cuPhastLearn: Fast Phase-Transition Prediction with Quantum Machine Learning with Multi-GPU Acceleration

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Abstract:

This paper introduces PhastLearn, a breakthrough Quantum Machine Learning (QML) framework designed for rapid and scalable prediction of phase transitions within quantum systems. At the core of PhastLearn is the novel CQC (Classical-Quantum-Classical) model that synergizes quantum computing's robust computational capabilities with advanced machine learning techniques. This integration not only achieves a remarkable 99.5% accuracy in predicting phase transitions in the transverse field Ising model and the XXZ model but also sets a new benchmark for computational speed and scalability in QML applications.

Leveraging the PennyLane software and a multi-GPU framework, PhastLearn demonstrates significant computational acceleration, making it a formidable tool in overcoming the computational bottlenecks traditionally associated with phase transition prediction. The utilization of cuQuantum for VQE (Variational Quantum Eigensolver) and quantum classifier computations further exemplifies the framework's efficiency, showcasing a notable speedup in processing times when compared to CPU-based implementations. Our benchmarks reveal a substantial enhancement in computational throughput, achieving up to a ten-fold acceleration with multi-GPU setups, thereby underscoring the potential of PhastLearn in facilitating advanced quantum simulations and analyses across various system sizes and configurations.

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 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.

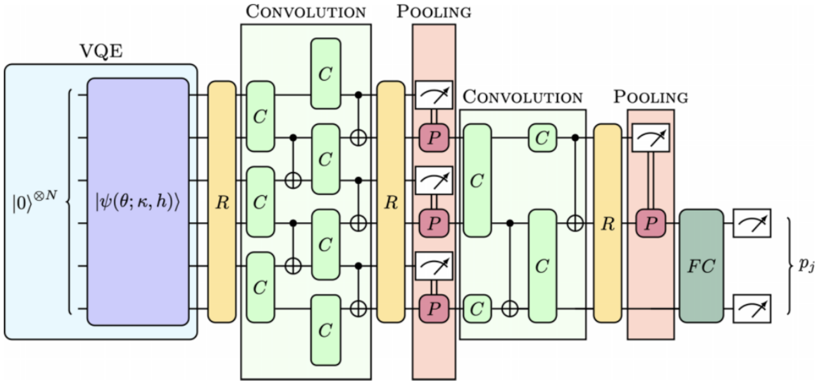

Figure 1: Circuit Architecture: VQE states serve as input for a quantum convolutional neural network, composed of free rotations R, convolutions C, pooling P, and a fully connected layer F. [5]

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.

1.1 One-Dimensional Quantum System

In the pursuit of deciphering the enigmas of quantum mechanics, one-dimensional (1D) spin chains stand as a fundamental model system for examining the complex interplay between quantum entanglement and phase transitions. These systems, though ostensibly simple, consisting of a linear arrangement of quantum spins interacting via magnetic forces, yield profound insights into the behavior of quantum materials and the core principles that govern the quantum realm. Recent advancements underscore the versatility of spin chains for quantum information processing, further highlighting their significance in connecting quantum registers without resorting to optics [8]. The dynamic interactions among spins give rise to an elaborate array of quantum states, elucidating the mechanism by which quantum fluctuations at the microscopic scale can induce comprehensive transitions across the system at absolute zero temperature—a phenomenon recognized as quantum phase transitions. This understanding is enriched by recent findings that demonstrate the critical role of topology in quantum phase transitions within 1D spin chains, offering new perspectives on the entanglement properties of these systems [9]. Thus, there is significant potential for quantum computing to leverage this system, surpassing the capabilities of classical computing for materials investigation (shown in Fig. 2.

