LHI-RC complexes of Rhodobacter Sphaeroides: Superradiance, high efficiency, and adaptability

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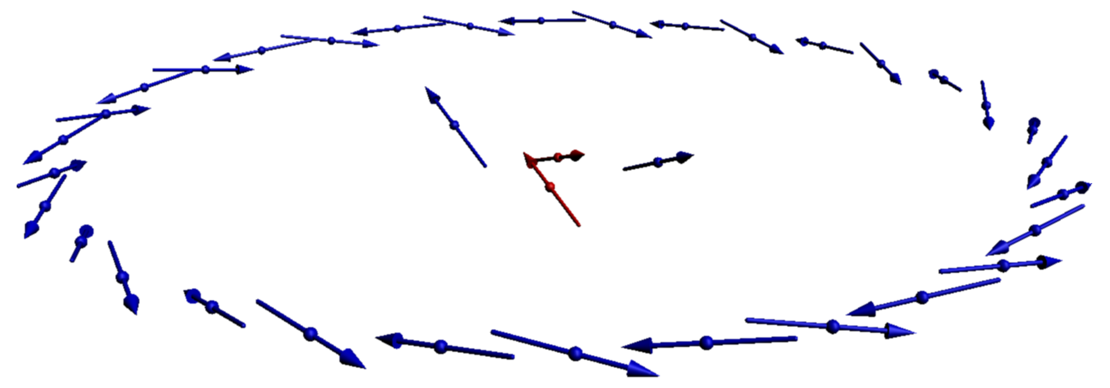
Abstract

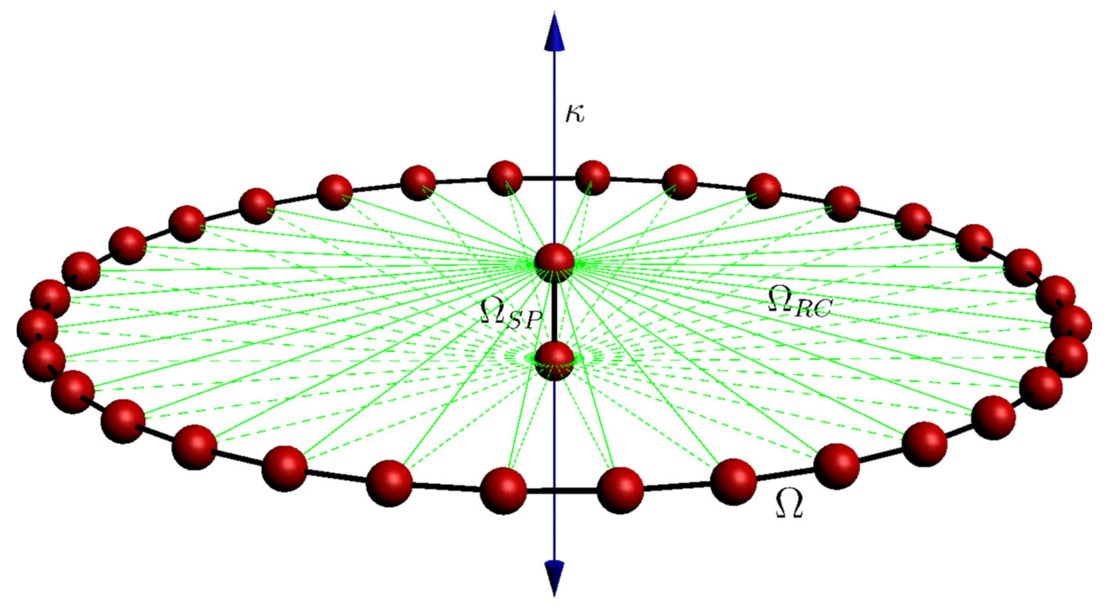
We study the Superradiance mechanism in different models for the Light Harvesting I-Reaction Center (LHI-RC) complex of purple bacteria, whose structure is shared by LH complexes of many organisms. At zero disorder a superradiant (small) and a subradiant (much larger) subspace of the single excitation state space can be characterized in terms of decay widths. As the static diagonal disorder increases, superradiance is destroyed, and subradiant states display a maximum in decay width and energy transfer efficiency. Interestingly, physiological values of the disorder lie around such a maximum, thus suggesting that Superradiance is exploited by nature to broaden the number of moderately efficient excited states, enhancing adaptability.

