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Quantum State Preparation for the Schwinger Model

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It is not possible, using standard lattice techniques in Euclidean space, to calculate the complete fermionic spectrum of a quantum field theory. Algorithms running on quantum computers have the potential to access the theory with real-time evolution, enabling a direct computation. As a testing ground we consider the 1 + 1-dimensional Schwinger model with the presence of a θ term using a staggered fermions discretization. We study the convergence properties of two different algorithms —adiabatic evolution and the Quantum Approximate Optimization Algorithm— with an emphasis on their cost in terms of CNOT gates. This is crucial to understand the feasibility of these algorithms, because calculations on near-term quantum devices depend on their rapid convergence. We also propose a blocked algorithm that has the first indications of a better scaling behavior with the dimensionality of the problem.

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1. Introduction

The successful implementation on a noisy intermediate-scale quantum (NISQ) device of a gate-based quantum algorithm depends critically on the limited and noisy quantum resources. The noise is not the only factor to take into account, but also the depth and width of a given implementation. In this proceeding we study two different algorithms for quantum state preparation —adiabatic evolution [1] and the Quantum Approximate Optimization Algorithm (QAOA) [2]— on a 1 + 1-dimensional quantum field theory, the Schwinger model [3] in the presence of a θ term [4]. The Schwinger model, i.e. Quantum Electrodynamics in 1 + 1 dimension, has been used in the past as a testing ground for simplified studies of QCD [5] and in the presence of a θ term for testing different computational approaches [6, 7]. This is because it enjoys properties such as spontaneous chiral symmetry breaking and confinement. After gauge fixing the photons become massive and there is a non-vanishing chiral condensate $\langle\overline{\psi}\psi\rangle$ similarly to QCD. The presence of a θ term is particularly interesting because direct simulations of QCD with a θ term in Euclidean space are not possible, the action being complex.

2. Model Description

The Lagrangian of the Schwinger model in 1 + 1 dimensions, with U(1) gauge fields A_μ, and the θ term can be written as

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

where the gamma matrices in 1 + 1 dimensions are $\gamma^0 = \sigma^3$, $\gamma^1 = i\sigma^2$, $\gamma^5 = \gamma^0\gamma^1$, the field tensor $F_{\mu\nu}$ takes the usual form and $\epsilon_{\mu\nu}$ is a totally antisymmetric tensor. The parameters of the theory are the gauge coupling g, which in 1 + 1 dimensions has the dimension of a mass, the fermion mass m and the θ angle. Using a $U(1)_A$ rotation, the θ-term can be absorbed into the mass term [8]. If we choose the timelike axial gauge $A_0 = 0$ the Hamiltonian reads [9]

$$H = \int dx \left[-i\bar{\psi}\gamma^1(\partial_1 + igA_1)\psi + m\bar{\psi}e^{i\theta\gamma_5}\psi - \frac{1}{2}\dot{A}_1\dot{A}^1\right], \tag{2}$$

where the electric field has only one component $E = F^{10} = -\dot{A}^1$. The equation of motion (Gauss's law) provides the additional constraint for the remaining gauge degrees of freedom $\partial_1 E = g\bar{\psi}\gamma^0\psi \implies \partial_1\dot{A}^1 + g\bar{\psi}\gamma^0\psi = 0$. Strictly speaking, in a finite volume this is true only with open boundary conditions, while periodic boundary conditions will still allow a remaining gauge degree of freedom.

2.1 Discretization and Pauli Hamiltonian

Following Ref. [10], in the Hamiltonian formalism we keep the time continuous and discretize the spatial dimension on a 1D lattice of N sites and lattice spacing a using staggered fermions [11, 12]

$$H = -i\sum_{n=1}^{N-1}\left(\frac{1}{2a} - (-1)^n\frac{m}{2}\sin\theta\right)\left[\chi_n^\dagger e^{-aigA^1(an)}\chi_{n+1} - \text{h.c.}\right] + m\cos\theta\sum_{n=1}^{N}(-1)^n\chi_n^\dagger\chi_n + \frac{g^2a}{2}\sum_{n=1}^{N-1}\Pi_n^2\,, \tag{3}$$

where $\Pi_n = -\frac{\dot{A}^1(an)}{g}$ is the rescaled conjugate momentum at the lattice point $x = an$. 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. In this formulation the Gauss's law becomes [13]:

$$0 = -(\Pi_n - \Pi_{n-1}) + \chi_n^\dagger \chi_n - \frac{1-(-1)^n}{2} \,. \tag{4}$$

