

<http://power.itp.ac.cn/~suncp/quantum.htm>





## *What is Life ?, Cambridge, 1946.*

"

"



Erwin Schrödinger  
1887-1961

DNA

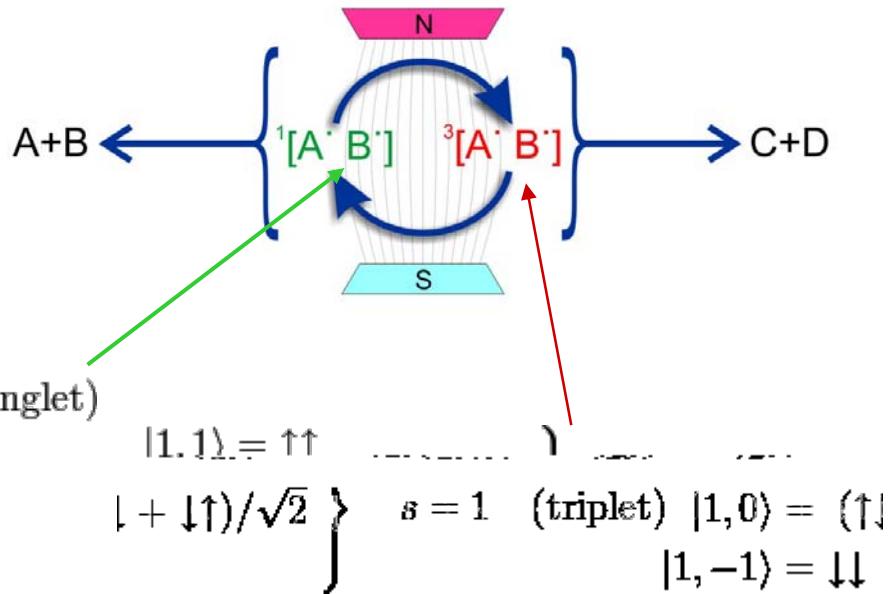
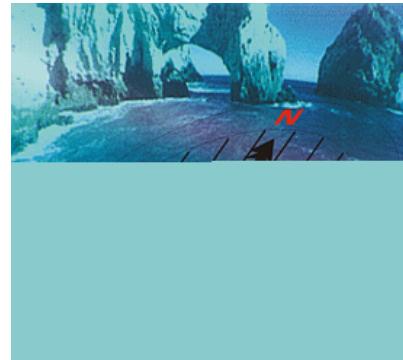
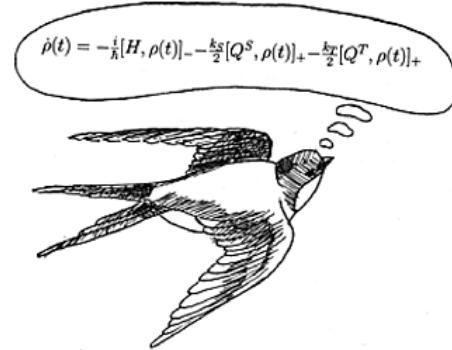


# free radical pair

Biophysical Journal Volume 78 February 2000 707–718

## A Model for Photoreceptor-Based Magnetoreception in Birds

Thorsten Ritz, Salih Adem, and Klaus Schulten



$$|0,0\rangle = (\uparrow\downarrow - \downarrow\uparrow)/\sqrt{2} \quad s = 0 \quad (\text{singlet})$$

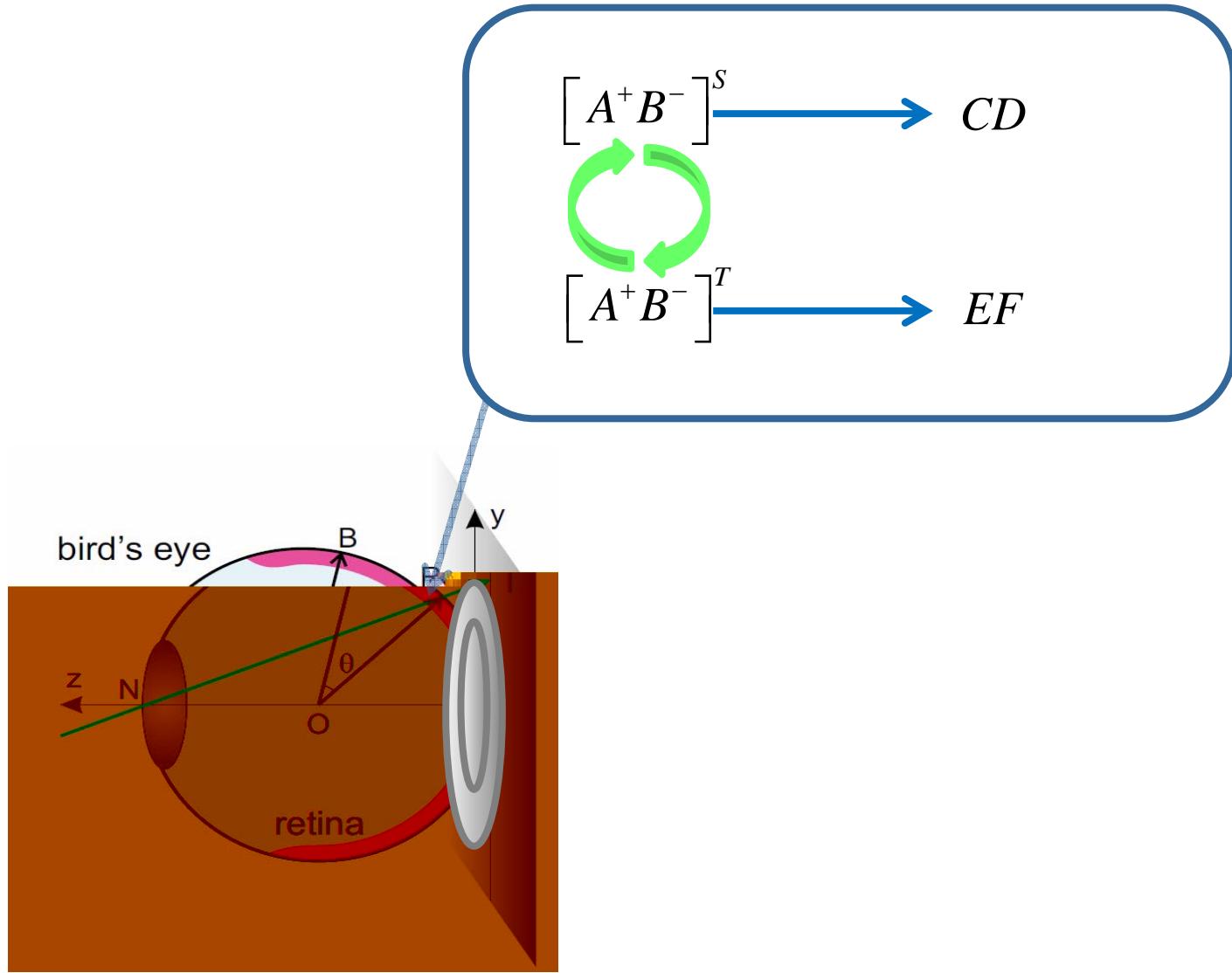
$$|1,1\rangle = \uparrow\uparrow$$

$$|\downarrow + \uparrow\uparrow\rangle/\sqrt{2}$$

$$s = 1 \quad (\text{triplet})$$

$$|1,0\rangle = (\uparrow\downarrow)$$

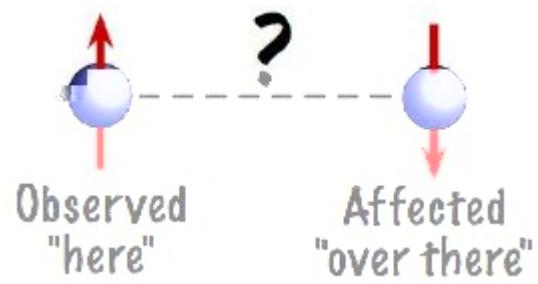
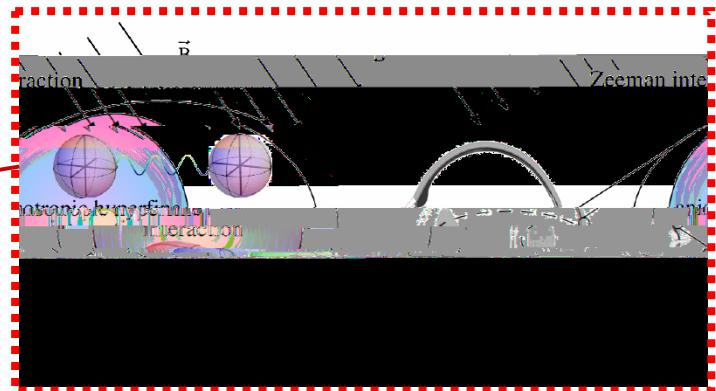
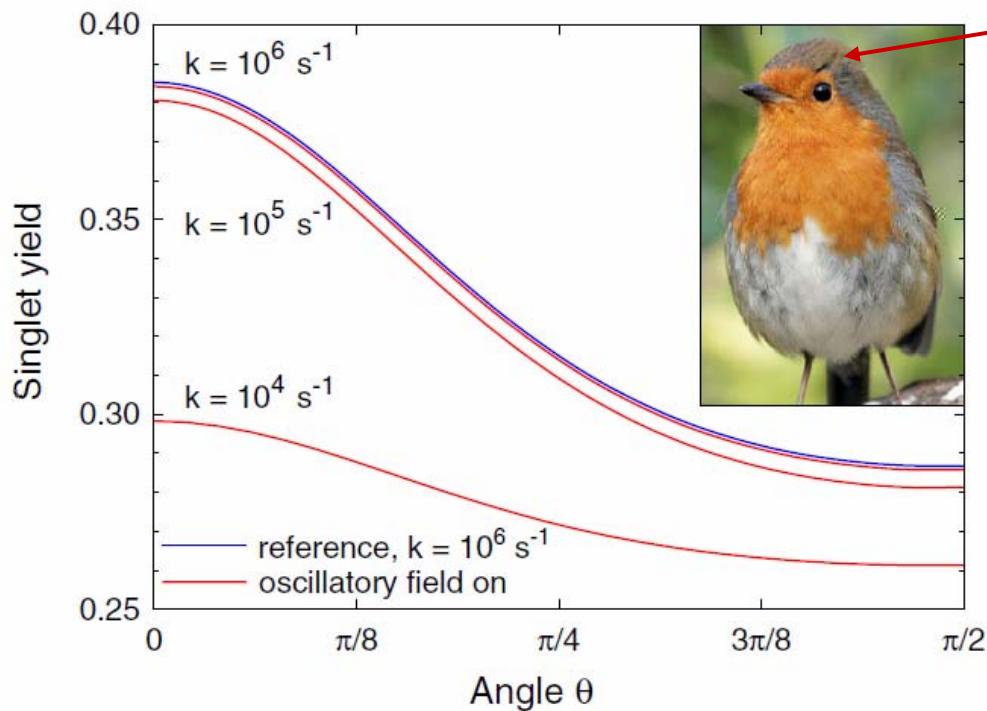
$$|1,-1\rangle = \downarrow\downarrow$$



