Title: Physics in Nature Presentation: Quantum Engtanglement in Photosynthesis

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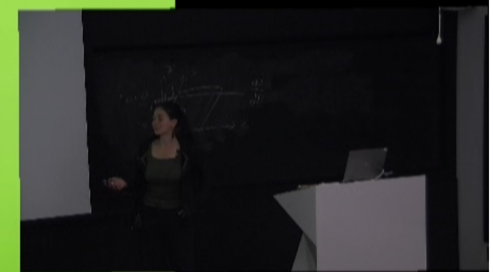
Abstract:



Quantum Entanglement in Photosynthesis

Yvonne Geyer

Perimeter Institute, PSI

August 19, 2011

Quantum Entanglement in Photosynthesis

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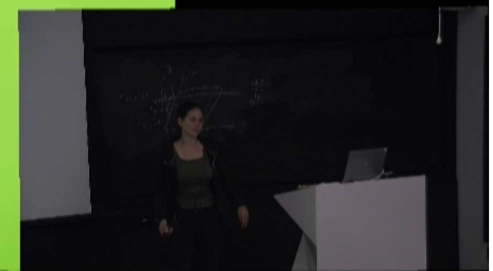
Overview



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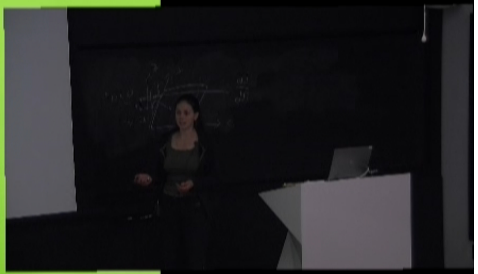
Biological Preliminaries

Photosynthesis



- Photosynthesis = chemical process converting energy of photons to chemical energy

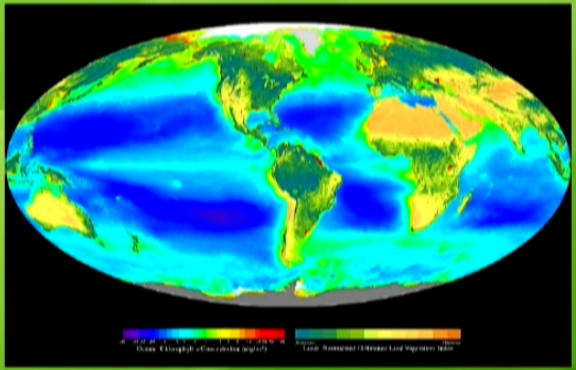


Figure: Global distribution of photosynthesis

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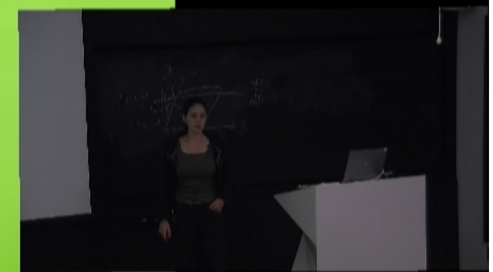


- Photosynthesis
  = chemical process converting energy of photons to chemical energy
- Appearance:
  plants, algae, bacteria
- Gathering of light via proteins, located in organelles called chloroplasts
  $\Rightarrow$ LHC

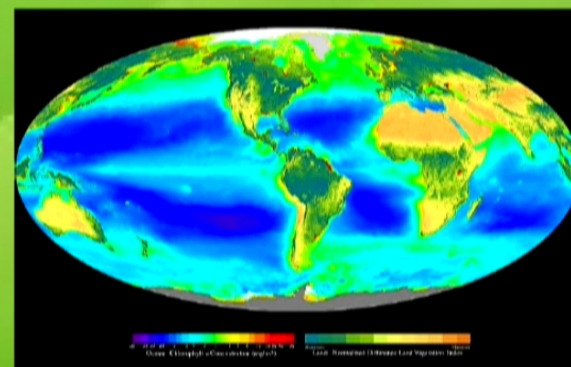
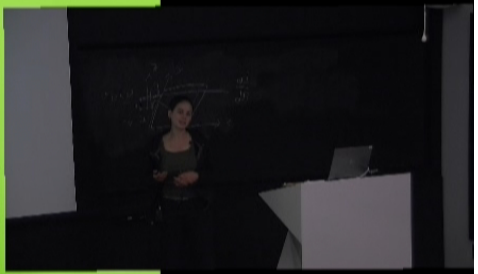


