PROCEEDINGS OF SCIENCE

Preparing ground states for quantum computation of gauge theories

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Simulation of adiabatic methods on a quantum computer has been successfully used to prepare ground states of gauge theories. However, this process requires a high number of quantum gates, which is inaccessible in the NISQ era. An alternative approach is to use variational methods, which utilise a hybrid of classical and quantum computation. We show how a particular example, the Quantum Approximate Optimisation Algorithm (QAOA), can be used to prepare ground states of the Schwinger Model, with an improved circuit depth compared to the adiabatic approximation that targets current devices. In addition, we discuss how, in principle, Permutational Quantum Computing can give us better optimisation beyond the NISQ era.

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1. Introduction

Lattice formulations provide a non-perturbative framework to perform gauge theory calculations in regimes with strong interactions. Whilst successful in many cases, there are issues when attempting to evaluate a path integral using typical Markov-Chain Monte Carlo methods if the integrand is highly oscillatory. This is known as the sign problem [1] and arises in many topics of interest, such as real time evolution, out-of-equilibrium dynamics, high fermionic density, and models with topological terms or chemical potentials. One option to circumvent the sign problem is to switch to the Hamiltonian formulation, however the memory required to store the full wave function is dependent on the size of the Hilbert space, which grows exponentially as the lattice is scaled up. This fast becomes infeasible for classical computation, however the outlook for quantum computation is promising, since qubits can more naturally represent these large Hilbert spaces.

An important consideration when designing a quantum computation is the resources required in comparison with the current hardware available. The so called Noisy Intermediate Scale Quantum (NISQ) era describes the class of present day quantum machines which have access to up to tens or hundreds of qubits, whilst being prone to error rates which limit the depth (quantum gate count) of a circuit [2]. For example, the adiabatic theorem can be used to guarantee preparation of the ground state (approximate) of a desired Hamiltonian from a known Hamiltonian, however the number of gates required to do so is infeasible to run without noise dominating [3]. Eventually it is hoped that technologies will develop to the point of fault tolerance, which will likely require us to perform quantum error corrections [4]. However, it is worth exploring the options for the quantum state preparation that are available in the near-term. One choice is to employ variational methods, which take a combined quantum and classical computation approach to reduce the resources required on the quantum side. We set out the method for a particular form of this, a version of the Quantum Approximate Optimisation Algorithm (QAOA) [5] which uses the S_n-CQA ansatz [6]. This has potential applications with many particle physics models as it is suitable for models with an $SU(d) symmetry$.

2. Translating gauge theory Hamiltonian for quantum computation

Before diving into specific quantum algorithmic methods, it is useful to briefly cover the basics of converting a particle physics problem into a form we can work with quantum computation. As an example, and the main model considered in this paper, we look at the Schwinger model (1 + 1 dimensional QED) with an added topological term θ which as discussed in the previous section, would cause a sign problem with Monte Carlo methods. Using the staggered fermion χ_n of mass m, the Hamiltonian for N sites is given by

$$H = -i \sum_{n=1}^{N-1} \left(w - (-1)^n \frac{m}{2} \sin\theta \right) \left[\chi_n^\dagger e^{i\phi_n} \chi_{n+1} - \text{h.c.} \right] + m \cos\theta \sum_{n=1}^{N} (-1)^n \chi_n^\dagger \chi_n + J \sum_{n=1}^{N-1} L_n^2, \quad (1)$$

where for lattice spacing a and coupling strength g, we have $w = 1/(2a)$ and $J = g^2 a/2$. ϕ_n lives on the nth site and is related to the gauge operator $\phi_n \leftrightarrow -agA^1(x)$, whilst L_n lives on the link

between sites n and $n+1$ and is related to the conjugate momentum $L_n \leftrightarrow -\Pi(x)/g$.