# Chemical compass model of avian magnetoreception

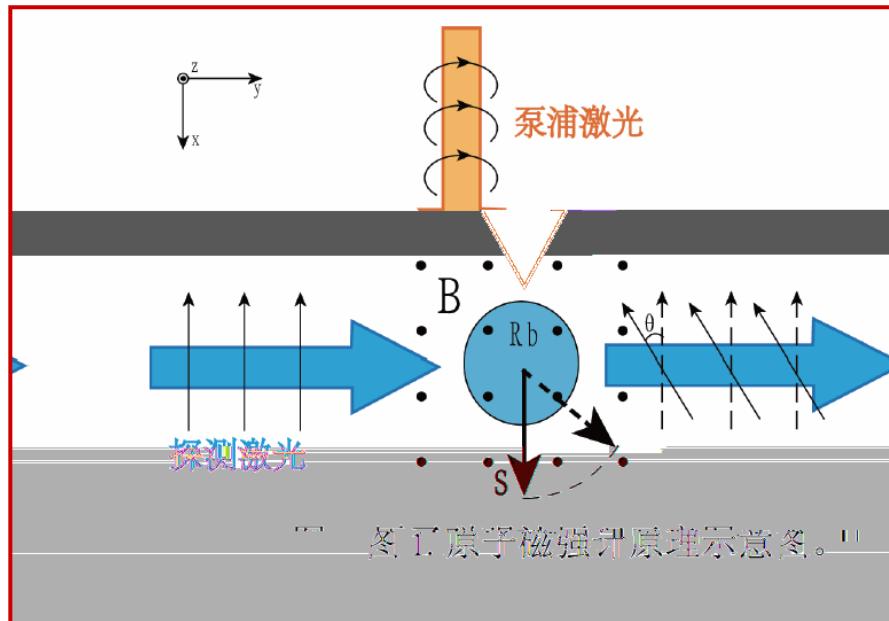
John A. D. Liddell<sup>3</sup>, Devens Gust<sup>3</sup>, Christiane R. Timmel<sup>1</sup> & P. J. Hore<sup>2</sup>                         

## Guager et al , Phys. Rev. Lett. 106, 040503 (2011)



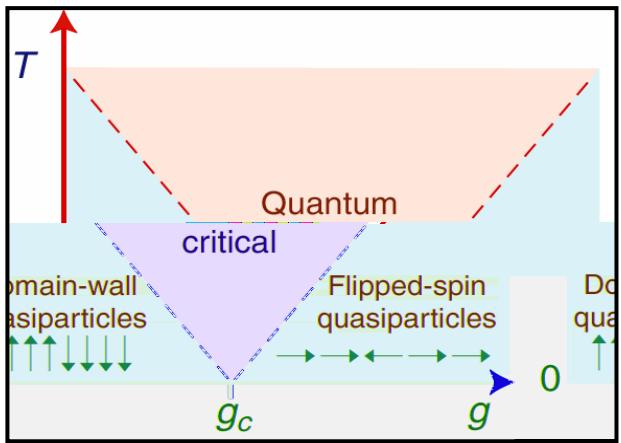
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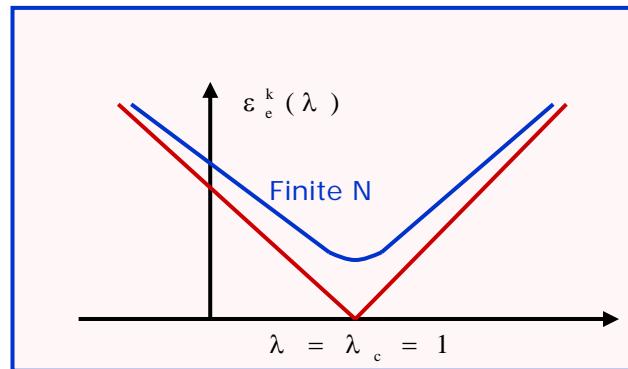


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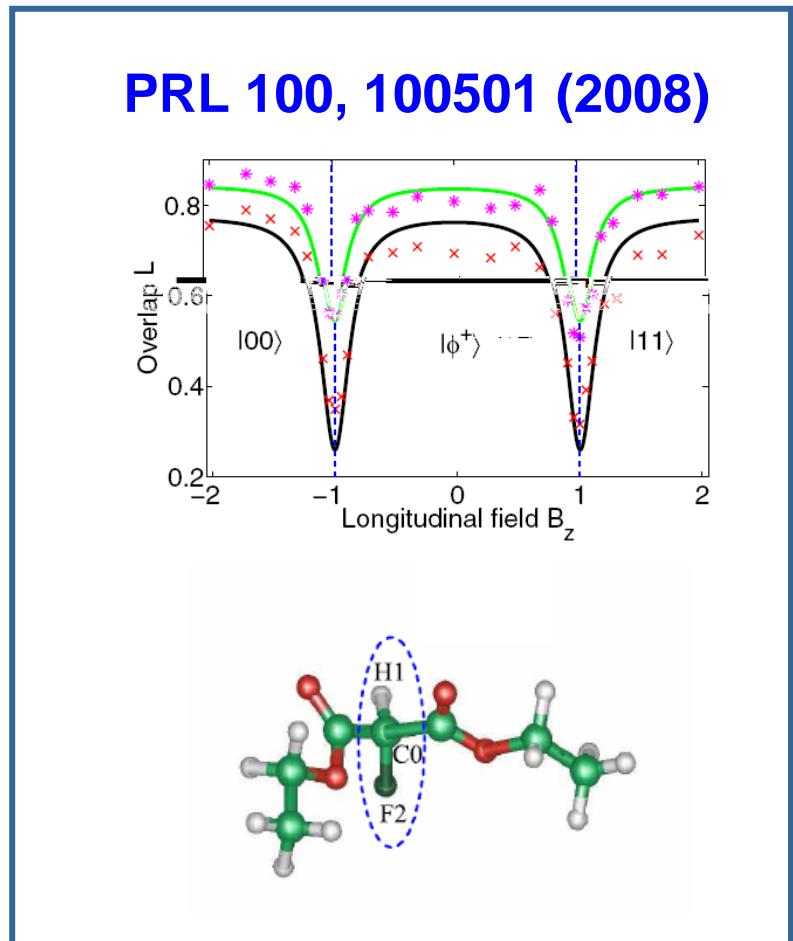
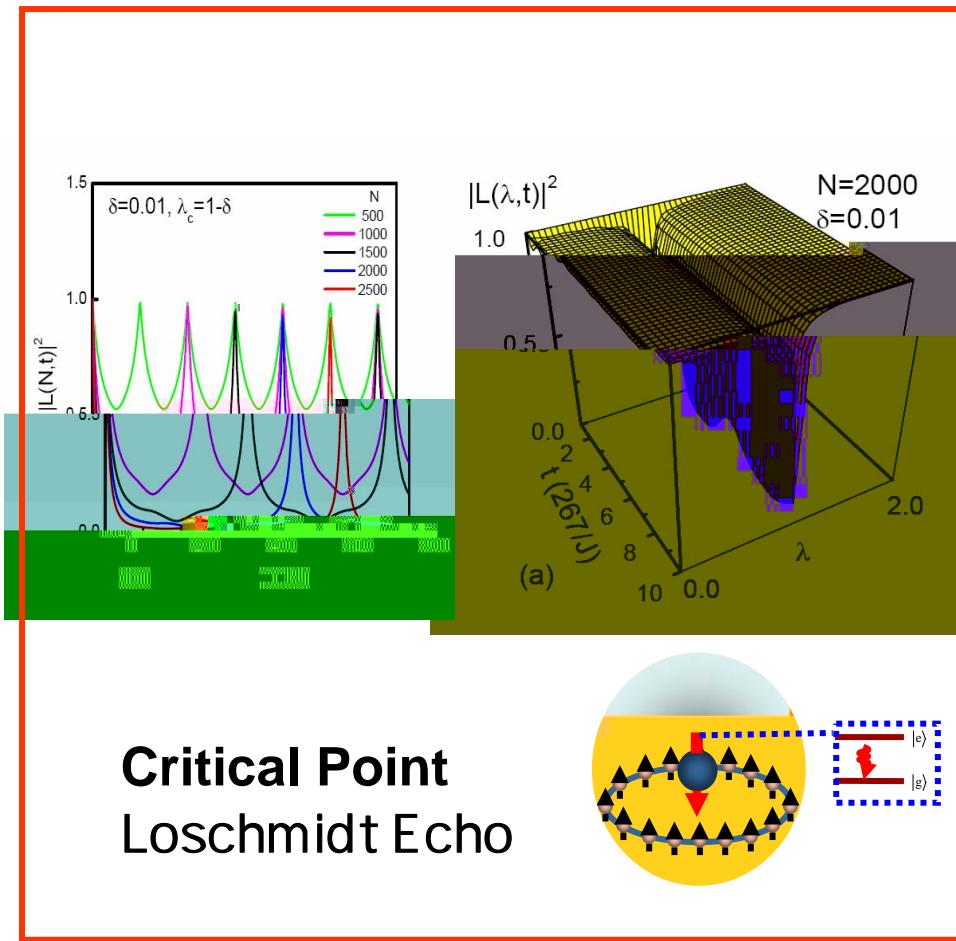


S Sachdev, (2000)  
Quantum Phase Transitions.  
Cambridge University Press



$$\varepsilon_e^k(\lambda) = 2J\sqrt{1 + \lambda^2 - 2\lambda \cos(ka)}$$

Quan, Song, Liu, Zanardi, Sun Phys. Rev. Lett. 96, 140604 (2006)



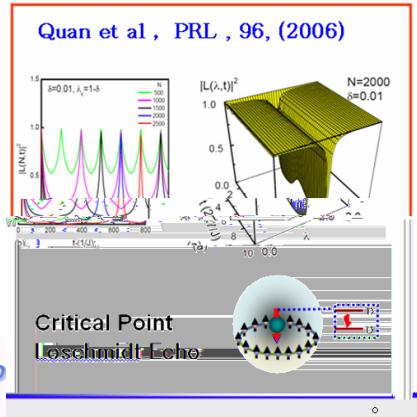
Quan et al , Phys. Rev. Lett. 96, 140604 (2006)-

[6]

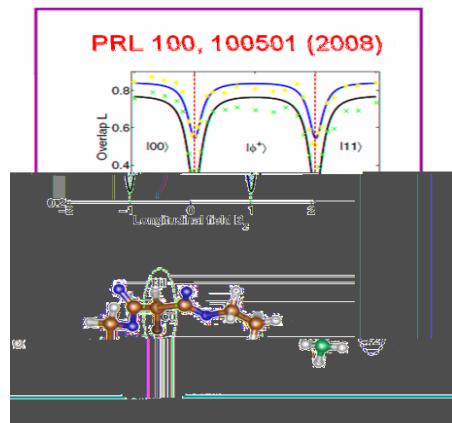
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我们的理论