Figure: Global distribution of photosynthesis

Biological Preliminaries

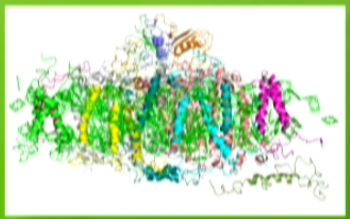
Photosystem and LHC



Photosystem

(i) Function:
photochemistry of photosynthesis

- absorption of light
- transfer of energy and electrons



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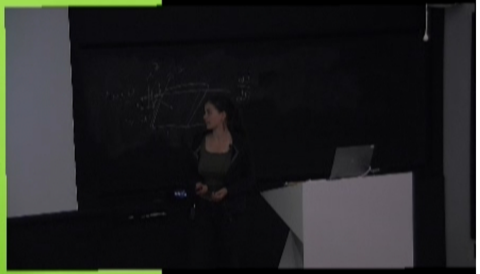


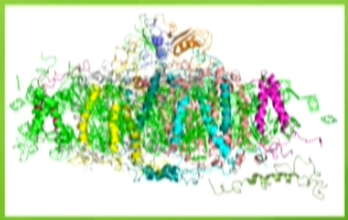
Photosystem

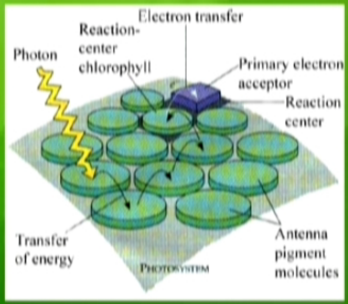
(i) Function:
photochemistry of photosynthesis

- absorption of light
- transfer of energy and electrons

(ii) Configuration of membrane complexes

- reaction center:
  enzyme using light to reduce molecules
- LHC (Light-Harvesting Complex):





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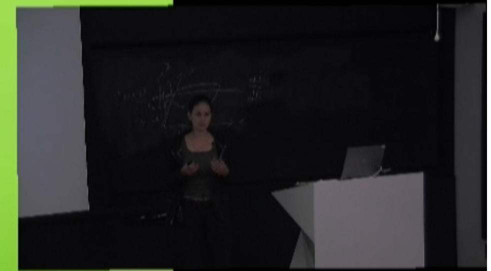
Photosystem and LHC



Photosystem

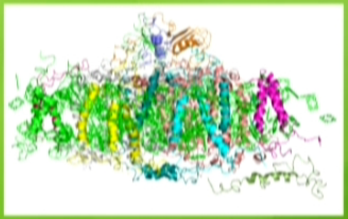
(i) Function:
photochemistry of photosynthesis

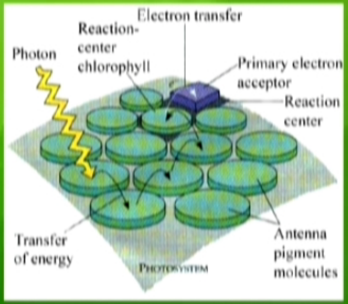
- absorption of light
- transfer of energy and electrons

(ii) Configuration of membrane complexes

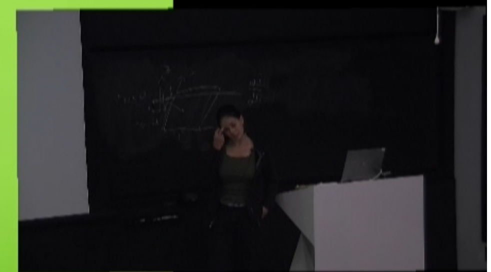
- reaction center:
  enzyme using light to reduce molecules
- LHC (Light-Harvesting Complex):
  - enhances absorption of light
  - transfers energy to reaction center

⇒ complex many-body system





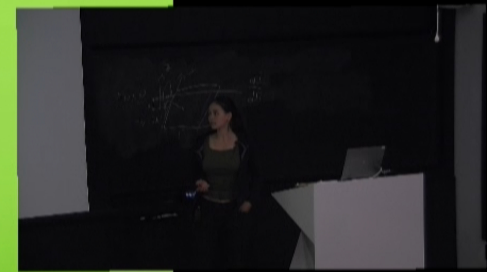
Quantum Entanglement



(i) General notion:
Quantum phenomena as explanation of energy transfer rates at LHC

- coherence and decoherence
- delocalization of excitations
- stabile entanglement