Three models for the LHI-RC complex

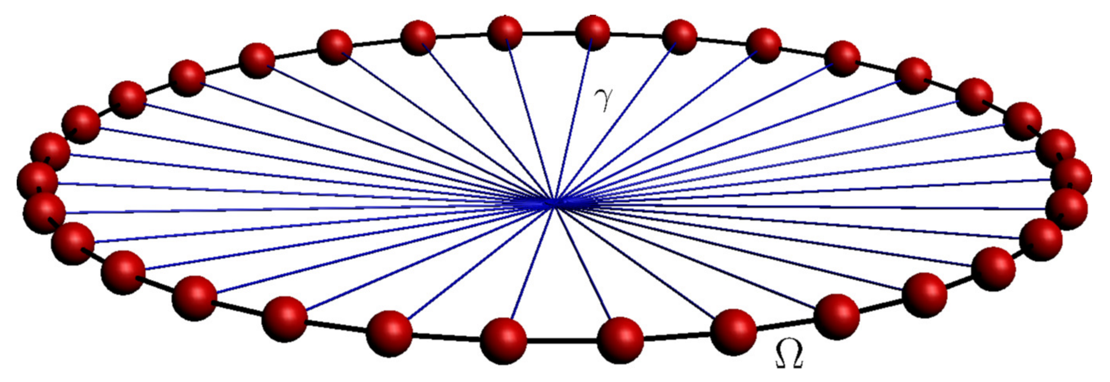
1) *n =32 two-level systems on LHI and 4 in RC*: experimental nearest neighbor and dipole interaction with opening on the RC special pair (red)



2) *32 two-level systems on LHI and 2 in RC*: tight binding ($\Omega = 600\,\mathrm{cm}^{-1}$, $\Omega_{rc} = 6\,\mathrm{cm}^{-1}$, $\Omega_{sp} = 1000\,\mathrm{cm}^{-1}$), opening $\kappa = 1\,\mathrm{cm}^{-1}$ on RC sites



3) *32 two-level systems on LHI*: tight binding model ($\Omega = 600\,\mathrm{cm}^{-1}$), *effective opening γ of each site towards the same channel*



Key features of Superradiance

segregation of decay widths: strong dependence of energy transfer efficiency on initial state

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interplay of opening and localization: different regimes as disorder strength increases

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superradiant subspace: higher efficiency up to critical disorder

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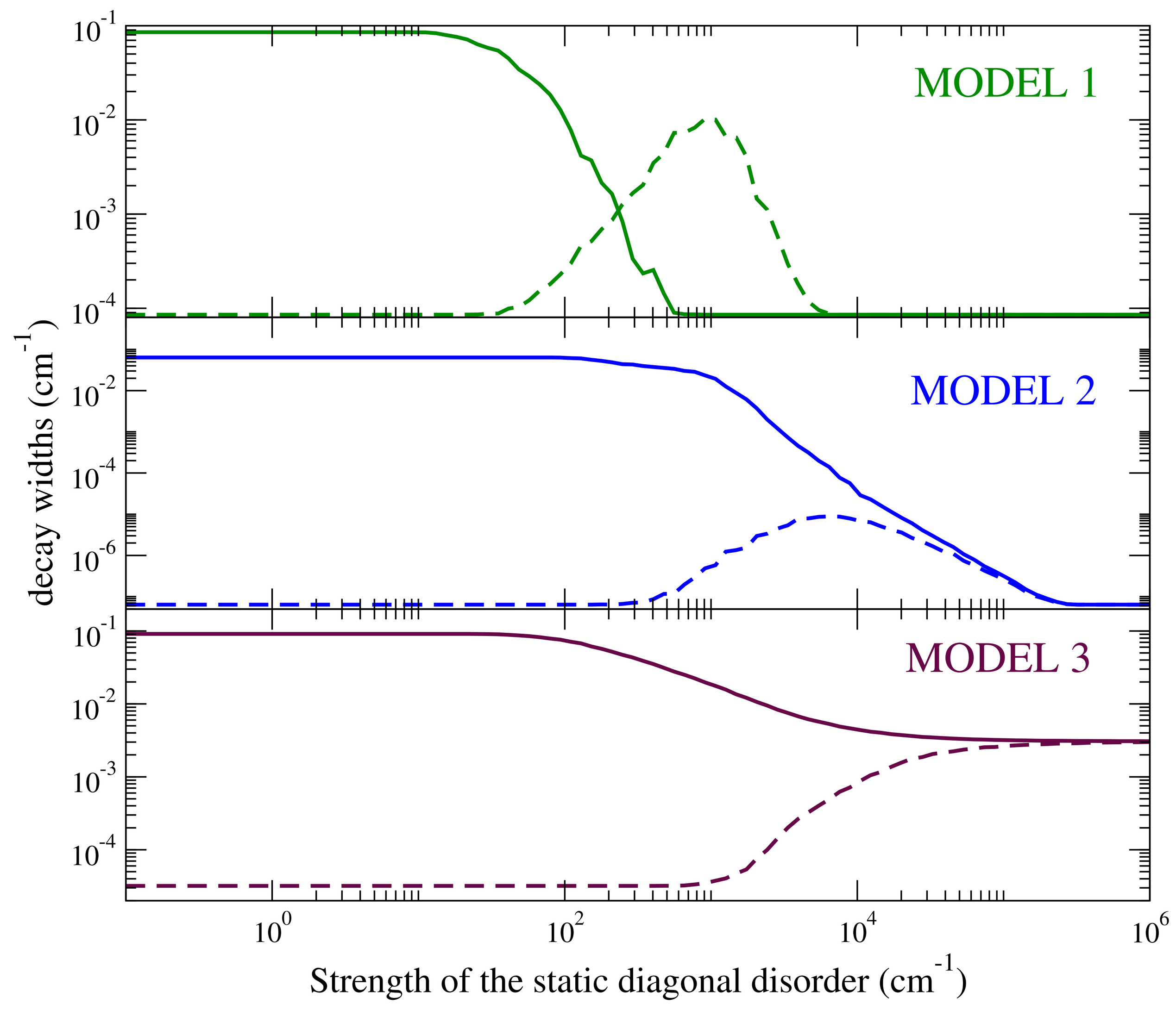
subradiant subspace: maximal efficiency at critical disorder

