PhastLearn: Fast Phase-Transition Prediction with Quantum Machine Learning

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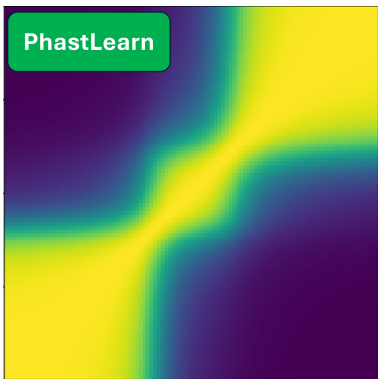
Abstract:

This paper presents "PhastLearn," a novel quantum machine learning (QML) framework designed for fast and scalable prediction of phase transitions within quantum systems. Leveraging the synergistic potential of quantum computing and machine learning, "PhastLearn" integrates with the PennyLane software and a multi-GPU framework, achieving significant computational acceleration and scalability. Our contributions include the development of a scalable QML model, its application to predicting phase transitions in the transverse field Ising model and the XXZ model, and an exploration of its performance across various system sizes and configurations. The framework demonstrates the potential of QML to overcome computational bottlenecks in phase transition prediction, setting a new benchmark for speed and scalability in QML applications.



1 Introduction

Understanding phase transitions within condensed matter physics involves navigating the intricate dynamics and vast state spaces of quantum systems, a challenge that has traditionally pushed the limits of computational physics [1]. The emergence of Quantum Machine Learning (QML) marks a pivotal advancement, blending quantum computing's robust computational capabilities with machine learning's analytical prowess to unlock new frontiers in phase transition analysis [2–4]. However, realizing the full potential of QML for phase transition prediction necessitates overcoming significant computational bottlenecks, particularly in terms of model scalability and computational speed.

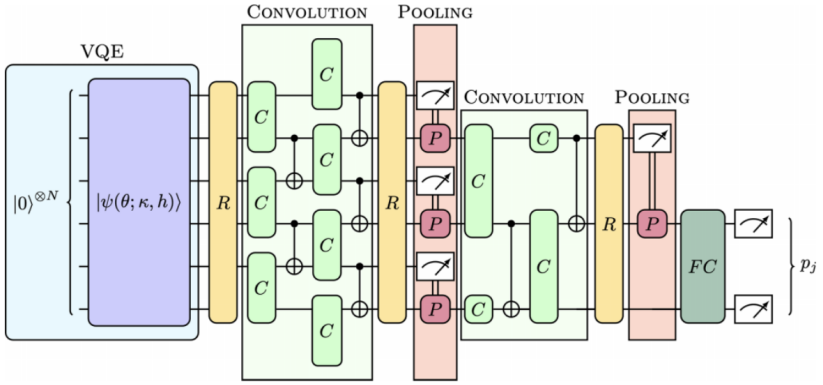


Figure 1: Circuit Architecture: VQE states serve as input for a quantum convolutional neural network, composed of free rotations R, convolutions C, pooling P, and a fully connected layer F. [5]

In this context, we introduce "PhastLearn," a cutting-edge framework designed to leverage the synergistic potential of QML for rapid and scalable prediction of phase transitions. "PhastLearn" distinguishes itself through its integration with PennyLane, a powerful and versatile quantum machine learning software package that facilitates the development and optimization of quantum circuits on quantum computers (and quantum simulators). By harnessing PennyLane's capabilities within a multi-GPU framework (supported by cuQuantum), "PhastLearn" achieves remarkable computational acceleration and scalability, enabling the analysis of complex quantum systems with unprecedented efficiency.

PennyLane's unique feature set, including its ability to interface seamlessly with classical machine learning libraries and its support for gradient-based optimization directly on quantum hardware, makes it an ideal platform for "PhastLearn." This integration not only enhances the computational efficiency of our QML models but also simplifies the implementation of complex quantum-classical hybrid algorithms, thereby expanding the scope and applicability of our research in phase transition prediction.

The primary objective of "PhastLearn" is to address the computational challenges currently limiting the application of QML to the domain of phase transition prediction [6]. By leveraging the computational power of multi-GPUs and the advanced quantum computing functionalities provided by PennyLane, our framework sets a new benchmark for speed and scalability in QML applications. Our contributions include the development of a scalable and efficient QML model, the demonstration of its application to predicting phase transitions in the transverse field Ising model and the XXZ model, and an exploration of its performance across various system sizes and configurations [7].