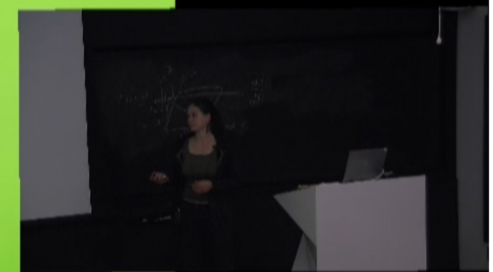
Quantum Entanglement



(i) General notion:
Quantum phenomena as explanation of energy transfer rates at LHC
- coherence and decoherence
- delocalization of excitations
- stabile entanglement

(ii) Growing experimental support

(iii) Quantum entanglement
$\Rightarrow$ simultaneous sampling of transfer pathways
$\Rightarrow$ choice of most efficient one



Quantum Entanglement

BUT:

(i) Biological system ⇒ irregular lattice
⇒ destructive interference
⇒ localization
= absence of diffusion in disordered media
⇒ NO full explanation of observed transfer rates

(ii) Dephasing noise

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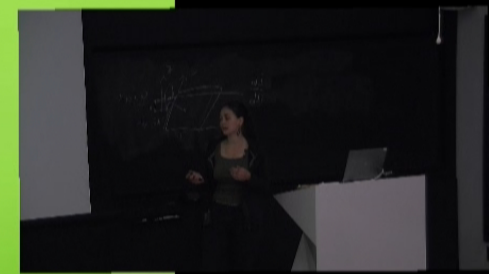
Quantum Entanglement



- coherent oscillation
  $\Rightarrow$ preservation of quantum coherence
  $\Rightarrow$ coherence surviving over large spacial distances and over long time scales

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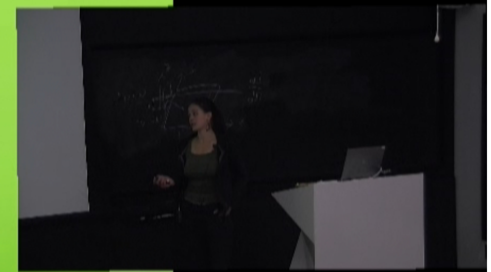
Quantum Entanglement

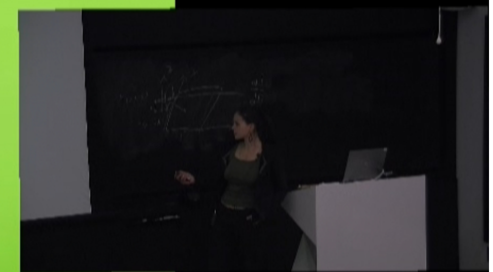


- coherent oscillation
  $\Rightarrow$ preservation of quantum coherence
  $\Rightarrow$ coherence surviving over large spacial distances and over long time scales
- LHC at most one excitation
  $\Rightarrow$ two-level system: $|0\rangle$, $|i\rangle$

$$|J\rangle = \sum_i c_i(J)\,|i\rangle \quad \text{eigenbasis}$$

$\Rightarrow \mathcal{H}$ restricted to subspace of zero/one excitation

Quantum Entanglement



- State in 1-excitation manifold

$$\rho(t) = \sum_{i=1}^{N} \rho_{ii}(t) \left|i\right\rangle \left\langle i\right| + \sum_{i=1}^{N} \sum_{j>i}^{N} \left(\rho_{ij}(t) \left|i\right\rangle \left\langle j\right| + \rho_{ij}(t)^* \left|j\right\rangle \left\langle i\right|\right)$$

$\left|i\right\rangle$: excitation on i^{th} site, other sites in ground state

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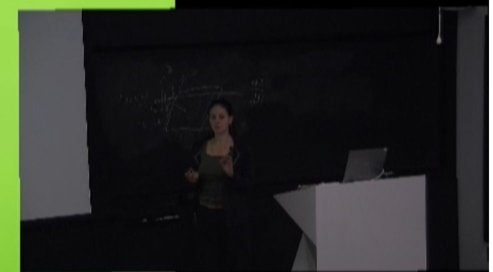
Quantum Entanglement

