Quantum coherence in biological processes: Case of avian magnetoreception

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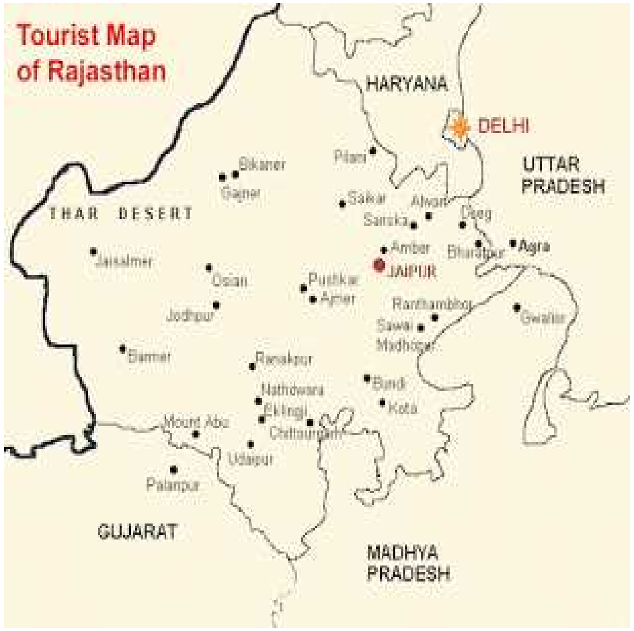
Tourist Map of Rajasthan
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Kota
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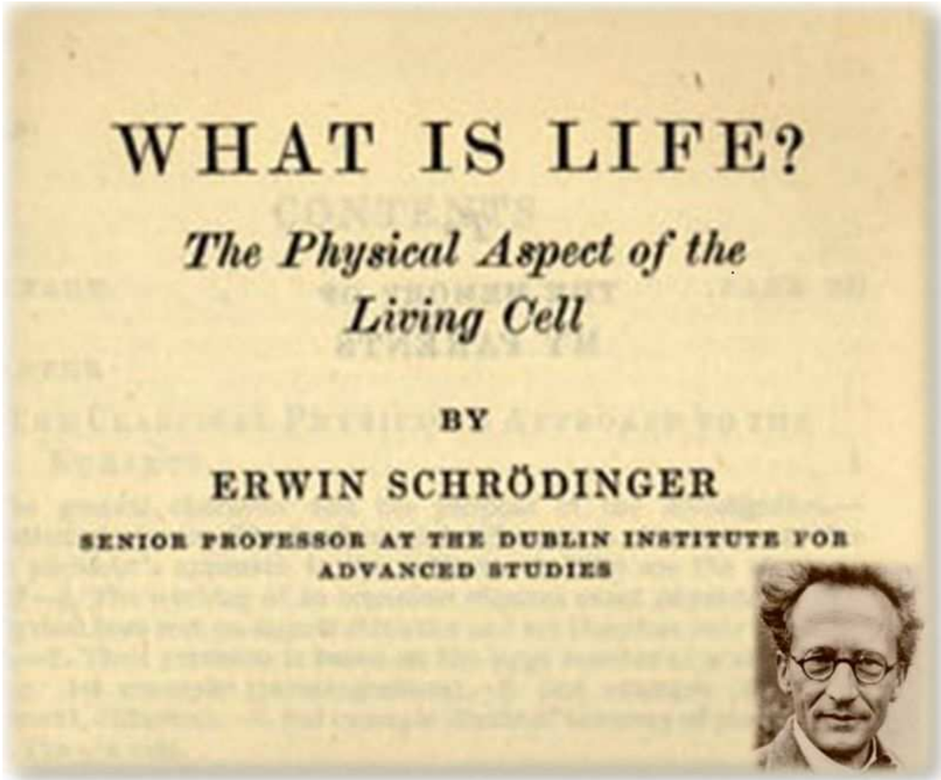
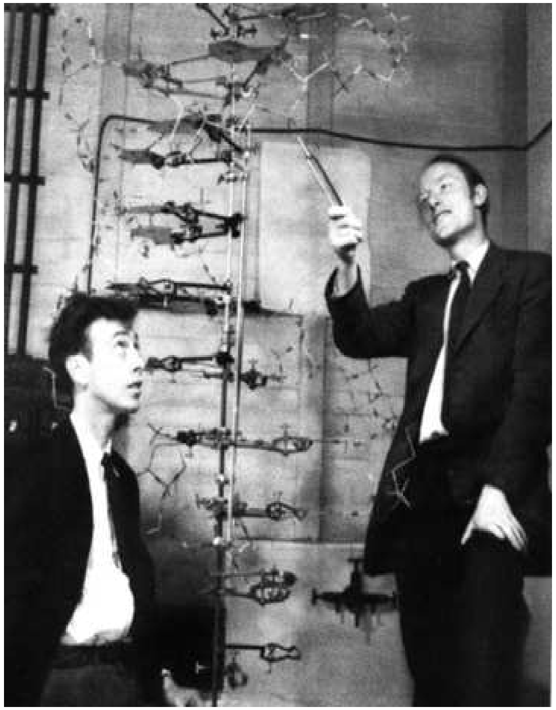
Palanpur
GUJARAT
MADHYA PRADESH

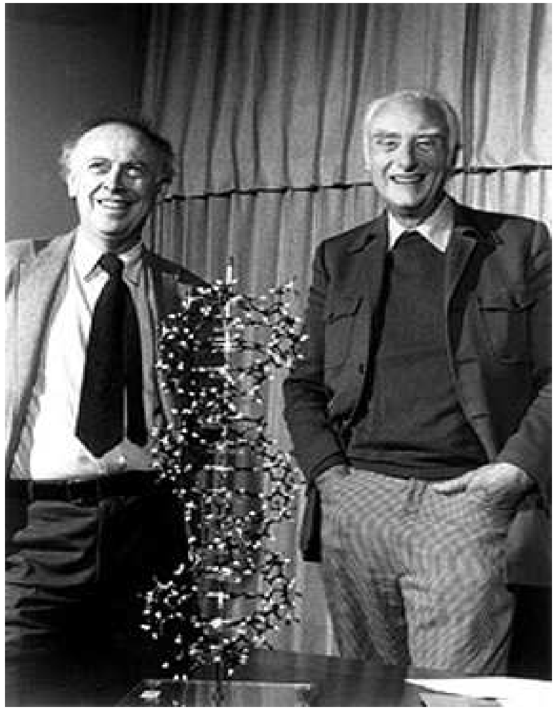
What is life? (1944)

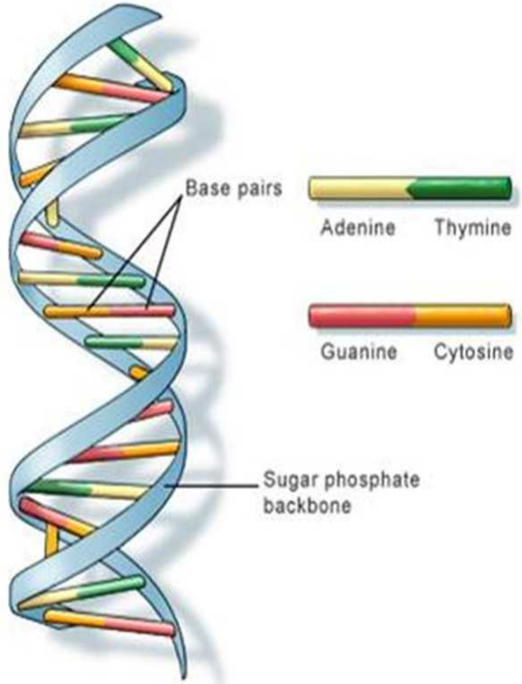


"....The mutations are actually due to quantum jumps in the gene molecule....In the light of present knowledge, the mechanism of heredity is closely related to, nay, founded on, the very basis of quantum theory....we may safely assert that there is no alternative to the molecular explanation of the hereditary substance...."

