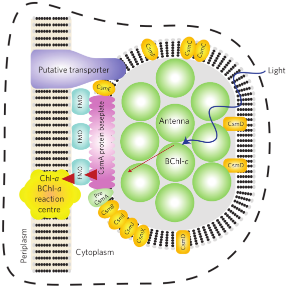
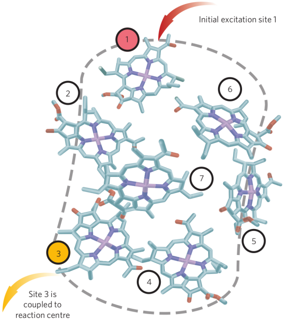
Time dynamics of multiparty quantum correlations in light-harvesting complexes





Titas Chanda

Harish-Chandra Research Institute, Allahabad, INDIA

February 24, 2015

Outline

Outline

- **Introduction**

  Quantum Biology

  Quantum Coherent Energy Transport in Photosynthesis

Outline

- **Introduction**
  - Quantum Biology
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- **Fenna-Matthews-Olson (FMO) Complex**
  - Dynamical Model

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- **Results**
  - Dynamics of Multipartite QC Measures
  - Classification of Chromophore Sites
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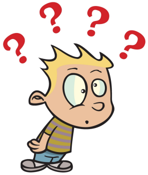
- **Conclusions**

Introduction

Quantum Biology

Introduction

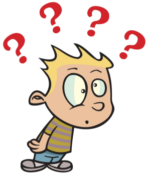
Quantum Biology



Biology!!!!

Introduction

Quantum Biology

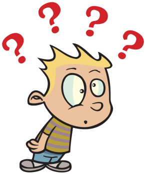


Biology!!!!

But it has a "Quantum" part too!!!!

Introduction

Quantum Biology



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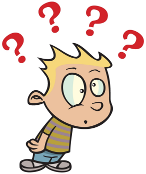
Biological process ⇒ combinations of chemical processes ⇒ inherently quantum.

Introduction

Quantum Biology



Biology!!!!

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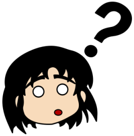
Biological process $\Rightarrow$ combinations of chemical processes $\Rightarrow$ inherently quantum.



What is "Quantum Biology"?

Introduction

Quantum Biology

- **"Biology" part :** Deals in complex biological systems (macroscopic).

Introduction

Quantum Biology

- **“Biology” part :** Deals in complex biological systems (macroscopic).
- **“Quantum” part :**

Introduction

Quantum Biology

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- **"Quantum" part :**
  - ✓ **Can these biological systems use quantum mechanics to perform a task that cannot be done classically?**

Introduction

Quantum Biology

- **"Biology" part :** Deals in complex biological systems (macroscopic).

- **"Quantum" part :**

  - ✓ **Can these biological systems use quantum mechanics to perform a task that cannot be done classically?**

  - ✓ **Is that task more efficient than the best classical one?**

Introduction

Quantum Biology

Introduction

Quantum Biology

Main directions of quantum biology:

1. **Quantum coherent energy transport in photosynthesis.**
2. **Avian magnetoreception.**
3. **Several others.**

Introduction

Quantum Biology

Main directions of quantum biology:

1. **Quantum coherent energy transport in photosynthesis.**
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For details see: Lambert *et al.*, Nature Physics (2012)

Introduction

Quantum Coherent Energy Transport in Photosynthesis

Introduction

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☞ **Photons are absorbed by light-harvesting antennas as electronic excitations.**

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Introduction

Quantum Coherent Energy Transport in Photosynthesis

- ☞ **Photons are absorbed by light-harvesting antennas as electronic excitations.**
- ☞ **The excitation transport: Antenna $\rightarrow$ Reaction center.**
- ☞ **The precise biological structures vary between organisms.**
- ☞ **Most well-studied example $\rightarrow$ The light-harvesting apparatus of green-sulphur bacteria (Fenna-Matthews-Olson (FMO) complex).**

Introduction

Quantum Coherent Energy Transport in Photosynthesis

☞ **FMO complex mediates the excitation transport.**

Introduction

Quantum Coherent Energy Transport in Photosynthesis

- ☞ **FMO complex mediates the excitation transport.**
- ☞ **Efficient excitation transport can not be explained by classical models.**

  Quantum models proposed.

  Caruso *et al.*, JCP (2009); Mohseni *et al.*, JCP (2008).