Measure of Entanglement

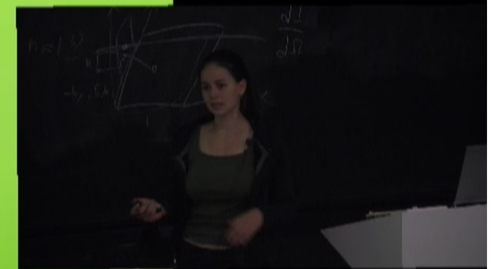


(i) Bipartite entanglement
concurrence $C(\rho) = \max(0,\, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4)$
with eigenvalues λ_i of the Hermitian matrix
$R = \sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}, \quad \tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$

$$\Rightarrow \; C_{ij} = 2|\rho_{ij}|$$

Quantum Entanglement

Measure of Entanglement



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$$\Rightarrow \; C_{ij} = 2|\rho_{ij}|$$

(ii) Global entanglement

$$E[\rho] = -\sum_{i=1}^{N} \rho_{ii} \log \rho_{ii} - S(\rho)$$

with the von Neumann entropy $S(\rho) = -\mathrm{tr}\rho \log \rho$

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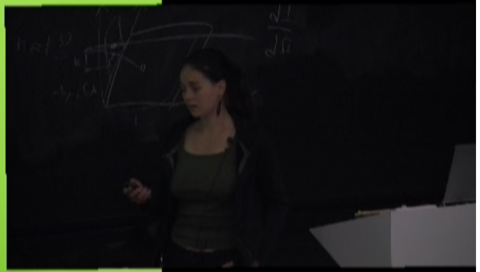
Quantum Entanglement

Numerical Simulation



(i) Model applying both LHC and quantum information

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Quantum Entanglement
Numerical Simulation

(i) Model applying both LHC and quantum information

(ii) Focus on FMO-complex (Fenna-Matthews-Olson)

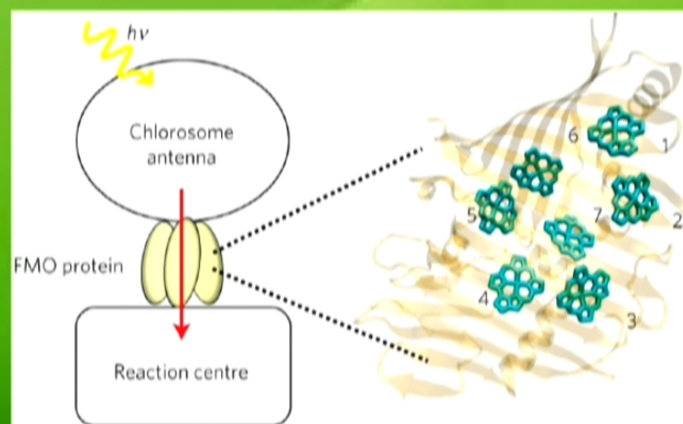

Figure: FMO-complex

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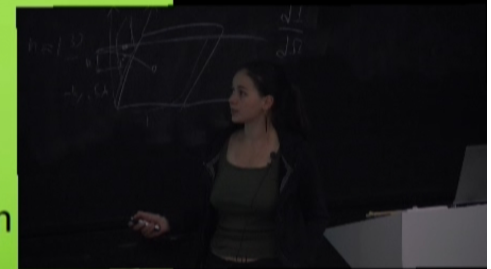
Quantum Entanglement

Numerical Simulation



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(iii) Non-perturbative, non-markovian quantum master equation