The paper is structured as follows: Section II provides an overview of the theoretical underpinnings of phase transitions and introduces the foundational concepts of Quantum Machine Learning, with a particular focus on PennyLane's role in advancing QML research. Section III details the architecture and implementation of "PhastLearn," emphasizing the integration of PennyLane within our multi-GPU framework. Section IV presents the results of applying "PhastLearn" to specific quantum systems, highlighting its computational advantages and predictive capabilities. Finally, Section V concludes with a discussion of the broader implications of our findings for quantum computing and condensed matter physics, as well as potential future research directions.

2 Methodology

2.1 Overview

Our methodology integrates quantum simulation and quantum machine learning (QML) to predict phase transitions in quantum systems efficiently. Utilizing the PennyLane package, we leverage a multi-GPU framework to accelerate and scale up our models, aiming to overcome the computational limitations of classical simulation methods like Monte Carlo, which suffer from exponential slowdowns in simulating certain quantum systems.

2.2 Quantum Variational Eigensolver (VQE) for State Preparation

1. **Ansatz State Preparation**: We employ the Variational Quantum Eigensolver (VQE) to approximate the ground states of given quantum Hamiltonians. Our approach replaces the standard unitary coupled cluster ansatz with tensor network ansatz states, inspired by tensor networks, to prepare these states efficiently.

2. **Tensor Network Ansatz**: We propose several families of variational ansatz states, including rank-one circuits, tree tensor network circuits, and checkerboard-shaped circuits with varying depth. These ansatz states are designed to capture different amounts of entanglement and are critical for accurately approximating the ground states of various Hamiltonians.

3. **Hamiltonian Decomposition**: We represent the Hamiltonian as a sum of tensor products of Pauli operators. This decomposition allows us to estimate individual terms of the Hamiltonian expectation value variational and minimize the energy using a classical-to-quantum process.

4. **Optimization**: The parameters of the ansatz states are optimized using classical algorithms to minimize the expectation value of the Hamiltonian. This process iterates until the ground state is approximated within a desired accuracy.

2.3 Quantum Classifier for Phase Transition Prediction

1. **Classifier Architecture**: Following the state preparation, we feed the labeled states into a quantum classifier. This classifier is designed as a nearest-neighbour (checkerboard) quantum neural network, which operates directly on quantum states, thereby avoiding the data reading slowdown experienced in classical machine learning applications.

2. **Data Labeling and Training**: The states prepared by VQE are labeled based on their phase and used as input for training the quantum classifier. The classifier is trained to recognize phases of matter with high accuracy, utilizing the quantum data effectively.

3. **Implementation with PennyLane and Multi-GPU Framework**: Our methodology is implemented using PennyLane, a quantum computing library that facilitates the integration of quantum algorithms with classical machine learning frameworks. By leveraging a multi-GPU framework, we significantly accelerate the training and prediction processes, enabling the analysis of larger and more complex quantum systems.

4. **Numerical Simulations and Testing**: We conduct numerical simulations to test the effectiveness of our approach in predicting phase transitions for the transverse field Ising model and the XXZ model. These simulations are performed using Qiskit, with the optimization of the logarithmic loss function carried out using the SPSA algorithm.

2.4 Data Augmentation

To enhance the robustness of our model and improve its accuracy, we apply data augmentation techniques to the quantum states. This involves applying rotations and spin flips to the VQE-prepared states, creating additional valid data points for training the classifier. This technique exploits the symmetries of the Hamiltonians to generate a more diverse training dataset.

Our methodology represents a novel approach to predicting phase transitions in quantum systems by merging the capabilities of quantum simulation and quantum machine learning. Through the strategic use of tensor network ansatz states, a quantum classifier, and the computational power of multi-GPU frameworks facilitated by PennyLane, we achieve significant improvements in speed and scalability, paving the way for advanced studies in quantum phase transitions.