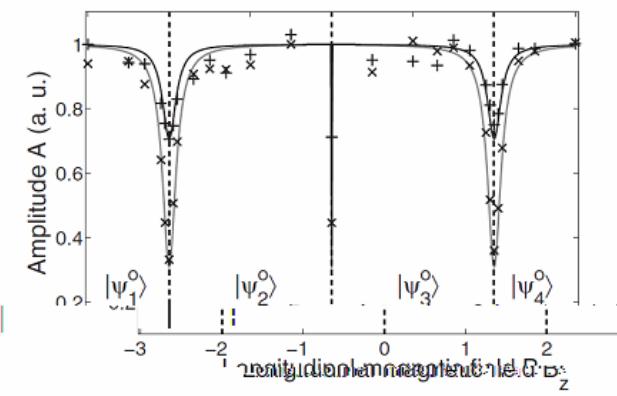
德国 Suter 小组的实验证实

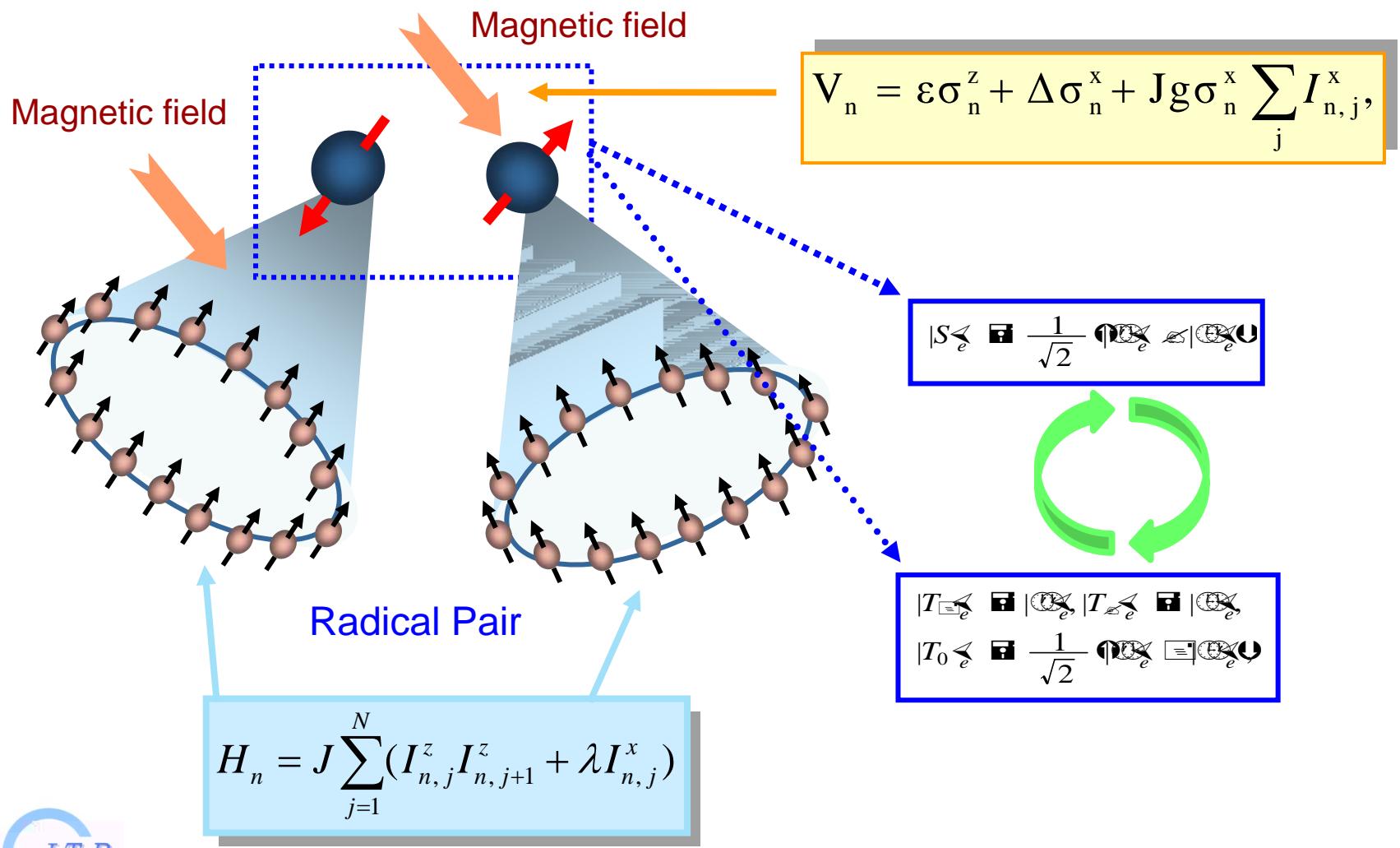


Laflamme

Phys. Rev. A 79, 012305 (2009)

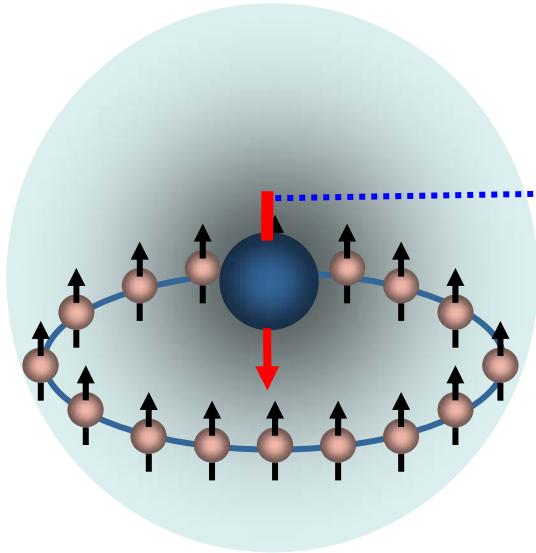
There has been a recent flurry of activity following the observation [6] that the proximity to a quantum critical point enhances the sensitivity of a system to external perturbations, as measured by quantum-information-theoretical quantities -



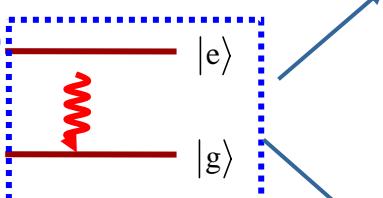


# Hepp-Col eman

$$H = H_0 + H_1 = -J \sum_j (\sigma_j^z \sigma_{j+1}^z + g \sigma_j^x + \delta |e\rangle\langle e| \sigma_j^x)$$



$$H_e = H_e(\lambda) = H_g + V_e$$



$$V_e = -J\delta \sum_j \sigma_j^x$$

$$H_g = H_0 = -J \sum_j (\sigma_j^z \sigma_{j+1}^z + g \sigma_j^x)$$

$$|\psi(0)\rangle = (c_g|g\rangle + c_e|e\rangle) \otimes |G\rangle_g \quad \rightarrow \quad |\psi(t)\rangle = c_g|g\rangle \otimes |\varphi_g(t)\rangle + c_e|e\rangle \otimes |\varphi_e(t)\rangle$$

$$\rho_s(t) = c_g c_g^* |g\rangle\langle g| + c_e c_e^* |e\rangle\langle e| + \langle \phi_e | \phi_g \rangle c_g c_e^* |g\rangle\langle e| + \langle \phi_g | \phi_e \rangle c_e c_g^* |e\rangle\langle g|$$

# Loschmidt echo

$$[\rho_s(t)]_{eg} = c_g c_e^* D(t)$$

$$D(t) = \langle \varphi_g(t) | \varphi_e(t) \rangle \quad \quad |\varphi_\alpha(t)\rangle = \exp(-iH_\alpha t) |G\rangle_g$$

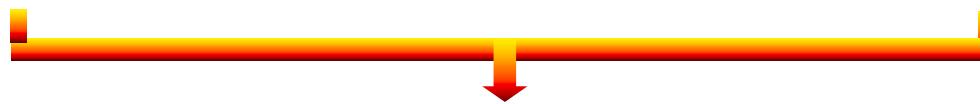
(Loschmidt echo)

$$L(\lambda, t) = \left| \langle \phi_g(t) | \phi_e(t) \rangle \right|^2 = \left| \langle G|_g \exp(iH_g t) \exp(-iH_e t) |G\rangle_g \right|^2$$

$$L(\lambda, t) = \prod_{k>0} [1 - \sin^2(2\alpha_k) \sin^2(\varepsilon_e^k t)].$$

$$\begin{aligned}
H_e &= -J \sum_j [\sigma_j^z \sigma_{j+1}^z + (g + \delta) \sigma_j^x] & H_g &= -J \sum_j (\sigma_j^z \sigma_{j+1}^z + g \sigma_j^x) \\
&= \sum_k \varepsilon_e^k (A_k^\dagger A_k - 1/2) & &= \sum_k \varepsilon_g^k (B_k^\dagger B_k - 1/2)
\end{aligned}$$

$$A_k |G\rangle_e = 0$$



$$B_{\pm k} = \cos(\alpha_k) A_{\pm k} - i \sin(\alpha_k) (A_{\mp k})^\dagger,$$

BCS-like ground state:

$$|G\rangle_g = \prod_{k>0} [i \cos(\alpha_k) + \sin(\alpha_k) A_k^\dagger A_{-k}^\dagger] |G\rangle_e$$

H. T. Quan, Z. Song, X. F. Liu, and C. P. Sun, PRL 96, 140604 (2006)

# Born-Oppenheimer

$$\begin{aligned} & |\text{electron} \text{ nucleus} \cos \frac{\gamma}{2} | \text{electron} \text{ nucleus} \sin \frac{\gamma}{2} | \\ & |\text{electron} \text{ nucleus} \sin \frac{\gamma}{2} | \text{electron} \text{ nucleus} \cos \frac{\gamma}{2} | \end{aligned}$$

$$\text{electron} \text{ nucleus} \frac{\gamma}{2} \text{tan}^{-1} \left( \frac{P}{\sqrt{E}} \right).$$

| ⟩

# Loschmidt Echo (I)

Loschmidt Echo

$$\rho_s(t) = \frac{1}{2} [ |+-\rangle\langle+-| + |--\rangle\langle--| - D(t)|+-\rangle\langle-+| - D^*(t)|-+\rangle\langle+-| ]$$