The χ field can be transformed into a qubit formulation using the well-known Jordan-Wigner transformation [14] that transforms the fermionic variables into spin variables

$$\chi_n = \prod_{l<n} iZ_l \frac{X_i - iY_i}{2} \,, \tag{5}$$

where the spin variables are the Pauli matrices located at each lattice point, $X_i = \sigma_i^x$, $Y_i = \sigma_i^y$, $Z_i = \sigma_i^z$. Using open boundary conditions, i.e. fixing the conjugate momentum Π at the boundary, and solving Gauss's law one obtains

$$\Pi_n = \Pi_0 + \frac{1}{2}\sum_{l=0}^{n} \left(Z_l + (-1)^l\right) \,, \tag{6}$$

and the value of Π_0 specifies the boundary conditions. Removing Π_0 is equivalent to shifting the θ angle by $2\pi\Pi_0$ [15], thus we can safely set $\Pi_0 = 0$. The parallel transport in the spatial direction can be reabsorbed in a redefinition of the fermion fields as an additional phase $\chi_n \to \prod_{l<n}\left[e^{-iagA^1(al)}\right]\chi_n$.

The final Hamiltonian, omitting constant terms, can be decomposed as $H = H_{ZZ} + H_\pm + H_Z$, where

$$\begin{aligned} H_{ZZ} &= \frac{J}{2}\sum_{n=2}^{N-1}\sum_{1\le k<l\le n} Z_k Z_l \\ H_\pm &= \frac{1}{2}\sum_{n=1}^{N-1}\left(w - (-1)^n\frac{m}{2}\sin\theta\right)\left[X_n X_{n+1} + Y_n Y_{n+1}\right] \\ H_Z &= m\cos\theta\sum_{n=1}^{N}(-1)^n Z_n - \frac{J}{2}\sum_{n=1}^{N-1}(n \bmod 2)\sum_{l=1}^{n} Z_l \,, \end{aligned} \tag{7}$$

where, using the same notation as Ref. [10], we denote the relevant couplings for the adiabatic evolution as $w = \frac{1}{2a}$ and $J = \frac{g^2}{2a}$.

3. Adiabatic State Preparation and the Quantum Approximate Optimization Algorithm

To study the properties of the system on a NISQ machine [16], one needs an efficient method to prepare the quantum state. The efficiency of a gate-based quantum algorithm depends on its depth (number of sequential gates) and width (number of qubits). Besides the optimization at compilation time, it is important to optimize the algorithm independently of the hardware used. In this work, we focus on the depth of two algorithms, trying to reduce the number of CNOT operations needed.

3.1 Adiabatic State Preparation

Adiabatic State Preparation (ASP) [1] is a well-established method for quantum state preparation. The basic idea is to first solve a system that is simpler than the target one, but for which state preparation is trivial. One then slowly (adiabatically) changes the Hamiltonian of the system to reach the target one. Following Ref. [10], we consider as the initial Hamiltonian $H_0 = H_{ZZ} + H_Z|_{m\to m_0,\theta\to 0}$, which has a ground state that can be easily identified as the product state of alternating spins up and down. The ground state of the Schwinger model is then obtained with an adiabatic Hamiltonian $H_A(t)$, which interpolates between $H_A(t=0) = H_0$ and the Schwinger model, i.e. $H_A(t=T) = H$.

