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Dissipative dynamics of a hole transfer in two-strand model of DNA

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The capability to generate DNA molecules of designed architectures has allowed scientists to explore novel applications in various fields, including structural biology, drug delivery and creating new DNA microelectronic devices. The last application requires developing models with a detailed account of both the electronic and structural properties of DNA, as well as its interaction with fluctuating environment. In this work, an electronic hole transfer through artificial DNA is studied based on the tight-binding model accounting a double-stranded structure of DNA chain [1].

As a specific object of application of this model, an artificially created DNA oligonucleotide chain with a homogeneous fragment composed of N identical adenine-thymine pairs (A-T)N is considered. This fragment of a variable length N is enclosed between guanine-cytosine (G-C) end sections, which play the role of donor and acceptor centers for a moving charge. Dissipative dynamics of a hole carrier in this model is described by solving the Lindblad equation for the density matrix of the system, taking into account two types of dissipative processes: (a) a slow attenuation of the wave function of a charged carrier moving from a photo-induced donor to an acceptor, which is due capturing of the carrier by the environment, and (b) the loss of coherence of the carrier wave function caused by the dephasing effect of thermal noise of the environment.

Numerical solutions of the Lindblad equation in the qubit representation are found using the open source LindbladMPO code, which simulates elements of a quantum algorithm on a classical computer [2]. The calculated results are compared to available experimental data [3].

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