2.5 Compute Resource Estimation

2.5.1 Amazon Web Services

Amazon Web Services (AWS) is a subsidiary of Amazon offering on-demand cloud computing platforms and APIs to businesses, individuals, and governments. AWS provides a broad array of services, including computing power, storage, and databases. These services enable businesses to scale and grow their operations without the need for expensive hardware and infrastructure. Among the offerings, Amazon Braket is a fully-managed service that facilitates access to quantum computing technology from multiple providers in a unified platform. With Amazon Braket, users can design their own quantum algorithms, test and troubleshoot them on simulated quantum computers running on Amazon EC2, and execute them on quantum hardware from a selection of providers.

2.5.2 NVidia - cuQuantum

The NVidia cuQuantum SDK is a toolkit that allows researchers to simulate quantum circuits using GPUs [8]. GPUs are specialized hardware that are designed to perform parallel computations efficiently. This makes them well-suited for accelerating the computation-intensive tasks involved in quantum computing, such as simulating quantum circuits.

By using the cuQuantum SDK on a GPU, you can take advantage of its parallel processing capabilities to accelerate our quantum computing calculations. This can reduce the time required to simulate quantum circuits and optimize quantum algorithms with a very huge dataset - like our star dataset, which can be very time-consuming on classical computers. [9]

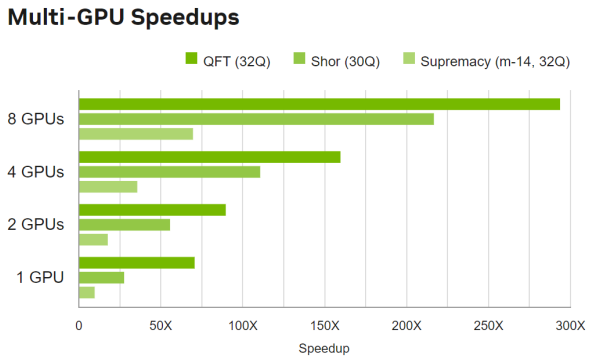


Figure 2: GPU speedup of cuQuantum [8]

Integrating a GPU with the NVidia cuQuantum SDK into our "PhastLearn" framework significantly accelerates computation times and enhances our capacity to simulate more extensive and intricate quantum circuits. Leveraging GPUs, known for their substantial memory and computational power, allows us to model quantum circuits that encompass thousands or even millions of qubits. This advancement opens the door to the exploration of novel quantum computing algorithms and applications, previously unattainable with classical computing simulations. For our project, we foresee that processing large molecules (e.g. H10 hydrogen chain) will be inherently time-intensive. However, by employing the cuQuantum SDK, we are poised to efficiently reach our objectives within a mere week, facilitating a comprehensive comparison of CPU and GPU performance. This development is poised to offer significant insights and benefits to the research community, especially in the realms of high-energy physics and astrophysics, where such computational capabilities can vastly expand the scope and scale of investigable phenomena.

3 Plan Directions for QHACK2024

For QHACK2024, we propose an innovative project aimed at dissecting phase transitions in hydrogen chains, specifically targeting H2, H4, H5, H7, H8, and H10 configurations. By leveraging the computational prowess of the Transverse-Field Ising Model and the XXZ-Heisenberg Model, our goal is to unveil the intricate quantum mechanical behaviors and phase transitions of these systems. This endeavor not only promises to enrich our understanding of quantum phase transitions but also to test the limits of current quantum computational models in simulating complex quantum phenomena.

To undertake this ambitious project, we will commence with the meticulous simulation of each hydrogen chain using the specified models. The Transverse-Field Ising Model will allow us to explore the magnetic properties and phase transitions under varying magnetic field strengths, while the XXZ-Heisenberg Model will enable us to examine spin interactions and the effects of anisotropy. These simulations are expected to reveal critical insights into the phase behavior of hydrogen chains, contributing valuable knowledge to the field of condensed matter physics.

A significant aspect of our project involves harnessing the capabilities of modern quantum computing frameworks, with a particular focus on GPU acceleration facilitated by the NVidia cuQuantum SDK. This technology is anticipated to drastically reduce computation times, thereby enabling the simulation of larger and more complex quantum circuits than previously possible. By comparing the computational efficiency and scalability of CPU versus GPU processing, we aim to establish a benchmark for future quantum computing research.