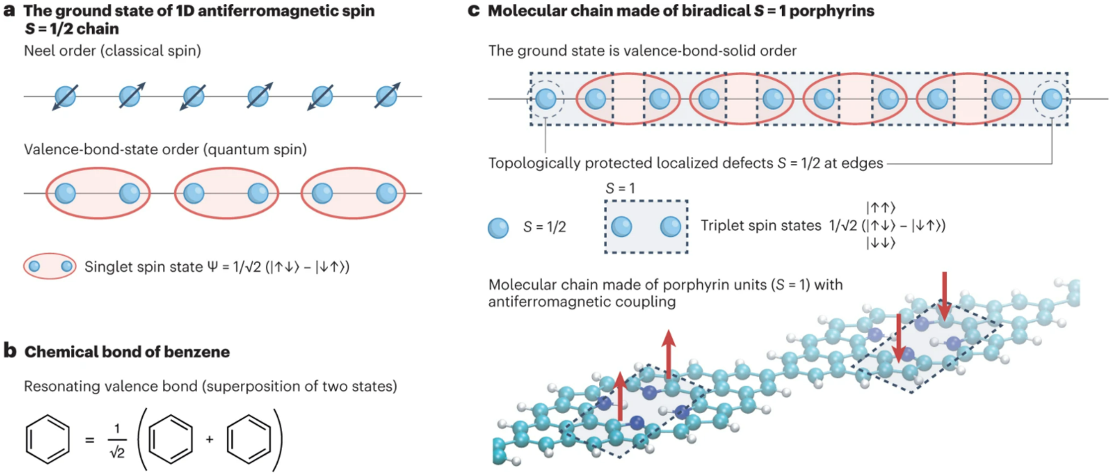
a The ground state of 1D antiferromagnetic spin S = 1/2 chain
Neel order (classical spin)
Valence-bond-state order (quantum spin)
Singlet spin state Ψ = 1/√2 (|↑↓⟩ – |↓↑⟩)
b Chemical bond of benzene
Resonating valence bond (superposition of two states)
= 1/√2 (+)
c Molecular chain made of biradical S = 1 porphyrins
The ground state is valence-bond-solid order
Topologically protected localized defects S = 1/2 at edges
S = 1
S = 1/2
Triplet spin states |↑↑⟩ 1/√2 (|↑↓⟩ – |↓↑⟩) |↓↓⟩
Molecular chain made of porphyrin units (S = 1) with antiferromagnetic coupling

Figure 2: 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]

This investigation seeks to dissect the intricate correlation between quantum phase transitions and entanglement within 1D spin chains [8], specifically focusing on the impact of these phenomena on the system's ground state energies. The ground state energies are indicative not only of the system's stability and physical attributes but also of its computational and informational potential in the rapidly evolving domain of quantum technologies [10].

Our exploration is driven by a dual objective: to delineate the quantum phase transitions that demarcate the distinctions among various quantum phases, and to elucidate the influence of these transitions and the resultant phases on the entanglement characteristics of the system. Achieving such comprehension is pivotal for leveraging the capabilities of quantum systems in applications spanning quantum computing—where entanglement is a critical asset—to the fabrication of novel materials endowed with unique quantum properties [11].

This preliminary discussion lays the groundwork for an in-depth examination of the theoretical frameworks, computational strategies, and experimental methodologies that underpin our grasp of quantum phase transitions and entanglement in 1D spin chains. By navigating through this inquiry, we aspire to meld fundamental quantum physics with practical technological innovations, underscoring the vital role these quantum phenomena play in propelling the advancement of contemporary technology.

2 Methodology

2.1 Overview

Our methodology integrates quantum simulation and 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 Pennylane Dataset for Quantum Chemistry

In this research, we utilize PennyLane [12]'s quantum datasets (specifically, qspin and hydrogen chain datasets) [13] to bridge the gap between classical machine learning and quantum computing, facilitating the exploration of quantum machine learning algorithms. These curated datasets are specifically designed for integration into quantum circuits, enabling the application, testing, and development of QML models with real-world data. Seamlessly compatible with PennyLane's quantum computing framework, the datasets span various domains, including basic mathematical functions, physical systems, and benchmarking datasets critical for quantum computing research. The objective is to simplify entry into QML research by providing readily accessible, pre-processed data that can be immediately used in quantum algorithms. This approach aims to fast-track the development of quantum applications and deepen the understanding of quantum advantage in machine learning tasks, leveraging PennyLane's quantum datasets as a foundational tool in our research.