Evidence of Superradiance in the three models

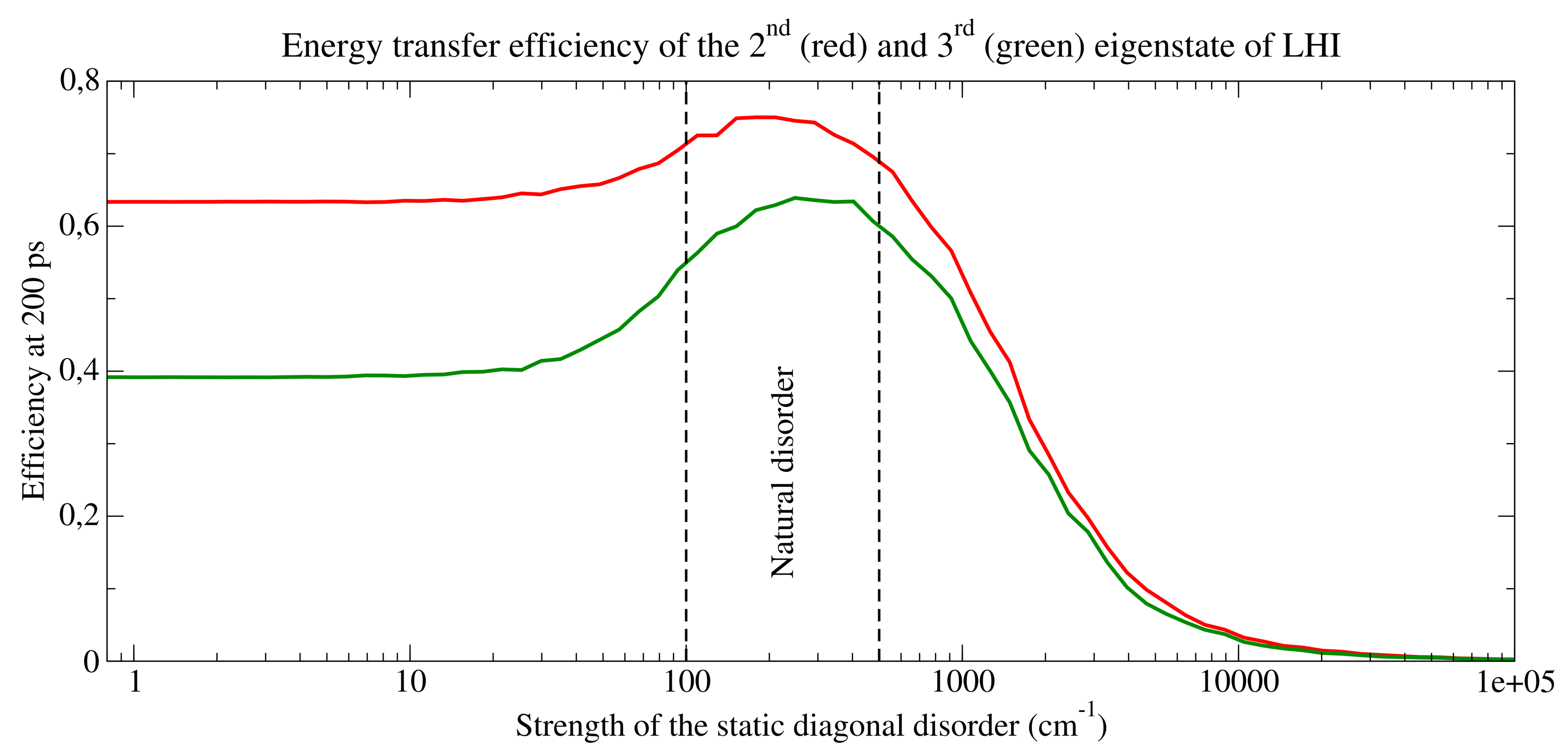
Decay widths of two paradigmatic states versus the strength of the static diagonal disorder: the completely **symmetric** superposition of the 32 excited sites on LHI (solid line) displays a typical **superradiant** behavior, whereas the completely **antisymmetric** superposition of the 32 excited sites on LHI (dashed line) displays a typical **subradiant** behavior.



