

Introduction

Using quantum computers to perform simulations of field theories has the potential advantage of enabling a direct computation of the fermionic spectrum. As a first step we simulate the Schwinger model Hamiltonian with a θ -term using staggered fermions. We consider adiabatic state preparation and the Quantum Approximate Optimization Algorithm, studying their convergence properties and costs in terms of CNOT gates. We conclude with results based on a blocked system that has a better scaling behavior with the dimensionality of the problem.

Model Description

We consider the Schwinger model [1], a $U(1)$ gauge theory in $1+1$ dimension, with the inclusion of a θ -term [2]. The Lagrangian can be written as

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{g\theta}{4\pi}\epsilon_{\mu\nu}F^{\mu\nu} + i\bar{\psi}\gamma^\mu(\partial_\mu + igA_\mu)\psi - m\bar{\psi}\psi$$

with the gamma matrices for $1+1$ dimensions being $\gamma^0 = \sigma^3$, $\gamma^1 = i\sigma^2$, $\gamma^5 = \gamma^0\gamma^1$ and the field tensor $F_{\mu\nu}$ takes the usual form. The gauge invariance of the Hilbert space is obtained by imposing the Gauss law: $0 = -\partial_1\dot{A}^1 - g\bar{\psi}\gamma^0\psi$

Discretization and Pauli Hamiltonian

We discretize the spatial direction on a 1D lattice of N sites and lattice spacing a using staggered fermions [3, 4] (a full description of the setup can be found in [5])

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

Where $\phi_n = -agA^1(an)$ and $L_n = -\frac{\dot{A}^1(an)}{g}$ while the fermions have been translated into a pair of one-component spinors such that: $\frac{\chi_n}{\sqrt{a}} = \psi_u(an)$ for n even and $\frac{\chi_n}{\sqrt{a}} = \psi_d(an)$ for odd n . Applying open boundary conditions and solving Gauss's law one obtains:

$$L_n = L_0 + \frac{1}{2}\sum_{l=0}^n(Z_l + (-1)^l).$$

At this point one can safely set $L_0 = 0$ by redefining θ and also absorb the gauge fields into the fermionic field as an additional phase: $\chi_n \rightarrow \prod_{l<n}[e^{-i\phi_l}]\chi_n$. The final hamiltonian in terms of spin variables can be written as: $H = H_{ZZ} + H_\pm + H_Z$ where:

$$H_{ZZ} = \frac{J}{2}\sum_{n=2}^{N-1}\sum_{1\leq k<l\leq n}Z_kZ_l$$

$$H_\pm = \frac{1}{2}\sum_{n=1}^{N-1}\left(w - (-1)^n\frac{m}{2}\sin\theta\right)[X_nX_{n+1} + Y_nY_{n+1}]$$

$$H_Z = m\cos\theta\sum_{n=1}^NZ_n - \frac{J}{2}\sum_{n=1}^{N-1}(n \bmod 2)\sum_{l=1}^nZ_l,$$

where we defined the constants $w = \frac{1}{2a}$ and $J = \frac{g^2}{2}$ and (X_n, Y_n, Z_n) are the Pauli matrices at site n

Adiabatic State Preparation and Quantum Approximate Optimization Algorithm

In order to study the properties of the system on a physical quantum hardware one needs an efficient method to prepare the wavefunction of states. Since the state preparation is just the first part of a quantum algorithm, it is important to make sure that to prepare the desired state one uses as few quantum operations as possible.

Adiabatic State Preparation

Adiabatic State Preparation (ASP) [6] is a well established method for state preparation. Its fundamental idea is to first solve a system that is simpler than the target one, but for which state preparation is trivial. One then slowly changes the Hamiltonian of the system to match that of the full problem. For example, in this work, following Ref. [5], we considered the initial hamiltonian $H_0 = H_{ZZ} + H_Z|_{m\rightarrow m_0, \theta\rightarrow 0}$, which is very simple to analyze. Its ground state is a product state of alternating spins up and down. To obtain the ground state of our Schwinger model one needs to repeatedly apply an approximate time evolution operator.

In the simplest case one defines this operator as $U(t) = e^{-iH_A(t)t}$ where $H_A(t)$ is the adiabatic hamiltonian, which interpolates between H and H_0 by making the constants w , θ and m time dependent.

