

Scalable Quantum Simulation of Molecular Energies

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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 too difficult for classical computers.

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.

Highlight boxes

The `\highlightbox` command inserts a coloured box, the default colour is a lighter version of the banner colour.

Qubit For representation, we describe information as qubit in quantum mechanics. It is an analogous concept of bit in information theory as we used in classical computer.

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.

Qubit

Techniques in Paper

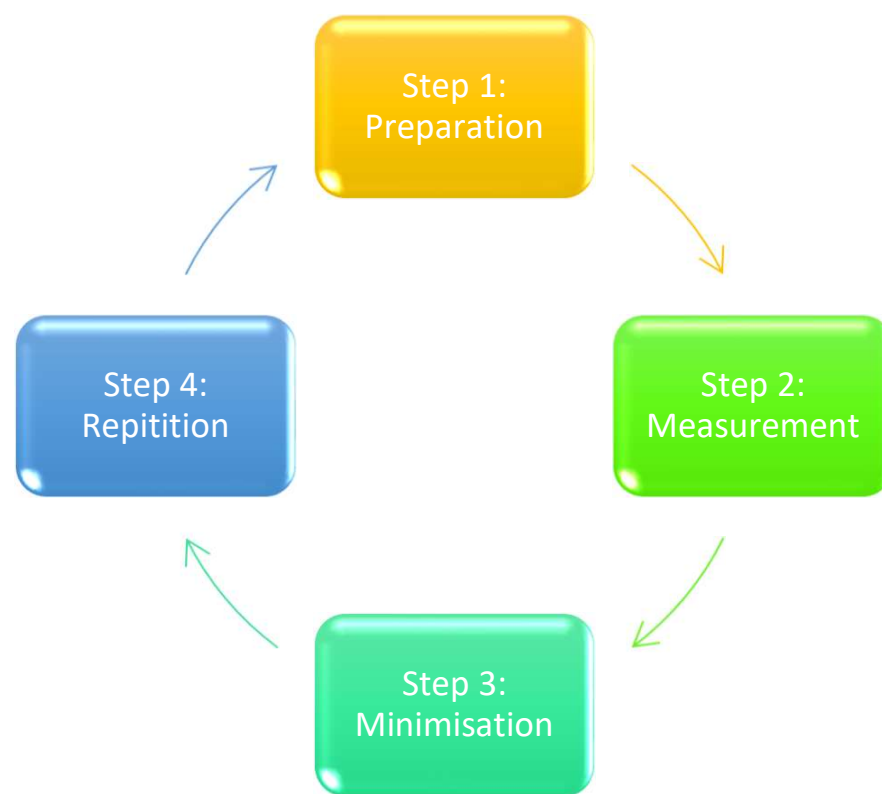


Figure 1: VQE

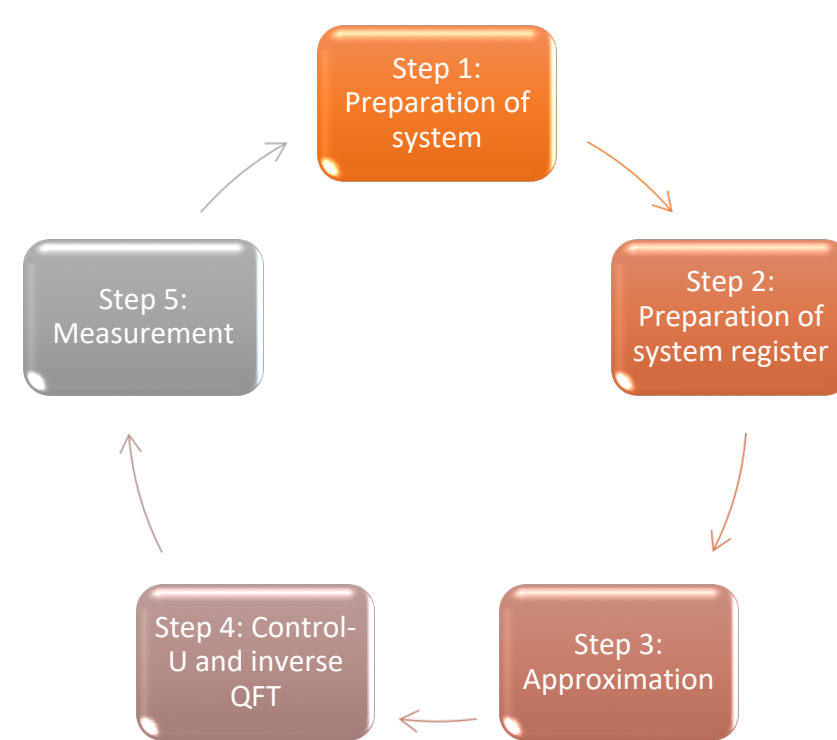


Figure 2: PEA

Conclusion and Outlook

The colour of a `\highlightbox` can also be changed.