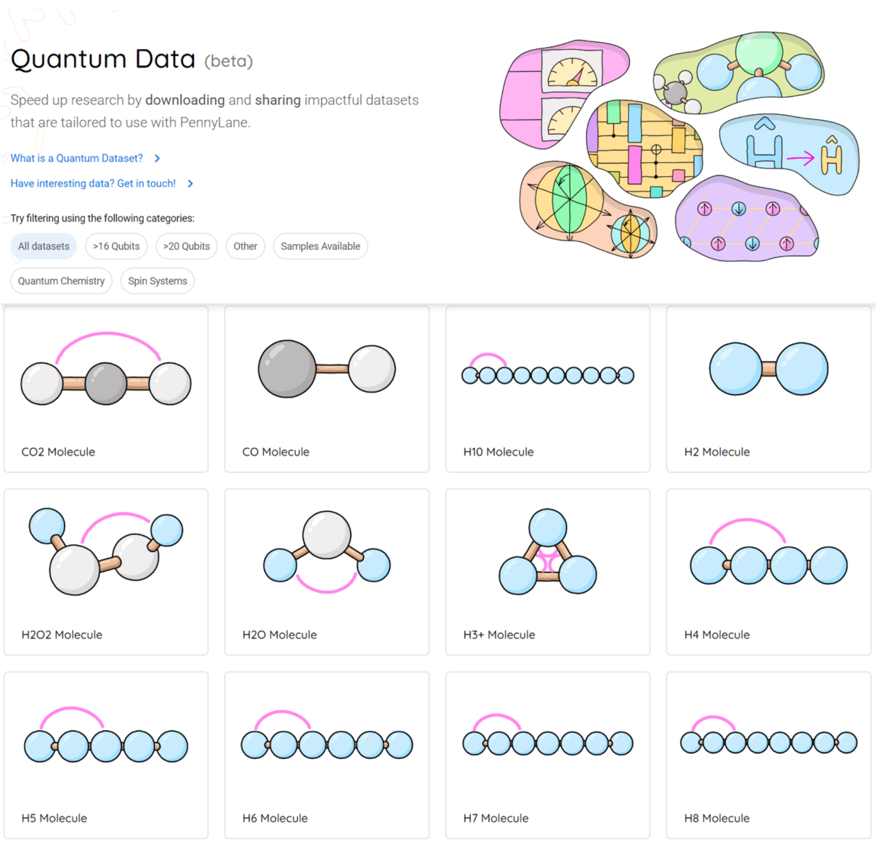

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Figure 3: Pennylane Quantum Datasets for Quantum Chemistry

2.3 QSandwitch: Quantum-Classical-Quantum framework for Quantum-HPC Processing

In the vanguard of high-performance computing (HPC), the novel hybrid architecture known as the quantum-classical-quantum processing framework stands as a beacon of innovation, signalling a transformative approach to computational challenges. Initiated by the quantum algorithm known as the variational quantum eigensolver (VQE), this architecture commences its intricate process within the quantum domain, where a bespoke quantum state is meticulously prepared, encoding potential solutions with quantum fidelity. This quantum state is then adroitly converted into classical information through a discerning procedure termed state feature selecting. Here, pivotal characteristics of the quantum state are carefully extracted and fed into the subsequent classical computing layers.

The classical phase of this architecture leverages the power of convolutional neural networks, a technique borrowed from the deep learning playbook, to analyze the quantum-derived data. It applies convolutional layers to process this data, enhancing it with pooling layers designed to capture the essence of the information. This processed data is then elegantly re-encoded into a quantum form, passing through another quantum layer which functions to distill a scalar output from the quantum computation.