Quantum gates in theory can be any unitary operation, however in practice, there are standard gate sets whose combinations can fully span the Hilbert space of the qubits [7]. Thus, we seek to translate the Hamiltonian above into a form easily implementable with fundamental quantum gates. The traditional approach is to map to a spin system, as the Pauli operators are the most common basic gates. There are different choices to map fermions to spins, we opt for the Jordan-Wigner transformation [8] given by

$$\chi_n = \left(\prod_{l<n} -iZ_l\right) \frac{X_n - iY_n}{2}, \tag{2}$$

where any (X_n, Y_n, Z_n) would indicate a corresponding Pauli gate on qubit n. We also have the advantage in one spatial dimension to solve the Gauss law

$$L_n - L_{n-1} = \chi_n^\dagger \chi_n - \frac{1-(-1)^n}{2}, \tag{3}$$

providing we specify open boundary conditions. This comes with the drawback of introducing non-local interactions to the final result, which may incur an extra cost depending on the connectivity between qubits of a quantum computer [9]. The full spin Hamiltonian ignoring constant terms is given by $H = H_{ZZ} + H_\pm + H_Z$, where

$$\begin{aligned} H_{ZZ} &= \frac{J}{2} \sum_{n=2}^{N-1} \sum_{1\le k\le l\le n} Z_k Z_l, \\ H_\pm &= \frac{1}{2} \sum_{n=1}^{N-1} \left(w - (-1)^n \frac{m}{2} \sin\theta\right) \left[Z_n Z_{n+1} + Y_n Y_{n+1}\right], \\ H_Z &= \frac{m\cos\theta}{2} \sum_{n=1}^{N} (-1)^n Z_n - \frac{J}{2} \sum_{n=1}^{N-1} (n \bmod 2) \sum_{l=1}^{n} Z_l. \end{aligned} \tag{4}$$

It is not uncommon to need to implement the exponential of this or similar Hamiltonians, for example with time evolution. And we use Suzuki-Trotter decomposition to evaluate the time evolution here -

$$e^{A+B} = \lim_{n\to\infty} \left(e^{A/n} e^{B/n}\right)^n, \tag{5}$$

and truncate at some n, a step called Trotterisation. Using fewer terms will naturally require a lower circuit depth, but the potential error incurred in doing so should be considered.

3. Variational Quantum Eigensolver

A general approach to utilising variational methods on a quantum computer is the Variational Quantum Eigensolver (VQE) [10]. Taking advantage of the fact that the ground state of a Hamiltonian will trivially have an equal or lower energy compared to an arbitrary state, we use a parametrised ansatz circuit to prepare a state and measure its energy. This energy becomes the cost function $C(\boldsymbol{\theta}) = \langle\psi(\boldsymbol{\theta})|H|\psi(\boldsymbol{\theta})\rangle$ which we optimise to a minimum using classical computation, as shown in Figure 1. Choice of ansatz is a key decision which involves many factors to consider. For

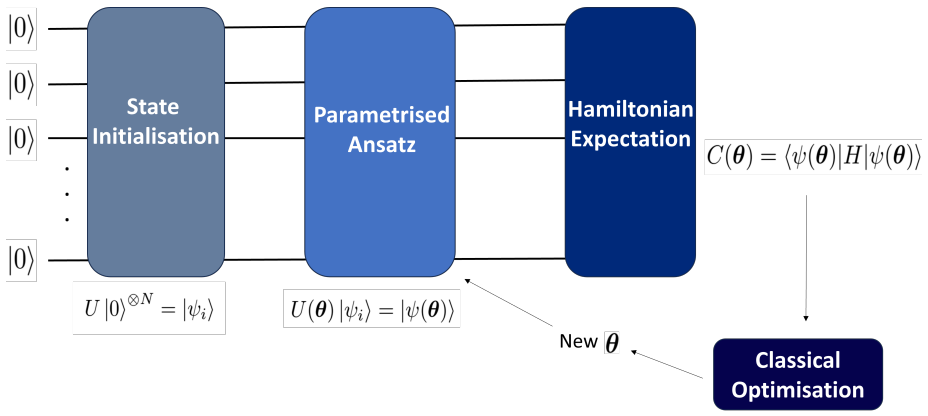

Figure 1: Circuit diagram showing the general structure of a VQE algorithm.