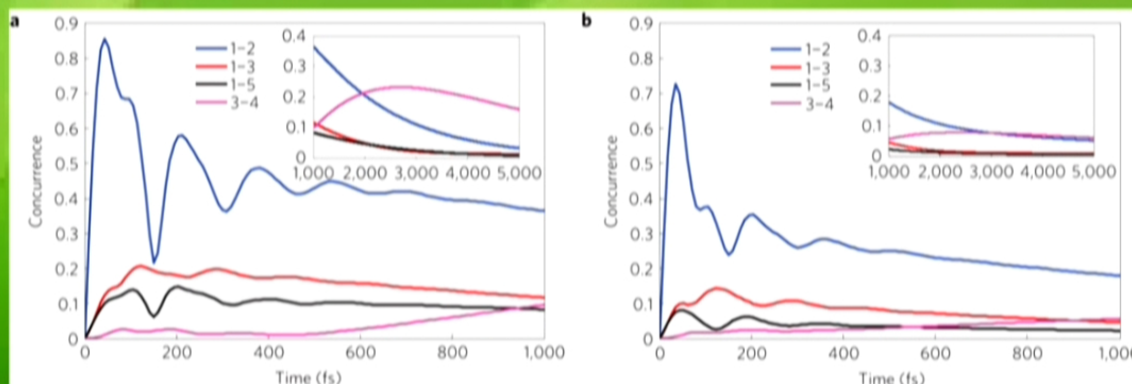

Figure: Bipartite entanglement

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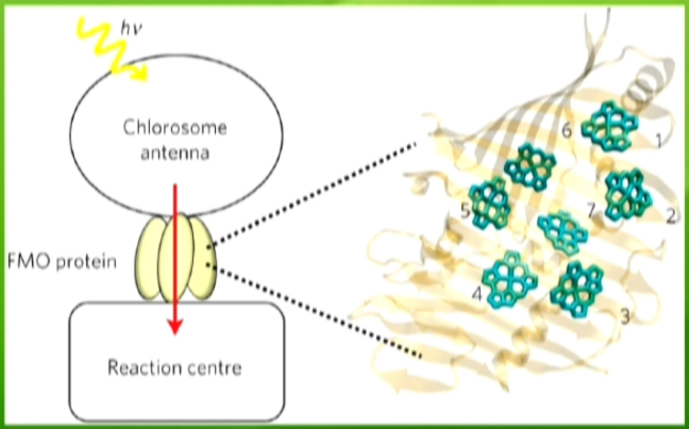

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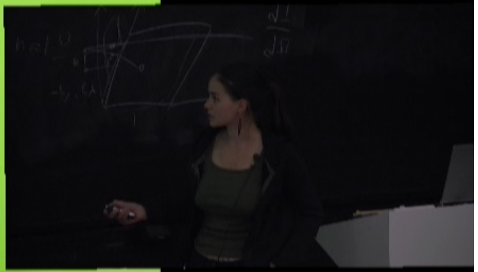

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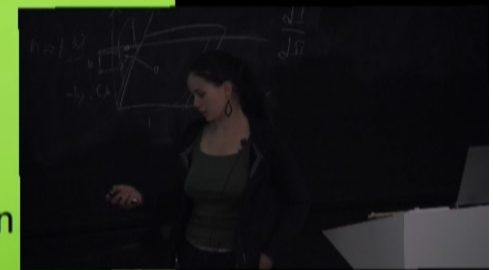

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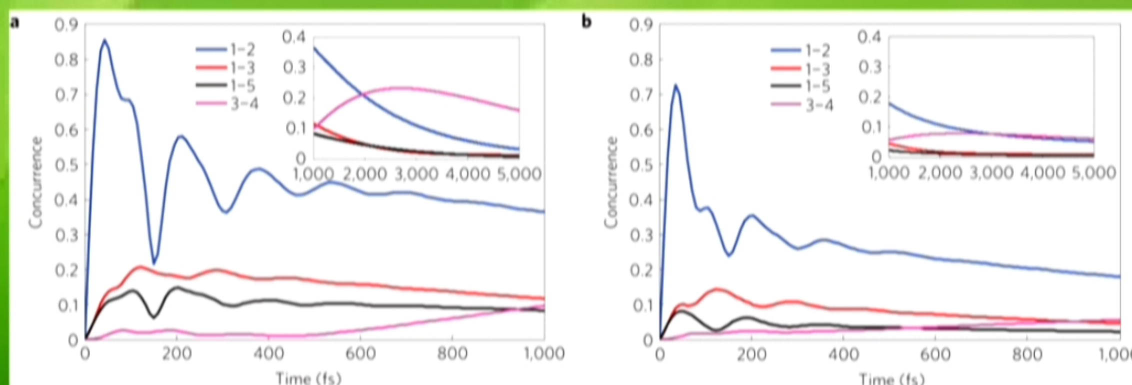
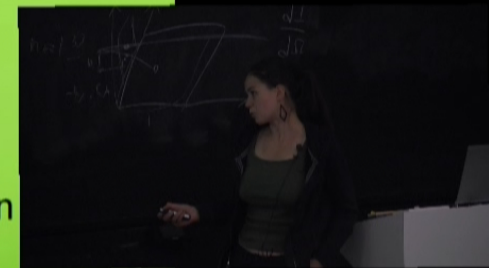


