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HIGHLIGHTING NEWS

BOOTSTRAP EMBEDDING ON A QUANTUM COMPUTER

This paper is talking about how they make molecular bootstrap embedding available to quantum computing. Embedding method allows problem of electronic structure form a large molecule to be solved by cutting the total system into fragments with part of them overlapped. Bootstrap is a method often used in statistics which works like this: each extracted sample has part overlapping with others.

Molecules can be applied on the devices available so far after embedding into smaller fragment. Originally, terms of the molecule grows exponentially with respect to the number of electronic orbitals. Embedding not only decreases the terms needed to be calculated in the same time, but also lets the terms only grow polynomially with the number of electronic orbital in a fragment. It achieve this by sacrificing some entanglement between the fragment and its environment. Bootstrap method comes to fix this problem.Bootstrap method is used in calculating molecule for making desired value of each fragment more precise by iterating the algorithm til the values of the overlapped region matched.

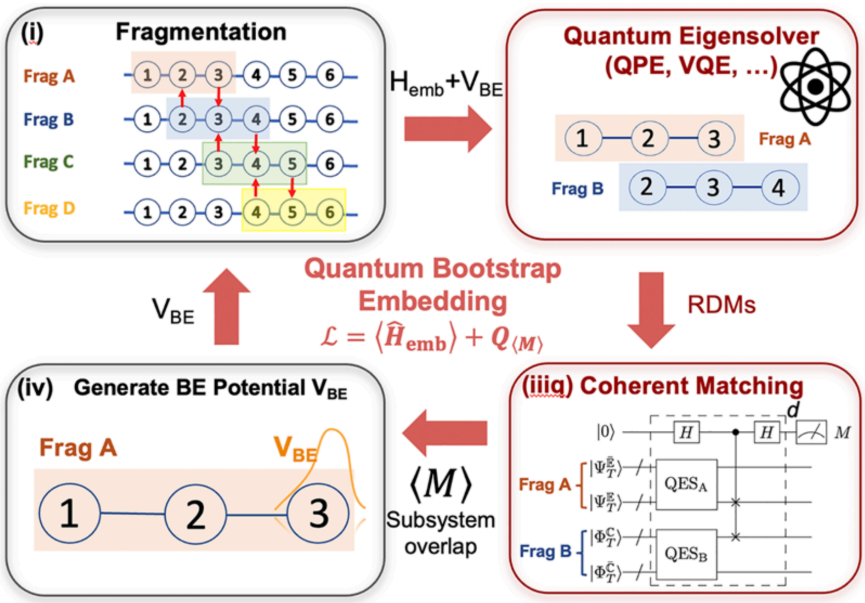

Figure form: Bootstrap Embedding on a Quantum Computer

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A VARIATIONAL QUANTUM COMPUTATIONAL CHEMISTRY SIMULATOR WITH MATRIX PRODUCT STATES

It is intuitively to think of applying quantum computing on chemistry, since they are both nature system. Nowadays, quantum computers are still developing, a large-scale, fully fault-tolerant quantum computer has not yet showed up to the world. Methods like variational quantum eigensolver (VQE) appear to solve the quantum chemistry problem on noisy intermediate-scale quantum (NISQ) devices. Classical simulating play an important role in the development of these algorithm and on validating result of NISQ. However, the memory needed to perform VQE on classical simulation grow exponentially with respect to the number of used qubits. This paper provides a VQE simulator based on the matrix product states (MPS) method from quantum many-body physics. With this method, memory requirement only grows polynomially when the number of required qubits increased.

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