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Optimization of quantum algorithms for near-term quantum computers

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Summary

A quantum processing unit or quantum computer is a device that uses the laws of quantum mechanics to perform calculations. The interest in quantum computation and quantum algorithms arises from the fact that these machines can solve some problems much faster than classical computers, what is commonly known as quantum speed-up. Contrary to what one might think, quantum computers will never replace classical computers. They will, most likely, become integrated within large supercomputers and will be used for purpose-specific tasks where the quantum speed-up can be exploited. In the past decade outstanding progress has been achieved in building prototypes of quantum computers, albeit small, fragile and error prone. While a large-scale, noise-free quantum computer is still years away, we expect to have access to quantum hardware sufficiently large to challenge the limits of classical supercomputer. This thesis covers most of the aspects that affect noisy quantum computers when combined with classical computers.

One of the most challenging aspects of existing quantum computers is the fact that they are extremely error-prone. If we aim at providing accurate calculations from such devices it is important to remove or mitigate errors as much as possible. In chapter 2 we develop the theory of a strategy to mitigate errors using the fact that problems in physics and chemistry have known properties that must remain unchanged, commonly known as symmetries (e.g. number of particles, number of spin-up/down particles, parity, amongst others). By measuring one or more of such properties and verifying that they remain unchanged from their known value we are able to identify when errors have occurred. The final computation is improved by removing the calculations in which the symmetries have been changed. In chapter 3 we put the theory of symmetry verification to work on a real two-qubit quantum device for the task of calculating the lowest energy of the hydrogen molecule. The proposed error mitigation strategy shows a ten-fold improvement in the accuracy of the calculation.

Even for a moderate size quantum computer of ≥ 50 qubits, the amount of classical memory required to store its full description is astronomical. As such it is unfeasible to extract all the information of a quantum computer. A quantum algorithm must, therefore, use only partial information

of the quantum state. In chapter 4 we explore what and how to extract the relevant information of a quantum computer for calculating properties of physical and chemical systems. Our main contribution is a proof on the minimum number of circuits required to extract properties beyond the energy for chemistry and physics problem from their reduced density matrices. Additionally, we provide a recipe to construct measurement circuits that exactly match the minimum number analytically calculated for 2-reduced density matrices.

The journey continues with the analysis of the performance of optimization algorithms in the context of variational quantum algorithms. An optimization algorithm is a piece of (classical) software that attempts at finding the set of parameters that minimize (or maximize) a mathematical function. Computer scientists have devoted decades of research to develop, study and benchmark optimization methods for a wide variety of (classical) problems. However, a systematic study of their performances when used in combination with quantum hardware is still lacking. Chapter 5 is an attempt of filling this gap by comparing some of the most used optimization algorithms in a subset of toy models in physics and chemistry.

In recent years public and private quantum computer laboratories have made small quantum computers accessible via internet services. Thanks to these cloud-based quantum devices research in quantum computation has democratized, showed by the fact that hundreds of articles are published every year from researchers all over the world. In chapter 6 we run a toy experiment with the Dutch public quantum computer infrastructure Quantum Inspire. We find that internet communication comes with large delays, which in turn affect the performance of the computation because of the short lifetime of the hardware, even for such a very small problem. Therefore we anticipate that performing large calculations on cloud-based quantum computers will be problematic.

In the last chapter of the thesis we explore an application of quantum computers in quantum chemistry, the calculation of energy derivatives. We describe a method to compute energy derivatives in near-term quantum hardware. The method is then used to optimize the geometry of the model of the hydrogen molecule as well as its polarizability with a real two-qubit device. Finally we verify the results of the experiment with extensive simulations finding a really good agreement in both, the simulation of the chemistry and the simulation of the experiment.