Design of Quantum-classical Computing Hybrid Algorithms for Materials Simulation

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Abstract

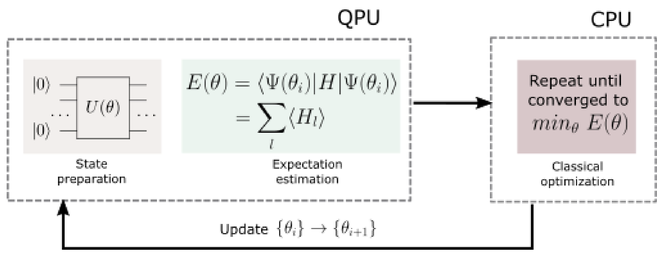
Accurately predicting properties of strongly correlated quantum materials is one of the grand challenges in many-body physics research. Classical methods for correlated materials simulation are computationally costly, in particular for complex materials with multi-orbitals and strong spin-orbit coupling. This complexity is intrinsic to the many-electron problem and arises from the exponential growth of the complexity of the electronic many-body wave function. To overcome these limitations, this project aims to leverage existing noisy intermediate-scale quantum (NISQ) computer technology to achieve highly accurate total energy calculations and to simulate quantum dynamics in correlated multi-orbital quantum materials. Specifically, we are determining the ground state solution quantum embedding Hamiltonians by implementing a **variational quantum eigensolver (VQE)**. This is feasible on NISQ devices, as it takes advantage of relatively shallow quantum circuits for error mitigation.

Background

- Finds eigenvalues of a (often large) Hamiltonian matrix
- Based on the **Variational principle**

$$E_0 \leq \langle\Psi|H|\Psi\rangle = \sum_{i=1}^{N} \lambda_i |\langle\Psi_i|\Psi\rangle|^2$$

- Takes advantage of NISQ-era devices as well as classical computing technologies.
  - ▷ Quantum subroutine is run inside of a classical optimization loop
  - ▷ Prepare and measure expectation value of the **ansatz**, $|\Psi(U(\boldsymbol{\theta})\rangle$
  - ▷ Optimize $\boldsymbol{\theta}$ until parameters converge and E_0 is reached
  - ▷ Variational methods have also been developed to target excited states $E_i,\ i > 0$ or time-evolved states $e^{-iHt}|\Psi_0\rangle$ [2]
- Models of interest include Hubbard and Heisenberg models.



Hamiltonian Variational Ansatz

- Different heuristic variational wavefunction ansätze have been proposed, often with physical insight such as keeping relevant excitations above a mean-field ground state (unitary coupled cluster ansatz UCC) or considering symmetry [3]
- The Hamiltonian Variational Ansatz (HVA) improves on unitary coupled cluster ansatz, which is a common ansatz used in quantum chemistry, by using rotations by terms in the Hamiltonian to reduce circuit depth [4]

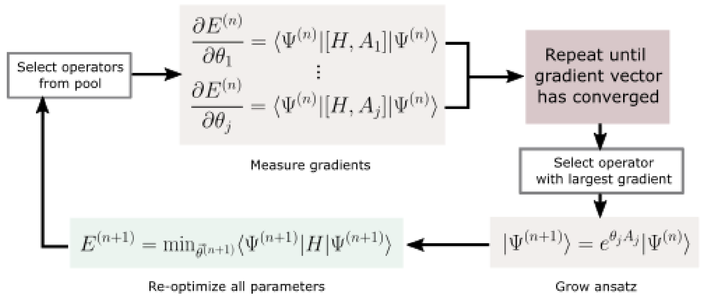
$$|\Psi_T\rangle = \prod_{b=1}^{S} \left(U_U\left(\frac{\theta_U^b}{2}\right) U_h(\theta_h^b) U_v(\theta_v^b) U_U\left(\frac{\theta_U^b}{2}\right) \right) |\Psi_I\rangle$$

- $U_x(\theta_x^b)$ approximates $e^{i\theta_x^b H_x}$ for $x \in \{U, h, v\}$, the interaction, horizontal, and vertical hopping terms
- Proposes two different optimization methods
  - ▷ **Global variational** optimizes all parameters for a fixed S
  - ▷ **Annealed variational** targets $H_{b/S}$ and optimizes the b ansatz step each iteration from $1, ..., S$

qubit-ADAPT

- Ansatz still might contain "useless" exponential terms. Can we alleviate that?
  - ▷ Dynamically build ansatz by selecting most important multi-qubit operators from an **operator pool**, $\{A_1, ..., A_j\}$ [5]
  - ▷ A new way of constructing the operator pool by exploiting the noncommutativity between different parts of the Hamiltonian.
  - ▷ $N_Y(O_{ij})$ is the number of Y gates in O_{ij}

$$\text{pool} = \{O_{ij} = [A_i, A_j] \text{ if } N_Y(O_{ij}) = 2k+1\}$$

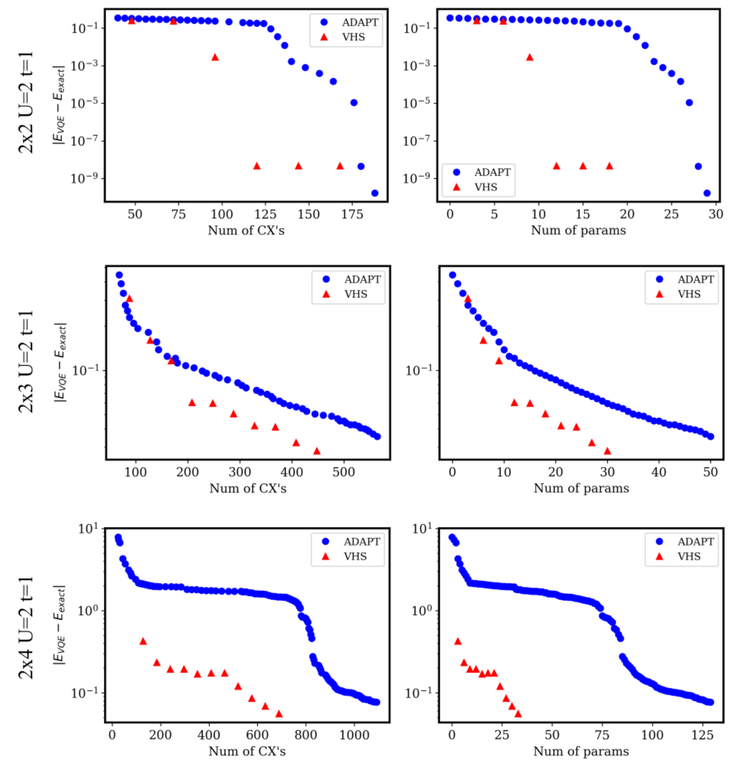


(Figure adapted from Ref. [6])

Results

- 4,6,8-site Hubbard model. Two-legged ladder with periodic boundary conditions

$$H = -t\ \Sigma_\sigma (c_\sigma^\dagger c_\sigma + h.c.) + U\ \Sigma_i n_{i\uparrow} n_{i\downarrow}$$



- Larger systems can be solved by solving two decoupled smaller systems and "stitching" them together with another VQE cycle
- Feasibility of running on NISQ devices is still in question due to the many measurements needed as well as the number of CNOT gates in the ansatz

References

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