_2^{\bullet -}$



- Anisotropic hyperfine couplings
- Radical pair lifetime is long $\sim \mu s$

Whether or not birds use entanglement for navigation is still an open question

For this mol … ntanglement does ont seem to be necessary to explain directional sensitivity of RPM/chemical compass.

Same or better senstivity can be obtained by some separable states!

Role of entanglement generally depends on its lifetime compared to reaction time.

--- APPENDIX ---

Entanglement vs. Coherence

Consider e.g. state resulting from depolarization of single qubits

$$\rho(t) = p_t \left|\Phi^+\right\rangle\left\langle\Phi^+\right| + (1-p_t)\frac{\boldsymbol{I}}{4}$$

$$p_t = e^{-\gamma t}$$

$$\left|\Phi^+\right\rangle = \frac{1}{\sqrt{2}}\left(\left|00\right\rangle + \left|11\right\rangle\right)$$

$$\rho(t) = \begin{pmatrix} \frac{1+p_t}{4} & & & \frac{p_t}{2} \\ & \frac{1-p_t}{4} & & \\ & & \frac{1-p_t}{4} & \\ \frac{p_t}{2} & & & \frac{1+p_t}{4} \end{pmatrix} \begin{matrix} 00 \\ 01 \\ 10 \\ 11 \end{matrix}$$

$$\begin{matrix} 00 & 01 & 10 & 11 \end{matrix}$$

Entanglement (e.g. concurrence):

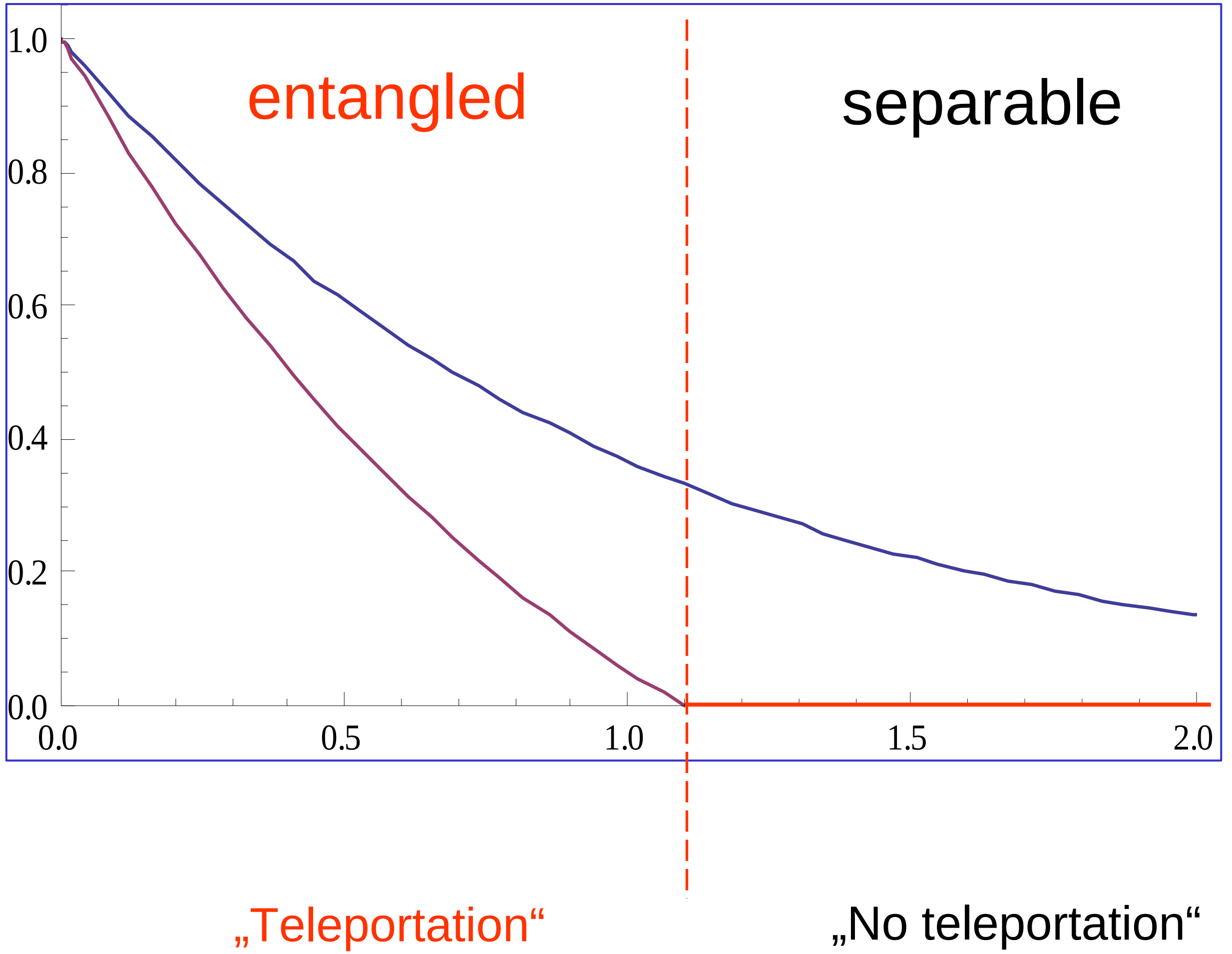
$$E(t) = \max\left\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\right\}$$