example, a hardware efficient ansatz [11] is generally applicable (i.e. agnostic to the target physics model) and only uses nearest neighbour two-qubit gates (which typical quantum computers will have connectivity to support.) However, the cost space is prone to suffer from vanishing gradients, called barren plateaus, which has crushing consequences if the optimiser gets stuck in such a region [12]. A logical consideration is to design problem specific ansatze, which can try to take advantage of known features or symmetries of the model [13]. This can, say, reduce the number of parameters needed to optimise over, which heuristically tends to mitigate the barren plateau problem. With this in mind we consider QAOA.

4. Quantum Approximate Optimisation Algorithm (QAOA)

Quantum Approximate Optimisation Algorithm (QAOA) [5, 10] is a quantum algorithm designed to generate a quantum state that represents a superposition of all potential solutions to a given problem. It operates by applying a series of unitary transformations to an initial state, where the number of transformations and their specific parameters are tailored to the problem for which the QAOA algorithm is implemented. That being said, for our purposes we will treat it as a standard VQE ansatz, which generates a state ψ_p parametrised by the two vectors of parameters $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ given as

$$\psi_p(\boldsymbol{\beta},\boldsymbol{\gamma}) = e^{-i\beta_p \hat{H}_M} e^{-i\gamma_p \hat{H}_C} \dots e^{-i\beta_1 \hat{H}_M} e^{-i\gamma_1 \hat{H}_C}, \tag{6}$$

where H_M and H_C are the so-called mixer and cost Hamiltonians respectively. The cost Hamiltonian is simply the problem Hamiltonian, for example that of the Schwinger model defined in equation 4. The mixer Hamiltonian is more flexible, with the only condition being that it does not commute with the cost Hamiltonian - this prevents the optimiser from getting stuck in a higher energy eigenstate. Note that this is an example of a layered ansatz with p layers, and thus $2p$ parameters. Choosing more layers requires more gates but the parametrised space may encapsulate the ground state with higher fidelity. As an example of this Figure 2 shows QAOA results for the Schwinger model from

1 to 5 layers, using a standard XY mixer,

$$H_M = \frac{1}{2}\sum_{n}^{N-1} X_n X_{n+1} + Y_n Y_{n+1}. \tag{7}$$

We choose to initialise the qubits in the ground state of the mixer Hamiltonian. Considering this, the motivation to choose an ansatz of this form is due to its similarity to using an adiabatic process. In the limit of infinite layers, convergence is guaranteed as we can choose parameters to be equivalent from adiabatically moving from the mixer Hamiltonian to the cost Hamiltonian.