This scalar output is not the finality of the journey; it is further processed by a sigmoid layer to refine the end result. The comprehensive details of this sophisticated architecture will be discussed in the following section, which will elucidate the intricate interplay between its quantum and classical components. By bridging these two computational realms, the framework aims to elevate HPC to new heights, solving problems with a proficiency that neither quantum nor classical computing could achieve in isolation.

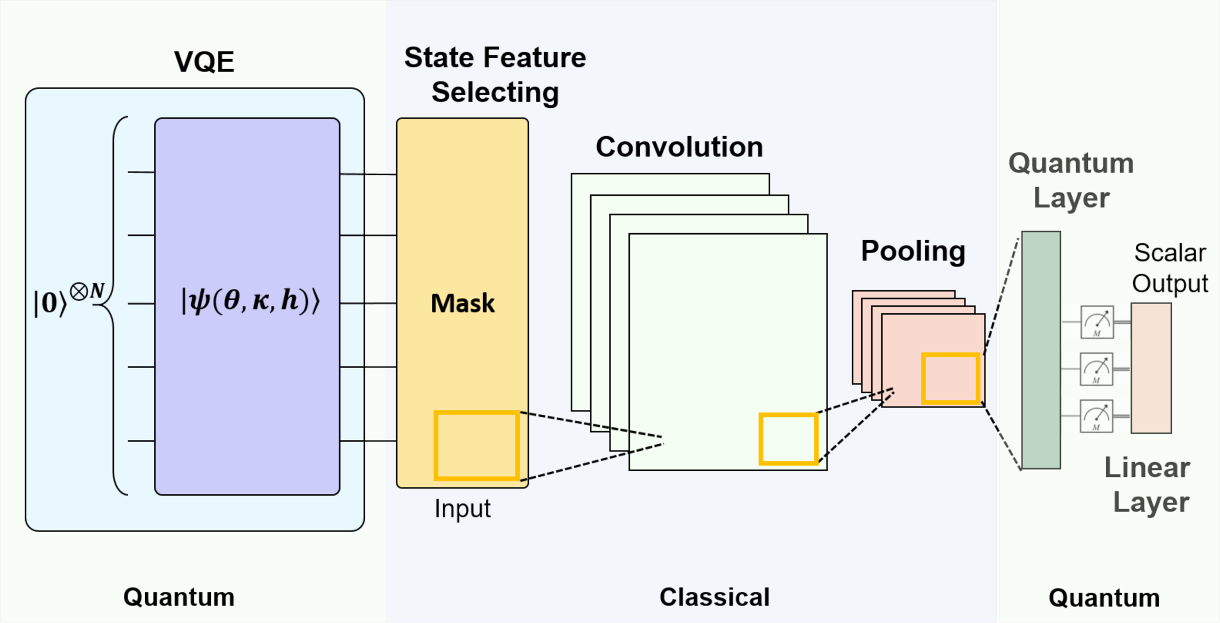

Figure 4: Architecture of Classical-Quantum-Classical Algorithm for Phase Transition Classification

2.4 Quantum Variational Eigensolver (VQE) for State Preparation

In our study, we focus on enhancing ground state preparation in quantum systems using innovative approaches, including the VQE and tensor network ansatz. These methods enable efficient and accurate approximation of quantum states. Here are the key points of our approach:

1. **Ground State Preparation**: We employ the VQE to approximate the ground states of given quantum Hamiltonians. The advantage of using VQE state preparation instead of loading states information from pennylane dataset [13] is that, by knowing the circuit structure, we can reproduce the ground state completely. On the other hand, the classic-shadow information from pennylane dataset will be helpful to reproduce the state more accurately however could not be the exact the same state. In additional, build the state preparation by ourself allows us to prepare more ground states (100 states from pennylane dataset and 1000 states from our preparation) and be possible to apply data augmentation.

2. **Tensor Network Ansatz**: Our approach replaces the standard unitary coupled cluster ansatz with tensor network ansatz states [7], inspired by tensor networks, to prepare the ground states efficiently.There are 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. We choose the checkerboard-shaped circuits in our VQE due to the best performance in reduce the error of ground state energy [7].