In the simplest case [10] one defines a "time" evolution operator $U(t) = e^{-iH_A(t)\,\delta t}$ where $\delta t = \frac{T}{M}$ is the elementary step of the adiabatic evolution made of M steps, and the remaining parts of the Hamiltonian are switched on making the parameters $w = \frac{1}{2a}$, θ and m time dependent

$$w \to \frac{t_n}{T} w \quad \theta \to \frac{t_n}{T}\theta \quad m \to \left(1 - \frac{t_n}{T}\right) m_0 + \frac{t_n}{T} m\,, \tag{8}$$

where $t_n = n\frac{T}{M} = n\delta T$, with $n = 0, \ldots, M$. It is clear that the initial time $t = 0$ corresponds to t_0 and the final time T corresponds to t_M. We label this linear discretization of the adiabatic evolution $L1$ or $L2$ depending on the order of the Trotter product formula we use to evaluate the evolution $U(t) = e^{-iH_A(t)\,\delta t}$. We have found more efficient discretizations of the adiabatic evolution that we discuss in Section 4.

3.2 Quantum Approximate Optimization Algorithm

The Quantum Approximate Optimization Algorithm (QAOA) [2] is a quantum optimization algorithm that can also be used for state preparation. It has the advantage of having a rather shallow depth of M layers and $2M$ total parameters. Just as ASP, it relies on the existence of a trivially solvable Hamiltonian H_0 with eigenstate $|\psi_0\rangle$. The ansatz for the eigenstate of the target Hamiltonian is then

$$|\psi_M(\vec{\gamma},\vec{\beta})\rangle = e^{-i\beta_M H_0} e^{-i\gamma_M H} \ldots e^{-i\beta_2 H_0} e^{-i\gamma_2 H} e^{-i\beta_1 H_0} e^{-i\gamma_1 H} |\psi_0\rangle \tag{9}$$

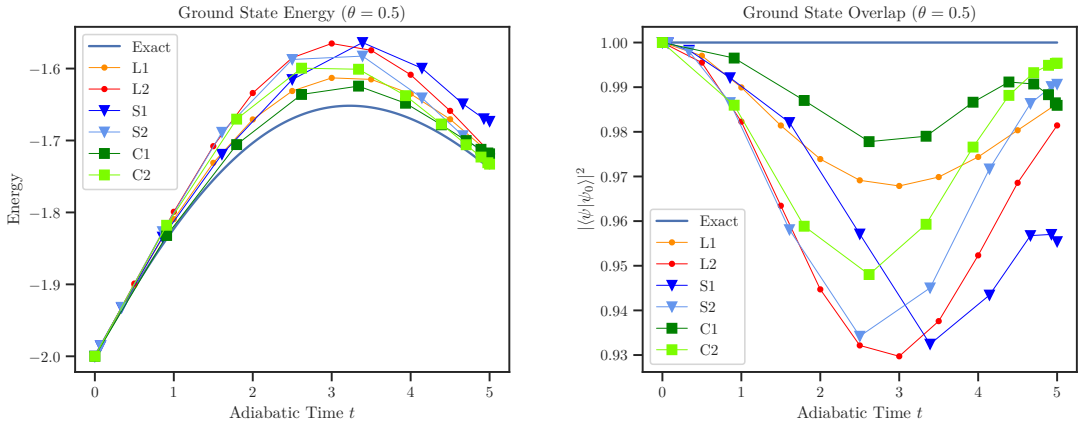
where $\vec{\beta}, \vec{\gamma}$ are $2M$ real coefficients. The problem is reduced to finding the optimal values for $\vec{\gamma}^*$ and $\vec{\beta}^*$ such that $|\psi_M(\vec{\gamma}^*,\vec{\beta}^*)\rangle$ is a good approximation of the desired state. The optimal parameters are found by solving the variational problem

$$\langle\psi_M(\vec{\gamma},\vec{\beta})|\, H\, |\psi_M(\vec{\gamma},\vec{\beta})\rangle \geq E_0, \tag{10}$$

with a minimizer of choice. In this work simulated annealing was used [17], as it is effective for multi-dimensional minimization even in the presence of multiple local minima.

4. Numerical Results

We summarize here first the results obtained using ASP and QAOA with a lattice of $N = 4$ points and then present preliminary results for a novel blocking procedure up to $N = 10$.