*Loschmidt Echo*

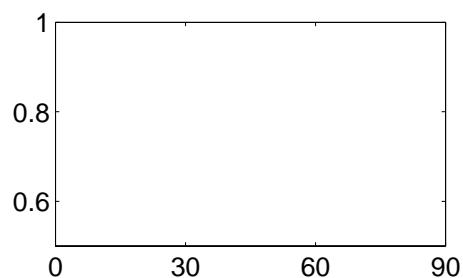
$$Lose-Dose \equiv \text{tr} |U^\dagger \rho U|^2$$

$$\rho_S(t) \equiv \frac{1}{0} r_c(t) \rho_S(0),$$

$$f_S(t) \equiv \text{tr} \rho_S(t)$$

$$r_c(t) \equiv k_S \exp(\Omega_S t)$$

$$\Lambda(\theta) = \frac{\partial \Phi_S}{\partial \theta}.$$

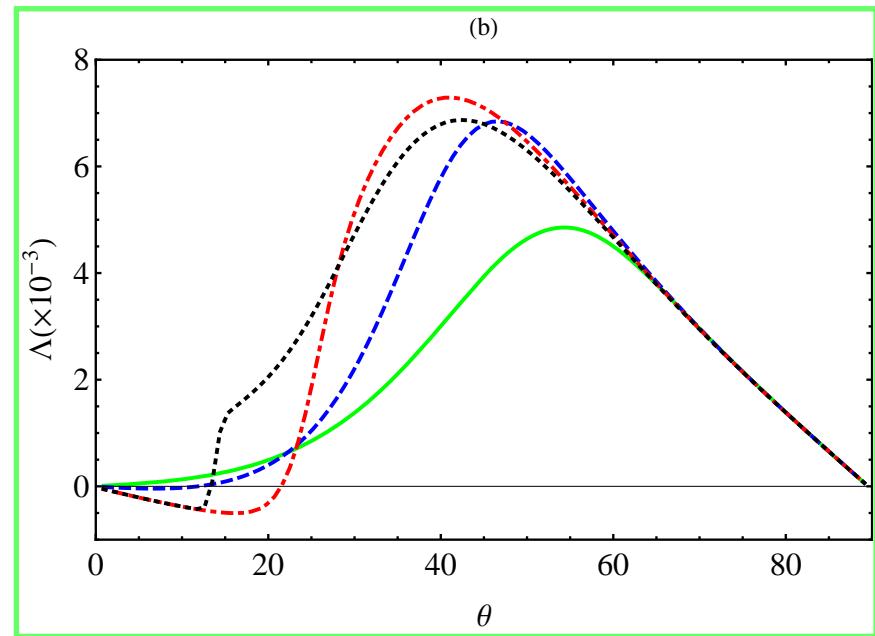
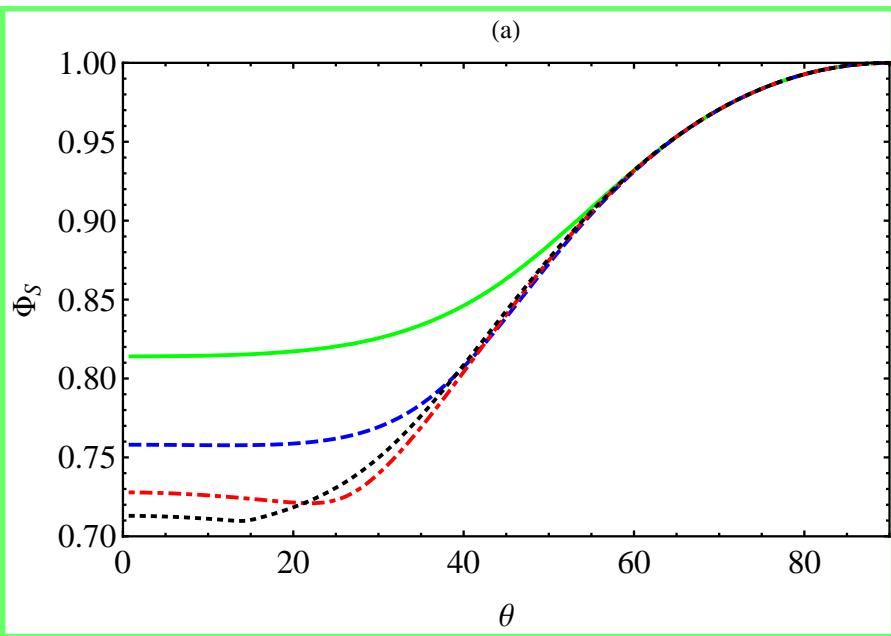


# Loschmidt Echo ( )

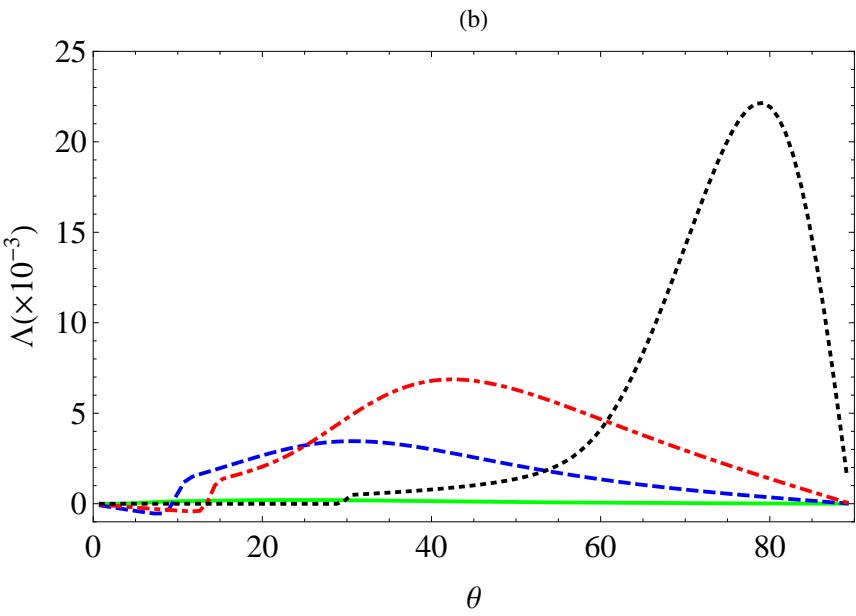
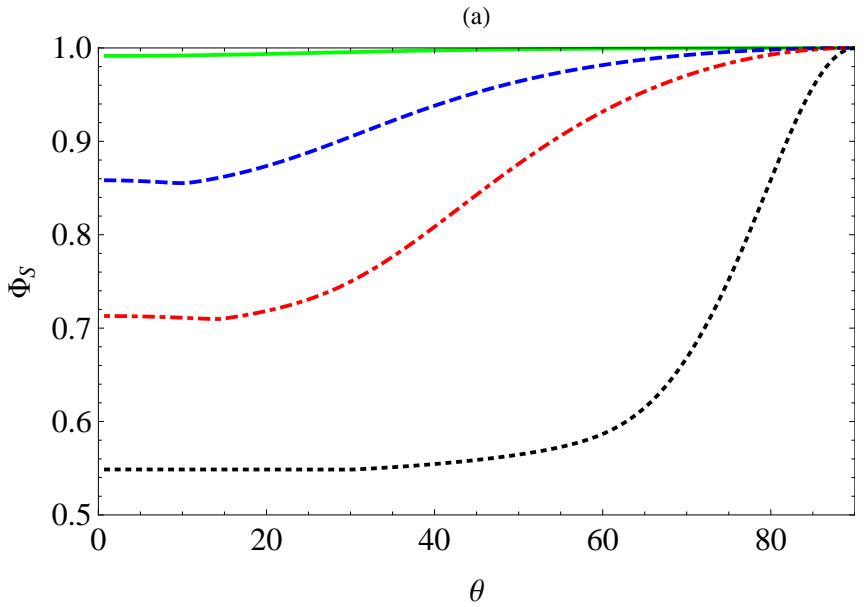
$$\star_S \quad \square \quad \frac{1}{2} \quad \equiv \frac{1}{2} k_S \quad \bigotimes_0^{\odot} L(t) e^{-k_S t} dt$$

$$f_S(t) \quad \square \quad \frac{1}{2} \leftarrow \equiv L(t) \rightarrow$$

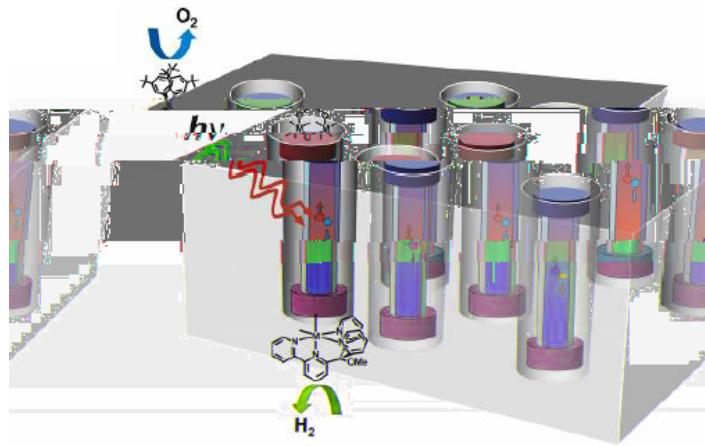
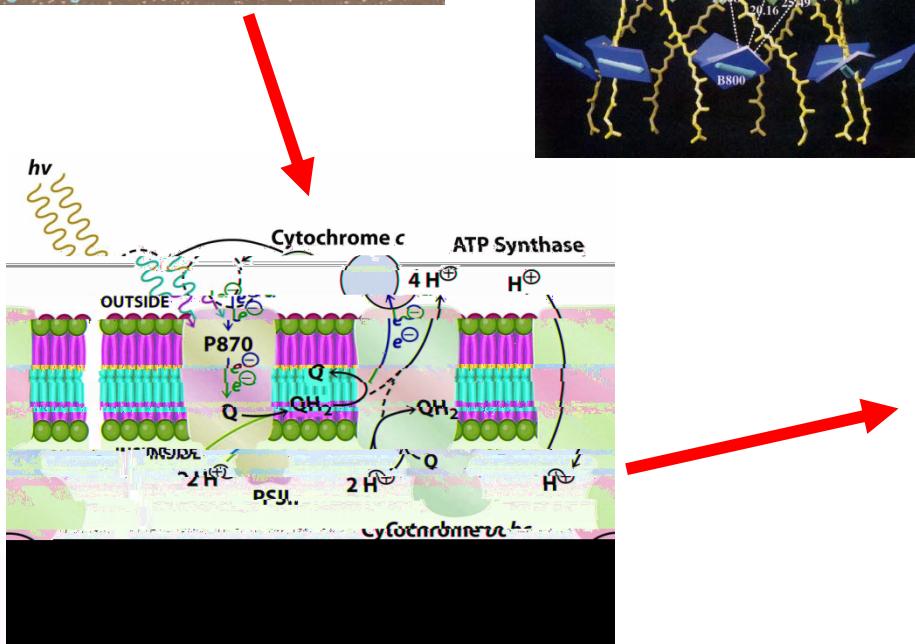
$$L(t) = \prod_{k>0} \frac{A_k^2 + B_k^2}{\left[ 1 + \cosh(\beta \varepsilon_k^-) \right]^2},$$
$$A_k = \left[ \cos^2 \alpha_k \cos(\varepsilon_k^+ - \varepsilon_k^-)t + \sin^2 \alpha_k \cos(\varepsilon_k^+ + \varepsilon_k^-)t \right] \cosh(\beta \varepsilon_k^-) + 1,$$
$$B_k = \left[ \cos^2 \alpha_k \sin(\varepsilon_k^+ - \varepsilon_k^-)t - \sin^2 \alpha_k \sin(\varepsilon_k^+ + \varepsilon_k^-)t \right] \sinh(\beta \varepsilon_k^-),$$
$$\alpha_k = \frac{1}{2} (\theta_k^- - \theta_k^+), \quad \theta_k^\pm = \tan^{-1} (\Delta_k / \eta_k^\pm),$$
$$\varepsilon_k^\pm = \sqrt{(\eta_k^\pm)^2 + \Delta_k^2}, \quad \eta_k^\pm = \eta_k (\lambda_\pm(\theta)).$$