Figure: Bipartite entanglement

Quantum Entanglement

Numerical Simulation



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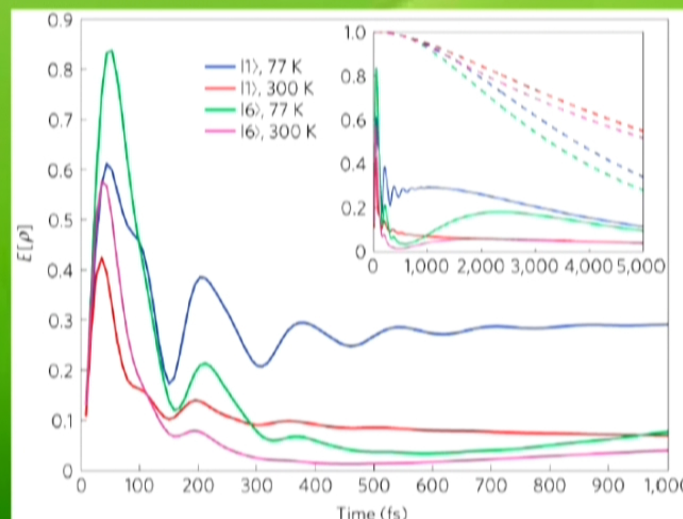
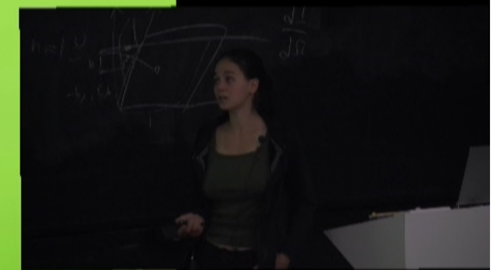


Figure: Global entanglement



Quantum Entanglement

Energy Transfer Dynamics

Formalization: Hamiltonian H for photosynthetic system

$$H_s = \sum_{i=1}^{N} \epsilon_i a_i^\dagger a_i + \sum_{j<i}^{N} V_{ij}(a_i^\dagger a_j + a_j^\dagger a_i)$$

$a_i^\dagger$, a_i:	creation/annihilation operators for excitons at site i
N:	number of sites
ϵ_i:	site energy
V_{ij}:	Coulomb coupling for transition densities of sites

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Quantum Entanglement

Energy Transfer Dynamics

Open system in contact with thermal phonon bath and radiation field

$\Rightarrow$ Interaction Hamiltonian $H_I = H_p + H_r$ with

$H_p = \sum_{i,j} q^p_{ij} a^\dagger_i a_j$	phonon coupling excitation manifold fixed
$H_r = \sum_i q^r_i (a^\dagger_i + a_i)$	excitation-phonon interaction transition between excitation manifolds

Quantum Entanglement

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Open system in contact with thermal phonon bath and radiation field

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$H_r = \sum_i q_i^r (a_i^\dagger + a_i)$	excitation-phonon interaction transition between excitation manifolds

$\Rightarrow$ Lindblad master equation

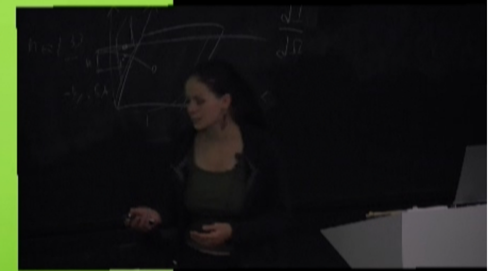
$$\frac{\partial \rho(t)}{\partial t} = -\frac{i}{\hbar}[H_{eff}, \rho(t)] + L_p(\rho(t)) + L_r(\rho(t))$$

with the Lindblad operators $L_p(\rho(t))$, $L_r(\rho(t))$ given by

$$L_k(\rho) = \sum_{i,j} \gamma_{ij}^k \left(A_i^k \rho A_j^{k\dagger} - \frac{1}{2} \left(A_i^k A_j^{k\dagger} \rho + \rho A_i^k A_j^{k\dagger} \right) \right)$$

Quantum Entanglement

Energy Transfer Efficiency



- Energy transfer efficiency
  = integrated possibility of excitation successfully leaving channel C to acceptor A

$$\eta := \frac{1}{\hbar}\int_0^\infty \mathrm{tr}(H_{C\mapsto A}\rho(t))dt$$

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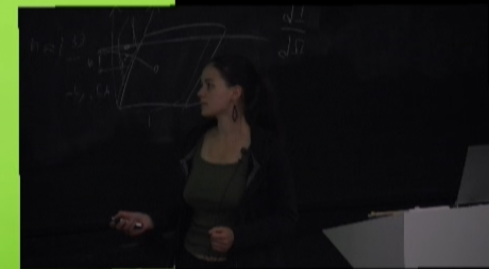
Quantum Entanglement