Quantum Approximate Optimization Algorithm

The Quantum Approximate Optimization Algorithm (QAOA) [7] is a quantum optimization algorithm that can be used also for state preparation. It relies, just as ASP, on the existence of a simple trivially solvable Hamiltonian to use as a starting point. The ansatz for the state is given by:

$$|\psi_N(\vec{\gamma}, \vec{\beta})\rangle = e^{-i\beta_N H_0} e^{-i\gamma_N H} \dots e^{-i\beta_2 H_0} e^{-i\gamma_2 H} e^{-i\beta_1 H_0} e^{-i\gamma_1 H}$$

The problem is reduced to finding the optimal values for $\vec{\gamma}^*$ and $\vec{\beta}^*$ such that $|\psi_N(\vec{\gamma}^*, \vec{\beta}^*)\rangle$ is a good approximation of the desired state. For this work we used simulated annealing, minimizing the energy of the system, as in a variational problem.

Numerical Results

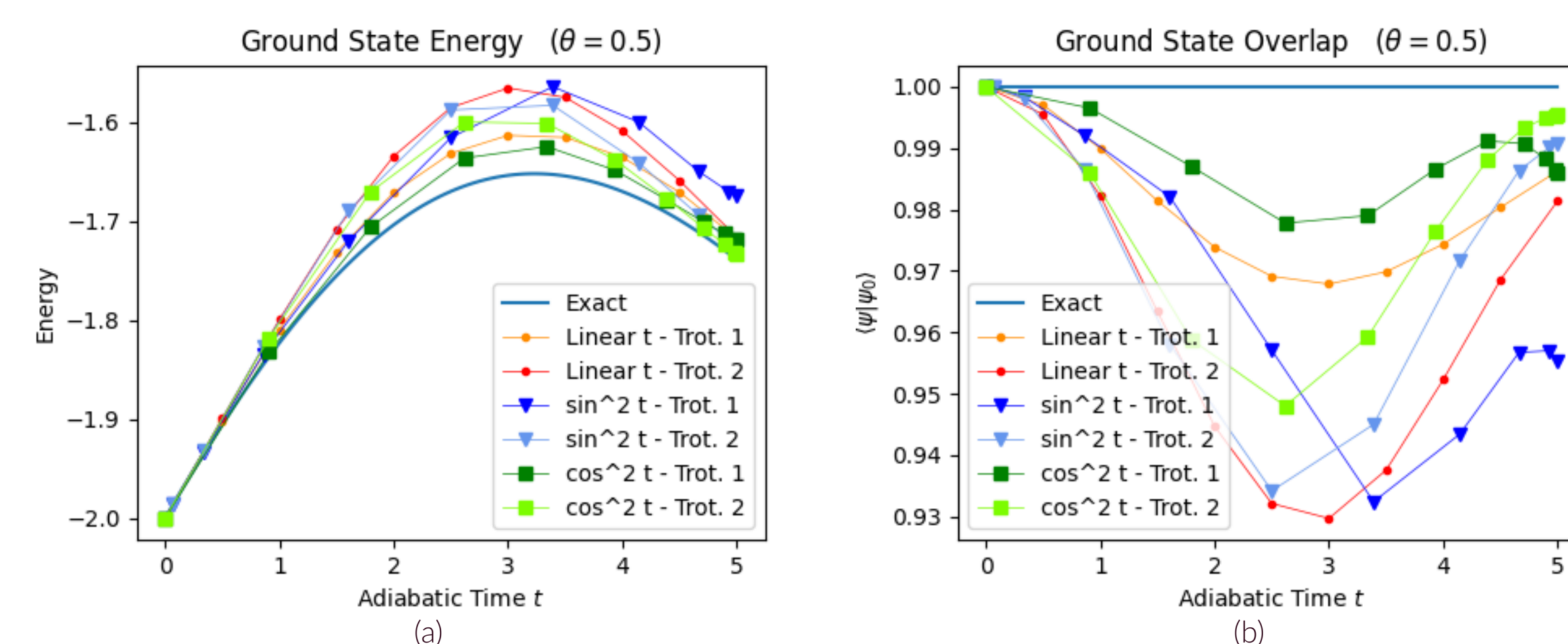


Figure 1. Simulation of ASP of a $N = 4$ system with $J = 0.5$, $m_0 = 0.5$, $m = 0$, $w = 1$, $\theta = 1$. The different series represent different adiabatic time spacings: linear, \sin^2 (taking more dense points at the beginning and end of the ASP) and \cos^2 (taking more dense points at the end of the evolution), with different trotterization scheme orders. The simulation is done using the Qiskit package from IBM. Left plot: energy of the system, the exact line represents the results obtained from exact diagonalization of the adiabatic hamiltonian at every time point. Right plot: overlap between the evolved state and the exact ground state of the adiabatic hamiltonian obtained from full diagonalization at every time t .