Introduction

Quantum Coherent Energy Transport in Photosynthesis

- ☞ **FMO complex mediates the excitation transport.**

- ☞ **Efficient excitation transport can not be explained by classical models.**

  Quantum models proposed.

  Caruso *et al.*, JCP (2009); Mohseni *et al.*, JCP (2008).

- ☞ **Presence of quantum coherence over appreciable length and time scales.**

  Even at room temperature.

  Engel *et al.*, Nature (2007); Fleming *et al.*, Science (2010).

Introduction

Quantum Coherent Energy Transport in Photosynthesis

What is the role of quantum correlation?

Introduction

Quantum Coherent Energy Transport in Photosynthesis

What is the role of "multipartite" quantum correlation?

Fenna-Matthews-Olson (FMO) Complex

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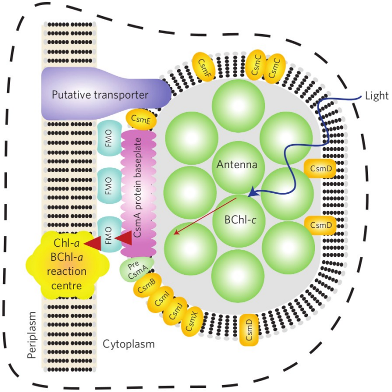
- **A water soluble pigment-protein complex (PPC), appears in green sulfur bacteria.**



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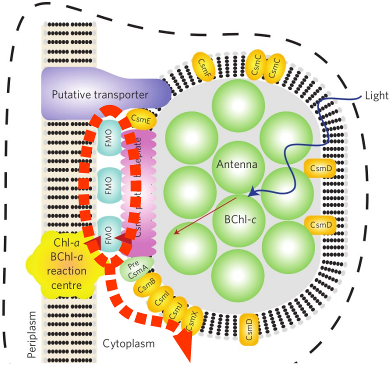

A trimer of three identical units

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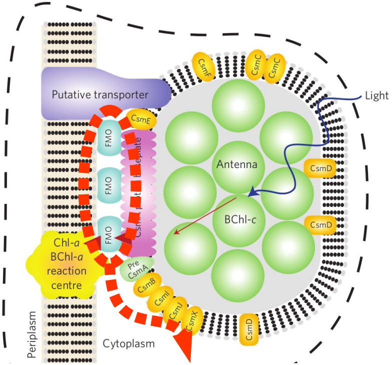

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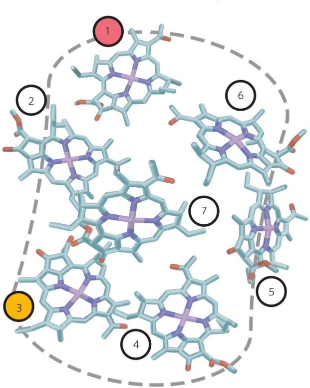

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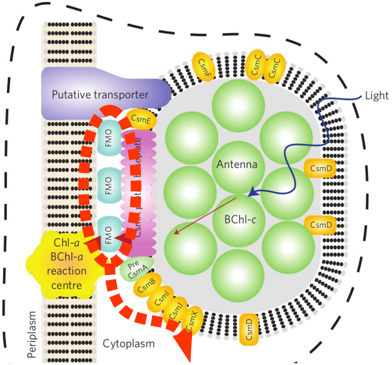

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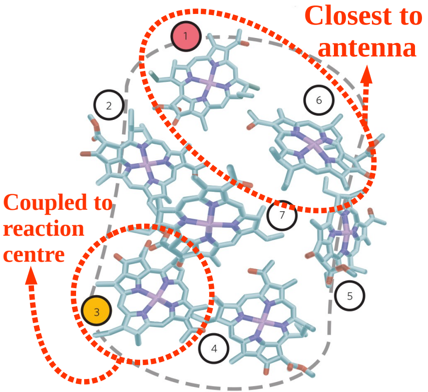

Fenna-Matthews-Olson (FMO) Complex

Dynamical Model

Fenna-Matthews-Olson (FMO) Complex

Dynamical Model

- **For coherent evolution of FMO complex :**

$$H = \sum_{j=1}^{7} \hbar\omega_j \sigma_j^+ \sigma_j^- + \sum_{\substack{i,j=1 \\ i \neq j}}^{7} \hbar v_{ij} (\sigma_i^+ \sigma_j^- + \sigma_j^+ \sigma_i^-)$$