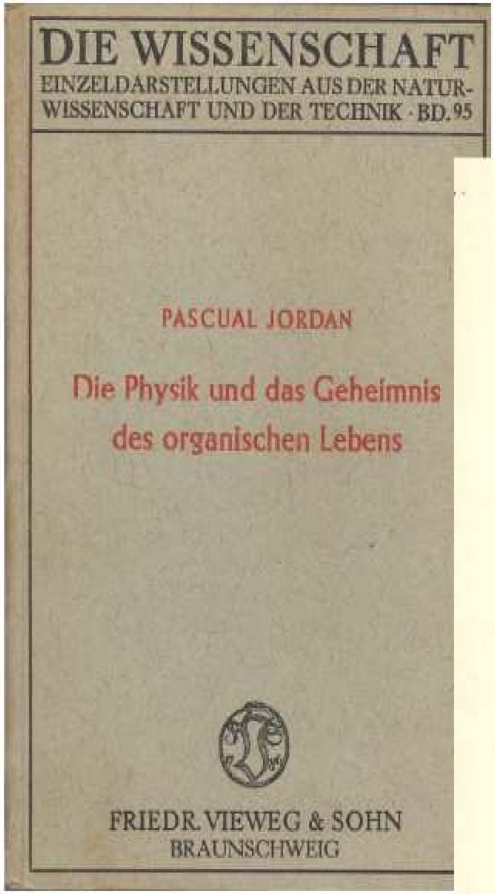
DNA double helix structure (1953)

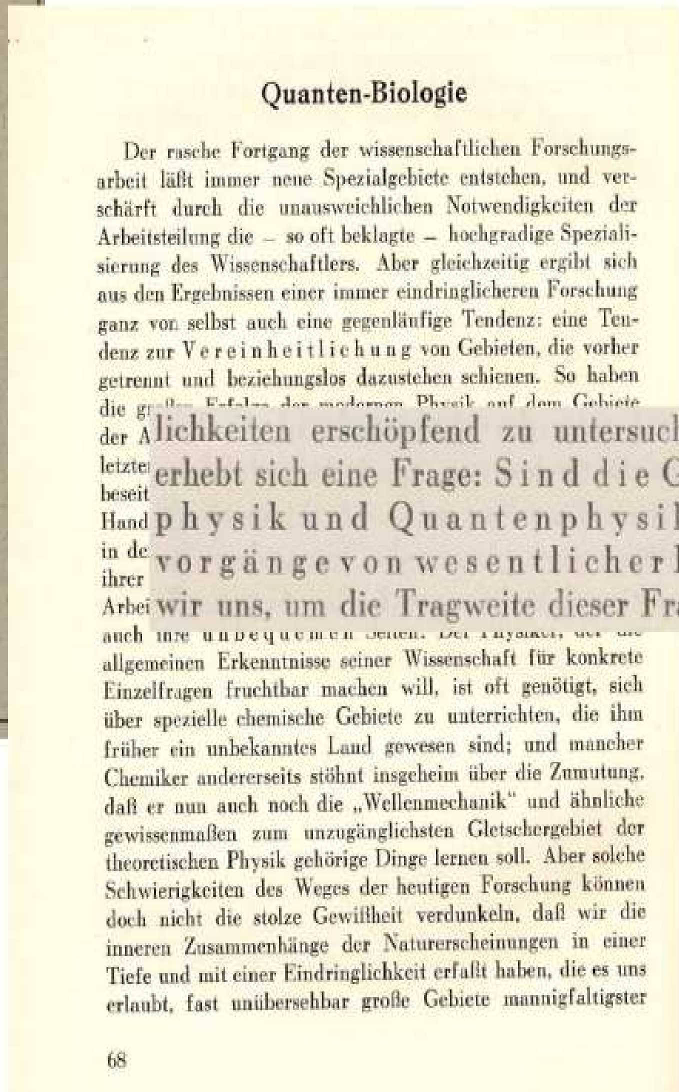






James D Watson and Francis Crick got Nobel Prize in 1962 (with Maurice Wilkins) *"for their discoveries concerning the molecular structure of nucleic acids and its significance for information transfer in living material"*





Quanten-Biologie

Der rasche Fortgang der wissenschaftlichen Forschungsarbeit läßt immer neue Spezialgebiete entstehen, und verschärft durch die unausweichlichen Notwendigkeiten der Arbeitsteilung die – so oft beklagte – hochgradige Spezialisierung des Wissenschaftlers. Aber gleichzeitig ergibt sich aus den Ergebnissen einer immer eindringlicheren Forschung ganz von selbst auch eine gegenläufige Tendenz: eine Tendenz zur Vereinheitlichung von Gebieten, die vorher getrennt und beziehungslos dazustehen schienen. So haben die gr... Erfolge der modernen Physik auf dem Gebiete der A...
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auch ihre unbequemen Seiten. Der Physiker, der die allgemeinen Erkenntnisse seiner Wissenschaft für konkrete Einzelfragen fruchtbar machen will, ist oft genötigt, sich über spezielle chemische Gebiete zu unterrichten, die ihm früher ein unbekanntes Land gewesen sind; und mancher Chemiker andererseits stöhnt insgeheim über die Zumutung, daß er nun auch noch die „Wellenmechanik" und ähnliche gewissenmaßen zum unzugänglichsten Gletschergebiet der theoretischen Physik gehörige Dinge lernen soll. Aber solche Schwierigkeiten des Weges der heutigen Forschung können doch nicht die stolze Gewißheit verdunkeln, daß wir die inneren Zusammenhänge der Naturerscheinungen in einer Tiefe und mit einer Eindringlichkeit erfaßt haben, die es uns erlaubt, fast unübersehbar große Gebiete mannigfaltigster

68

...lichkeiten erschöpfend zu untersuchen strebt. Dabei aber erhebt sich eine Frage: Sind die Gesetze der Atomphysik und Quantenphysik für die Lebensvorgänge von wesentlicher Bedeutung? Machen wir uns, um die Tragweite dieser Frage zu ersehen, bewußt,

REVIEWS OF MODERN PHYSICS VOLUME 35, NUMBER 3 JULY 1963

Proton Tunneling in DNA and its Biological Implications*

PER-OLOV LÖWDIN
Quantum Chemistry Group, Uppsala University, Uppsala, Sweden
Quantum Theory Project, University of Florida, Gainesville, Florida

“the electronic and protonic structure of biologically interesting molecules and systems has to be treated by quantum chemistry. This has lead to the opening of a new field which has been called sub-molecular biology or **“quantum biology”**....the genetic code is essentially contained in the hydrogen bonds....after a DNA replication, the protons are necessarily in nonstationary states which implies that there is a certain probability for “quantum jumps"..... which will show up and get manifested at the next DNA replication. This mechanism may be responsible for the occurrence of spontaneous mutations...."

“I want to suggest that for many years to come the student of living matter will have much more need for an understanding of physical chemistry than for a knowledge of quantum mechanics....This distinction is useful because ‘quantum effects’ are only noticeable when the quanta of energy exchanged between different parts of a system are large compared to kT....when a biochemist begins to use quantum-mechanical language in this nebulous way, we may justifiably suspect that he is talking nonsense"

—H. C. Longuet-Higgins

(Theoretical Chemist & Cognitive Scientist)

“Quantum Mechanics and Biology"

