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E. Faraji - Quantum state transfer in protein α-helices.

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The Davydov model describes energy transfer in the hydrogen-bonded spines that stabilize protein α-helices. Its Hamiltonian has three parts: $\hat{H}$ =$\hat{H}$ ex+$\hat{H}$ ph+$\hat{H}$ int, where $\hat{H}$ ex is the exciton Hamiltonian (describing the internal amide-I excitations of the peptide groups), $\hat{H}$ ph is the phonon Hamiltonian (describing deformational oscillations of the lattice) and $\hat{H}$ int is the interaction Hamiltonian (describing the interaction of amide-I excitation with the motions of the lattice sites). The primary goal of the thesis project is to go beyond the energy transfer and study the full state transfer along the α-helix by considering the Hamiltonian $\hat{H}$ as corresponding to a spin network. Preliminary investigations on the phase dynamics, which only account for $\hat{H}$ ex, show the possibility of perfect state transfer between distant qubit. We suspect however that the addition of $\hat{H}$ ph+$\hat{H}$ int can wash out the coherence, and we are currently estimating the time scale of this effect. Subsequently, we will pursue the same goal by modifying the Davydov model. In particular, we plan to introduce physically motivated anharmonic terms in $\hat{H}$ ph and site-dependent coupling constants in $\hat{H}$ int. These could lead to coherence recovery and hence facilitate the quantum state transfer through the protein α-helices.