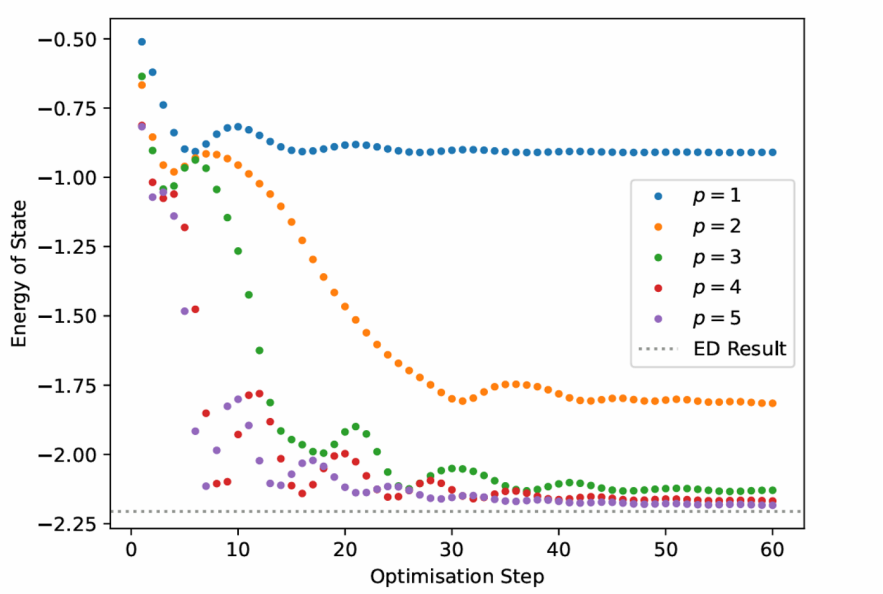

Figure 2: Results of QAOA with 1-5 layers for the Schwinger model. The dotted line is the result obtained from exact diagonalisation. $N = 4$, $m = 0.35$, $w = 0.6$, $J = 5/12$.

5. S_n Convolutional Quantum Alternating Ansatz

The lack of theoretical guarantees of convergence for finite layers is a current downside of QAOA, but only encourages exploring the practicality of the algorithm at varying levels. The S_n Convolutional Quantum Alternating Ansatz takes the same form of equation 6, but uses a specially designed mixer.

To introduce the S_n Convolutional Quantum Alternating (S_n-CQA) ansatz, it is first necessary to cover the topic of the Schur basis. Typical quantum computation involves measuring qubits in the basis of the eigenstates of the Pauli Z operator, commonly referred to as the computational basis. However this is not the only model of quantum computation, and the alternative we consider is permutational quantum computing. Here, we instead work in the state-space of qubits coupled via Clebsch-Gordan coefficients, and measure in the basis of eigenstates of the total spin and angular momentum operators, Z and S^2 respectively. We choose the particular coupled qubit subsets of

$$\{1,2\} \subseteq \{1,2,3\} \cdots \subseteq \{1,2,3 \ldots N-1\} \subseteq [N], \tag{8}$$

where $[N] = \{1, 2, 3, ..., N\}$. This choice is such that the simultaneous eigenstates of $S^2_{[2]}, S^2_{[3]}, \ldots, S^2_{[N]}, Z_{[N]}$ form a complete basis for an N-qubit Hilbert space, which we denote the Schur basis. We can use the relevant Clebsch-Gordan coefficients to map computational basis states to Schur basis states (to some arbitrary order) by implementing an algorithm for the quantum Schur transform [14].

The name permutational quantum computing comes from the fact that instead of using quantum gates, qubits are permuted before measurement. The central operations used in the S_n-CQA ansatz are Young-Jucys-Murphy (YJM) elements, which are defined as a sum of transpositions

$$X_k = (1, k) + (2, k) + (3, k) + \cdots + (k - 1, k), \tag{9}$$

where $1 < k \leq N$ and $X_1 = 0$ is set as a convention. All YJM-elements are diagonal in the Schur basis. Finally we are able to define the mixer Hamiltonian used in the (S_n-CQA) ansatz, which takes the form

$$H_M = \sum_{k<l} \beta_{kl} X_k X_l, \tag{10}$$

where the β_i's are parameters to be optimised over and the X_i's are the YJM elements.

6. Discussion

Our study explores quantum algorithms for preparing ground states in gauge theories, focusing on the Schwinger model. Classical methods face challenges like the sign problem, making quantum computation a promising alternative, particularly with variational approaches suited for NISQ-era devices.

We investigated QAOA as a method for ground-state preparation and found it significantly reduces circuit depth compared to adiabatic methods, making it more feasible for current hardware. However, its convergence at finite depth remains uncertain. To enhance optimisation and mitigate barren plateaus, we are currently testing the S_n Convolutional Quantum Alternating Ansatz (S_n-CQA) for the Schwinger model. This ansatz leverages the Schur basis and permutational quantum computing to encode problem-specific symmetries, potentially improving convergence. Our goal is to determine whether this method consistently outperforms standard QAOA or at what limits it provides better and faster convergence. Challenges remain, particularly in implementing Schur-based operations on quantum processors and optimising variational parameters efficiently.

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