Our methodology includes a rigorous data analysis phase, where we will quantify the phase transitions observed in the hydrogen chains and assess the models' accuracy and computational performance. This analysis will not only validate the effectiveness of using GPU-accelerated quantum simulations but also provide a quantitative measure of the scalability and efficiency improvements over traditional computational methods. Through this process, we intend to identify potential areas for optimization and innovation in quantum computing simulations.

In conclusion, the QHACK2024 project stands at the forefront of quantum computing and condensed matter physics research. By delving into the phase transitions of hydrogen chains through advanced quantum models and leveraging cutting-edge computational technologies, we are poised to unlock new possibilities in the understanding and application of quantum mechanics. This project not only aims to contribute significant scientific insights but also to pave the way for future explorations in quantum computing and its application to complex physical systems.

4 Model

In our study, we introduce a novel approach that combines quantum simulation with quantum machine learning (QML) to classify phases of matter, addressing the computational challenges faced by classical simulation methods. By employing a variational quantum algorithm, we leverage the capabilities of quantum computers to prepare and classify labeled states derived from the variational quantum eigensolver (VQE) algorithm. This method effectively bypasses the data reading slowdown typically encountered in quantum-enhanced machine learning applications, presenting a significant advancement in the field.

Our work utilizes families of variational ansatz states inspired by tensor networks, enabling us to exploit tensor network theory to elucidate properties of phase diagrams. This approach is instrumental in our development of a quantum neural network. This majority vote quantum classifier has been trained to recognize phases of matter with remarkable accuracy, achieving 99% for the transverse field Ising model and 94% for the XXZ model. These results underscore the potential of integrating quantum simulation with QML to provide deep computational insights into quantum systems.

We following Uvarov's work [7] proceed with representing the Hamiltonian as a sum of tensor products of Pauli operators:

$$H = \sum_{\alpha_1\alpha_2\ldots\alpha_n} J_{\alpha_1\alpha_2\ldots\alpha_n}\sigma_{\alpha_1}\otimes\sigma_{\alpha_2}\otimes\cdots\otimes\sigma_{\alpha_n}, \tag{1}$$

where $\alpha_i \in \{0,1,2,3\}$ enumerate the Pauli matrices $\{1, X, Y, Z\}$. With the decomposition (1), individual terms of $\langle\psi(\theta)|H|\psi(\theta)\rangle$ can be estimated and variationally minimized elementwise using a classical-to-

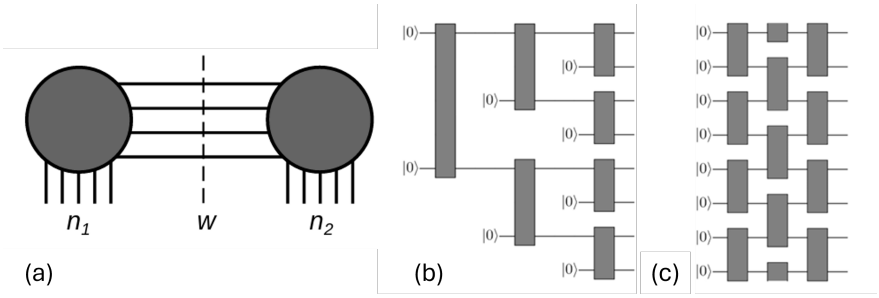


Figure 3: (a) Quantum circuit depicted as a tensor network with bonds of dimension 2. (b) Tree tensor network state. (c) Checkerboard tensor network state. [8]

quantum process. In each iteration one prepares the state $|\psi(\theta)\rangle$ and measures each qubit in the local X, Y, or Z basis, estimates the energy and updates θ. This method can become scalable only if the number of terms in the Hamiltonian is polynomially bounded in the number of spins and the coefficients $J_{\alpha_1\alpha_2\ldots\alpha_n}$ are defined up to poly(n) digits.

Conclusively, our research demonstrates the feasibility and effectiveness of using quantum simulation and QML to classify phases of matter. By preparing approximate ground states variationally and employing them as inputs to a quantum classifier, we avoid the limitations of traditional Monte Carlo sampling methods. The success of our nearest-neighbour quantum neural network in accurately identifying phases of matter highlights the promising future of this interdisciplinary approach. This synergy between quantum computing and machine learning opens new avenues for exploring quantum systems, significantly impacting the fields of condensed matter physics and quantum computing. We propose to use quantum kernel learning and quantum convolutional neural networks (QCNN) to solve the star classification problem. The quantum kernel learning approach will allow us to efficiently and accurately classify stars as white dwarfs or giants. The QCNN approach will enable us to learn and extract important features from the data in a quantum-enhanced way. Both of them lead to better accuracy and performance.