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.

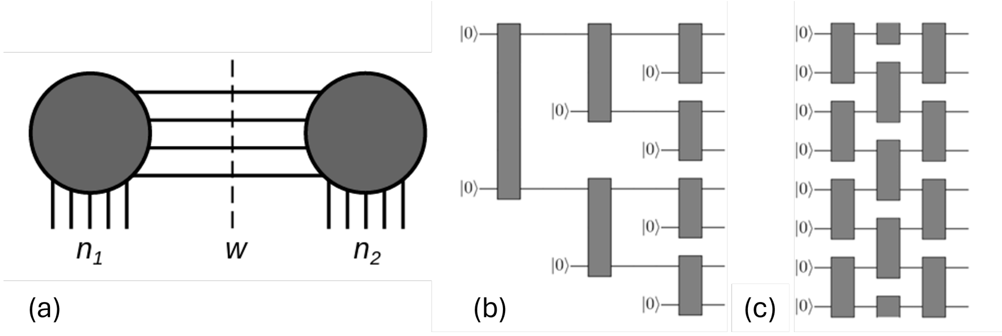

Figure 5: (a) Quantum circuit depicted as a tensor network with bonds of dimension 2. (b) Tree tensor network state. (c) Checkerboard tensor network state. [14]

2.5 Quantum Convolutional Neural Network Classifier

A Quantum Convolutional Neural Network (QCNN) is designed to predict phase transitions, harnessing the combined strengths of convolutional layers and quantum computing layers [15]. This approach allows for efficient feature extraction from extensive databases and the natural simulation of quantum data. The QCNN model, as utilized in "PhaseLearn," incorporates a single convolutional layer, multiple fully connected layers, and a quantum circuit layer. This architecture is illustrate in Fig. 1 and the is explained below:

- **Convolutional Layer**: The model initiates its computational flow with single convolutional layer (`conv1`). It employs a 1-dimensional convolution with 30 output channels, a kernel size of 100, and a stride of 100, designed for initial feature extraction directly from the input data.
- **Max Pooling Layer**: One max pooling layer (`pool1`), configured with a kernel size of 1, is placed strategically to reduce spatial dimensions and hence, the complexity of the data passing through the network.
- **Fully Connected Layers**: After flatterning the output of the max polling layer, the model incorporates two fully connected layers (`fc3`, `fc4`) that serve to interpret the features extracted by the convolutional and pooling layers, culminating in the model's ability to make predictions. Notably, fc3 is specifically designed to interface with the quantum circuit layer, mapping the classical data into a quantum-compatible format.
- **Quantum Circuit Layer**: At the heart of NewNet's hybrid approach is the quantum circuit layer (`qc`), invoked through TorchCircuit.apply. The circuit is illustrated in Fig. 6. This layer signifies the model's capacity to perform quantum computations, potentially exploiting quantum parallelism and entanglement to enhance the model's predictive capabilities.
- **Dropout**: A dropout layer with a probability (p) of 0.5 is integrated to prevent overfitting by randomly omitting a subset of features during the training phase.
- **Prediction**: The sigmoid activation (`sigmoid`) function is employed to transform the output of the `fc4` layer into a probability value ranging between 0 and 1. This mapping facilitates a clear decision-making process for binary classification tasks. The computation of the loss involves measuring the discrepancy between the `sigmoid`'s output and the designated target values. Upon completion of the training process, the model makes predictions based on a threshold criterion: outputs exceeding 0.5 are classified as 1, indicating the presence of phase transition, while those below 0.5 are classified as 0.