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- **The matrix form (in units of cm^{-1}):**

$$H = \begin{pmatrix} 215 & -104.1 & 5.1 & -4.3 & 4.7 & -15.1 & -7.8 \\ -104.1 & 220 & 32.6 & 7.1 & 5.4 & 8.3 & 0.8 \\ 5.1 & 32.6 & 0 & -46.8 & 1.0 & -8.1 & 5.1 \\ -4.3 & 7.1 & -46.8 & 125 & -70.7 & -14.7 & -61.5 \\ 4.7 & 5.4 & 1.0 & -70.7 & 450 & 89.7 & -2.5 \\ -15.1 & 8.3 & -8.1 & -14.7 & 89.7 & 330 & 32.7 \\ -7.8 & 0.8 & 5.1 & -61.5 & -2.5 & 32.7 & 280 \end{pmatrix}.$$

J. Adolphs and T. Renger, Biophysical Journal (2006)

Fenna-Matthews-Olson (FMO) Complex

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- **For the dissipation of excitons to environment:**

$$\mathcal{L}_{diss}(\rho) = \sum_{j=1}^{7} \Gamma_j \left[2\sigma_j^- \rho \sigma_j^+ - \{\sigma_j^+ \sigma_j^-, \rho\} \right]$$

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$\Gamma_j = \Gamma_{diss} = 1/(2 \times 188)$ $\mathbf{cm}^{-1}$.

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$\gamma_j = \{0.157, 9.432, 7.797, 9.432, 7.797, 0.922, 9.433\}$ $\mathbf{ps}^{-1}$.

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$$\mathcal{L}_{sink}(\rho) = \Gamma_8 [2\sigma_8^+ \sigma_3^- \rho \sigma_3^+ \sigma_8^- - \{\sigma_3^+ \sigma_8^- \sigma_8^+ \sigma_3^-, \rho\}]$$

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$\Gamma_8 = 62.8/1.88$ **cm**$^{-1}$.

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Caruso et. al. JCP (2009)

Quantum Correlation Measures

Quantum Correlation Measures

What is the role of "multipartite" quantum correlation?

Quantum Correlation Measures

What is the role of "multipartite" quantum correlation?

Motivation: **Multipartite quantum correlations capture global perspective of the entire system.**

Quantum Correlation Measures

- **Problem** $\rightarrow$ **Unavailability of computable multipartite measures.**

Quantum Correlation Measures

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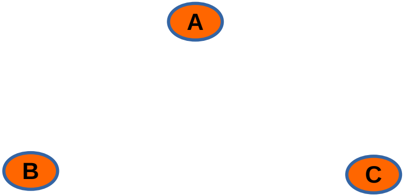

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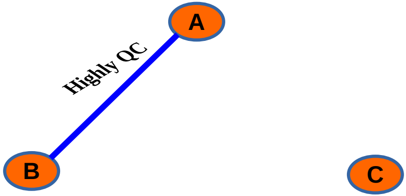

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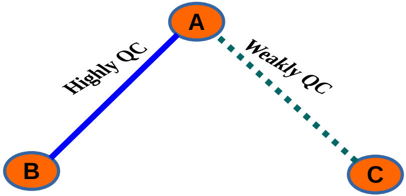

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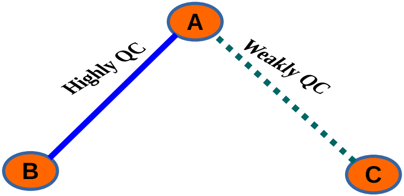

If $\mathcal{Q}$ is monogamous,

$$\mathcal{Q}(\rho_{A:BC}) \geq \mathcal{Q}(\rho_{A:B}) + \mathcal{Q}(\rho_{A:C})$$

Coffman, Kundu, Wootters, PRA (2000)

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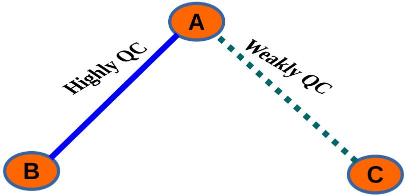

3 party case $\Rightarrow$ **Monogamy score of** $\mathcal{Q}$**:**

$$\delta\mathcal{Q}_A = \mathcal{Q}_{A:BC} - (\mathcal{Q}_{A:B} + \mathcal{Q}_{A:C})$$

Prabhu *et al.*, PRA (2012)

