Scalable Quantum Simulation of Molecular Energies

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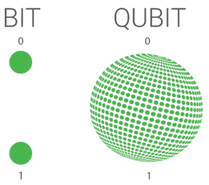
A new era for computing

Quantum computing is a rapidly advancing field predicted to have important applications, some of which are encryption, communication and the development of new medicines and materials.

Quantum computers are not considered to be a replacement for classical computers; they will only be useful for certain types of problems which are too difficult for classical computers to solve, such as simulating quantum systems in chemistry.



Such quantum simulations would enable a leap forward in our understanding of fundamental chemistry, and reduce the need for lengthy and expensive trial-and-error techniques used to develop new medicines and materials.

Key terms

Qubit A quantum bit of information. A classical bit represents classical information and is encoded in ‘0’s and ‘1’s.

Superposition A qubit can be in two states (‘0’ and ‘1’) simultaneously. In contrast, a classical bit is either just a ‘0’ or ‘1’.

Quantum simulations in chemistry Quantum theory describes phenomena happening at the smallest scales imaginable. A quantum computer uses quantum phenomena to boost computing power in simulating chemistry processes.

Algorithm A set of instructions, usually ran using a computer, used to find solutions to a problem.

What are the techniques?

The work done in the paper ‘Scalable Quantum Simulation of Molecular Energies’ uses qubits kept at very low temperatures to run two different algorithms, the variational quantum eigensolver (VQE) and the phase estimation algorithm (PEA), to find information about the fundamental properties of molecules. A special type of qubit known as an Xmon is used to run the algorithms; it runs using a superposition of “charge” states.

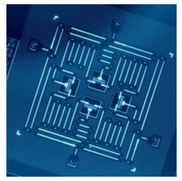


Figure 1: IBM qubit

The qubits used to run the algorithms were a type of charge qubit that is kept at very low temperatures and is similar to this IBM qubit.

Algorithms for Quantum Chemistry

VQE uses the averages of the total energy to calculate the energy of a molecule.

1. Prepare a starting state.
2. Measure the total energy for each distance between the molecules. We must select the lowest value (the ground energy).
3. Use a tool to find more lower values of the total energy.
4. Repeat until we reach the smallest value possible.

PEA estimates the index value over exponential coefficients to calculate energy of a molecule.

1. Prepare a starting state, and encode information onto an exponential coefficient.
2. Some equipment must be set up in a superposition of states - this will make it possible to measure the state.
3. Use operations to set up the state and the apparatus so that it is ready to be measured.
4. Measure the state to find the lowest value of the total energy. We repeat this process until find an accurate value of the total energy.

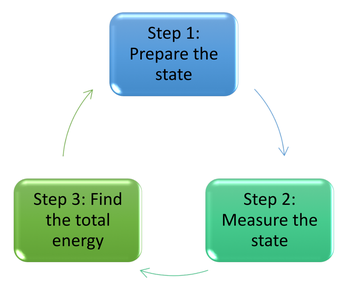


Figure 2: VQE

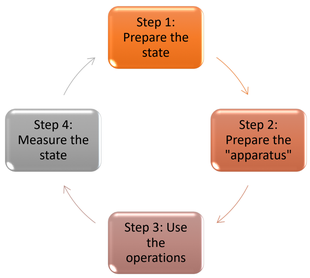


Figure 3: PEA

Outlook

VQE works better than PEA because it gives more accurate results, as shown in Figure 4. The ability to simulate the quantum behaviour of atoms and molecules could offer new avenues for increasing our understanding of the world around us, and our ability to develop new medicines and materials!

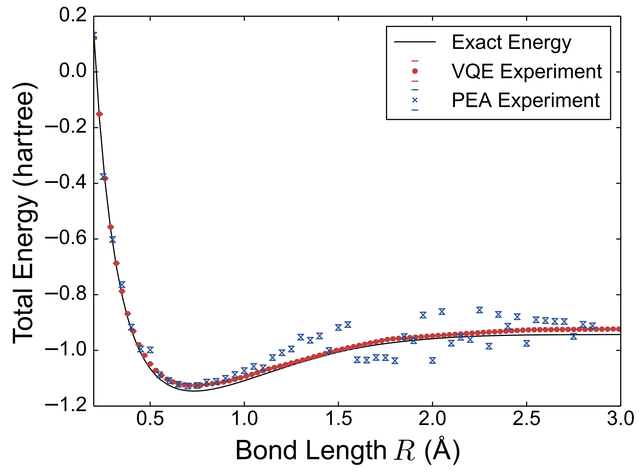


Figure 4: Computed H_2 energy curve, energy surface of molecular hydrogen as determined by both VQE and PEA