The role of symmetry in the photosynthetic antenna complex of Green Sulphur Bacteria

UNIVERSITÀ DEGLI STUDI FIRENZE

Author: Alessia Valzelli

Department of Information Engineering

Laboratory: CSDC

PhD program in Information Engineering

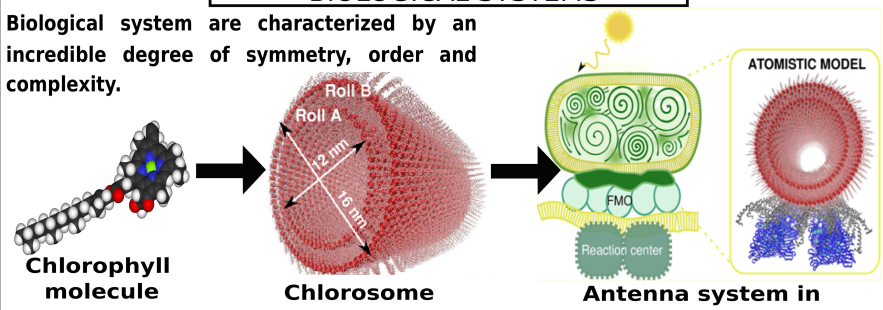
Abstract

Nanotubular molecular self-aggregate are characterized by a high degree of symmetry and considered to be fundamental systems in natural **light-harvesting complexes**, artificial nanostructures for energy transport and in other several biological systems such as microtubules. They are extremely efficient structures for absorbing sunlight and transporting photo-excitation energy. While coherent effects are though to be at the basis of their high efficiency, the relationship between **structure**, **coherence** and **functionality** is still an open problem. Here we compare the disposition of the chlorophyll networks in natural photosynthetic complexes of **Green Sulphur Bacteria (GSB)** with other mathematical models, showing that the natural chlorophyll networks are able to support a coherence length which is an order of magnitude larger than the coherence length of mathematical models at room temperature [1].

QUANTUM BIOLOGY

ROLE OF QUANTUM MECHANICS IN BIOLOGICAL SYSTEMS

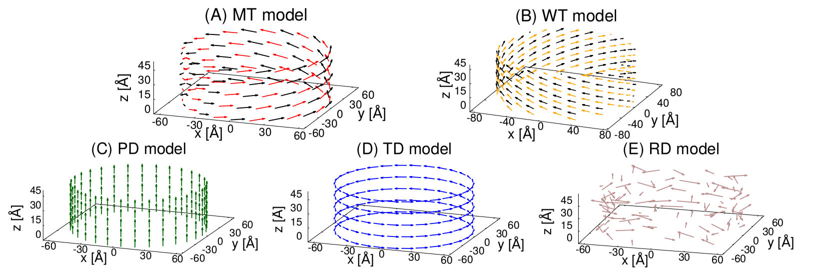
Biological system are characterized by an incredible degree of symmetry, order and complexity.



1- What is the **relationship** between **structure** and **functionality**?
2- Can QM have a functional role in such large aggregates?
COOPERATIVE EFFECTS (**SUPERRADIANCE** AND **SUPER-TRANSFER COUPLING**) AND **INTERNAL EFFICIENCY** 100%

The models and the Hamiltonian

NATURAL VS MATHEMATICAL MODELS



The **effective Non-Hermitian Hamiltonian**, which is commonly used to model the interaction with the EMF in several systems, such as natural light-harvesting complexes and cold atomic clouds, reads:

$$\hat{H} = e_0 \sum_{i=1}^{N} |i\rangle\langle i| + \sum_{i\neq j} \Delta_{ij}|i\rangle\langle j| - i \sum_{i,j=1}^{N} Q_{ij}|i\rangle\langle j|$$

Each molecule: **two-level system** with an excitation energy e_0 and a transition dipole moment $\boldsymbol{\mu}_i$. The parameters are:

$e_0 = 15390\,cm^{-1}$ $\lambda_0 = 650\,nm$

$|\boldsymbol{\mu}_i| = \sqrt{30}\,D$ $\gamma = 1{,}821 \cdot 10^{-4}\,cm^{-1}$

Single excitation manifold: the ith molecule is excited while all the others are in the ground state.

Single cylinders: Superradiance and Coherence length

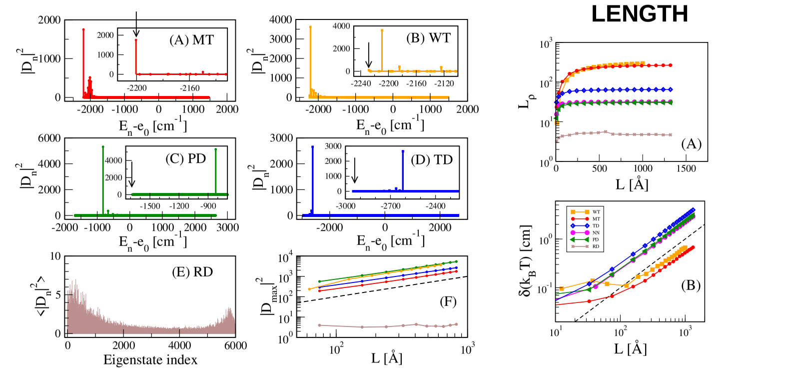
If N is the total number of molecules, then we will express the transition dipole moment $\boldsymbol{D}_n$ associated with the nth eigenstate as follows:

$$\boldsymbol{D}_n = \sum_{i=1}^{N} C_{ni}\boldsymbol{\mu}_i \quad \text{with} \quad |E_n\rangle = \sum_{i=1}^{N} C_{ni}|i\rangle$$

The dipole strength of the nth eigenstate is defined by $|\boldsymbol{D}_n|^2$

Below $N_{max} = 9600$ and $L_{max} \approx 1320$ Å.