**$N = 11$**   
 **$N = 21$**   
 **$N = 101$**   
 **$N = 1001$**

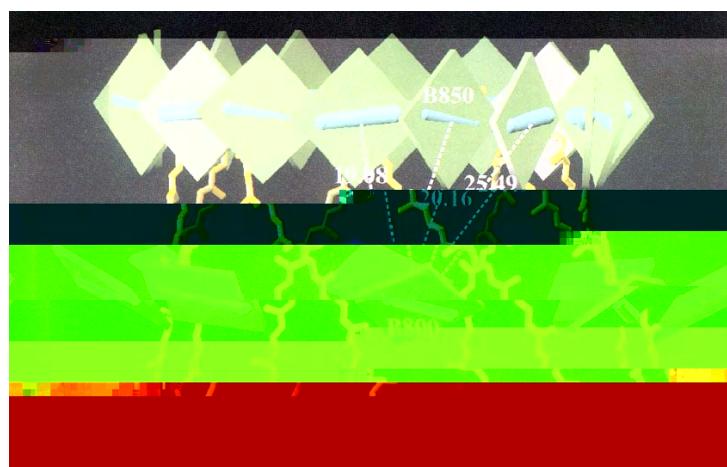
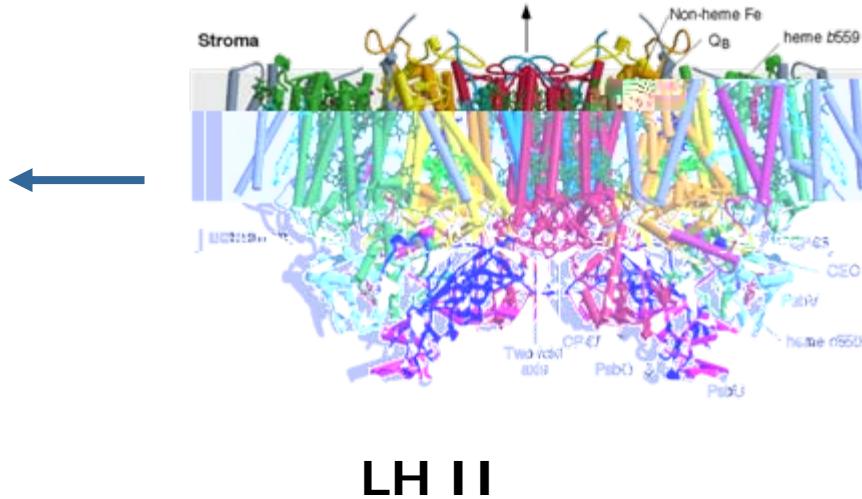
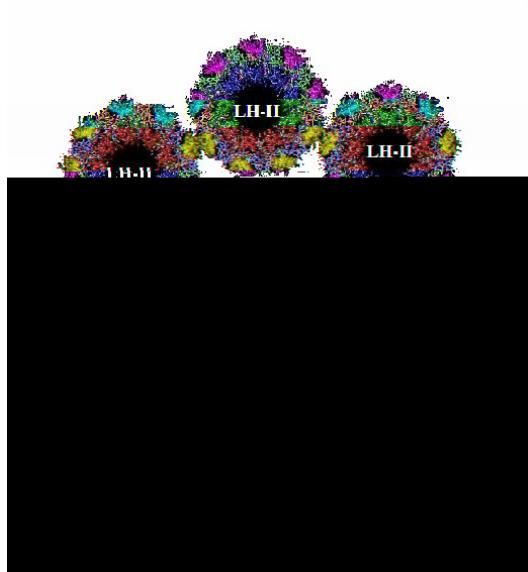


$g_0 = 0.1$   
 $g_0 = 0.5$   
 $g_0 = 1$   
 $g_0 = 5$

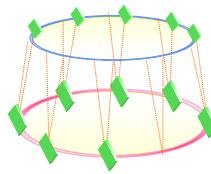


2009

# LH II      LH I

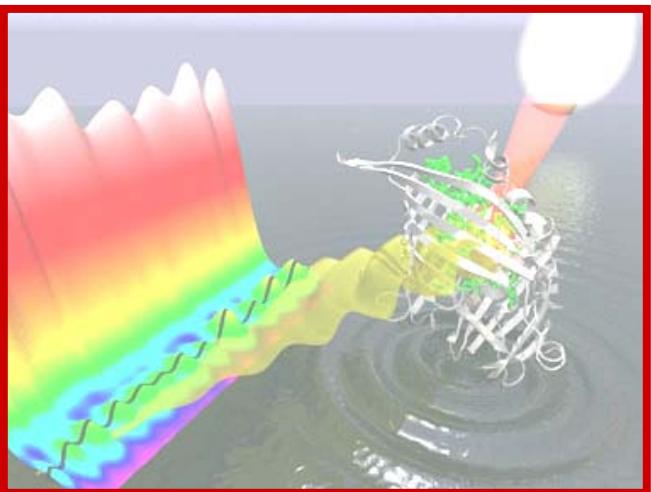


**purple bacteria  
(photosystem II)**



## Coherence Dynamics in Photosynthesis: Protein Protection of Excitonic Coherence

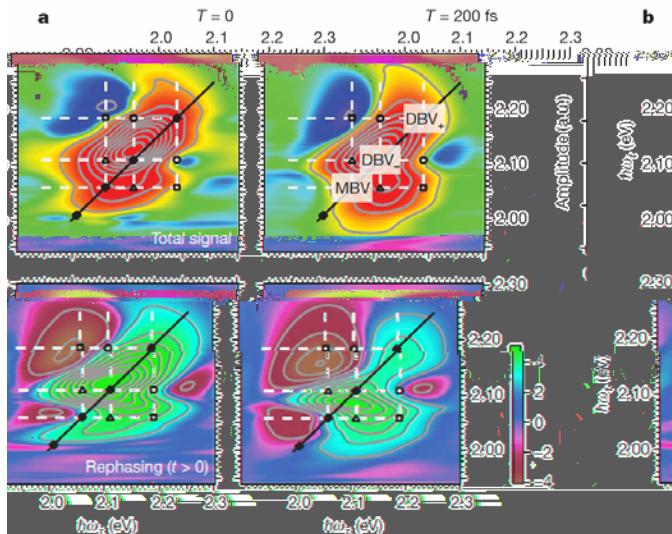
Science 8 June 2007: Vol. 316. no. 5830, pp. 1462



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# Coherently wired light-harvesting in photosynthetic marine algae at ambient temperature