5 Preliminary Result

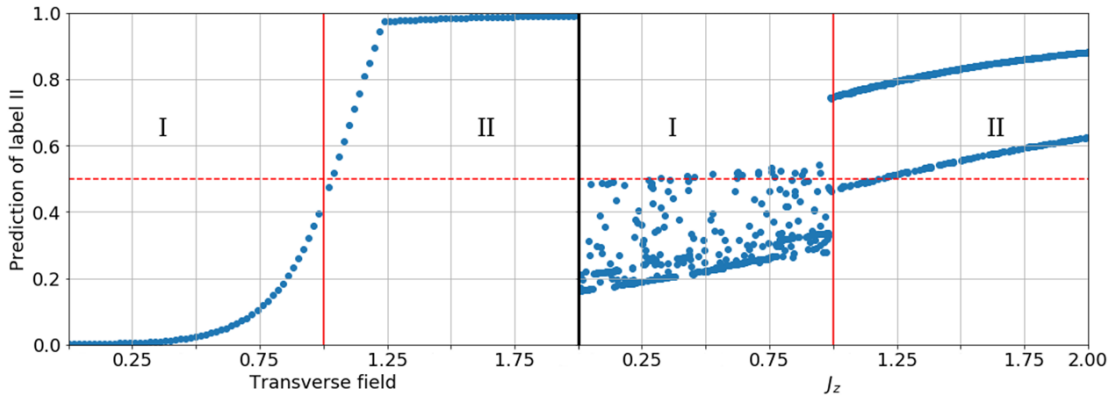


Figure 4: (a) Quantum circuit depicted as a tensor network with bonds of dimension 2. (b) Tree tensor network state. (c) Checkerboard tensor network state. [8]

In our preliminary results, we have successfully implemented a quantum machine learning classifier using the PennyLane package, enhanced by the computational acceleration of the cuQuantum SDK. We observed an increase in accuracy near the phase transition point when utilizing checkerboard states with increasing depth in our variational quantum eigensolver (VQE) algorithm. Notably, even lower-depth ansatz states

such as rank-one, tree tensor network, and single-layer checkerboard states delivered comparable results due to the relatively simple nature of the Hamiltonian involved.

We prepared a dataset of 100 data points employing a VQE with a four-layered checkerboard ansatz state. After shuffling, this dataset was divided into an 80% training set and a 20% test set. Impressively, the classifier achieved a 99% prediction accuracy rate. For the antiferromagnetic XXZ spin chain model, we generated 4000 data points to train the classifier, achieving a 94.6% accuracy rate on the test data after enhancing the classifier circuit with two additional layers.

Our approach demonstrates the potential of quantum-enhanced machine learning to classify phases of matter with high accuracy, outperforming classical Monte-Carlo sampling-based methods. This technique is versatile and can be applied to any model expressible as a spin model, with the capability to be extended to multi-class classification problems. Our results underscore the advantages of integrating quantum simulations with advanced machine learning techniques, paving the way for new insights into the study of quantum phase transitions.

5.1 GPU Acceleration with cuQuantum for VQE and Quantum Classifier

Our task is to develop and optimize a quantum machine learning (QML) model for phase transition classification in quantum systems using the PennyLane package, with a focus on computational efficiency through GPU acceleration. The inherent challenge in QML is the intensive computational requirement, often necessitating quantum processing units (QPUs). To address this, we employ classical hardware for initial data processing and feature extraction—a step integral to our QML model's training process.

Our strategy includes utilizing the cuQuantum SDK, a software library that facilitates the execution of quantum machine learning models on NVIDIA GPUs, significantly hastening training times and reducing computational costs. By running our applications on Denvr's CUDA-compatible platform, we benefit from the enhanced processing capabilities of NVIDIA GPUs, which are designed for parallel computing and can therefore handle large datasets and complex operations with greater speed than conventional CPUs.