SUPERRADIANCE IN NANOTUBES — THERMAL COHERENCE LENGTH



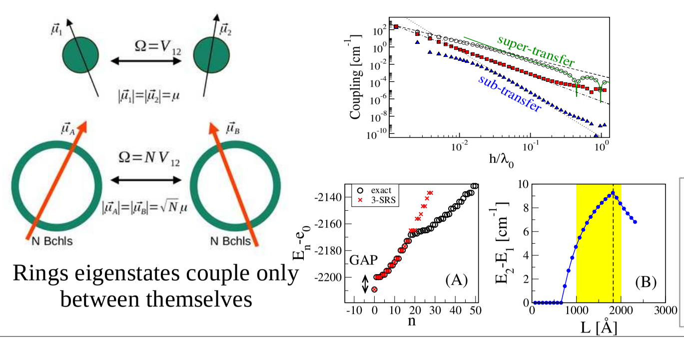
Given a quantum state specified by the density matrix $\boldsymbol{\rho}$ it is possible to define its coherence length L_ρ in the single excitation manifold defined by the basis states i:

$$L_\rho = \frac{1}{N}\frac{(\sum_{ij}|\rho_{ij}|)^2}{\sum_{ij}|\rho_{ij}|^2} \quad 1/N \le L_\rho \le N \quad \rho_{ij} = \sum_n \frac{e^{-\beta E_n}}{Tr(e^{-\beta \hat{H}})}\langle i|E_n\rangle\langle E_n|j\rangle$$

Super-transfer

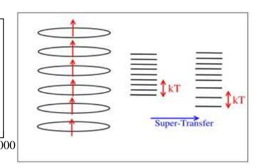
WHAT IS THE CONNECTION BETWEEN A SUPERRADIANT STATE CLOSE TO THE GROUND STATE AND A LARGER COHERENCE LENGTH?

SUPER-TRANSFER — Emergence of an energy gap



Rings eigenstates couple only between themselves

Super-transfer coupling: mechanism that explains the large thermal coherence length in natural models

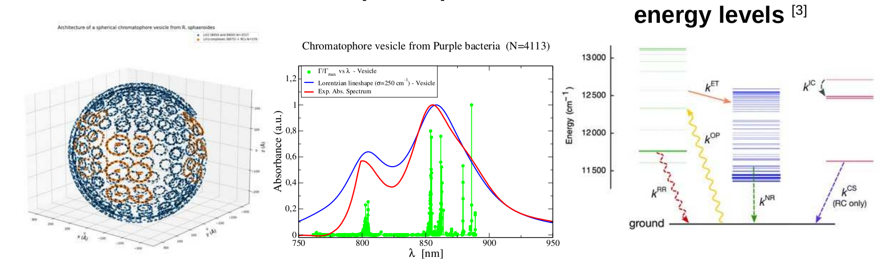


Future perspectives and ongoing collaborations

1. What is the role of geometry in the **high-efficient energy transfer** of the excitation to the reaction centers? What is the role of QM in the energy-transfer?

Application to the light-harvesting system of **Purple Bacteria** ***Rhodobacter sphaeroides*** [2].

The model — Absorption spectrum — Transfer rates and energy levels [3]



Ongoing collaboration with the CSDC group and prof. G. Battistelli of the Dep. of Information Engineering

2. Development of a **bio-mimetic sunlight-pumped laser** using the antenna systems of Purple bacteria to enhance the pumping on the gain medium to achieve inversion population under natural sunlight pumping.

Ongoing collaboration with the experimental groups of the Photonic Material Area at LENS

Conclusions

Molecular nanotubes are fundamental structures in biological systems to be used in quantum devices. The most important message which can be extracted by our analysis is the fact that **specific geometric features**, connected to symmetries, allows to **control the cooperative effects** in molecular aggregates. Indeed it is due to the presence of such cooperatively enhanced coupling (Super-Transfer) inside the molecular aggregates that macroscopic coherent states are allowed to survive at room temperature. This is an emergent property of such structures which cannot be reduced to the intensity of the coupling between the molecules, neither to their interaction range.

References

[1] Gullì M., et al. Macroscopic coherence as an emergent property in molecular nanotubes. New Journal of Physics 21.1 (2019): 013019.

[2] Şener Melih K., et al. Atomic-level structural and functional model of a bacterial photosynthetic membrane vesicle. Proceedings of the National Academy of Sciences, 2007, 104.40: 15723-15728.

[3] Baghbanzadeh S.; Kassal I. Distinguishing the roles of energy funnelling and delocalization in photosynthetic light harvesting. Physical Chemistry Chemical Physics, 2016, 18.10: 7459-7467.

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