Biophysical Journal, 1962

CURRENT STATUS OF THEORETICAL CHEMISTRY IN INDIA

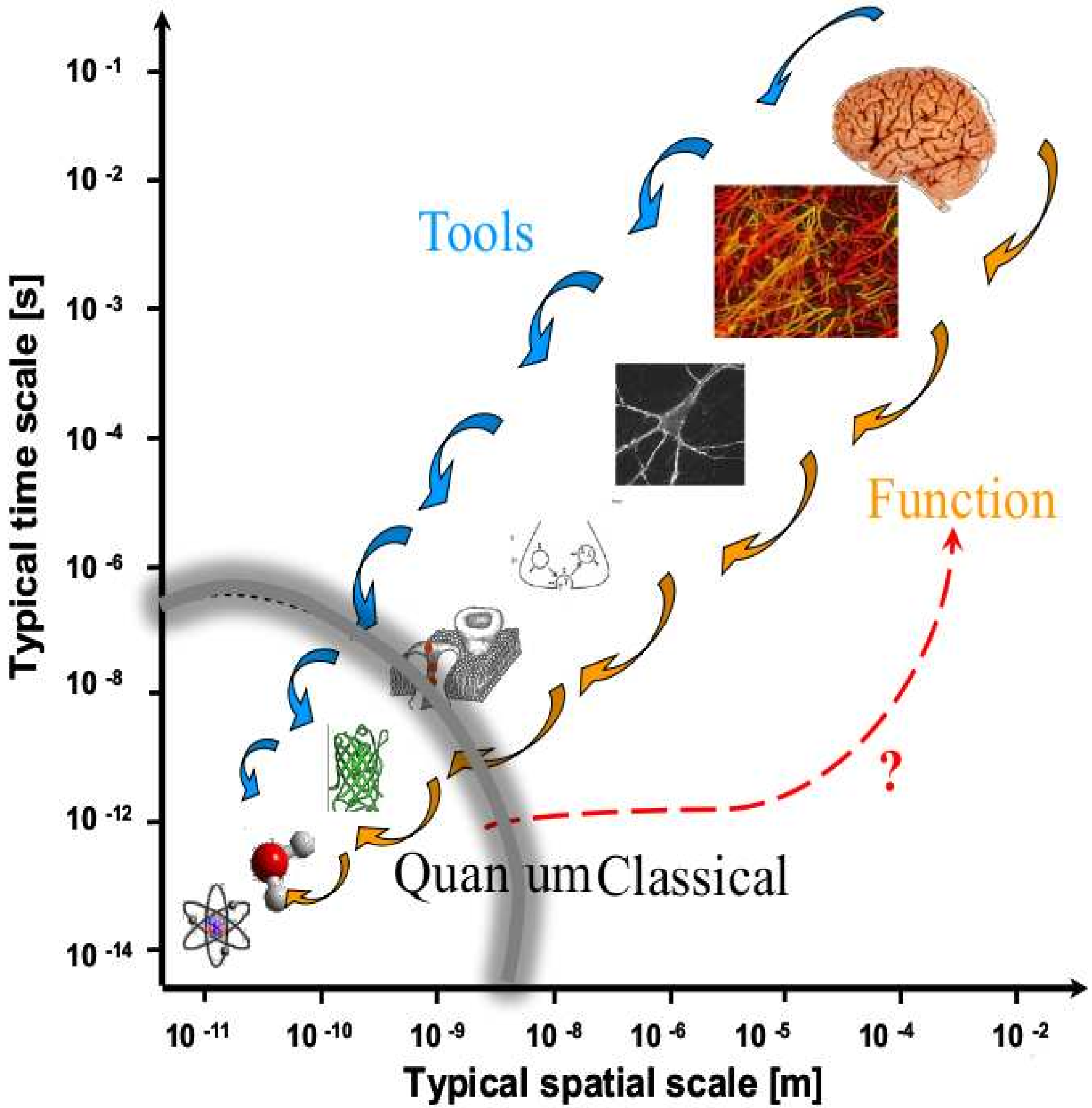
B. M. DEB
Department of Chemistry and Group of Theoretical Studies,
Indian Institute of Technology, Bombay 400 076, India.

ABSTRACT

In spite of nearly 35 years' activity in theoretical chemistry, India is not one of the leading countries in the subject. This report identifies the *strengths* and *weaknesses* of theoretical chemistry research in India, listing various topics in *quantum chemistry* (including *quantum biology*), *statistical mechanics* and *non-equilibrium thermodynamics*, which are either pursued or ought to be pursued. Quantum chemistry is relatively the strongest in our country, while the other two are very weak. The *main* weaknesses in theoretical chemistry are: (a) lack of *original* concepts and mathematical formalisms, and (b) lack of indigeneous large-scale computer programs. The reasons for these are mentioned and the strongest institutions in the country identified. For rapid development of theoretical chemistry in India, 4 *advanced interlinked multi-role* centres of research are proposed, one each for the eastern, western, northern and southern zones. Explicit suggestions are made to improve the teaching of the subject in our universities. Finally, a representative bibliography, consisting mostly of recent papers, is presented.

A satisfactory growth of theoretical chemistry is vital for the overall growth of chemical sciences as well as large areas in physics and biology. With careful marshalling of critical masses, India can rapidly become one of the frontrunners in the subject.

Current Science, 1984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Typical spatial scale [m]
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Three classes of QM effects on biological processes

- The trivial: Fundamentally QM dictates the atomic/molecular details of bio-systems, eg. molecular orbitals, energy levels are determined by QM
- Chemical kinetics: Chemical reactions are also fundamentally QM processes, but classical descriptions using mol. dynamics and chemical kinetics are very accurate. Exceptions - reactions involving quantum tunneling of protons/heavy atoms, etc.
- Functional necessity: QM effects (coherence, entanglement, etc.) are relevant for proper functioning of bio-systems. This is interesting because here QM influences emergent biological properties.
    - "Quantum Biology" deals mainly with the last category, and partially with the second category

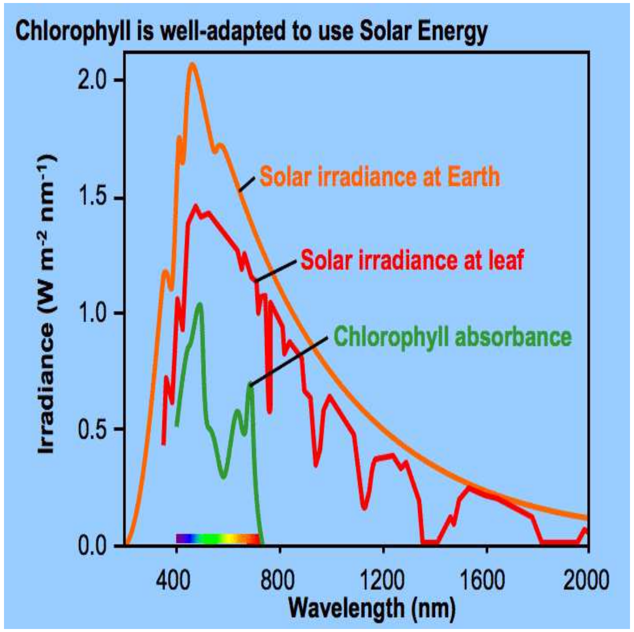
Plan of this talk

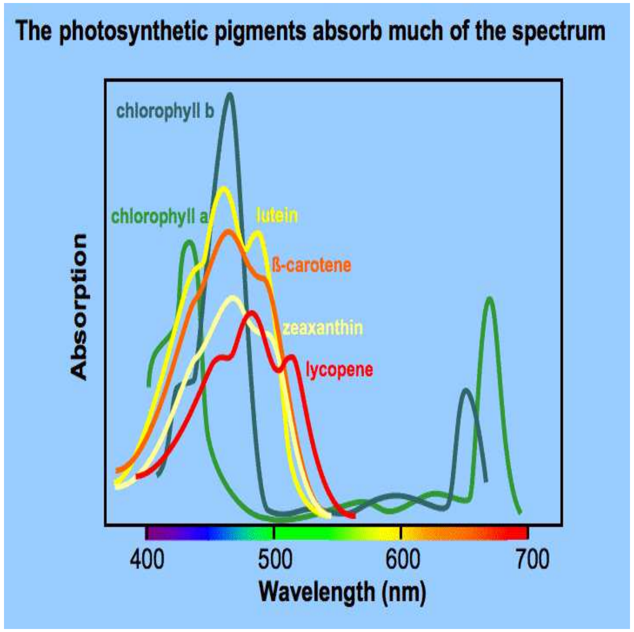
- Functional role of Quantum coherence in different biological processes
  - Photosynthesis
  - Olfaction process

