ANALOG QUANTUM SIMULATION OF MOLECULAR DYNAMICS AND SPECTROSCOPIC OBSERVABLES

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Modern computational techniques used to simulate quantum chemistry are on the boundary of tractability due to the exponential growth of the molecular wavefunction, requiring a careful balance between molecule size and simulation accuracy. In recent years, quantum computing has risen in popularity as a potential alternative to conventional (classical) techniques; however, most methods rely on access to "digital" quantum computers composed of qubits and quantum gates, which at present are severely limited by noise. We have developed a real-time, analog approach to simulate vibronic chemical dynamics with existing quantum technology. Our approach uses an intuitive mapping of molecular electronic and vibrational degrees of freedom onto quantum resonators and qudit (d-level system) states, with controllable couplings between degrees of freedom. The measurement output can be mapped onto different time-dependent observables, including the time-domain simulation of vibronic spectra. Our approach can also incorporate controlled sources of noise to simulate system-bath interactions and dissipative dynamics at a minimal cost. We present experimental results using a trapped-ion device, thus showing the potential for near-term simulation of chemical dynamics in complex environments beyond the abilities of classical computers.