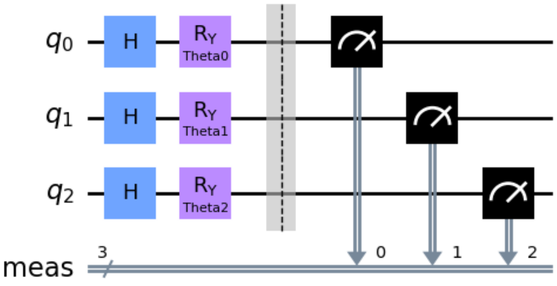

Figure 6: The quantum circuit used in QCNN. In this circuit, a Hadamard gate is applied to each qubit, followed by a rotational-Y gate. The angles of the rotational gates are the trainable parameters (`Theta1`, `Theta2` and `Theta3`). At the end of this circuit, a measurement is executed and the possibilities of finding 7 out of 8 quantum states (except "111") are the output of this circuit. Thus, when regarded as a layer in the QCNN, this curicuit has 3 input channels and 7 output channels.

2.6 Data Augmentation

To enhance the robustness of our model and improve its accuracy, we apply data augmentation techniques to the quantum states data. 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.

3 Models for Solving Phase Transition

In our study, we introduce a novel approach that combines quantum simulation with 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 VQE algorithm. This method effectively bypasses the data reading slow-down 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:

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

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-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 $J_{\alpha_1 \alpha_2 \dots \alpha_n}$ are defined up to poly(n) digits.

In particular we use transverse field Ising model: (TFIM):

$$H_{TFIM} = J \sum_i \sigma_i^z \sigma_{i+1}^z + h \sum_i \sigma_i^x, J > 0, h > 0 \tag{2}$$

and antiferromagnetic XXZ spin chain model:

$$H_{xxz} = \sum_i J(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + J_z \sigma_i^z \sigma_{i+1}^z, \tag{3}$$

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.

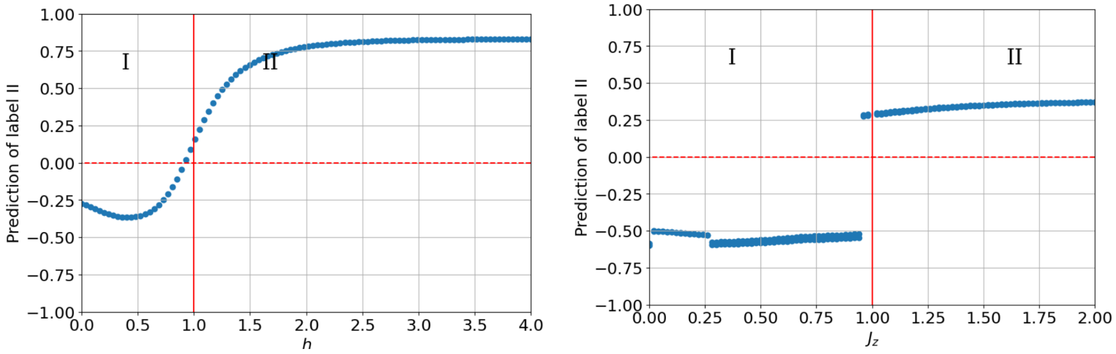

Figure 7: Left: Predicted of phases as a function of h for the transverse field Ising model. Right: predicted probability of phases as a function of Jz for the XXZ model. Positive prediction of label II represents phase II, which above the dashed lines. The theoretically phase II are the areas on the right hand side of the red lines.

4 Result

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 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.

