

Quantum Advantage in Predicting Ground State Properties Beyond Constant Gaps

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I. INTRODUCTION

Ever since the idea of quantum computers was introduced, one of the central goals of the field was to develop hardware and algorithms to deepen our understanding of material science or chemistry, as well as provide predictive tools to those fields. However, a question that has become more apparent in recent years is "when do we *really* need quantum computers?" Constant competition between quantum engineers and classical simulation specialists have lead to a back and forth between quantum demonstrations, and classical simulations of those demonstrations. Clever developments in general purpose techniques like tensor network algorithms[1], or density functional theory[2] for calculating many-body properties have also provided insights to new materials and chemical behaviour without needing quantum computers. In the modern data-driven world, such quantum advantages can be expected to even more unlikely, especially when the data provided is quantum in origin. One may be tempted to intuit that ground states properties are natural candidates for quantum advantage in machine learning. However, within the regime of gaped phases of matter, predicting expectation values and classical shadows of ground states within a single phase has been solved using classical machine learning algorithms [3–6]. Quantum data has explicitly been shown to elevate classical algorithms to perform computations beyond purely classical resources [7]. Therefore it is important to understand the if quantum advantage is present for any new quantum algorithm.

In this work we explore the possibility of advantages beyond the gap property. Prior results [3–6] demonstrated that if we violate the constant gap condition, or equivalently learning within a single phase, then resource costs do not remain classically efficient. In this work we take the first steps towards the development of quantum learning of ground state properties across multiple phases. We further address the question of provable quantum advantage by demonstrating a task our algorithm solves that cannot be learnt by a classical algorithm even when given access to the same set of quantum generated data. This quantum advantage extends to both learning from the training data, as well as inferring properties of hitherto unseen states.

To construct this algorithm we combine recent work on learning quantum dynamics[8] with new results we developed regarding the quantum adiabatic state preparation algorithm (see ref [9] for review of adiabatic state preparation). We extend the results of Bachmann et al [10, 11] by developing technical error tracking tools to show under what conditions we can get away with shorter evolution times for adiabatic state preparation when the gap is order $\Delta \in \Omega(\text{polylog}(n)^{-1})$. This algorithm allows us to predicting ground state properties of a family of Hamiltonians with non-constant gaps, to accuracy $\epsilon \in \Omega(\text{polylog}(n)^{-1})$. Previous classical learning algorithms predict that these properties could lead to super-polynomial sample complexity.

II. PROBLEM STATEMENT

Prior examples of classical learning from quantum data [3–5] learnt ground state properties of some smooth family of Hamiltonian $H(x)$ with constant gap. Here we go beyond this using a family of Hamiltonians with poly-log gaps.

Problem 1 (Poly-logarithmic gaped learning problem). *Consider a family of geometrically local Hamiltonians defined on a n -qubit lattice Λ and specified by an input $x \in \mathcal{X}$, and an unknown parameter $\vec{\alpha} \in \mathbb{R}^d$ defined*

$$H(x, \vec{\alpha}) = \sum_j h_j(x) + \sum_{k=1}^d \alpha_k P_k, \quad (1)$$

where each P_k is a geometrically local operator with a Pauli-operator spectrum (equal number of ± 1 eigenvalues). Assume that for all $x \in \mathcal{X}$ and $\alpha \in \mathbb{R}^d$, there exists a Hamiltonian path H_s , $s \in [0, 1]$ with $H_1 = H(x, \vec{\alpha})$ with ground state $|\psi(x, \vec{\alpha})\rangle$, H_0 having a unique ground state $|\psi^*(x)\rangle$, and all H_s having a spectral gap $\Delta \in \Omega(\text{polylog}(n)^{-1})$.

Given a polynomial number of training samples $\{(x_k, \sigma_T[|\psi(x_k, \vec{\alpha})\rangle\langle\psi(x_k, \vec{\alpha})|])\}_k$ for fixed $\vec{\alpha}$, where $\sigma_T[\rho]$ is a classical shadow of ρ , determine $\vec{\alpha}$.

Depending on the formulation of the problem, we can also replace the classical shadows, $\sigma_T[|\psi(x_k, \vec{\alpha})\rangle\langle\psi(x_k, \vec{\alpha})|]$, in the training data with expectation values of operators A_k , which may vary with x_k (and for some Hamiltonians may have to vary).

