Scalable Quantum Simulation of Molecular Energies

Shuhao Yang[1], James Mills[1], and Shanice St John[1]

[1]Department of LaTeX Studies, UCL

Introduction

Quantum computing is a rapidly advancing field predicted to revolutionise many areas of science and technology. It is predicted to have important real-world applications in encryption and communication systems and in the development of new medicines and materials to name but a few. An important point is that these quantum computers are not considered a replacement to classical computers, they will only be brought to bear on certain types of problems which are too difficult for classical computers to solve. Classical computers is a term used to describe all everyday computational computing devices which rely on classical (non-quantum) phenomena to compute.

Highlight boxes

Qubit For representation, we describe information as qubit in quantum mechanics. It is an analogous concept of the classical bit in which classical information is encoded in 0s and 1s. For the information stored in a qubit can be represented by a state.

Superposition A qubit has extraordinary property, which can be in both states of '0' and '1' at the same time, but a classical bit is either '0' or '1'.

Algorithm A set of instructions used to solve a problem, especially by a computer. The instructions are created so that it can be understood by the computer. This is then sent to the quantum computer. The computer then follows the instructions using some program or software. The end of the process provides an answer or even many possible answers.

Quantum simulations in chemistry Quantum theory is our best description of phenomena happening at the smallest scales imaginable. Simulating quantum systems with classical computers is extremely difficult, and becomes increasingly difficult as the size of the system increases. Quantum simulations with quantum computing hardware are much easier, as we are using quantum phenomena (the same phenomena that make the system difficult to describe with a classical computer) to boost our computing power.

Techniques in Paper

VQE and PEA are two types of algorithm which is performed by a special type of computer known as the quantum computer.

VQE

- Firstly, we start by preparing a state using a "special" method. This method makes it possible for the algorithm run in the way that we want.
- Secondly, we measure the total energy for each value of the distance. We must select the lowest value as we are focusing on the ground energy.
- After that, a tool is then used to find more lower values of the total energy.
- All steps are repeated until we reach the smallest value possible.

PEA

PEA is the algorithm estimate the value of index over exponential coefficient in order to work out molecule energy.

- Similarly to the VQE algorithm, we must prepare a state using another "special" method since these are two different algorithms.
- Next, some "magical" equipment must be set up in a superposition of states - this will make it possible to measure the state.
- Then, we use some operations to set up the state and the apparatus so that it is ready to be measured.
- Finally, we 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.

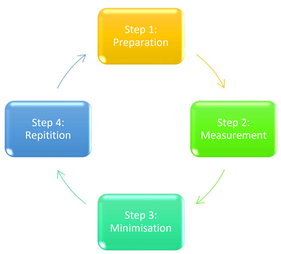

Figure 1: VQE

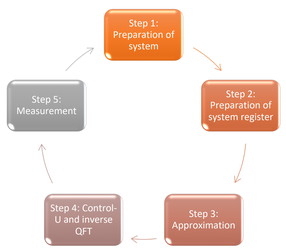

Figure 2: PEA

Conclusion and Outlook

Simulating systems in quantum chemistry is one of those problems too difficult for classical computers. If we can efficiently simulate quantum chemistry experiments it would enable a dramatic leap forward in our understanding of fundamental chemistry, and be hugely impactful to a number of fields of endeavour. For example it would significantly reduce the need for cumbersome and expensive trial-and-error techniques in the development of new medicines and materials.