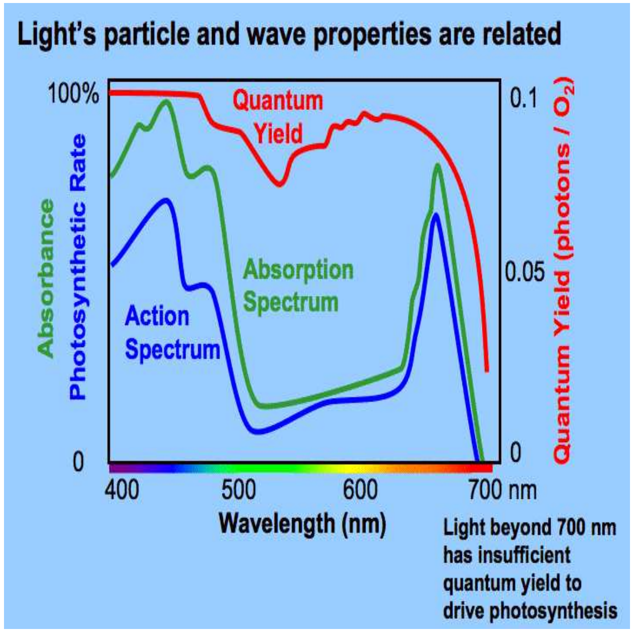
$$\vdots$$

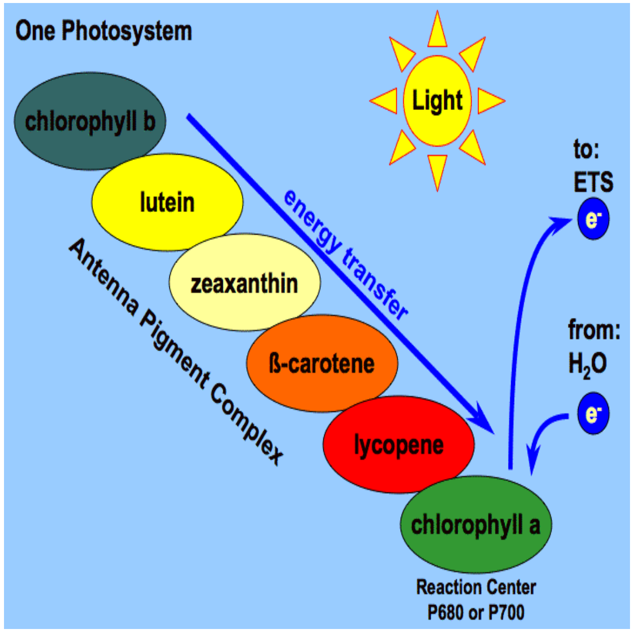
- Magnetoreception process in Migratory Birds (Avian Magneotreception)
  - Behavioral experiments with European Robin
- Biochemical model for avian magnetoreception
- Theoretical model
- Results
- Conclusion and future directions

Photosynthesis

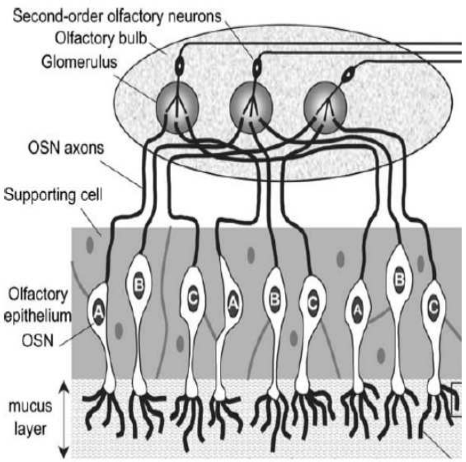


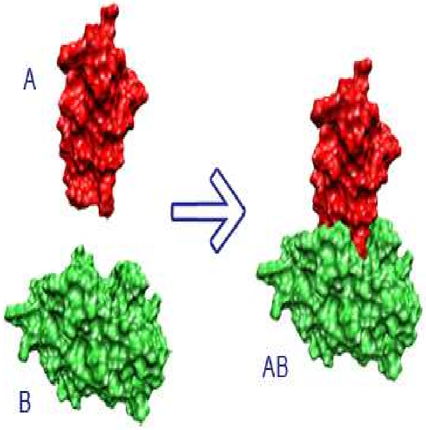


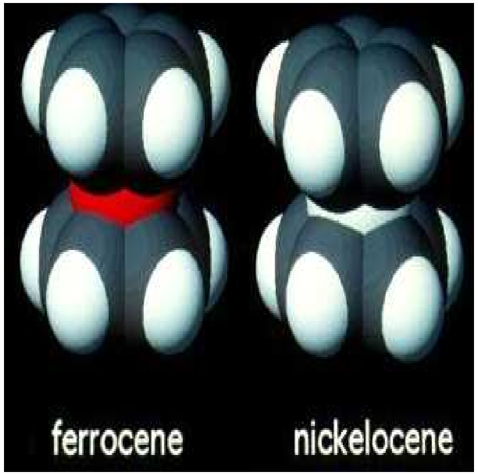




Olfaction process







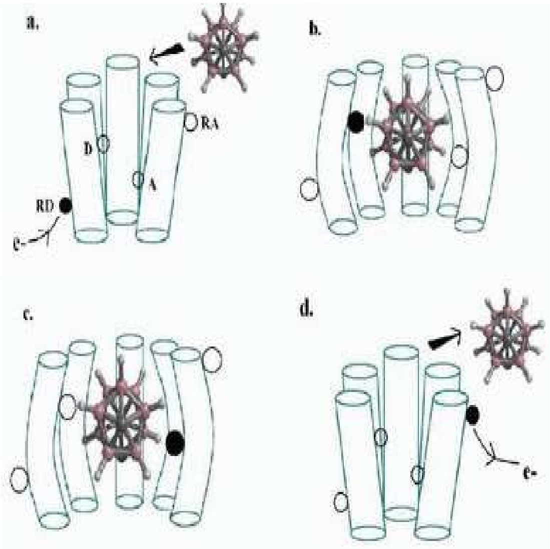
Smell Process

Molecular docking

(Lock-Key mechanism)

$C_6H_{10}Fe \mid C_6H_{10}Ni$

(Identical shape)



