Uncovering Resonance and Interference effects in Donor-Acceptor Reactions with a Bosonic Processor

Delmar G. A. Cabral,¹ Pablo E. Videla,¹ Brandon Allen,¹ Pouya Khazaei,² Rodrigo G. Cortiñas,^{4,5} Jorge Chávez-Carlos,³ Michel H. Devoret,^{4,5} Lea F. Dos Santos,³ Eitan Geva,² Victor S. Batista^{1,5}

¹Department of Chemistry, Yale University, New Haven, CT 06520, USA;
²Department of Chemistry, University of Michigan, Ann Arbor, MI 48109, USA;
³Department of Physics, University of Connecticut, Storrs, CT 06511, USA;
⁴Department of Applied Physics and Physics, Yale University, New Haven, CT 06520, USA; ⁵Yale Quantum Institute, Yale University, New Haven, CT 06511, USA;

Understanding the dynamics of reactions in open quantum systems remains an outstanding challenge of great current interest, relevant to a various donor-acceptor applications, including energy transfer, proton transfer, and electron transfer in molecular systems. In this study, we investigate the capabilities of bosonic quantum devices described by a Kerr-cat Hamiltonian for exploring quantum dynamics across a donor-acceptor barrier. Our findings reveal that the transfer dynamics from reactants to products exhibit intriguing resonances and interference effects, dependent on parameters that characterize the energetics and dissipative behavior of the system. Notably, the strength of dissipation significantly impacts the kinetics and efficiency of the reaction, suggesting the potential for engineering dissipative control of chemical reactions as an alternative to coherent control strategies. We demonstrate simulations utilizing the Kerr-cat Hamiltonian to model the dynamics of proton and electron transfer in molecular systems.