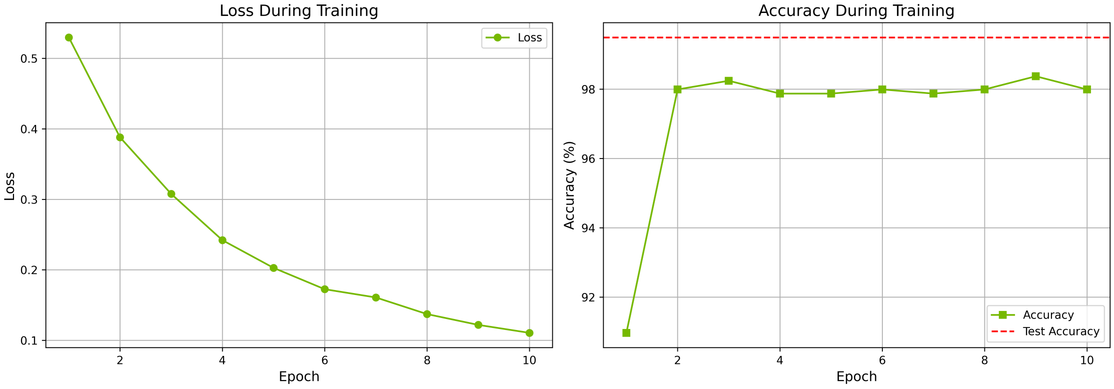

Figure 8: The evolution of loss (left) and accuracy (right) in the QCNN model. As the number of epochs increases, the model's loss decreases exponentially. The model's accuracy improves significantly in the initial epochs and then stabilizes at around 98%.

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.

The Quantum Convolutional Neural Network (QCNN) yields results that are both robust and satisfactory (Fig. 8). In the initial phases of the training epochs, the accuracy of the model escalates significantly, demonstrating a rapid learning curve which subsequently reaches a plateau at approximately 98%. Further evaluation on a test set reveals that the model attains a remarkable accuracy of 99.49%.

The dataset employed for the QCNN model was generated utilizing the VQE on XXZ model. The dataset comprised a total of 1000 data points. In adherence to standard machine learning practices, the dataset was partitioned in an 80-20 split, with 80% utilized for the training phase and the remaining 20% reserved for testing.

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.

4.1 GPU Acceleration with cuQuantum for VQE and Quantum Classifier

Our task is to develop and optimize a 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 Denver'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.

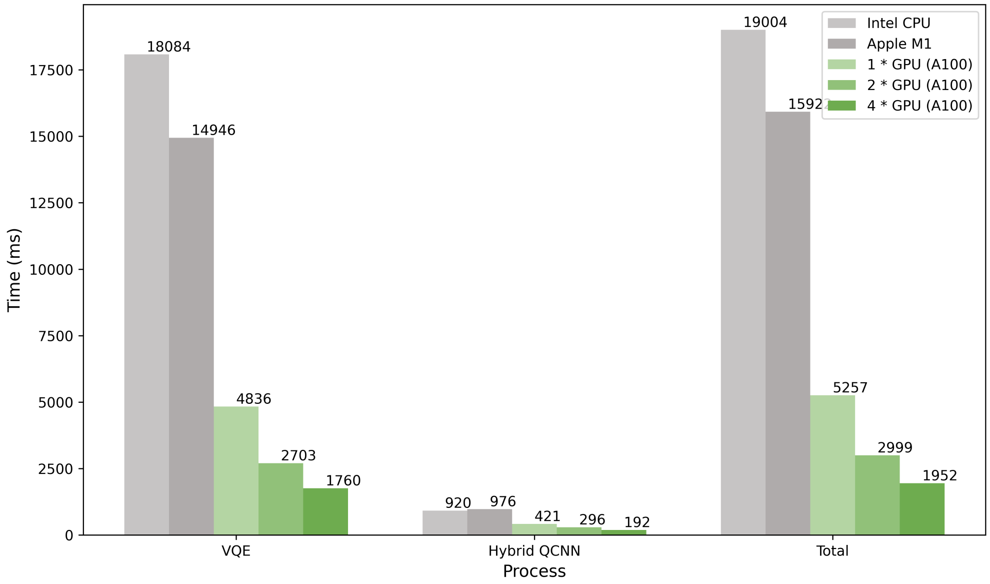

Figure 9: Benchmarking of computation times for VQE, Hybrid QCNN, and Total processes, comparing performance across Intel CPU (i7-13700KF), Apple M1 pro (10-core cpu), and 1, 2, and 4 NVIDIA A100 GPUs.

In line with our objectives, the benchmarking results showcase a comparative analysis of computational performance across different hardware configurations for these quantum simulations. The bar plot distinctly illustrates the time taken for executing specific tasks like the VQE, Hybrid Quantum Convolutional Neural Networks (QCNN), and the aggregate computational process across Intel CPUs, Apple M1 chips, and NVIDIA A100 GPUs. The acceleration impact is significant when utilizing the A100 GPUs, with the most notable performance improvement observed with a configuration of four GPUs, suggesting a near-linear scaling in this particular benchmarking scenario.