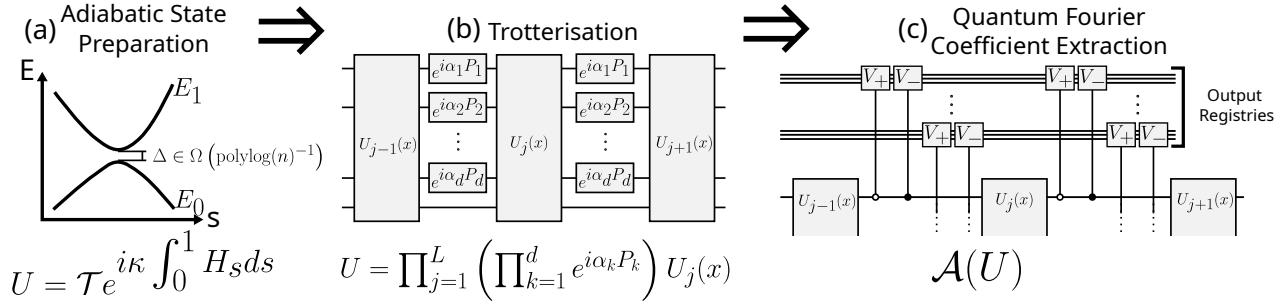


Figure 1. A demonstration of our procedure. (a) We take any geometrically local Hamiltonian that can be written as $H_1(x, \alpha) = \sum_j h_j(x) + \sum_{k=1}^d \alpha_k P_k$ and consider the adiabatic preparation from some fixed Hamiltonian $H_0(x, \vec{\alpha}) := H_0(\vec{\alpha})$. Assuming we know a smooth family of Hamiltonians $H_s(x, \vec{\alpha})$, $s \in [0, 1]$ with spectral gap $\Delta = E_1 - E_0 \in \Omega(\text{polylog}(n))$ adiabatic evolution, $U = \mathcal{T} e^{i \kappa \int_0^1 H_s ds}$, for time $\kappa \in O(\text{polylog}(n))$. (b) We can Trotterise to obtain the quantum circuit shown. The structure shown repeats $O(\text{polylog}(n))$ times and the Pauli operators P_k may act on more than 1 qubit, or on the same qubit, we show it here as P_k acts only on the k^{th} qubit for graphical simplicity. The circuit structure satisfies the assumptions in quantum Fourier coefficient extraction [8]. (c) Using the approach in ref [8], we convert each exponential $e^{i \alpha_k P_k}$ to a pair of control gates acting on the eigenspaces of P_k , one incrementing a registry when in the $+1$ eigenspace and the other decrementing it when in the -1 eigenspace.

This problem is in essence very similar to the problems posed in refs [3–6], however with a few key differences. The first is that only expectation values are considered rather than classical shadows. In our context, where we have access to a quantum computer during the inference stage, classical shadows are redundant since we may simply prepare a quantum state and measure the relevant operator expectation values. Second, the Hamiltonians we consider may have a spectral gap of $\Delta \in \Omega(\text{polylog}(n)^{-1})$ instead of only constant gaps $\Delta \in \Omega(1)$. Spectral gaps of this size are predicted to require super-polynomial classical resource costs in the prior methodologies, which we confirm in order to prove a quantum advantage for this task over *any* classical approach. Our algorithm also extends to when O is of poly-logarithmic support, as well as if we wish to reduce the error in expectation value estimation to be within $\epsilon \in \Omega(\text{polylog}(n))$ accuracy.

III. QUANTUM LEARNING ALGORITHM

The approach we propose is built upon two key components, the first is quantum Fourier coefficient extraction, a quantum algorithm with provable quantum advantage first proposed in [8]. The second component is adiabatic state preparation, a well developed quantum algorithm used for ground state preparation. To use adiabatic state preparation, we extended the results of Bachmann et al. [10, 11], which demonstrated a shorter evolution time is sufficient when there is constant gap, to work when $\Delta \in \Omega(\text{polylog}(n)^{-1})$. Finally, we make atypical use of Trotterisation to convert the adiabatic state preparation algorithm into a valid quantum circuit for quantum Fourier coefficient extraction.