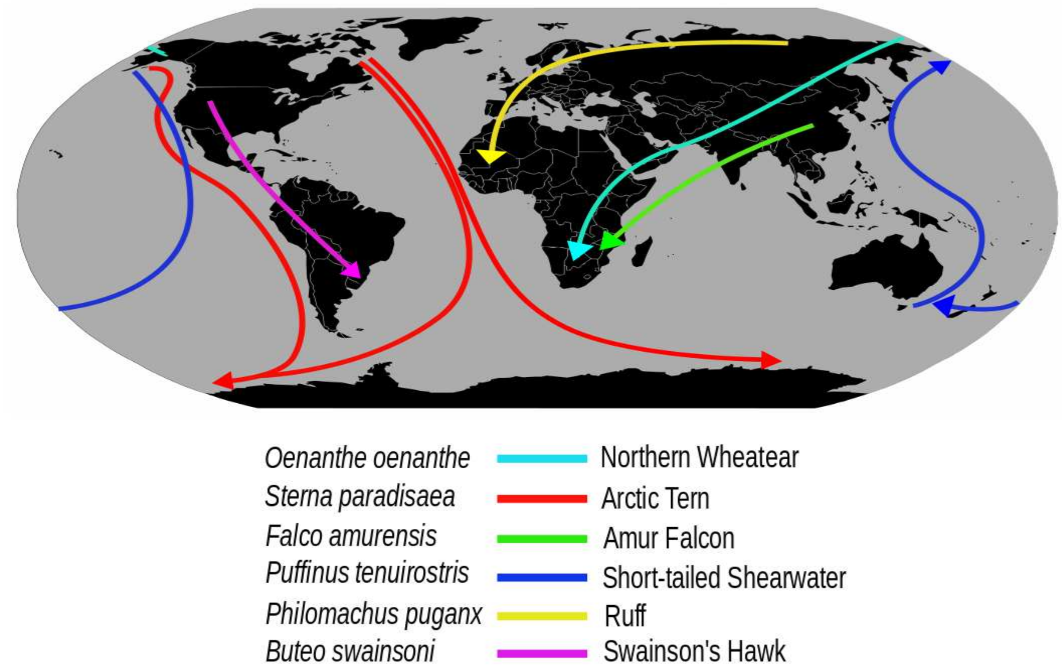
New model

Molecular Docking

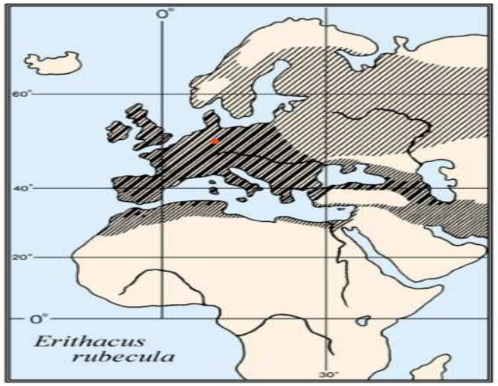
+

Vibration assisted electron tunneling

Avian Magnetoreception



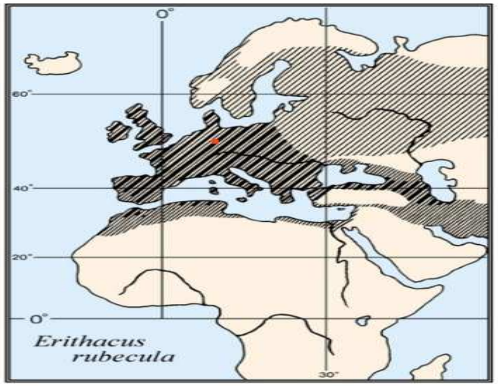
Behavioral Experiments



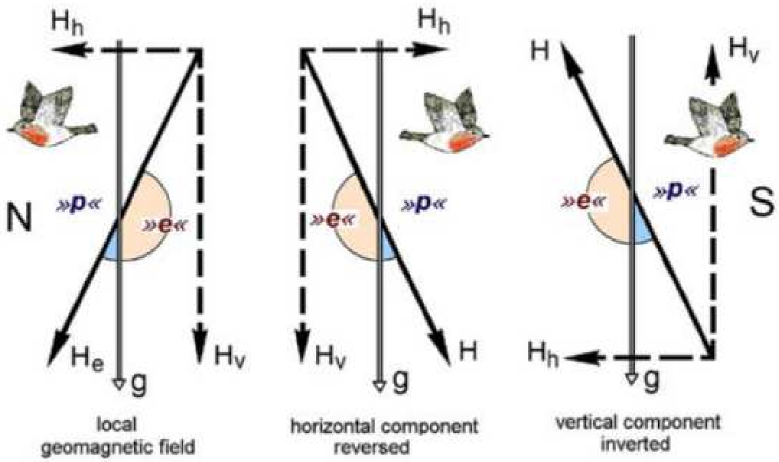
European Robin

Frankfurt

Behavioral Experiments



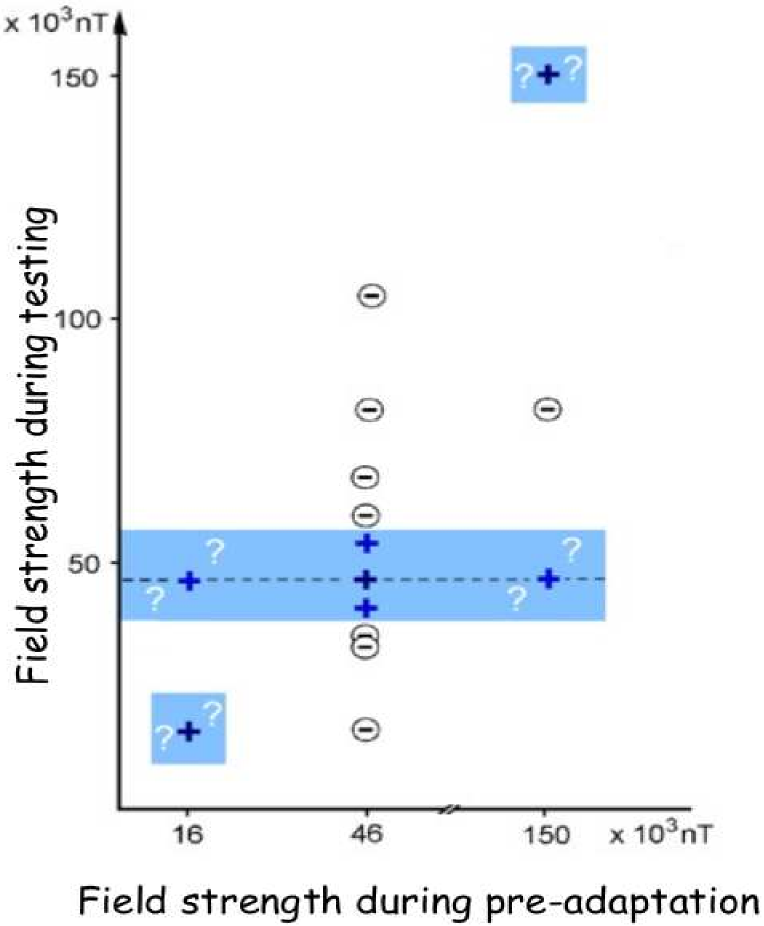
European Robin Frankfurt



Inclination Compass

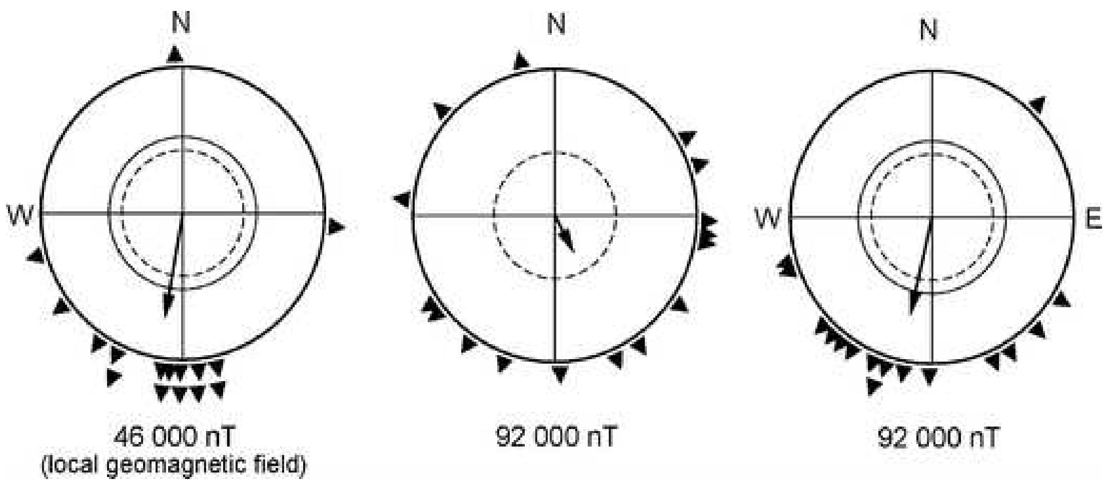
Ref. Wiltschko & Wiltschko, Science **176**, 62 (1972)

Behavioral Experiments (Contd.)



- Avian magnetic compass operates in a narrow functional window that adapts to local magnetic field conditions: $\pm 20 - 30\%$ of local geomagnetic field

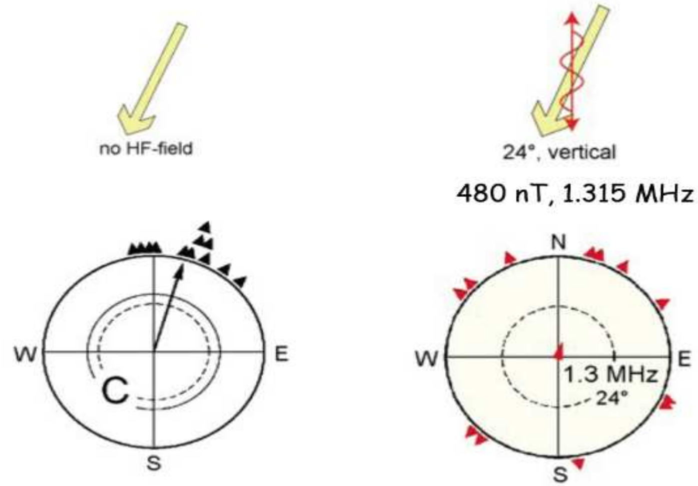
Behavioral Experiments (Contd.)



- They regain their ability after spending some time in that stronger/weaker magnetic field

Ref. Wiltschko *et. al.*, Naturwissenschaften **93**, 300 (2006)

Behavioral Experiments (contd.)