NATURE | Vol 463 | 644 | 2010



(marine cryptophyte algae)  
(  
(two dimensional photon echo  
spectroscopy),

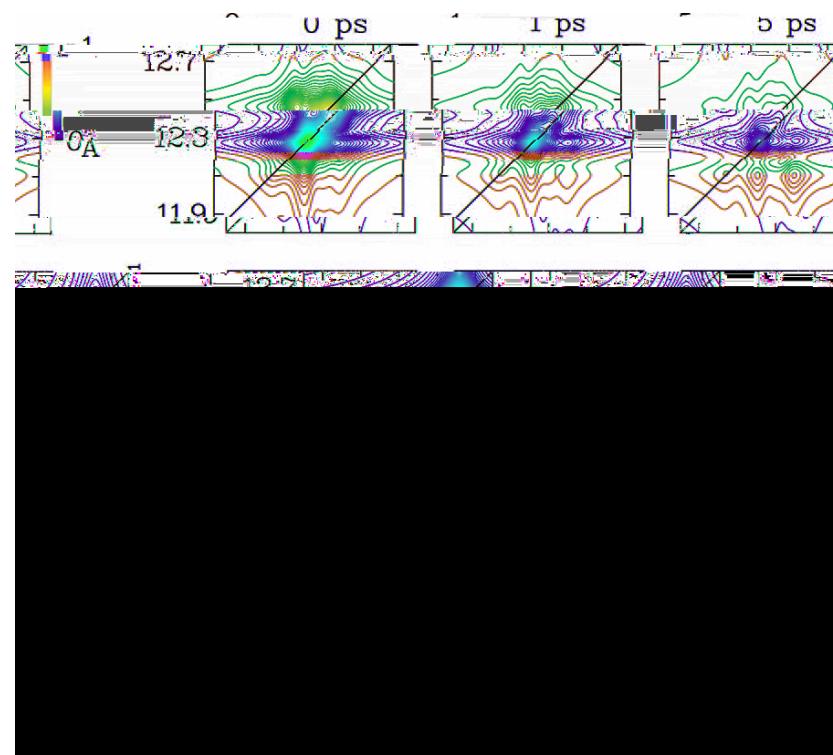
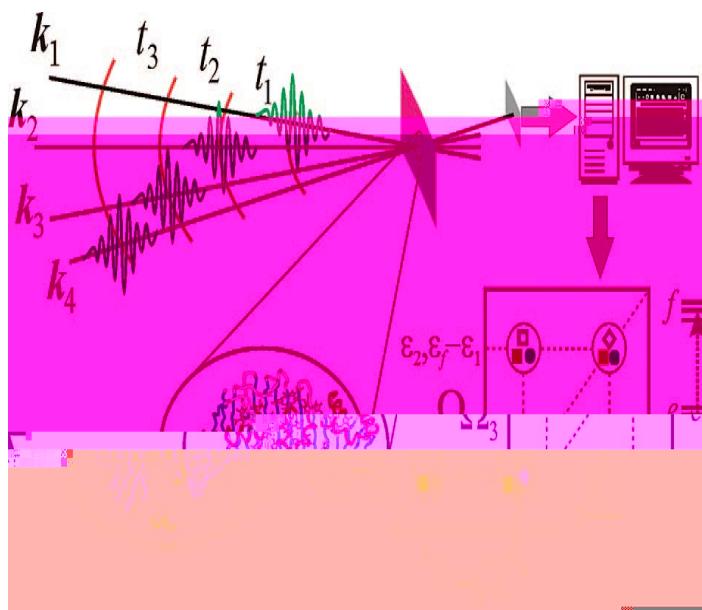
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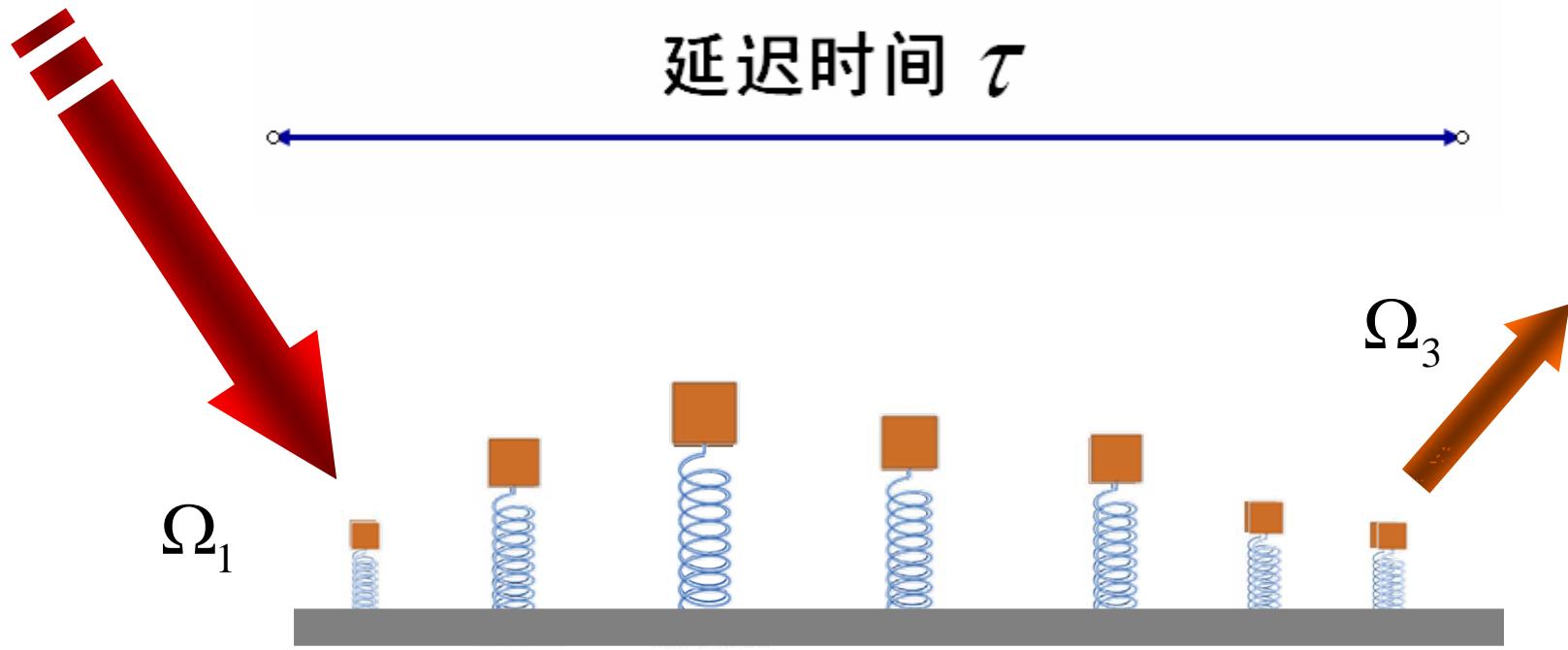
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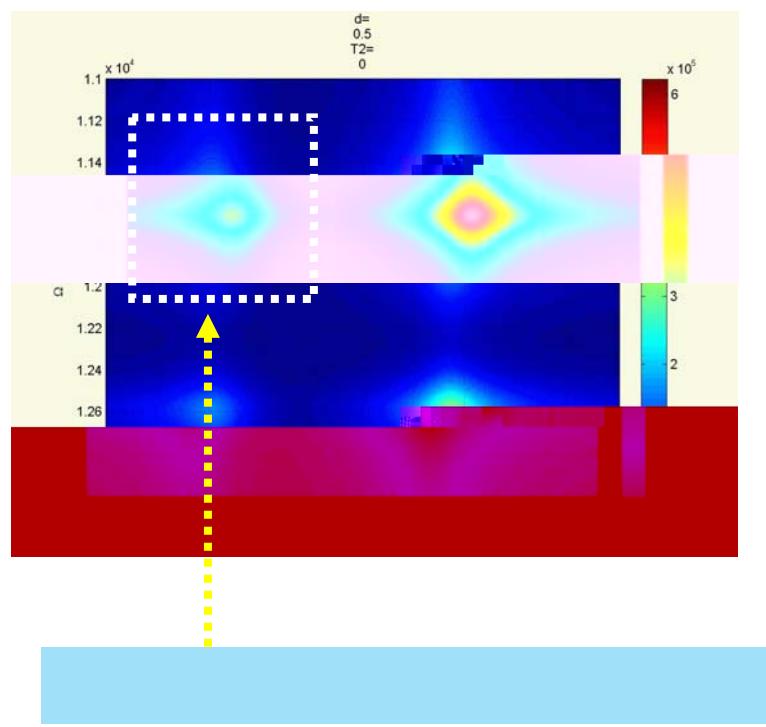
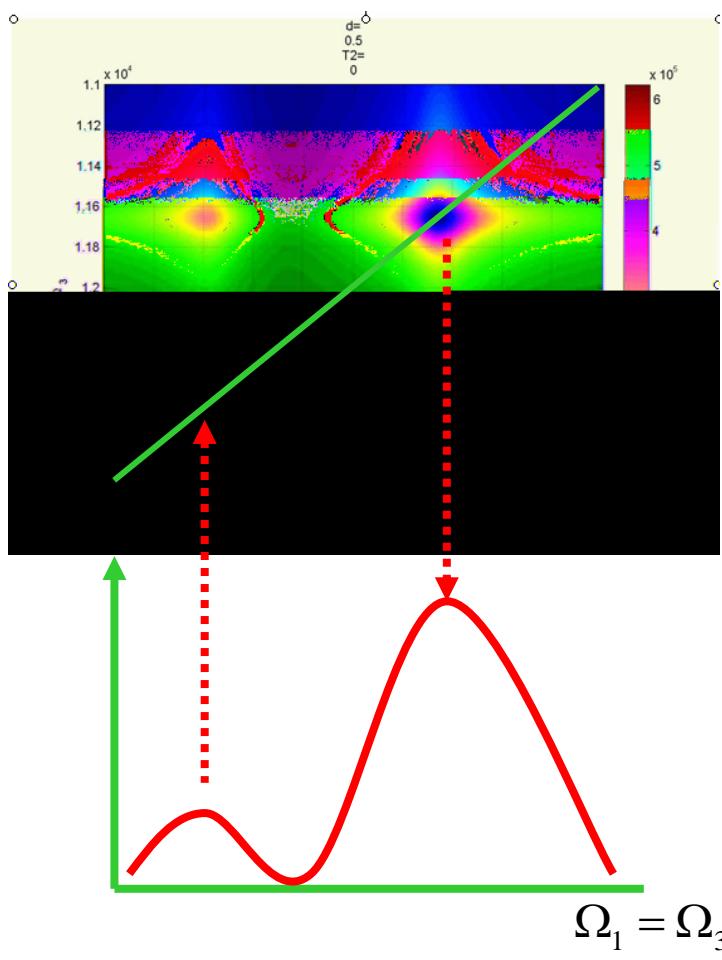
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Fleming et. al, 2007

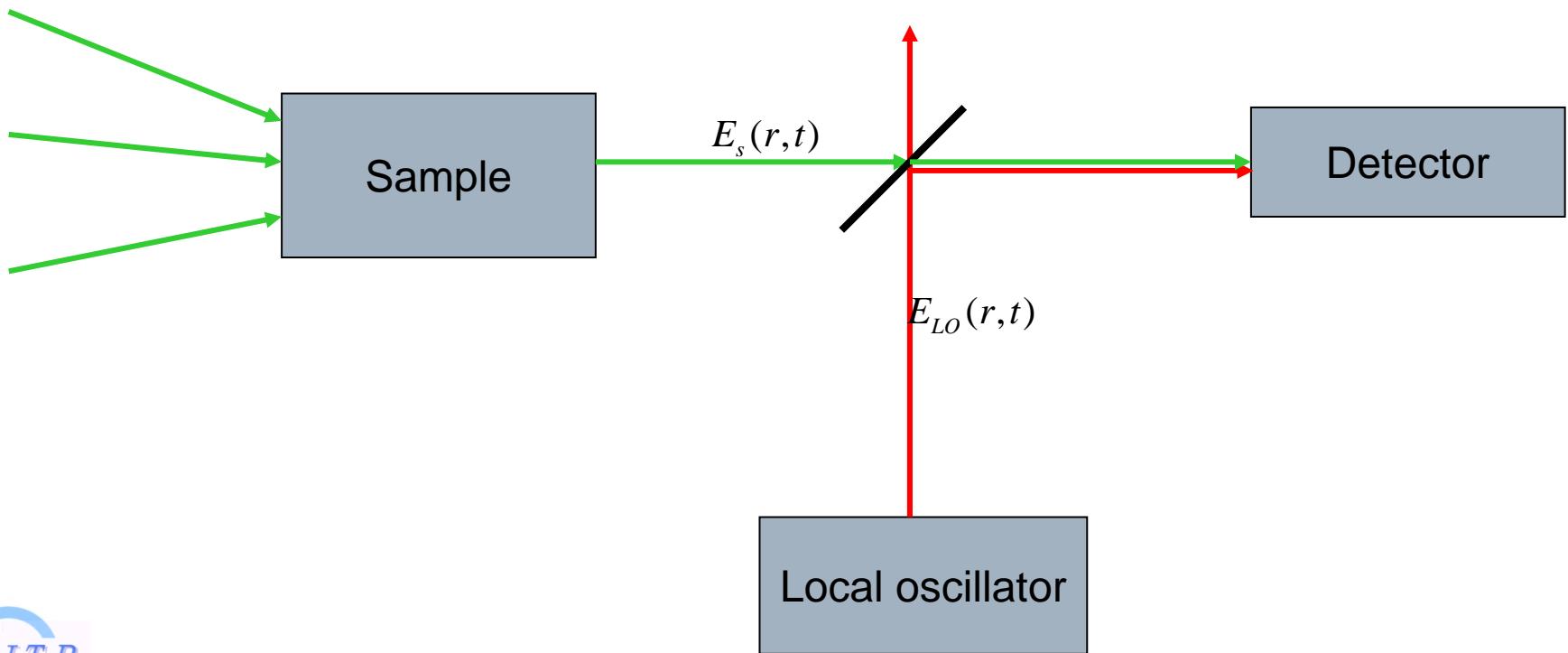


$$I_{k_s}(\Omega_3, \tau, \Omega_1)$$



# Heterodyne detected signal

- Experimental setup for heterodyne detection



# Dimerization-assisted energy transport in light-harvesting complexes

21 JUNE 2010

VOLUME 132 NUMBER 23

## THE JOURNAL OF CHEMICAL PHYSICS



AIP

THE JOURNAL OF CHEMICAL PHYSICS 132, 234501 (2010)

### Dimerization-assisted energy transport in light-harvesting complexes

S. Yang,<sup>1</sup> D. Z. Xu,<sup>1</sup> Z. Song,<sup>2</sup> and C. P. Sun<sup>1(a)</sup>

<sup>1</sup>Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, China

<sup>2</sup>School of Biological Sciences, Tsinghua University, Beijing 100084, China