Energy Transfer Efficiency



- Energy transfer efficiency
  = integrated possibility of excitation successfully leaving channel C to acceptor A

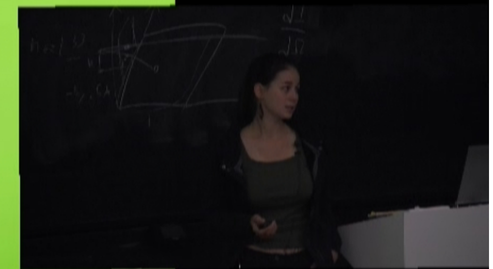
$$\eta := \frac{1}{\hbar}\int_0^\infty \mathrm{tr}(H_{C\mapsto A}\rho(t))dt$$

- Transfer time

$$\tau := \frac{1}{\eta}\int_0^\infty t\mathrm{tr}(H_{C\mapsto A}\rho(t))dt$$

Quantum Entanglement

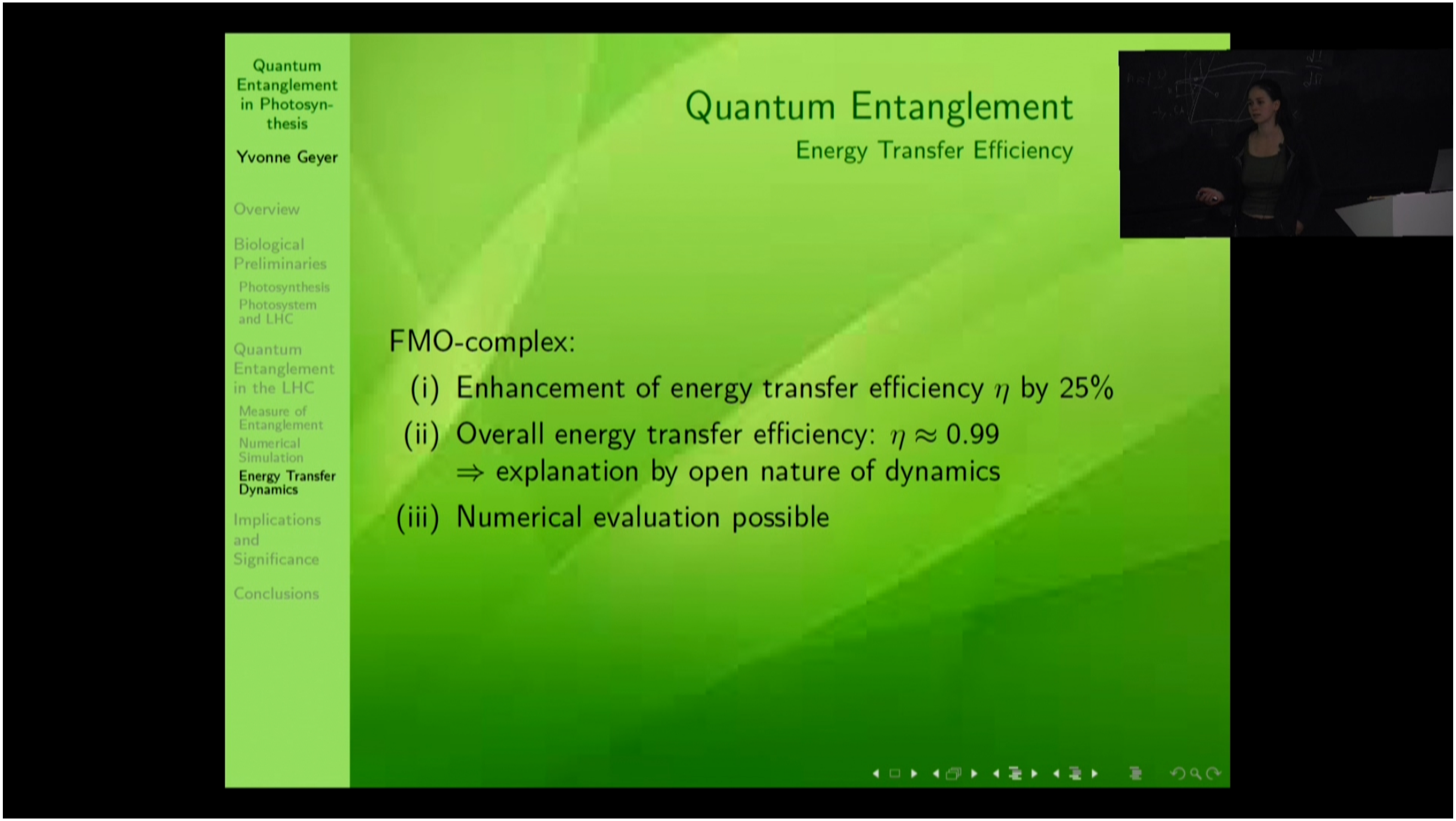
Energy Transfer Efficiency



FMO-complex:

(i) Enhancement of energy transfer efficiency η by 25%

(ii) Overall energy transfer efficiency: $\eta \approx 0.99$
$\Rightarrow$ explanation by open nature of dynamics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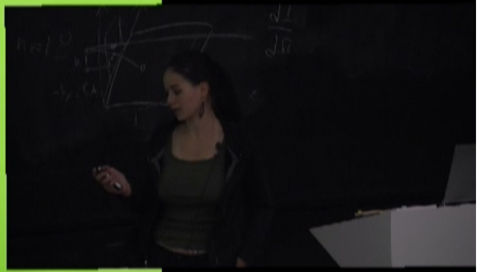
(iii) Numerical evaluation possible



Implications and Significance

Implications for

(i) understanding of biological structures

(ii) link between quantum physics and biology

(iii) artificial photosynthetic systems

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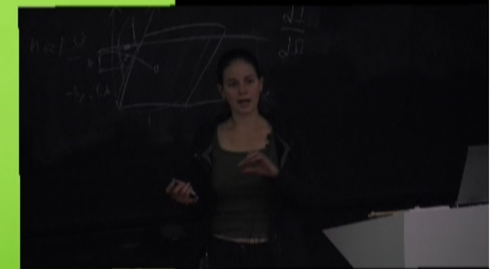