Quantum Correlation Measures

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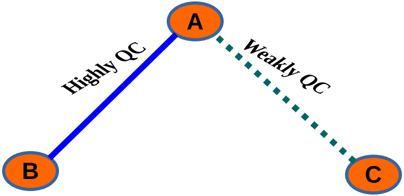

N party case ⇒ Monogamy score of $\mathcal{Q}$:

$$\delta\mathcal{Q}_i = \mathcal{Q}(\rho_{i:R}) - \sum_{j=1, j\neq i}^{N} \mathcal{Q}(\rho_{j:i})$$

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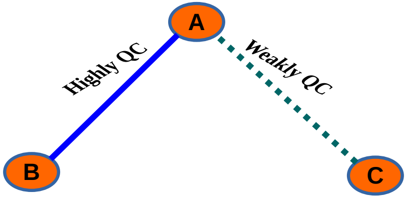

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For details: Asutosh Kumar's talk

Quantum Correlation Measures

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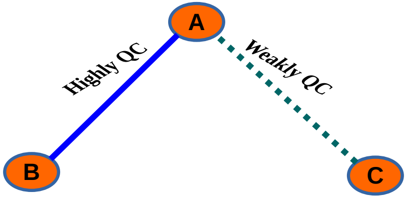

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Prabhu *et al.*, PRA (2012)

For details: Asutosh Kumar's talk

Monogamy scores for negativity (N) and quantum discord (D).

Quantum Correlation Measures

Negativity $\rightarrow$ **absolute sum of the negative eigenvalues of the partial transposed state.**

Quantum Correlation Measures

Negativity $\rightarrow$ **absolute sum of the negative eigenvalues of the partial transposed state.**

Quantum Discord $\rightarrow$ $$D_{A:B} \equiv D(\rho_{A:B}) = \mathcal{I}(\rho_{AB}) - \mathcal{J}(\rho_{AB})$$

$\mathcal{I}(\rho_{AB}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}) \longleftarrow$ **Quantum mutual information, measure of total correlation**

$\mathcal{J}(\rho_{AB}) = \mathrm{Max}[S(\rho_B) - S(\rho_{B|A})] \longleftarrow$ **Measure of classical correlation**

$S(\rho_{B|A}) = \sum p_i S((\Pi_i \otimes I)\rho_{AB}(\Pi_i \otimes I)/p_i) \longleftarrow$ **Quantum conditional entropy**

Quantum Correlation Measures

Negativity $\rightarrow$ **absolute sum of the negative eigenvalues of the partial transposed state.**

Quantum Discord $\rightarrow$ $D_{A:B} \equiv D(\rho_{A:B}) = \mathcal{I}(\rho_{AB}) - \mathcal{J}(\rho_{AB})$

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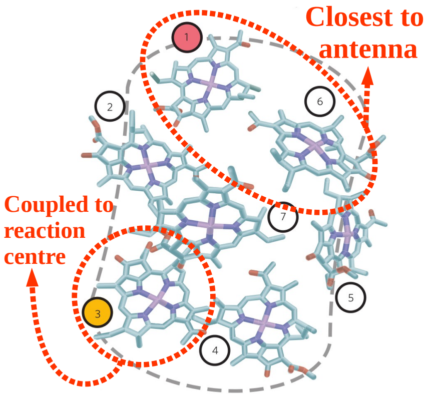
Now back to the FMO complex

Results

Dynamics of Multipartite QC Measures

Results

Dynamics of Multipartite QC Measures



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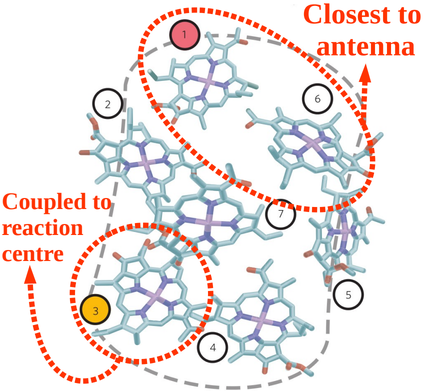

Set initial state:

1. $|1\rangle\langle 1|$
2. $|6\rangle\langle 6|$
3. $(|1\rangle\langle 1| + |6\rangle\langle 6|)/2$.