20 February 2010; accepted 5 May 2010; published online 15 June 2010

(Received

The role of the dimer structure of light-harvesting complex II (LH2) in excitation transfer H2 [without a reaction center (RC)] to the LH1 (surrounding the RC) or from the LH2 LH2. The excited and unexcited states of a bacteriochlorophyll (BChl) are modeled by a In the framework of quantum open system theory, we represent the excitation transfer as a kage of the LH2 system and then calculate the transfer efficiency and average transfer time with various quantum superposition properties. We study how the dimerization of the B850 BChl ring can enhance the transfer efficiency and shorten the average transfer time. © 2010 American Institute of Physics. [doi:10.1063/1.3435213]

#### INTRODUCTION

To face the present and forthcoming global energy crisis, much research has been done on energy sources. Recently the investigations on the basic energy science for photosynthesis have received great attention and experienced impressive progress based on the fundamental physics.<sup>1–2</sup> In synthetic process, the structural elegance and chemical efficiency of the natural system based on pigment molecule in transferring the energy of sunlight have stimulated those driven investigation,<sup>3–13</sup> finding artificial analogs phyrin-based chromophores. These artificial systems imitate the natural process of photosynthesis<sup>3</sup> so that the higher efficiencies could be gained than that obtained conventional solid systems.<sup>4</sup> It is because one of the attractive features of photosynthesis is that the light can be captured and transferred to the reaction center within about 100 fs and with more than 95% efficiency.<sup>4,14</sup> In most of the plants and bacteria, the joint processes of photosynthesis are almost simultaneous.<sup>15–18</sup> Light harvested by antenna proteins can many chromophores, their electronic excitations stored in the RC sequentially, where photoinduced electron flow gives rise to convert the excitation energy into energy. Most recent experiments have been able to determine the time scales of various transfer property the ultrafast laser technology.<sup>16–18</sup> These great

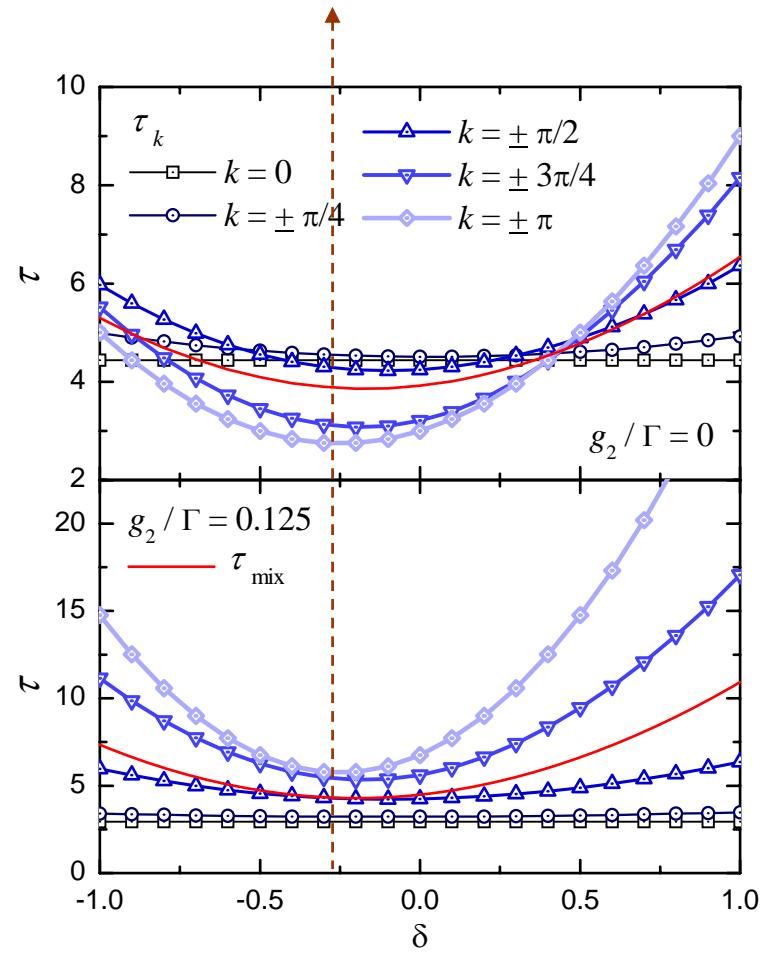
its induced decoherence could affect on the efficiency of the primary photosynthetic event. The present paper will similarly study the influences of spatial structure on the primary processes of photosynthesis for the light-harvesting complexes.<sup>19,20,21,22</sup>

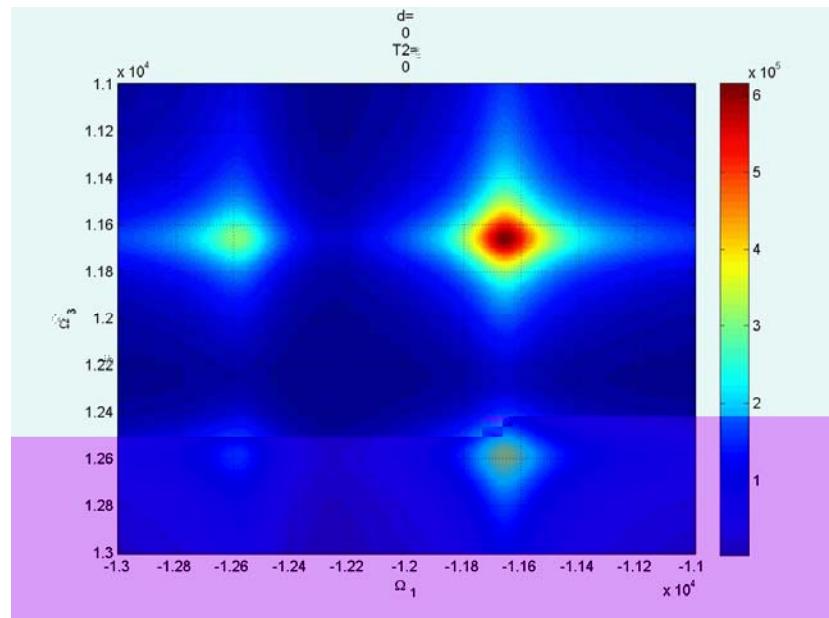
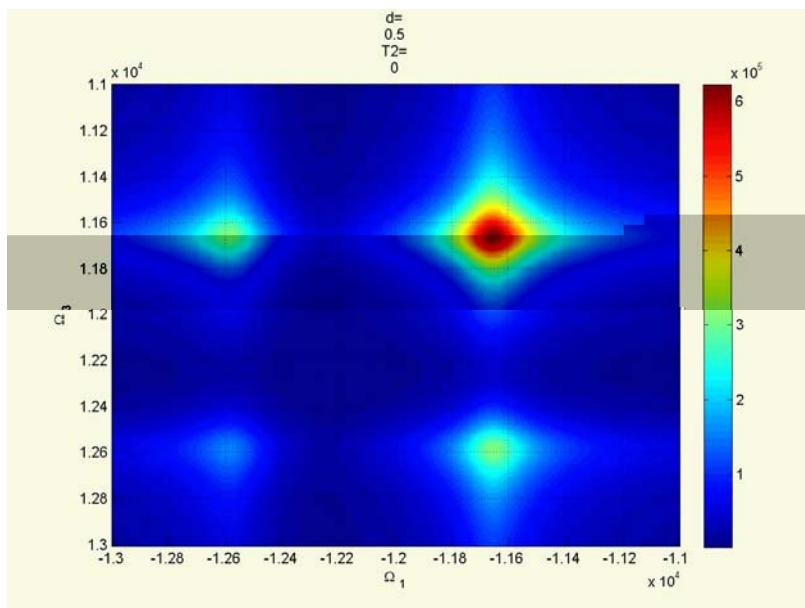
In the past, by making use of the x-ray crystallographic techniques, the structure of light-harvesting system has been elucidated.<sup>3,19</sup> In the purple photosynthetic bacteria, there exist roughly two types of light-harvesting complexes, referred to as light-harvesting complex I (LH1) and LH2. In LH1, the RC is surrounded by a B875 bacteriochlorophyll (BChl) ring with maximum absorption peak at 875 nm. The LH2 complex, however, does not contain the RC but can transfer energy excitation to the RC indirectly through LH1. In the purple bacteria, LH2 is a ring-shaped aggregate built up by eight (or nine) minimal units, where each unit consists of an  $\alpha\beta$ -heterodimer, three BChls, and one carotenoid. The

recently reported structure of LH2, while the BChls are embedded in the methylidene bridge, the carotenoids are located in the periphery of the ring. The top ring, including 16-β,16'-β-methylene camphorane (B850), has the lowest-energy absorption maximum at 850 nm. The bottom ring, with eight BChls, is called B850' because it mainly absorbs light at 850 nm. In every minimal unit, the carotenoid connects B850 BChl with one of the two B850' BChls. Excitation is transferred from one pigment to the neighbor one through the Förster mechanism,<sup>23</sup> while the electron is spatially transferred via the Marcus mechanism.<sup>20</sup> Generally, it is independent of the global geometry configuration of the system.

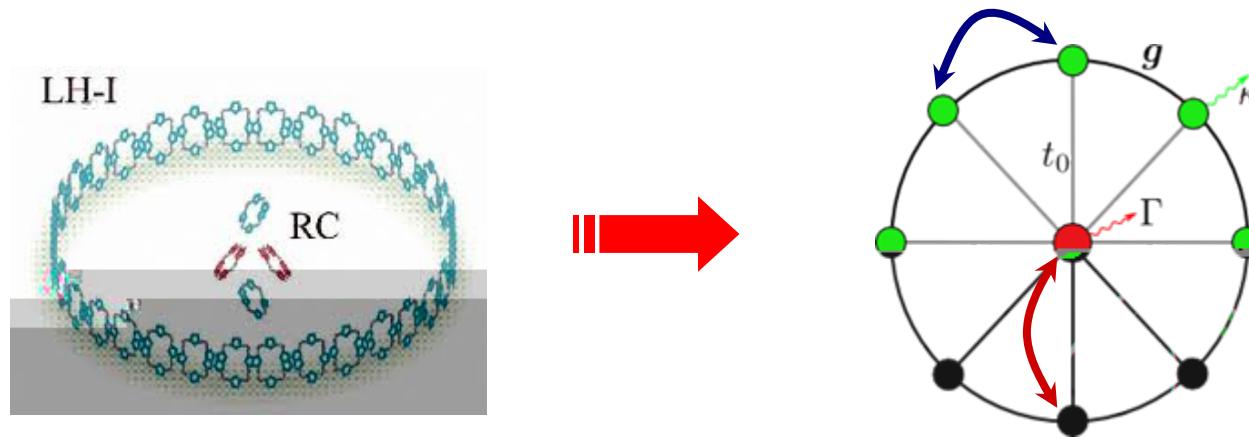
S. Yang, D. Z. Xu, Z. Song, CPS, JCP, 132, 234501 (2010)