A. Quantum Fourier coefficient extraction

The quantum Fourier coefficient extraction is an algorithm introduced in [8] for quantum circuits of the form:

$$U(x, \vec{\alpha}) = \prod_{j=L}^1 \left(U_j(x) \left(\prod_{k=1}^d e^{i \alpha_k P_k} \right) \right) U_0(x), \quad \Rightarrow \quad \langle 0 | U(x, \vec{\alpha})^\dagger O U(x, \vec{\alpha}) | 0 \rangle = \sum_{\ell \in [-2L, 2L]^d} a_\ell(x) e^{i \vec{\alpha} \cdot \ell} \quad (2)$$

for arbitrary choice of Pauli strings P_k and arbitrary unitaries $U_j(x)$. Quantum Fourier extraction allows us to convert any unitary of this form into a second unitary by replacing the exponents $e^{i \alpha_k P_k}$ with a pair of projectors onto the $+1/-1$ eigenbasis of P_k that control an incrementor/decrementor on some ancillary register. We call this updated circuit $\mathcal{A}(U)$. The algorithm $\mathcal{A}$ is shown in fig 1, between (b) and (c), and gives rise to the resulting action

$$\mathcal{A}(U, O) | 0 \rangle | 0 \rangle = \frac{1}{\|a(x)\|} \sum_{\ell \in [-2L, 2L]^d} a_\ell(x, O) | \ell \rangle | 0 \rangle + | \cdots \rangle | 0^\perp \rangle. \quad (3)$$

If $[-2L, 2L]^d$ is a polynomial sized set, then we can extract every $a_\ell(x, O)$ and determine which $\vec{\alpha}$ results in the training expectation values $\langle \psi(x, \vec{\alpha}) | O | \psi(x, \vec{\alpha}) \rangle$. Therefore, we consider $L \in O(\text{polylog}(n))$ and $d \in O\left(\frac{\log(n)}{\log \log(n)}\right)$.

B. Adiabatic state preparation

Adiabatic state preparation allows us to take the ground state $|\psi_0(x)\rangle$ (independent of $\vec{\alpha}$) and prepare ground state $|\psi(x, \vec{\alpha})\rangle$ of target Hamiltonian $H_0(x, \vec{\alpha})$. Given a continuous deformation of Hamiltonians from H_0 to H_1 , denoted H_s , $s \in [0, 1]$, we can use the evolution

$$|\psi(x, \vec{\alpha})\rangle \approx \mathcal{T} e^{i\kappa \int_0^1 H_s(x, \vec{\alpha}) ds} |\psi_0(x)\rangle, \quad (4)$$

where $\mathcal{T}$ is the time ordering operator. The approximation is valid so long as the time taken to perform the operation, κ is sufficiently large relative to the spectral gap $\Delta_s = E_1 - E_0$ of the Hamiltonians $H_s(x, \vec{\alpha})$.

Normally, for many-body quantum states, κ must scale with the system size in order to suppress the error to a constant [9]. This is too long for the quantum Fourier coefficient extraction algorithm. So, in order to combine this with the quantum Fourier coefficient extraction algorithm, we extend results of Refs [10, 11] on shortcuts to adiabaticity. This prior work showed a constant κ is sufficient if the gap is bounded by $\Delta_s \in \Omega(1)$ if we only want to be accurate for expectation values on operators of constant support. We show that if the gap is bounded by $\Delta_s \in \Omega(\text{polylog}(n)^{-1})$, then runtime $\kappa \in O(\text{polylog}(n))$ when restricted to the same expectation values. This is summarised in the following theorem that we proved to construct our algorithm,

Theorem 1. *Consider a family of geometrically local Hamiltonians H_s , $s \in [0, 1]$ defined on a lattice of constant spatial dimension, and with gaps lower bounded by $\Delta_{\min} \in \Omega(\text{polylog}(n)^{-1})$. If we have the ground state of H_0 to be $|\psi_0\rangle$, then we can produce a quantum state $|\tilde{\psi}_1\rangle$ which agrees with the ground state of H_1 for the expectation value of operators O with support $|\text{supp}(A)| \in O(\text{polylog}(n))$ up to error $\|O\|_\infty \epsilon$ if we perform adiabatic time evolution for time $\kappa \in O(\text{poly}(\log(n), \epsilon^{-1}))$.*