- Very weak (1% of local geomagnetic field strength) radio-frequency field can disrupt avian compass, provided:
  - The RF field is not parallel to the local geomagnetic field direction
  - Frequency of the RF field resonant with the energetic splitting due to local geomagnetic field

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

- Strong resonance at Larmor Frequency has been observed in 4 species

European Robin

Chicken

Wiltschko et al.,
J Exp Biol 210 (2007)

Zebra Finch

Keary et al.,
Front. Zool. 6 (2009)

Mole-rats: no effect

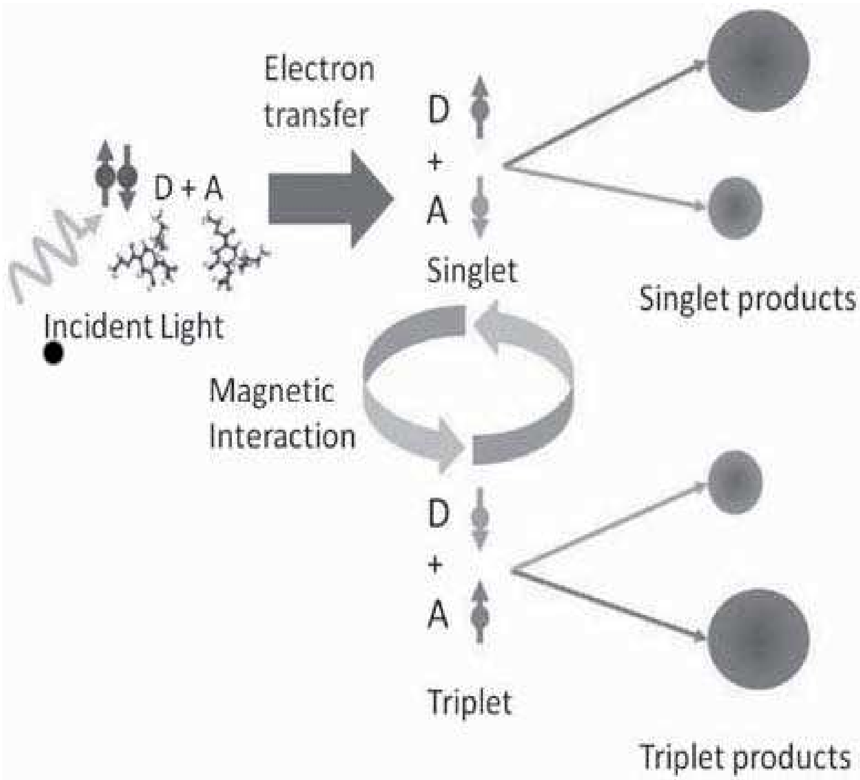
Thalau, Ritz et al. (2006),
J. R. Soc. Interface 3

cockroach

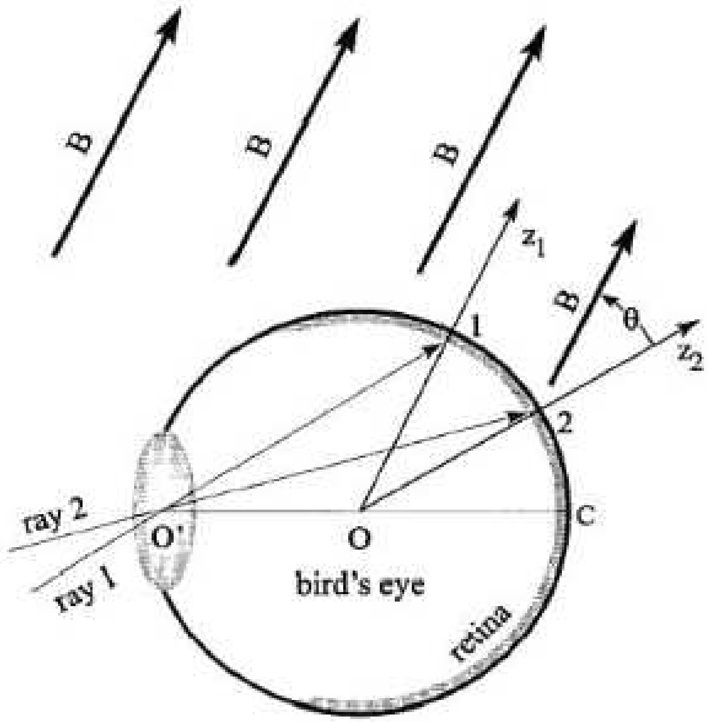
Vacha et al.,
J Exp Biol 212 (2009)

Radical Pair based chemical model

Ref. Ritz, Adem, & Schulten, Biophys. J. **78**, 707 (2000)



Where does this reaction take place?



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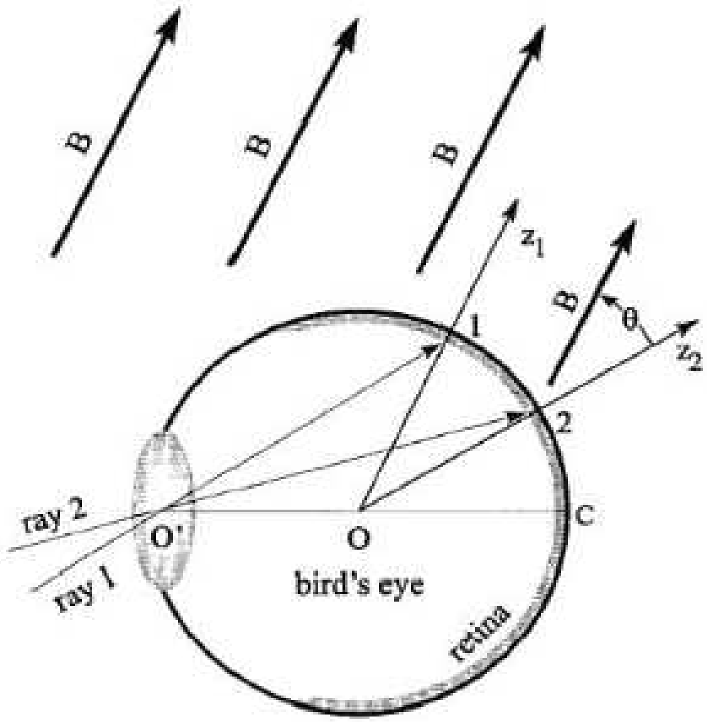
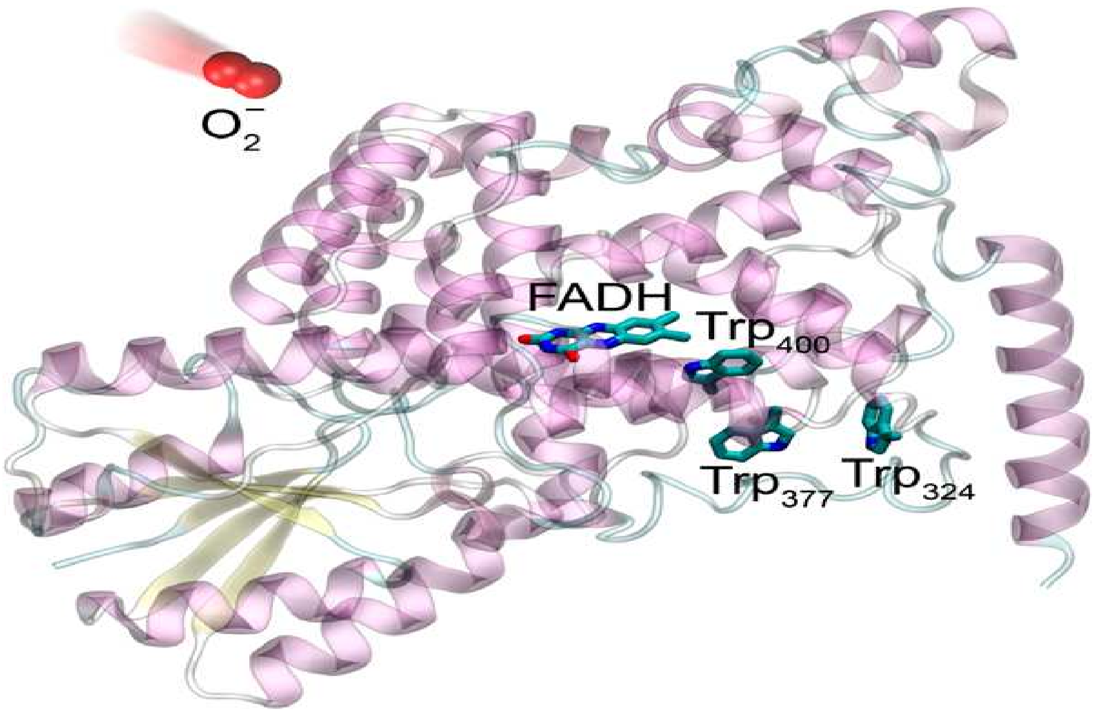