Our findings using ASP are that with 10 time steps one can easily find the ground state of the system with 99% accuracy. It is also worth noticing that the \cos^2 time spacing seems to give the overall best results already with first order trotterization, meaning that is more important to evolve more precisely the state in the last steps, where the hamiltonian is closer to the full one. However, as seen from table 1, the number of quantum gates required are presently too large for any practical purpose.

QAOA Results

The QAOA method has the advantage to permit to set the number of steps in the evolution to a very small number, provided one can find the optimal parameters for such evolution. For instance, for the same systems shown before we obtained comparable results with just two steps, table 1.

| Method | # of Steps | Trotter Scheme | # of CNOT/Qubit | E_0 | GS Overlap |
|--------------|------------|----------------|-----------------|---------|------------|
| ASP linear | 10 | 1st order | 45 | -1.7140 | 0.9827 |
| ASP \sin^2 | 10 | 1st order | 45 | -1.6751 | 0.9599 |
| ASP \cos^2 | 10 | 1st order | 45 | -1.7144 | 0.9827 |
| ASP linear | 10 | 2nd order | 75 | -1.7089 | 0.9729 |
| ASP \sin^2 | 10 | 2nd order | 75 | -1.7204 | 0.9847 |
| ASP \cos^2 | 10 | 2nd order | 75 | -1.7260 | 0.9880 |
| QAOA | 2 | 2nd order | 18 | -1.7353 | 0.9975 |
| QAOA | 3 | 2nd order | 27 | -1.7357 | 0.9977 |

Table 1. Comparison of final states from ASP and QAOA for the same system as in fig. 1. Calculation are performed using the Qiskit software package from IBM [8].

The issue with QAOA is that the minimization problem needs to be solved either classically or with a quantum algorithm. Solving it classically is feasible only for small systems, solving it on quantum hardware can be expensive and limited by noise. Therefore, to make the algorithm scale better an option is to use custom optimized 2-qubit gates [9]. However, since the hamiltonian is non local because of the interaction and boundary term, this cannot be done trivially.

Our proposal is to first solve a blocked system, then stack such blocks and use them as a starting point for further optimization. For example the $N = 4$ case would be composed of 2 non interacting blocks of 2 qubits each, thus providing a much better starting Hamiltonian than just H_0 , and consequently improving scaling considerably. In table 2 we report the results for an optimized blocked $N = 4$ system and the results for larger ones obtained using the optimal parameters of the $N = 4$ case without further optimization. These simulation consist of 2 steps of blocked QAOA (which can be turned into just 2 optimal gates per step) and a final step with the full hamiltonian.

| N | # CNOT/qubit | E_0 | E_0/E_{Exact} | GS Overlap |
|----|--------------|---------|-----------------|------------|
| 4* | 19 (10.5) | -1.7263 | 0.9931 | 0.9924 |
| 6 | 24 (16.6) | -3.4072 | 0.9926 | 0.9872 |
| 8 | 28.5 (21) | -5.6292 | 0.9926 | 0.9780 |
| 10 | 32.8 (23.2) | -8.3265 | 0.9930 | 0.9676 |

Table 2. QAOA Blocked with $2+1$ steps, meaning 2 blocked and 1 fully connected step, for the same parameters as in table 1. The results for the $N = 4$ are obtained after parameter optimization, the results for $N = 6, 8, 10$ are have been computed using the same optimal parameters for $N = 4$. The number of qubits in parenthesis represents the amount of CNOTs gates required if optimal custom gates are used.

Summary and Outlook

We found that it is possible to efficiently prepare the ground state of a Schwinger model with θ -term using both Adiabatic State Preparation and Quantum Approximate Optimization Algorithm. With the first method one is limited by the number of two-qubit gates in the quantum algorithm, which becomes quickly prohibitively large for current quantum hardware. Better adiabatic time discretizations can help improve convergence in fewer steps. QAOA on the other hand requires considerably less gates to achieve comparable results.

To circumvent the increasing complexity of the optimization problem for QAOA we proposed a blocking procedure that produces good candidates for the ground state of a system given the optimized parameters of a smaller sized one.

We intend to apply these findings as a starting point for further studies such as implementing the Rodeo algorithm [10] to obtain the spectrum of the theory.

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