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Simulated Quantum Computation of non-equilibrium charge transport in a cyclic molecule.

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Molecular electronics may provide novel functionalities out of the scope of the traditional silicon-based electronics. This work is aimed at a study of a charge transport in a benzene molecule that is a representative member of a broad class of cyclic molecules. Due to many pathways for a charge propagation, quantum interference effects determine peculiar transport properties in these molecules, thus giving rise to new design principles in molecular electronics. At the same time, because the microelectronic molecular device is an opened quantum system, coupling of the molecule to its environment switches on several dissipation mechanisms and processes, which is expected to strongly influence the charge transport. To study this problem, the dissipative transport is described by the Lindblad master equation for the density matrix of the molecule coupled to a Markovian bath environment. The model of "molecule + bath"is represented in term of interacting qubits. Numerical solutions of the Lindblad master equation in qubit representation are obtained with the use of open-source solver based on matrix product operators (MPO) representation and called lindbladmpo (Qiskit Community GitHub (2022)).
Numerical solutions for charge transport characteristics are analyzed and interpreted. It is shown that interference effects may be weakened‘ due to dissipative processes, but still they survive if the coupling of the molecule to the bath environment is not too strong.

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