Simulating electronic structure on bosonic quantum devices

Rishab Dutta,[a] **Nam P. Vu,**[b] **Ningyi Lyu,**[a] **Chen Wang,**[c] **Victor S. Batista**[a,d]

[a]*Department of Chemistry, Yale University, New Haven, CT 06520, USA*
[b]*Department of Chemistry, Lafayette College, Easton, PA 18042, USA*
[c]*Department of Physics, University of Massachusetts-Amherst, Amherst, MA 01003, USA*
[d]*Yale Quantum Institute, Yale University, New Haven, CT 06511, USA*

Demonstrating the capabilities of quantum computers as applied to molecular electronic structure calculations is a subject of great current interest. Significant efforts have already been reported using conventional qubit-based quantum computers, mostly based on the variational quantum eigensolver (VQE) methodology. However, calculations on bosonic quantum devices have yet to be reported. Here, we show how to map Slater determinants of fermionic systems and fermionic Hamiltonians into the corresponding states and Hamiltonians of bosonic quantum devices. Our findings open the door for a wide range of electronic structure calculations, and simulations of fermionic systems by harnessing the capabilities of bosonic quantum computers in general. A specific example of a bosonic device where near-term variational electronic structure calculations could be implemented is the 3-Dimensional circuit Quantum Electrodynamics (3D cQED) architectures. These are particularly attractive platforms where the quantum states are represented as states of microwave photons in the unbounded Hilbert space of the circuit bosonic modes. The nonlinearity necessary for control and readout procedures is provided by ancillary Josephson junctions. These devices offer favorable platforms for quantum error correction codes due to the well understood dominant source of errors in oscillator modes, namely, the single-photon loss. We anticipate that the larger volume of the bosonic Hilbert space should enable more flexible and efficient variational algorithms than the corresponding calculations in the subspace of fermions.