Excited state relaxation in vibronic model for bacterial reaction center

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Bacterial reaction center (BRC) is an important complex for photosynthesis. During photosynthesis charge separation occurs in this complex. Unsurprisingly it is an object of great interest for researchers. This complex is made up of 6 pigments. The whole complex looks mostly symmetrical, with two branches, but during charge separation one of the branches is favored. This makes excited state relaxation in BRC complex interesting.

The usual way to calculate relaxation rates needed to describe excited state relaxation is through the second order approximation together with Markov approximation, where the bath is averaged over. In vibronic model[1] a part of bath's degrees of freedom is included in Hamiltonian explicitly as harmonic oscilators (Fig. 1). The rest of the bath is treated approximately to second order. Thus vibronic model should provide a more accurate description.

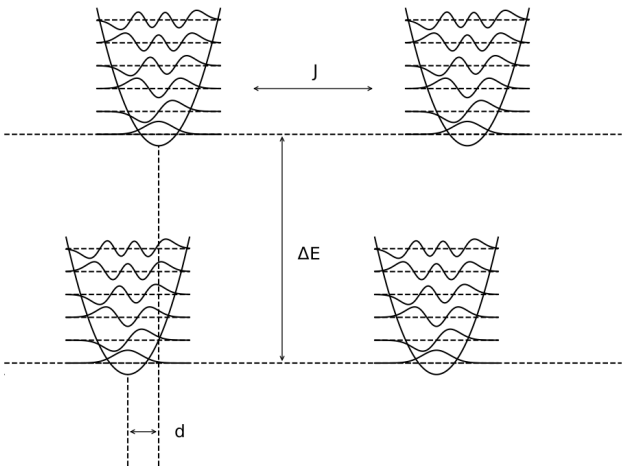

Fig. 1. Dsplaced harmonic oscilators vibronic model, J is electronic coupling amd d is displacement of harmnic oscilators in excited and ground states. .

Vibronic model application for BRC complex will be presented and excitation relaxation and relaxation pathways in BRC complex will calculated.

References:

[1] V. Butkus, L. Valkunas, D. Abramavicius, Vibronic phenomena and exciton-vibrational interference in two-dimensional spectra of molecular aggregates, J. Chem. Phys. 140, 034306 (2014).