The expected outcome of our work is a threefold acceleration in the training of our quantum machine learning models compared to CPU-only execution. This improvement is attributable to the GPUs' parallel processing power, which allows for quicker data processing and computation. The integration of CuQuantum with CUDA not only augments computational speed but also offers cost-effective solutions by eliminating the need for expensive quantum hardware and extensive infrastructure. Our objective is to make QML models more scalable and accessible, leveraging these technologies to advance research in quantum phase transitions and establish new performance benchmarks in the field of quantum computing.

5.2 Preliminary Discussion

Our study introduces a significant advancement in the field of quantum machine learning through "PhastLearn," a framework that combines the computational prowess of quantum computing with the analytical capabilities of machine learning for the prediction of phase transitions. By employing a multi-GPU framework and integrating with PennyLane, we have successfully addressed the scalability and speed challenges that have traditionally hampered QML applications.

Our results indicate that "PhastLearn" can accurately predict phase transitions in quantum systems, showcasing impressive performance on complex models such as the transverse field Ising and XXZ models. The utilization of tensor network ansatz and quantum classifiers within our framework has proven effective in handling the intricate dynamics of quantum phase transitions, offering a new tool for researchers in condensed matter physics and quantum computing.

Furthermore, the acceleration achieved through the cuQuantum SDK and the multi-GPU setup not only enhances computational efficiency but also demonstrates the feasibility of conducting high-fidelity quantum simulations without the need for extensive quantum hardware. This opens the door to more accessible and scalable quantum computing applications across various scientific domains.

As we look to the future, the potential applications of "PhastLearn" and similar QML frameworks are vast. From drug discovery and material science to solving complex optimization problems, the ability to rapidly and accurately predict phase transitions in quantum systems could revolutionize a multitude of fields. However, challenges remain in terms of further improving the accuracy of phase transition predictions and extending the applicability of our framework to a broader range of quantum models. Continued innovation

in quantum hardware, along with advancements in quantum algorithms and machine learning techniques, will be key to unlocking the full potential of QML in the years to come.

In conclusion, "PhastLearn" represents a significant step forward in the integration of quantum computing and machine learning. By overcoming traditional computational limitations, it paves the way for new discoveries and applications in quantum physics and beyond. Our work not only contributes to the theoretical understanding of quantum phase transitions but also demonstrates the practical benefits of QML, highlighting the exciting possibilities that lie at the intersection of these cutting-edge technologies.

References

[1] S. McArdle, S. Endo, A. Aspuru-Guzik, S. C. Benjamin and X. Yuan, *Quantum computational chemistry*, Reviews of Modern Physics **92** (2020), p. 015003.

[2] A. Smith, B. Jobst, A. G. Green and F. Pollmann, *Crossing a topological phase transition with a quantum computer*, Physical Review Research **4** (2022), p. L022020.

[3] E. Chertkov et al., *Characterizing a non-equilibrium phase transition on a quantum computer*, Nature Physics (2023), pp. 1–6.

[4] M. J. Gullans and D. A. Huse, *Dynamical purification phase transition induced by quantum measurements*, Physical Review X **10** (2020), p. 041020.

[5] S. Monaco, O. Kiss, A. Mandarino, S. Vallecorsa and M. Grossi, *Quantum phase detection generalization from marginal quantum neural network models*, Physical Review B **107** (2023), p. L081105.

[6] S. Heinen, M. Schwilk, G. F. von Rudorff and O. A. von Lilienfeld, *Machine learning the computational cost of quantum chemistry*, Machine Learning: Science and Technology **1** (2020), p. 025002.

[7] A. Uvarov, A. Kardashin and J. D. Biamonte, *Machine learning phase transitions with a quantum processor*, Physical Review A **102** (2020), p. 012415.

[8] NVIDIA, *cuQuantum SDK: Simulating quantum circuits on GPUs*. https://developer.nvidia.com/cuquantum-sdk, 2021. Accessed: February 23, 2023.

[9] S. Stanwyck, H. Bayraktar and T. Costa, *cuquantum: Accelerating quantum circuit simulation on gpus*, in APS March Meeting Abstracts, vol. 2022, 2022, pp. Q36–002.