C. Trotterisation

Since adiabatic state preparation is not presented in a quantum circuit, we must convert it to a quantum circuit of the form of eq (2). For a Hamiltonian in the form of eq. (1) we can get $e^{i\alpha_k P_k}$ if we Trotterise the unitary in eq. (4) so that each term in H_s is now exponentiated separately. However this leads to a polynomial deep circuit, and leads to more than $L \in O(\text{polylog}(n))$ instances of $e^{i\alpha_k P_k}$ appearing. Instead, we first Trotterise the terms that depend on x and those that depend on α . This produces an error of $O\left(\kappa^2 \frac{\|\sum_j h_j(x), \sum_k \alpha_k P_k\|_2^2}{N}\right)$ when we Trotterise into N steps. Since d is less than logarithmic, and $h_j(x)$ are geometrically local terms, then the total error from Trotterisation is order $O\left(\frac{\text{polylog}(n)}{N}\right)$ and we only need to alternate between the x dependent terms and the α dependent terms a poly-logarithmic number of times. Finally we can Trotterise $e^{i\sum_k \frac{\alpha_k}{N} P_k}$ to exponentiate each P_k individually. This will mean each P_k will appear no more than $L \in O(\text{polylog}(n))$ times and quantum Fourier coefficient extraction becomes viable.

IV. PROVABLE QUANTUM-CLASSICAL SEPARATION

To demonstrate a provable quantum advantage for our algorithm, it is sufficient to consider a geometrically local poly-logarithmic depth BQP quantum circuit. A BQP problem corresponds to measuring a particular qubit (say qubit 1) after some circuit, so to this qubit we append X_1^α , which will make the expectation value give either the correct or incorrect response for this BQP circuit depending on the value of α . We can formulate this as an instance of our problem by using the geometrically local Feynman Hamiltonian construction of our circuit proposed by Oliveira and Terhal[12]. Then the input data, x , is specification of a poly-log depth BQP circuit that is classically hard to simulate (e.g. requiring super-polynomial classical resources) with label, y , that is the correct output for the circuit specified by x if $\alpha = 0$ and the opposite output if $\alpha = 1$. If the prior distribution of α is uniform between $\{0, 1\}$, then the label y is completely uncorrelated from the circuit specified by x . Therefore, determining α is as hard as simulating the classically hard BQP circuit specified by x . Furthermore, determining the label y' for any new classically hard BQP circuits, x' , would still require super-polynomial classical resources even when α is known. Demonstrating quantum advantage in both the training stage and the inference stage of the learning protocol.

- [2] R. O. Jones, [Rev. Mod. Phys.](#) **87**, 897 (2015).
- [3] H.-Y. Huang, R. Kueng, G. Torlai, V. V. Albert, and J. Preskill, *Science* **377**, [10.1126/science.abk3333](#) (2022).
- [4] L. Lewis, H.-Y. Huang, V. T. Tran, S. Lehner, R. Kueng, and J. Preskill, *Nature Communications* **15**, [10.1038/s41467-024-45014-7](#) (2024).
- [5] M. Wanner, L. Lewis, C. Bhattacharyya, D. Dubhashi, and A. Gheorghiu, [Predicting ground state properties: Constant sample complexity and deep learning algorithms](#) (2024), [arXiv:2405.18489 \[quant-ph\]](#).
- [6] C. Rouzé, D. Stilck França, E. Onorati, and J. D. Watson, *Nature Communications* **15**, [10.1038/s41467-024-51439-x](#) (2024).
- [7] H.-Y. Huang, M. Broughton, M. Mohseni, R. Babbush, S. Boixo, H. Neven, and J. R. McClean, *Nature Communications* **12**, [10.1038/s41467-021-22539-9](#) (2021).
- [8] A. Barthe, M. Y. Rad, M. Grossi, and V. Dunjko, [Quantum advantage in learning quantum dynamics via fourier coefficient extraction](#) (2025), [arXiv:2506.17089 \[quant-ph\]](#).
- [9] T. Albash and D. A. Lidar, [Rev. Mod. Phys.](#) **90**, 015002 (2018).
- [10] S. Bachmann, W. De Roeck, and M. Fraas, *Physical Review Letters* **119**, [10.1103/physrevlett.119.060201](#) (2017).
- [11] S. Bachmann, W. De Roeck, and M. Fraas, [Communications in Mathematical Physics](#) **361**, 997–1027 (2018).
- [12] R. Oliveira and B. M. Terhal, [The complexity of quantum spin systems on a two-dimensional square lattice](#) (2008), [arXiv:quant-ph/0504050](#).