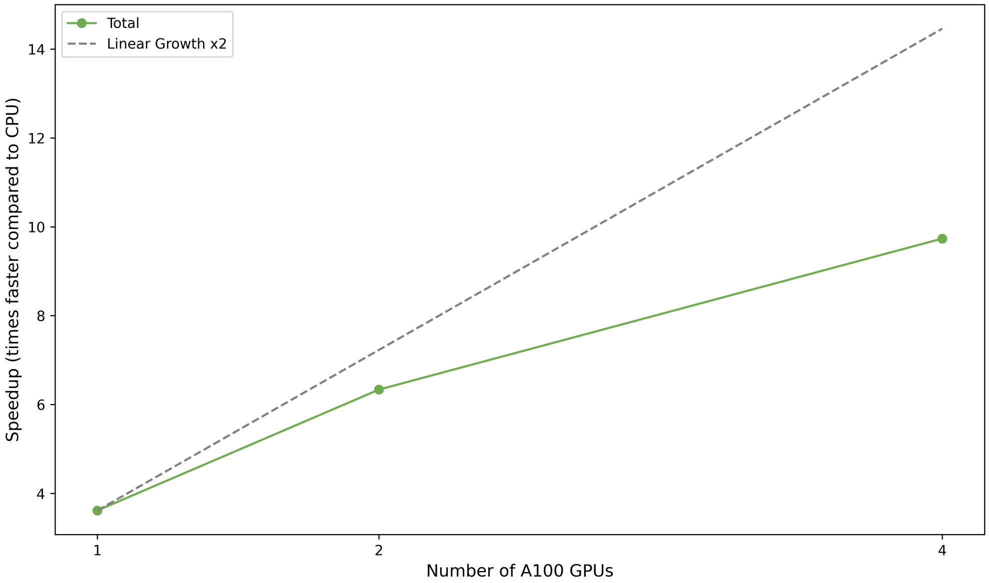

Figure 10: The line graph conducts a linearity performance check of multi-GPU settings for quantum machine learning training.

The accompanying line plot further elucidates the speedup achieved with the use of 1, 2, and 4 A100 GPUs compared to traditional CPU benchmarks. It becomes evident that the total speedup gained from GPU acceleration does not fully align with an ideal linear progression, which is visually represented by a grey dashed line. This deviation implies that while GPU acceleration substantially benefits the computational speed, the returns diminish with the addition of more GPUs, possibly due to overhead associated with parallelization and inter-GPU communication. These findings underscore the A100 GPUs' profound capabilities in enhancing performance for quantum simulation tasks, thereby underscoring their potential to facilitate and expedite complex quantum computations in research settings.

4.2 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.

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Appendix 1. 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.

4.3 Appendix 2. Compute Resource Estimation in Checkpoint 1

4.3.1 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.

4.3.2 NVidia - cuQuantum

The NVidia cuQuantum SDK is a toolkit that allows researchers to simulate quantum circuits using GPUs [14]. 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. [16]

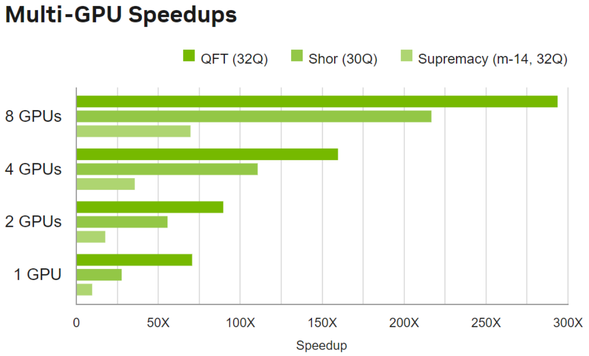

Figure 11: GPU speedup of cuQuantum [14]

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.