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Simulating Quantum Systems Using the D-Wave Quantum Computer

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Simulating complex quantum systems is an inherently difficult task for classical computers due to the exponentially increasing computational costs of solving the Schrödinger equation. To overcome this challenge, quantum computers were proposed to naturally simulate quantum systems as qubits, enabling larger systems such as molecules to be accurately simulated. We here demonstrate how such simulations are possible on D-Wave Systems' quantum computer, although we find that our current algorithm is not an improvement over calculations on classical computers.

While quantum computation is still in its infancy, pioneering computers such as the D-Wave have shown promise in their ability to outperform classical computers for well-suited problems. The D-Wave machine is based on a quantum annealing design, as opposed to a universal-gate design. As such, the D-Wave is most useful for solving optimization problems, and any problem must be written in the form of a quadratic, unconstrained, binary optimization (QUBO) problem in order for the D-Wave to be used.

As a demonstration of the techniques used, we have chosen to start with a relatively simple quantum system consisting of two electrons in an external magnetic field, which has been used as a simple model for the entanglement of the H_2 molecule. Such a system has the benefit of having a Hamiltonian of the form of tensor products of Pauli spin variables, allowing the calculation of the ground state energy to easily be transformed into a QUBO as demonstrated in Xia et al. [J. Phys. Chem. B 2018, 122, 13, 3384-3395]. In the future, we plan on extending our work to small molecules such as H_2 and H_3^+ with few valence electrons. Such systems have the added complication that the Hamiltonian must first be discretized by writing it in second quantized form. The STO-nG basis sets are particularly useful for the orbitals, as the overlap integrals are relatively easy to calculate. Then, using either a Jordan-Wigner or Bravyi-Kitaev transformation, the Hamiltonian can be written as a tensor product of Pauli spin variables, as in our example system.

To write the example Hamiltonian in the form of a QUBO, we first transform it into a tensor product of Pauli spin variables of the same direction. Such a transformation is only approximate and necessarily introduces ancillary qubits, the number of which determine the accuracy of the approximation. The Hamiltonian then must be reduced to a quadratic form with the same ground state. Finally, the Pauli spin variables are then converted to binary variables with another simple transformation. The coefficients of the resultant Hamiltonian can then be fed to the D-Wave as a QUBO.

After simulating the example system on the D-Wave, we find that the calculated ground state energy aligns well with the exact value, which can be found by diagonalizing the original Hamiltonian. The majority of the computational cost for the procedure lies in transforming the Hamiltonian into a QUBO. The number of terms required to represent the Hamiltonian as a QUBO rapidly increase as the complexity of the system and desired accuracy increases. For this reason, we believe it necessary improve the transformation process or find an alternative transformation to simplify the problem before such calculations on the D-Wave truly outperform classical computers.