

Simulation of Electron Transfer on Noisy Quantum Computers

We present a framework [1] for the digital-analog simulation of open quantum systems governed by Hamiltonians with linear-vibronic coupling (LVC) and structured vibrational environments. Our approach exploits the intrinsic dissipation of qubits in near-term quantum hardware as a resource to emulate vibrational relaxation, combined with a model-specific error mitigation scheme to filter out noise sources incompatible with the target open system. We validate our strategy by resolving the vibronic transfer spectra of a one-dimensional donor-acceptor chain on IBM superconducting processors, reproducing non-Markovian dynamics and scaling the chain length up to 10 electronic sites, an unprecedented scale for chemical dynamics on quantum computers. Our model of vibronic electron transfer offers a portable, application-oriented benchmark for simulating long-lived entangled states on NISQ computers.

[1] Gajewski et al, Nat. Comm. 17, 4779 (2026)