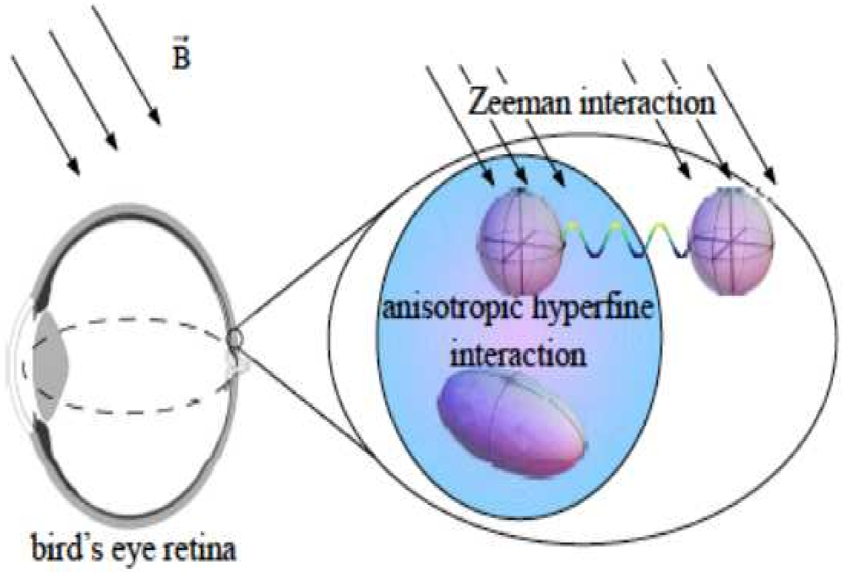
Probable photo-pigment

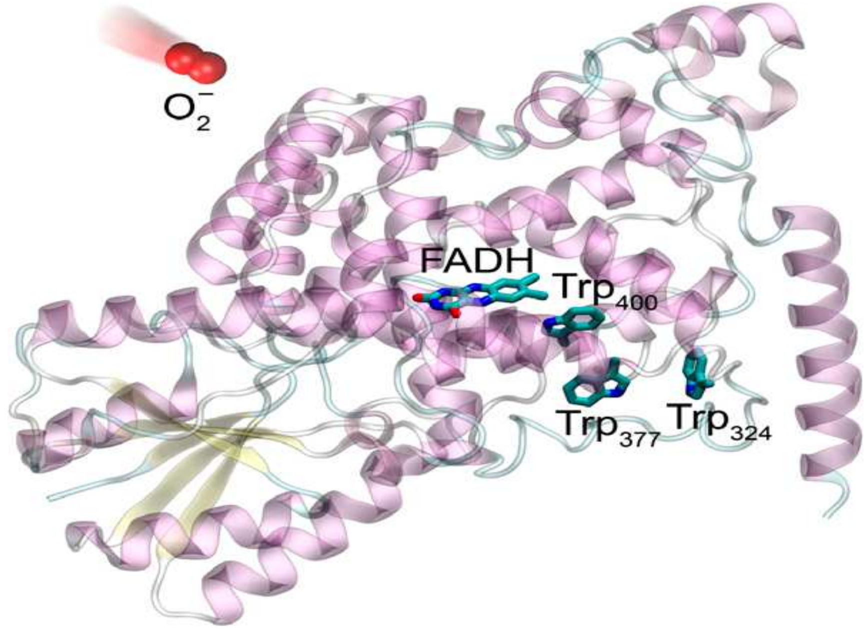


Cryptochrome

- FAD = Flavin Adenine Di-nucleotide
- FADH = Semi-reduced form of FAD
- Trp = Tryptophan

Theoretical modelling





Hamiltonian : $H_S = \widehat{I} \, . \, \overleftrightarrow{\mathbf{A}} \, . \, \widehat{S}_1 + \gamma \, [\overrightarrow{B} + \overrightarrow{B}_{RF}(t)] \, . \, (\widehat{S}_1 + \widehat{S}_2)$

where : $\widehat{S}_i \equiv \{\sigma_x^{(i)}, \, \sigma_y^{(i)}, \, \sigma_z^{(i)}\}$; $\gamma = \frac{1}{2}\mu_0 g;$

$\overleftrightarrow{\mathbf{A}} = \text{diag}\{A_x, \, A_y, \, A_z\}$ with $A_x = A_y = a = \frac{1}{2}A_z;$

$\overrightarrow{B} = B \, \{\sin\theta, 0, \cos\theta\}$ [Azimuthal symmetry]; $B = 47 \, \mu T$

$\overrightarrow{B}_{RF}(t) = B_{RF} \, \cos(\omega t) \, \{\sin\alpha, 0, \cos\alpha\}$

Theoretical modelling (contd.)

- Initial state (density matrix) : $\rho(0) = \frac{1}{2}\mathbb{1}_N \otimes |S\rangle\langle S|$
  - The nuclear spin is in completely mixed state
  - The electron pair is in pure singlet state:

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

- Dynamics (Coherent evolution + Recombination) :

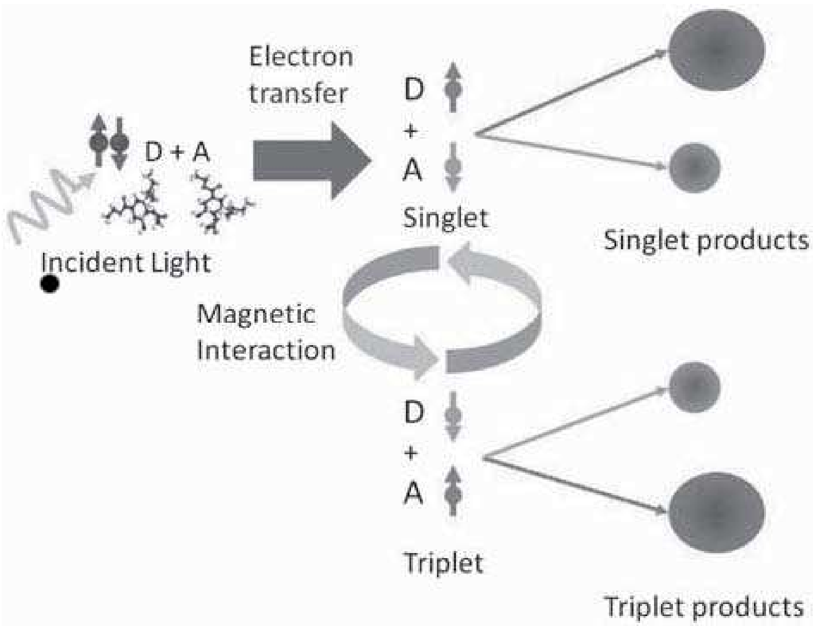
$$\frac{d\rho}{dt} = -i[H_S, \rho] - \frac{k_\mathsf{S}}{2}\left(Q_\mathsf{S}\rho + \rho Q_\mathsf{S}\right) - \frac{k_\mathsf{T}}{2}\left(Q_\mathsf{T}\rho + \rho Q_\mathsf{T}\right)$$

Singlet projection operator:

$$Q_S = |S\rangle\langle S|$$

Triplet projection operator:

$$Q_T = \mathbb{1} - Q_S$$

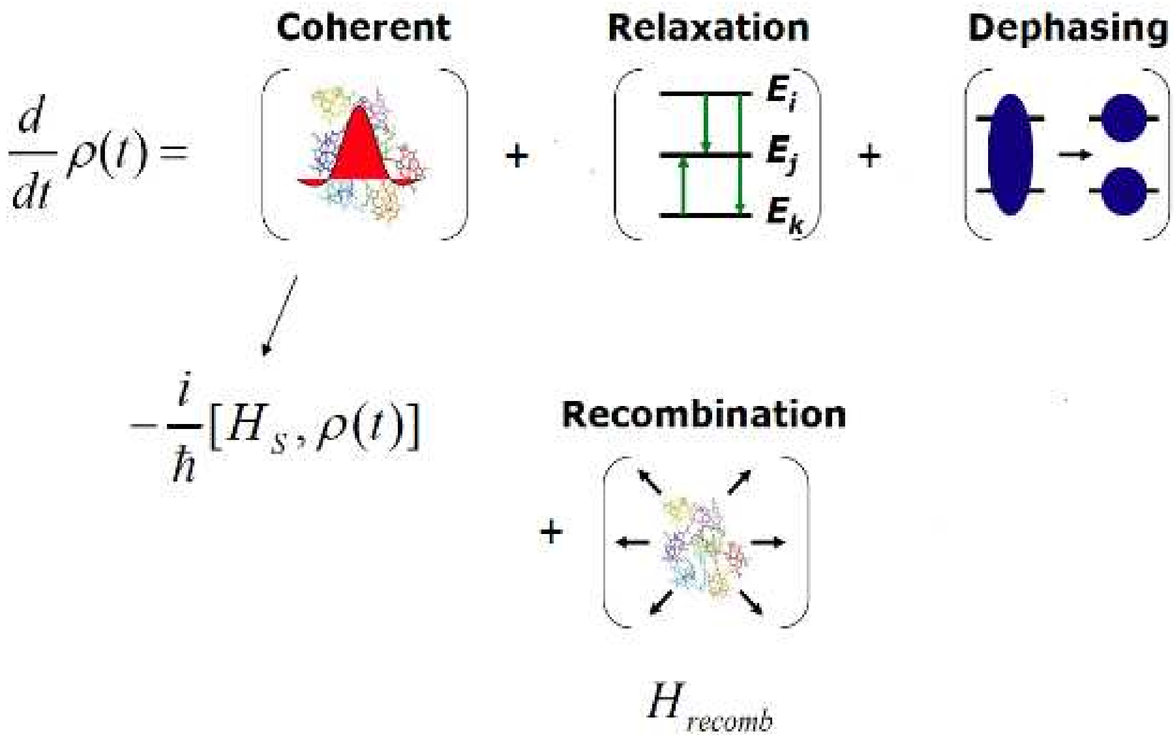


Theoretical modelling (contd.)

- Model for the effect of environment on the system:

$$\frac{d\rho}{dt} = -i[H_S,\, \rho] - \frac{k_{\mathsf{S}}}{2}\left(Q_{\mathsf{S}}\rho + \rho Q_{\mathsf{S}}\right) - \frac{k_{\mathsf{T}}}{2}\left(Q_{\mathsf{T}}\rho + \rho Q_{\mathsf{T}}\right)$$

$$+ \sum_i \Gamma_i \left[L_i \rho L_i^\dagger - \frac{1}{2}\left(L_i^\dagger L_i \rho + \rho L_i^\dagger L_i\right)\right]$$



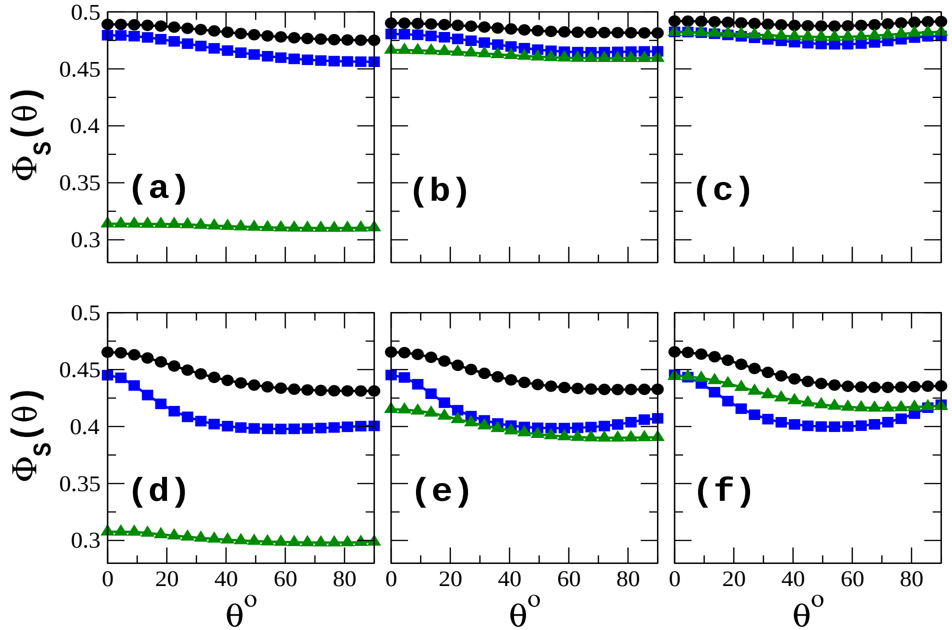
Theoretical modelling (contd.)

- Singlet product yield $[\Phi_S(\theta)]$: The amount of product decaying via the singlet channel (as a function of angle)
  - $\Phi_S(\theta) = k_S \int_0^\infty \langle S|\text{Tr}_N \rho(t)|S\rangle \, dt$

    $\text{Tr}_N =$ Partial trace over nuclear subspace
  - $\langle S|\text{Tr}_N \rho(t)|S\rangle$: probability (quantum) of the electronic state to be in singlet
  - $k_S \, dt$: probability (classical) of the RP to recombine and to produce singlet product within the time interval $[t,\, t + dt]$

Results

Define : $\bar{a} \equiv \sqrt{A_x^2 + A_y^2 + A_z^2}$; Here : $\bar{a} = \sqrt{6}a$



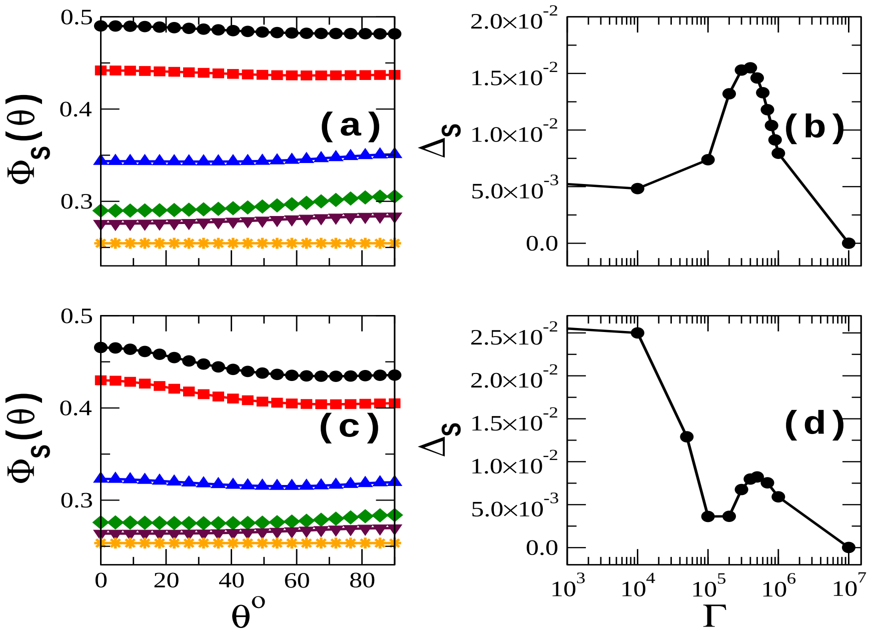
$\leftarrow \ \bar{a} = 1.0\,\mu s$

$\leftarrow \ \bar{a} = 0.5\,\mu s$

- Only geomagnetic field $B = 47\,\mu T = 0.76\,\mu s$ (●); 30% weaker magnetic field (■); Geomagnetic + RF field (▲)
- $k = 10^5$ (a); $k = 5 \times 10^5$ (b); $k = 8 \times 10^5$ (c)
- $k = 10^5$ (d); $k = 4 \times 10^5$ (e); $k = 6 \times 10^5$ (f)

Results (contd.)

- We estimate : $k \simeq 5 \times 10^5$ for $\overline{a} = 1.0\,\mu s$ case
  $k \simeq 4 \times 10^5$ for $\overline{a} = 0.5\,\mu s$ case
- Mean life time : $\tau \simeq 2.0 - 2.5\,\mu s$ $\{\times 4\}$ (Reasonable, experimentally observed in plant cryptochrome)
- Compass Sensitivity : $\Delta_S \equiv \Phi_S^{\max} - \Phi_S^{\min}$



$\leftarrow \quad \overline{a} = 1.0\,\mu s$

$\leftarrow \quad \overline{a} = 0.5\,\mu s$

- (a) & (c) : Singlet yield profile for different Γ

Conclusion

- We have incorporated results of both the behavioral tests into our model
- Our estimated mean life time of the RP is of the order of micro-seconds (reasonable)
- Estimated coherence time is also about few micro-seconds...This is also acceptable value
- Most interestingly, we have found a parameter regime where environmental influence is actually enhancing the sensitivity of avian compass....and long coherence time is not at all needed....

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