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Steps:

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1. **Choose one initial state. E.g. $|1\rangle\langle 1|$.**

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3. **Calculate $\delta\mathcal{Q}_i,\ \mathcal{Q}_{i:R}$ and $\mathcal{Q}_{R_i}$ throughout the dynamics.**

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2. **Evolve the state according to master equation.**
3. **Calculate** $\delta\mathcal{Q}_i,\ \mathcal{Q}_{i:R}$ **and** $\mathcal{Q}_{R_i}$ **throughout the dynamics.**

$\Rightarrow$ **We can classify the results into three groups.**

Results

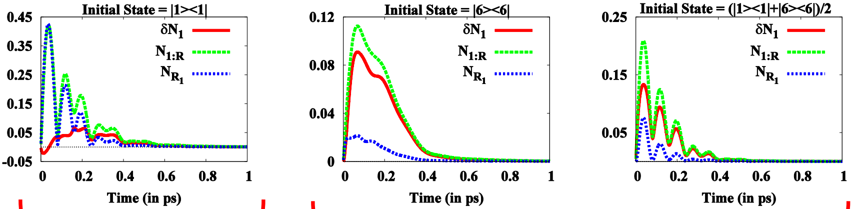
Dynamics of Multipartite QC Measures

Sites 1 and 2 as nodal observers

Results

Dynamics of Multipartite QC Measures

Sites 1 and 2 as nodal observers



$\delta N_i < N_{R_i}$; $t < 0.2$ ps

$\delta N_i > N_{R_i}$; otherwise

$\delta N_i > N_{R_i}$

Results

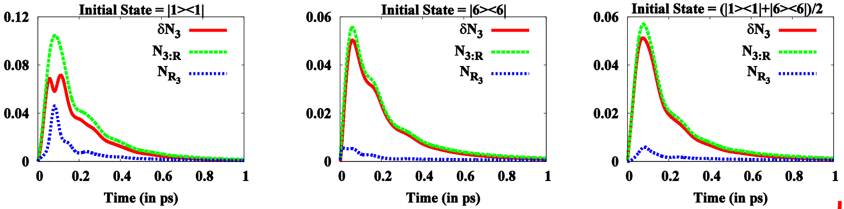
Dynamics of Multipartite QC Measures

Sites 3, 4 **and** 7 **as nodal observers**

Results

Dynamics of Multipartite QC Measures

Sites 3, 4 and 7 as nodal observers



$$\delta N_i > N_{R_i}$$

Results

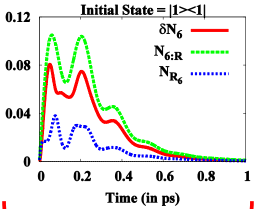
Dynamics of Multipartite QC Measures

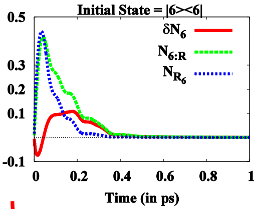
Sites 5 **and** 6 **as nodal observers**

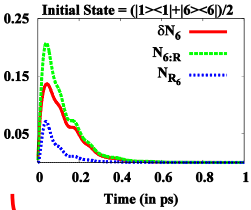
Results

Dynamics of Multipartite QC Measures

Sites 5 and 6 as nodal observers







$\delta N_i > N_{R_i}$

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Results

Classification of Chromophore Sites

Results

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Based on the observation:

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- **Group I: Sites 1 and 2.**
- **Group II: Sites 5 and 6.**
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Can we predict the structure of FMO complex?

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Known: **Sites 1 and 6 closest to antenna, site 3 coupled to reaction center.**

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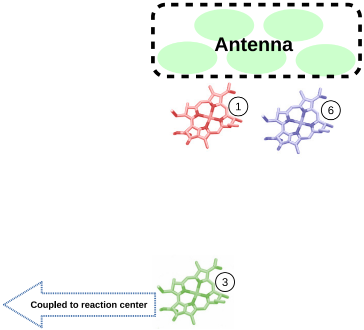

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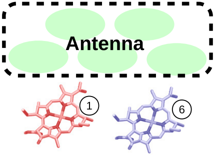

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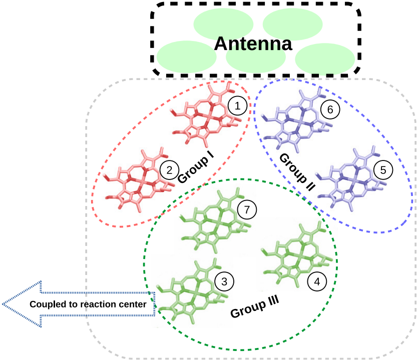

