Scaling Up Dynamics Simulation of Open Quantum Systems on NISQ computers

Marvin Gajewski[1,2]
Alejandro D. Somoza[1,2], Gary Schmiedinghoff[3], Pascal Stadler[4], Michael Marthaler[4] and Birger Horstmann[1,2,5]

[1]*Institute of Engineering Thermodynamics, German Aerospace Center (DLR), Wilhelm-Runge-Str. 10, 89081 Ulm, Germany*
[2]*Helmholtz Institute Ulm, Helmholtzstr. 11, 89081 Ulm, Germany*
[3]*Institute of Software Technology, German Aerospace Center (DLR), Linder Höhe, 51147 Köln, Germany*
[4]*HQS Quantum Simulations GmbH, Rintheimer Straße 23, 76131 Karlsruhe, Germany*
[5]*Department of Physics, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany*
marvin.gajewski@dlr.de

We analyse the performance of noisy, gate-based, digital quantum computers in simulating the dynamics of open quantum systems with electronic-vibrational (vibronic) interactions [1], where simulating large systems with local, vibrational environments remains a fundamental challenge [2]. We simulated a microscopic model of electron-transfer with a single donor and many acceptor sites (Figure 1), as relevant for electrochemical reactions and solar cells. Our approach takes advantage of the intrinsic dissipation in the quantum processor to simulate the nonequilibrium dynamics of the target physical system [3]. Our results reveal a probability of ET that is well aligned with numerically exact calculations where electronic and vibronic resonances can be identified at the expected driving forces (Figure 2). To access various regimes of electron transfer in quantum simulations, we discuss strategies to engineer the lifetime of vibrational motion and lay out the hardware requirements for scaling up simulations on NISQ computers.

References

[1] Manuscript in preparation
[2] A. D. Somoza et.al., Comm. Phys. Vol. 6: 65 (2023); doi: 10.1038/s42005-023-01179-z
[3] J. Leppäkangas et.al., Phys. Rev. A 108, 062424 (2023); doi: 10.1103/PhysRevA.108.062424

Figures

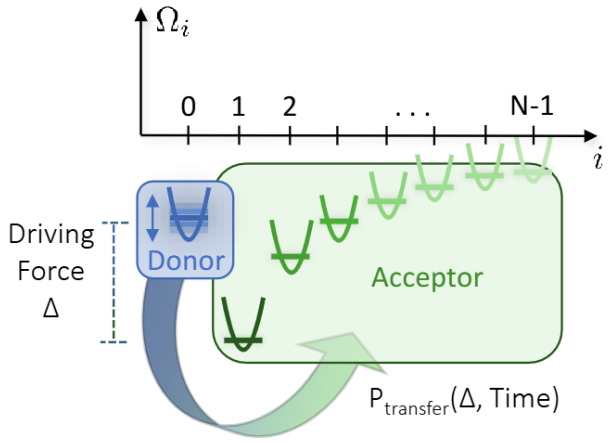

Figure 1: One-dimensional model of a donor-acceptor interface with nearest-neighbour interactions and local coupling to high-frequency quantized oscillators. We investigate the influence of vibronic coupling on electron transfer as a function of the driving force.

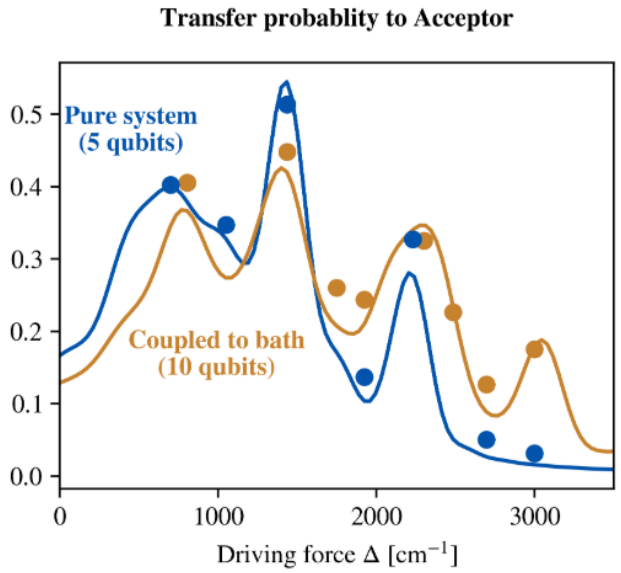

Figure 2: Emulated results for the time-integrated transfer probability $P_{transfer}$ (t) extracted from quantum dynamics simulations based on calibration data of IBM Heron chips, compared against numerically exact simulations of the open system in orange, and the system without vibronic coupling in blue.