$$\Lambda = \rho\left(\sigma_y \otimes \sigma_y\right)\rho^*\left(\sigma_y \otimes \sigma_y\right)$$

for this simple example:

$$E(t) = \frac{3p_t - 1}{2}$$

Entanglement vs. Coherence



Entanglement and magnetic field sensitivity

Since entanglement seems to play a role in the RPM

- Can we give a quantitative description of its evolution and role?
- Can we use it as signature?

Two-qubit measure of entanglement. (e.g. concurrence)

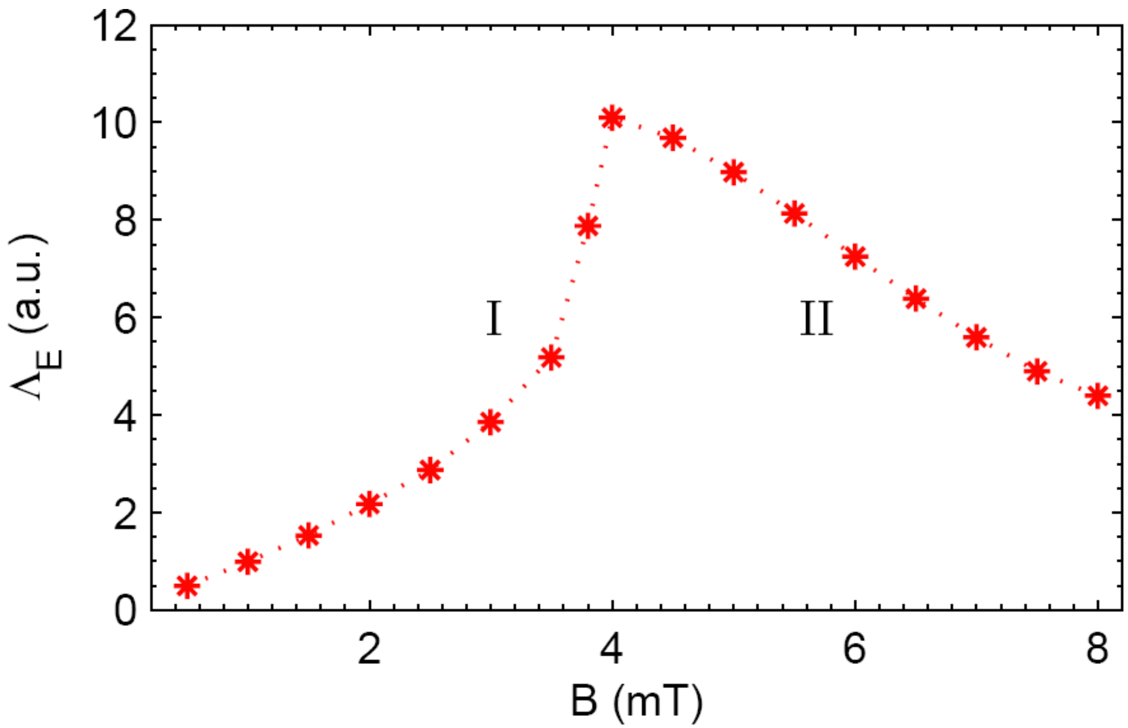
Similar to activation yield, define $$\Phi_E = \int_0^\infty r_c(t) E(t)\, \mathrm{d}t$$