# LH-I Model (I)



$$H_{DA} = \sum_{i=1}^N [e_i^\dagger e_i - \omega_i (e_{i+1}^\dagger + h.c.)]$$

$$+ \epsilon_A A_1^\dagger A_1 + \sum_{i=1}^N \omega_i (e_i^\dagger A_i + e_i^\dagger A_i)$$

$\Gamma$ : Usage rate of excitation

$\kappa$ : Decay rate of excitation

## LH-I Model (II)

Fourier Transf:

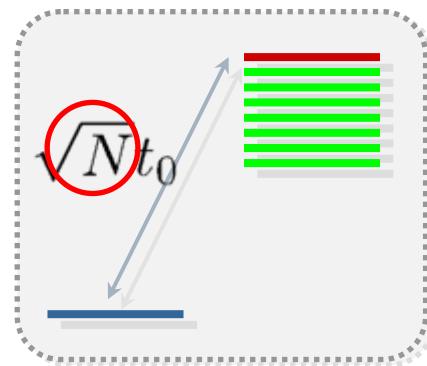
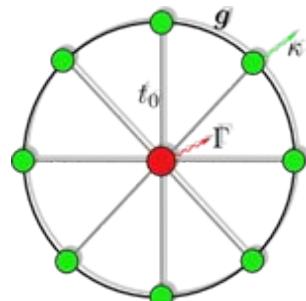
$$\sum_k e^{i k \phi} e_k e_j = \frac{i k \delta_{kj}}{\sqrt{N}}$$

=0 mode:

$$|1_{k=0}\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^N |1_i\rangle$$

Effective Hamiltonian:

$$H_{eff} = \epsilon_0 A_F (\epsilon_{eff} - 2g) (\tilde{c}_0^\dagger \tilde{c}_0 + y f c_0^\dagger c_0) + t_A \sqrt{N} t_0 (\tilde{c}_0^\dagger A^\dagger c_0 + \tilde{c}_0 A c_0)$$



# Transfer Properties

Transfer Efficiency:

$$\eta = \frac{\int_0^\infty 2\Gamma |v(t)|^2 dt}{\dots\dots\dots}$$

Population on Acceptor

Average transfer time:

$$\tau = \frac{1}{\eta} \int_0^\infty 2\Gamma t |v(t)|^2 dt$$

Average output power:

$$\mathcal{P} = \eta/\tau$$

# From Donor to Acceptor

## Initial Excitation on Donor ring

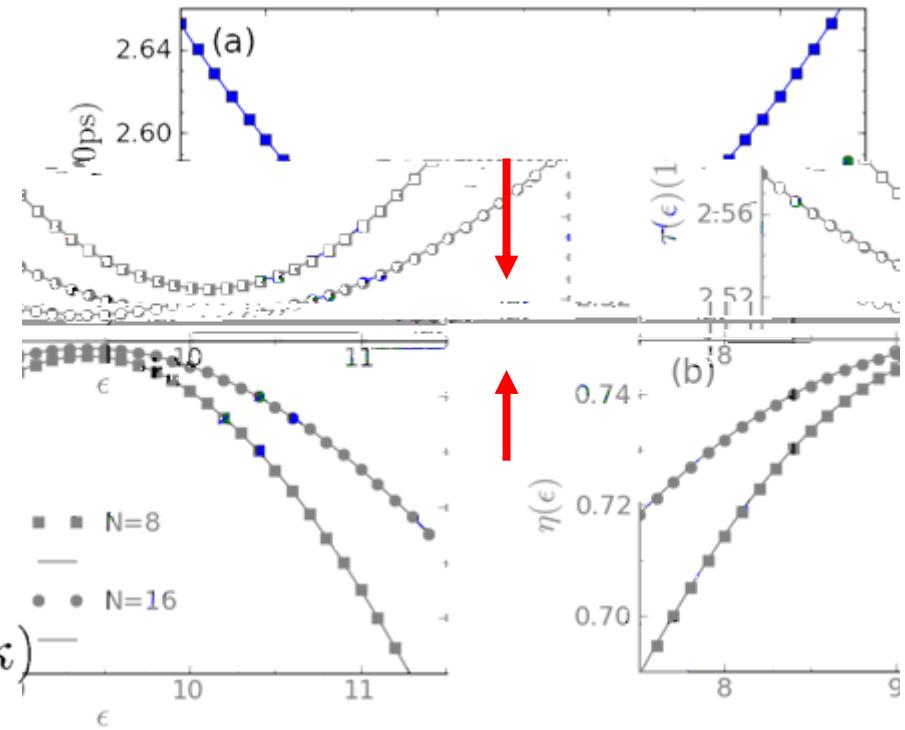
Optimal case:

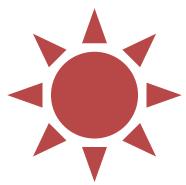
$$\epsilon + 2g = \epsilon_A$$

$\max \eta$

$\min \tau$

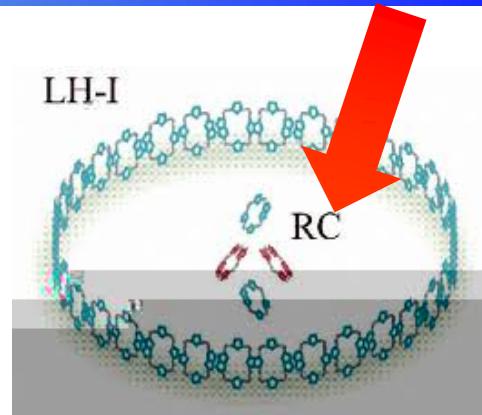
$$\eta_{\max} \leq \Gamma / (\Gamma + \kappa)$$





# There should be light...

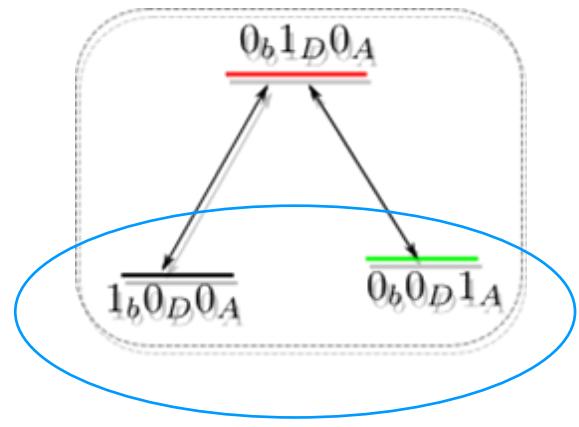
Visible light-wavelength  $\sim 500\text{nm}$   
LH-I radius  $\sim 4\text{-}6\text{nm}$



Photon-Donor interaction:

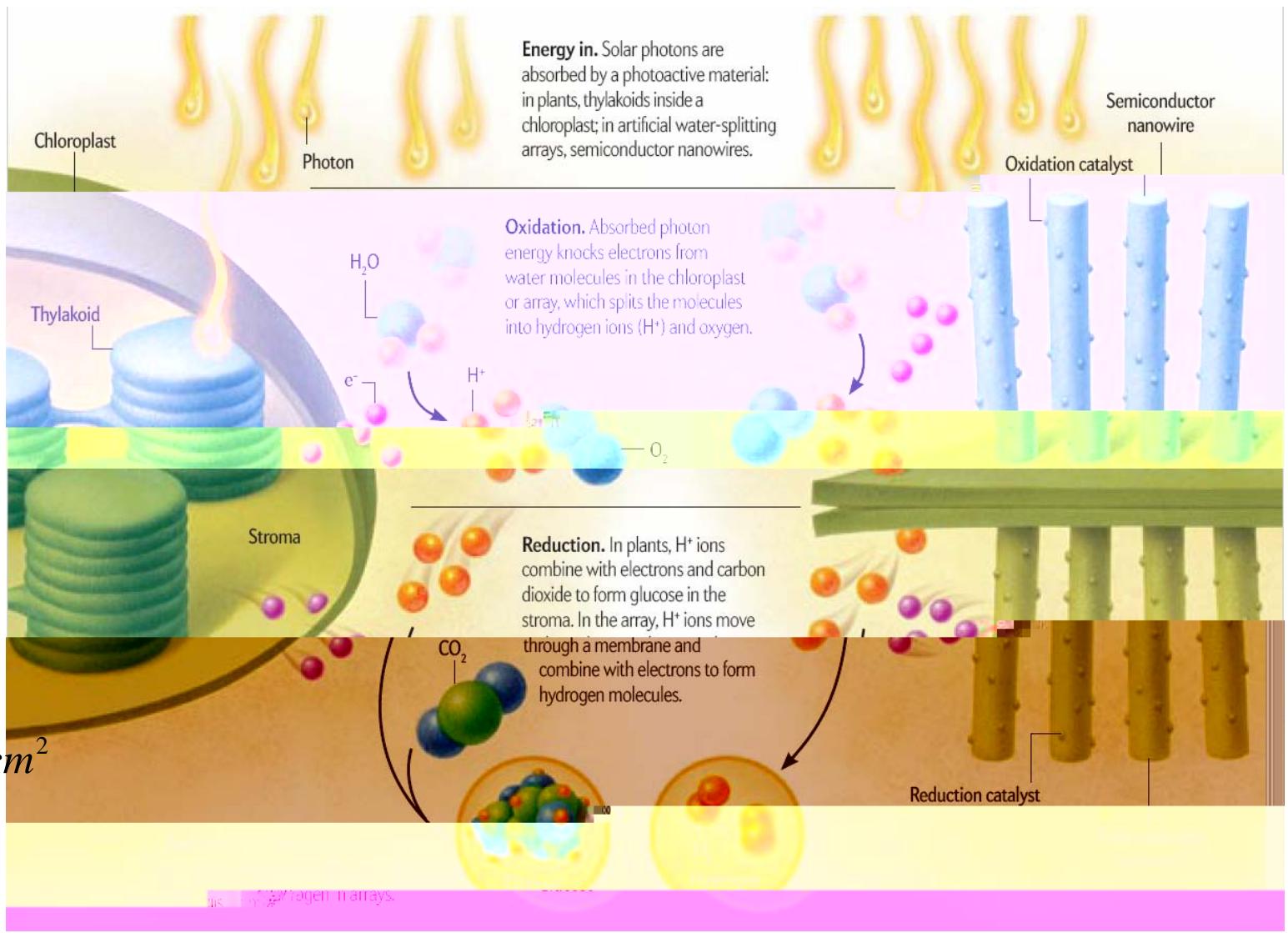
$$H_{pD} = J \sum_{i=1}^N (e_i^+ b + \text{h.c.})$$

$$\begin{aligned} H_{\text{eff}} = & \omega_0 \tilde{e}_0^\dagger \tilde{e}_0 + \omega b^\dagger b + \omega_A A^\dagger A \\ & + \sqrt{N} [(t_0 \tilde{e}_0^\dagger A + J \tilde{e}_0^\dagger b) + \text{h.c.}] \end{aligned}$$



$\overline{0_b 0_D 0_A}$

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# Grand challenges in basic energy sciences

Graham R. Fleming and Mark A. Ratner

Research focused in five related areas will allow unprecedented control over the microscopic world and could be the key to a sustainable future.

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**Thank You!**