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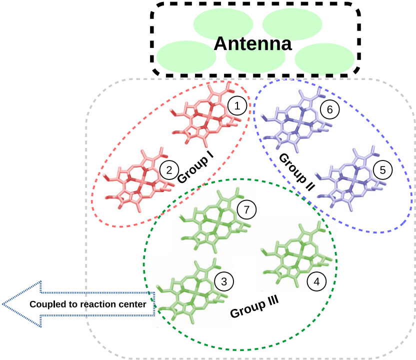

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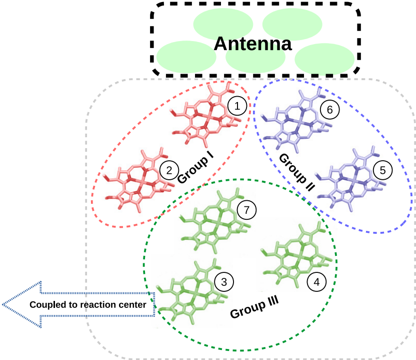

Can we predict the structure of FMO complex? **YES!!**

Take-Home Message : **Multiparty QC measures infer structural geometry of the system.**

Results

Detection of Energy Transfer Route

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Can we detect energy transfer route in FMO complex?

Results

Detection of Energy Transfer Route

Procedure :

- **Choose one initial state. E.g.** $|1\rangle\langle 1|$**.**
- **Investigate dynamics of the** $\{D_{i:R}\}$ **as functions of time.**

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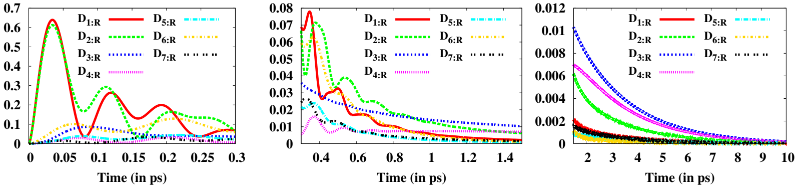

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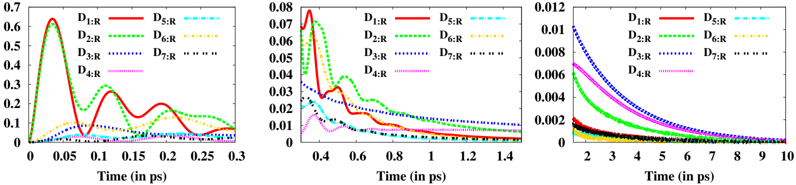

Time	Max$\{D_{i:R}\}$
0 – 0.4 ps	$D_{1:R}$ or $D_{2:R}$
0.4 – 0.8 ps	$D_{2:R}$
0.8 – 5 ps	$D_{3:R}$
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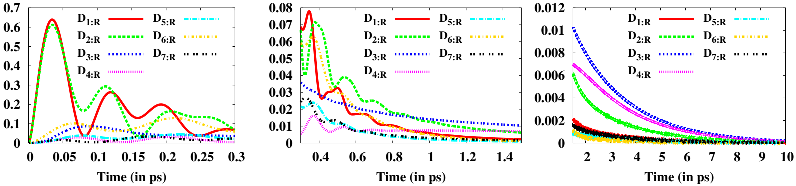

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- **Inference $\Rightarrow$ Primary energy transfer route: $1 \leftrightarrow 2 \leftrightarrow 3 \leftrightarrow 4$.**

Results

Detection of Energy Transfer Route

Similarly when the initial excitation is at site 6, we infer...

Primary energy transfer route: $6 \leftrightarrow 5 \leftrightarrow 4 \leftrightarrow 3$.

Results

Detection of Energy Transfer Route

Can we detect energy transfer route in FMO complex?

Results

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Yes!!! The primary one.

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Note : Other QC measures can also detect the route.

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Summarizing Results

1. **In general, multiparty correlations are more than bipartite one for negativity, opposite for quantum discord.**
2. **Discord monogamy scores decay faster than that of negativity. Opposite is true for bipartite contributions.**
3. **Discord monogamy score is negative most of the time, W-state like behavior.**
4. **Categorized seven chromophore sites into three distinct groups. $\Rightarrow$ Structural arrangements of different sites.**
5. **Primary energy transfer pathways detected by dynamics of multipartite quantum correlations.**

Collaborators

Ref : TC, Utkarsh Mishra, Aditi Sen(De), Ujjwal Sen, arXiv:1412.6519 [quant-ph]

Thank You!!!