Effective amount of entanglement present in active radical pairs during reaction

$$\Lambda_E = \frac{\partial \Phi_E}{\partial B}$$

„Entanglement sensitivity“

Entanglement sensitivity *vs.* magnetic field

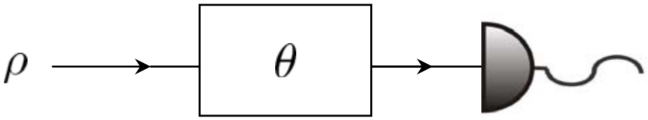


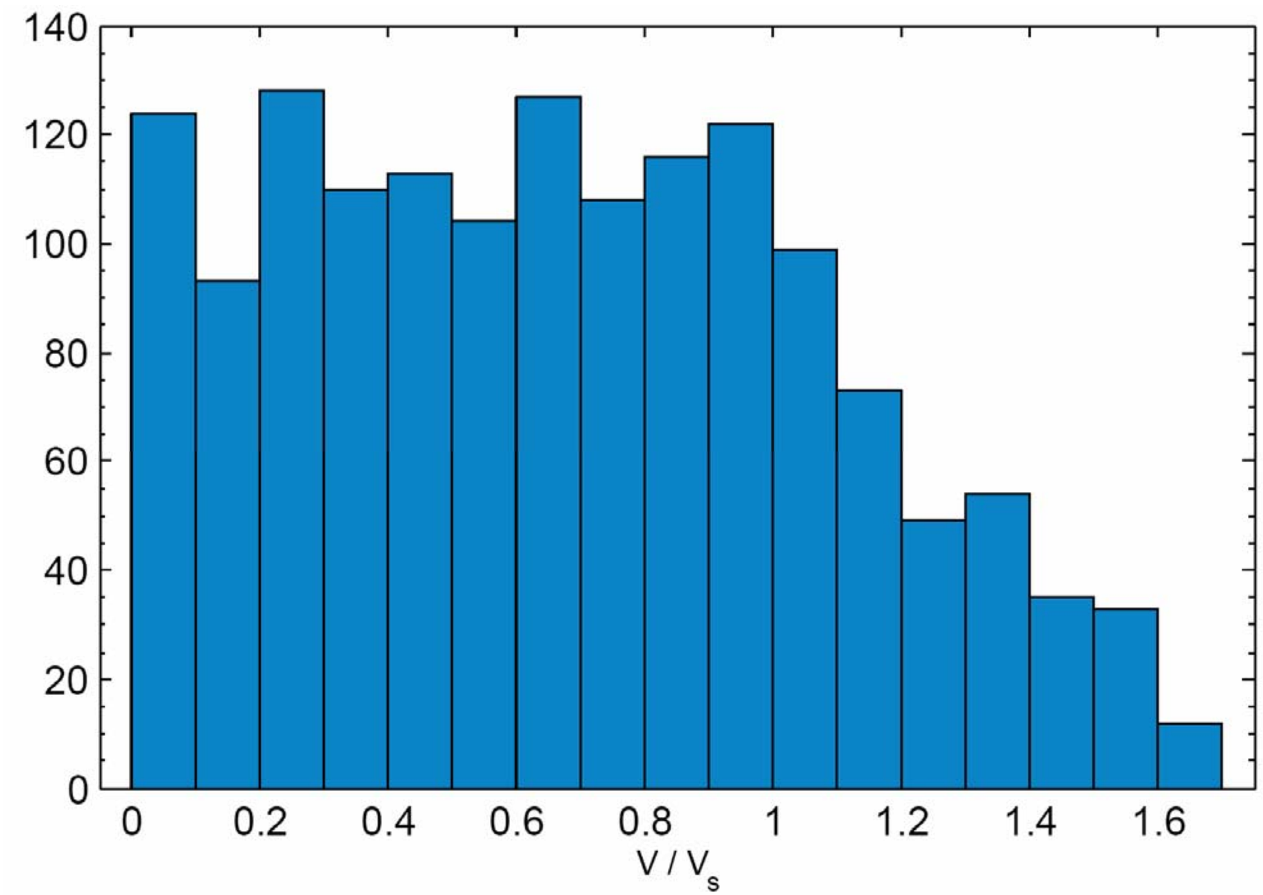
Entanglement sensitivity shows a **sharp discontinuity** (crusp) at B ~ 4mT

Figure 2: (Color online) Entanglement sensitivity Λ_E of a radical pair reaction [Py-$h_{10}^{\cdot -}$ DMA-$h_{11}^{\cdot +}$] as a function of the magnetic field B. The recombination rate constant is $k = 5.8 \times 10^8 s^{-1}$ [2].

Is entanglement necessary for avian compass?

1500 product states vs. entangled states





- A substantial part of separable states can give a high angular dependence
- Here entanglement seems not to play a significant role $\mathrm{FADH}^{\bullet} - \mathrm{O}_2^{\bullet -}$