Implications and Significance

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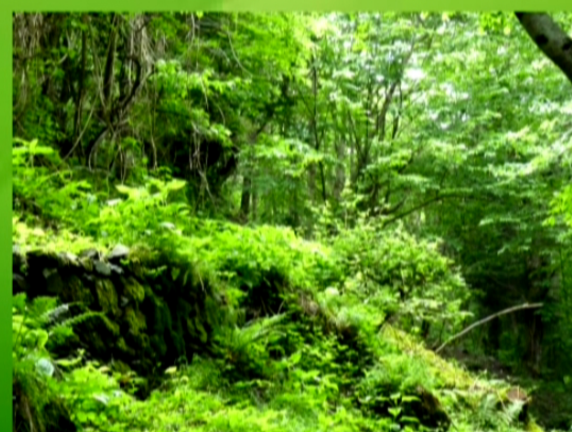
(i) understanding of biological structures
(ii) link between quantum physics and biology
(iii) artificial photosynthetic systems
(iv) quantum-based technologies



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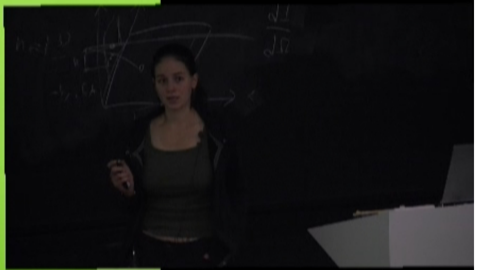

- Connection between quantum mechanics and biology
- Quantum phenomena crucial for photosynthesis
- Development of theoretical framework in Lindblad form
- Role of quantum effects in energy transfer dynamics

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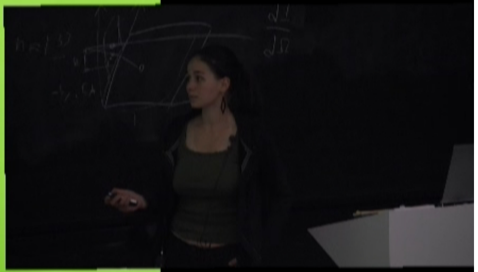

Conclusion

- Connection between quantum mechanics and biology
- Quantum phenomena crucial for photosynthesis
- Development of theoretical framework in Lindblad form
- Role of quantum effects in energy transfer dynamics

⇒ Quantum effects form an important part of other sciences.

⇒ Sometimes you might find physics where you least expect it!