Two relevant hybrid states in model 1

Due to the thermal environment, the **most likely populated** ring eigenstates are on the 2nd and 3rd energy level. It is then believed that the energy transfer associated with those states is the most relevant.

As it happens for most states, the 2nd and 3rd ring eigenstates are a superposition of super- and subradiant states, thus displaying a hybrid behavior: efficiency is relatively high at zero disorder, and remains independent of the disorder strength up to the transition region (*superradiant behavior*); in the transition region efficiency increases up to a maximum before eventually decreasing (*subradiant behavior*).



It is also very important to note that the **maximum of efficiency** is reached in a region which lies within the range of disorder strength (100–500 cm^{-1}) which is estimated to characterize the LHI-RC complex **in physiological situations**.

Effective opening γ of the reduced ring model for LHI

In model 2, within the single excitation approximation **at zero disorder**, 31 out of 34 energy eigenstates coincide with energy eigenstates of model 3: those states have no superposition with the open RC sites and no decay width is associated to them. Moreover, the antisymmetric combination of the RC site states is another eigenstate: it is clearly decoupled from the LHI ring and cannot be responsible for excitation transfer.

The two remaining eigenstates, the sole responsible for the excitation transfer, are a superposition of the completely symmetric combinations of LHI site states and RC site states. On the basis defined by such states, the two-dimensional coupling Hamiltonian H^c has matrix elements $H^c_{11} = 2\Omega$, $H^c_{22} = \Omega_{sp} - i\kappa$, and $H^c_{12} = \sqrt{2n}\Omega_{rc}$. In the regime $\Omega_{rc}/\Omega \ll 1$, the effective decay widths of the completely symmetric combination of LHI site states is given by

$$\Gamma_{LHI} = 2\min\{-\mathrm{Im}\,\epsilon_1, -\mathrm{Im}\,\epsilon_2\}\,,$$

where the ϵ_i's are the complex eigenvalues of H_c. Hence the effective opening strength in model 3 can be chosen as $\gamma = \Gamma_{LHI}/2n$.

Using model 3 with that effective opening, it is possible to obtain analytical estimates for the limits of the transition region in which Superradiance is destroyed in model 2.

The role of the geometric structure

The **cyclic organization** of chromophores in the LHI complex is crucial, since it allows for the onset of the Superradiant regime at zero disorder *for any opening strength*. To induce a superradiant behavior in linear assemblies, a critical opening strength must be reached, even at zero disorder.

The **breaking of cyclic symmetry** in the realistic model, due to the dipole coupling with the RC, is able to set the superradiant subspace of the system at low energies, so that they are likely to be excited even at high temperatures. On the contrary, in the cyclically symmetric tight binding models the superradiant states have the highest energy.

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