The power of one qubit in quantum simulation algorithms

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Summary

Quantum computing is an emerging technology, holding the potential to simulate complex quantum systems beyond the reach of classical numerical methods. Despite recent formidable advancements in quantum hardware, constructing a quantum computer capable of performing useful calculations remains a challenging task. In the absence of a reliable quantum computer, the study of potential applications relies on mathematical methods, ingenious approximations, and heuristics derived from the application fields. This thesis focuses on the development of quantum algorithms with applications in the simulation of complex quantum systems.

The introductory chapter outlines the challenges of quantum simulation, identifies and formalizes key simulation targets, and reviews successful quantum and classical simulation algorithms. Using the simulation of chemical systems as a prototypical example, the chapter then guides the reader through the quantum simulation development pipeline.

Subsequent chapters introduce and detail novel algorithms for quantum simulation, all connected by the common thread of introducing a single auxiliary qubit into the simulation algorithm. This qubit (a fundamental unit of quantum information) plays an active role in each algorithm, serving as a key element in their constructive design. The significance of working with a simple system, such as a qubit, becomes evident throughout the thesis, proving essential from both fundamental and applicative perspectives.

Chapter 2 explores simulating cooling through a single-qubit emulated fridge. In Nature, systems cool down by interacting with large cold environ-

ments, where they can dissipate heat and entropy. While simulating such baths is theoretically possible, it comes with a significant computational burden. We propose to substitute the environment with a single auxiliary qubit, which is periodically reset to its low-energy state allowing to extract heat and entropy from the system, analogous to the functioning of a fridge. Our investigation of single-qubit fridges leads us to introduce a category of algorithms designed for preparing low-energy states of simulated systems, which we name quantum digital cooling. We describe various possible approaches to quantum digital cooling, characterizing them with analytical and numerical tools.

The following three chapters relate to Echo Verification – a novel error mitigation technique first introduced in chapter 3. Quantum devices present a significant challenge due to their inherent noise, leading to the gradual corruption of stored and processed data and ultimately causing computation errors. Quantum hardware research aims to reduce noise levels, with long-term prospects for quantum error correction to solve this problem. Meanwhile, any effective quantum algorithm must be designed with resilience to noise in consideration. Error mitigation techniques play a crucial role in providing this resilience.

The error mitigation technique introduced in chapter 3 prescribes to measure a single bit of information from a state of the simulated system, while using the remaining quantum information to detect errors and contrast their effect. This approach is implemented through a method reminiscent of Loschmidt's echo, as the single-qubit measurement is sandwiched between two computations which mirror each other in time. Echo verification is readily applicable to a wide variety of quantum algorithms tailored to near-term devices. We explore its application to expectation value estimation and single-control quantum phase estimation, conducting numerical benchmarks on simulations of small quantum chemistry and magnetism models. The adoption of this technique resulted in the most extensive experimental test of a variational quantum algorithm for chemistry.

In chapter 4, we study the theoretical limits of the measurement model imposed by echo verification, wherein a single bit of information is extracted per state preparation. This model aligns to the general category of binary measurements, representing yes-no questions that can be posed about a quantum state, holding theoretical significance beyond the scope of echo verification. We develop a framework to optimize measurements of expectation values within this model, and demonstrate a substantial improvement in performance compared to a naive approach.

In Chapter 4, we explore the utilization of echo verification in a distinctly

different context: mitigating algorithmic errors in the adiabatic algorithm. The adiabatic algorithm is an important technique utilized to prepare fundamental states of a simulated system. While the adiabatic theorems ensure its success in the limit of infinite computation time, practical finite-time computations are susceptible to systematic errors. This error is of different nature from the stochastic hardware error typically addressed by mitigation techniques. We introduce a technique that allows to convert the systematic error into a stochastic one, enabling the application of echo verification to suppress its effect.

Finally, chapter 6 explores a potential application of near-term quantum computers in quantum chemistry: the detection of conical intersections in a molecular model. Much of quantum chemistry relies on the Born-Oppenheimer approximation, which separates the description of nuclei and electrons. Conical intersections are significant points in the geometry of a molecule, where the Born-Oppenheimer approximation breaks down. This facilitates processes like non-radiative relaxation, holding particular significance in the study of photochemical reactions. Conical intersections are characterized by a property called Berry phase, which can only take the discrete values of 0 or π. We design a quantum algorithm that allows to discern these two values, represented in a single bit of information. The inherent discreteness of the result renders the algorithm resilient to a certain amount of noise. We provide analytical proof of this resilience, and we conduct numerical testing on a molecular toy model designed to reproduce some behaviors of the biochemical system responsible for light perception.