(a) **(b)**

Figure 1: Simulation of ASP of a $N = 4$ system with $J = 0.5$, $m_0 = 0.5$, $m = 0$, $w = 0.5$, $\theta = 0.5$. The different series represent different adiabatic time spacings: linear, $L1$ and $L2$, $S1$ and $S2$ (taking more dense points at the beginning and end of the ASP), and $C1$ and $C2$, (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, that is $|\langle\psi(t)|\psi_0(t)\rangle|^2$.

4.1 Results with ASP

We have simulated an $N = 4$ Schwinger model with $g^2 = 1$, $m_0 = 0.5$, $m = 0$, $a = 1$ and $\theta = 0.5$, using different discretizations for the adiabatic evolution and different orders for Trotter's product formula for the time evolution. For the adiabatic evolution, besides the linear discretizations in Eq. (8), we have considered the following discretizations

$$t_n = 2\frac{T}{M}\sum_{k=0}^{n}\sin^2\left(\pi\frac{k}{M}\right), \tag{11}$$

and

$$t_n = 2\frac{T}{M}\sum_{k=0}^{n}\cos^2\left(\pi\frac{k}{2M}\right), \tag{12}$$

which we call respectively $S1$ (or $S2$) and $C1$ (or $C2$) again whether for the adiabatic time evolution we use a first order or a second order Trotter product formula. In Fig. 1a we show the evolution with ASP of the energy of the ground state using ASP with several discretizations of the time evolution. As a comparison, we also plot the result for the exact ground state determined for each time value. We generally observe a very good agreement for the ground state using only 10 steps of ASP. We do observe that the $S1$ discretization is the worst at reproducing the ground state, while the best discretizations are $C1$ and $C2$. These discretizations adapt the time interval to be smaller towards the end of the evolution indicating that it is more relevant to evolve more precisely the state in the last steps, where the Hamiltonian is closer to the target one, rather than at the beginning. These

Method	# of Steps	# of CNOT/Qubit	E_0	GS Overlap
ASP $L1$	10	45	-1.7140	0.9827
ASP $S1$	10	45	-1.6751	0.9599
ASP $C1$	10	45	-1.7144	0.9827
ASP $L2$	10	75	-1.7089	0.9729
ASP $S2$	10	75	-1.7204	0.9847
ASP $C2$	10	75	-1.7260	0.9880
QAOA	2	18	-1.7353	0.9975
QAOA	3	27	-1.7357	0.9977

Table 1: Comparison of final states from ASP and QAOA for the same system as in Fig. 1. For reference, the ground state energy from exact diagonalizaition is $E_0 = -1.7386$. Calculations are performed using the Qiskit software package from IBM [18].

results are summarized in Table 1. In Fig. 1b we show the results for the overlap with the ground state as a function of the adiabatic time. The overlap confirms the result of the energy with the best discretization being $C2$. The results obtained with all the discretizations considered here are summarized in Table 1.

The drawback of the ASP is that the number of quantum gates required is presently too large for any practical purpose. Each first-order Trotter step contains 18 CNOT gates, while a second-order step contains 30. This means that for 10 steps, as in Fig. 1 the total number of CNOTs per qubit is on average ≈ 45 and ≈ 75 for first and second order Trotterization respectively. These numbers (summarized in Table 1) are too large for current quantum hardware.

4.2 QAOA Results

The QAOA method relies on finding the optimal values for the parameters $\vec{\beta}, \vec{\gamma}$ introduced in Sec. 3.2, and it has the advantage to allow setting the number of steps in the evolution to a relatively small number, provided one can find the optimal parameters for such an evolution. For instance, for the same Schwinger model for $N = 4$ and same parameter values, we obtained comparable results for the energy of the ground state with only 2 steps, see Table 1.

The success of the QAOA algorithm depends on the solution of the optimization (minimization) problem that needs to be solved either classically or with a quantum algorithm. Solving it classically is feasible only for small systems, but solving it on quantum hardware can be expensive and limited by noise. One option to improve the scaling of the algorithm would be to use custom optimized 2-qubit gates [19]. However, since the Hamiltonian is nonlocal due to the interaction and boundary term, this cannot be done trivially.

Another option we propose here is to first solve a blocked system, then stack such blocks and use them as a starting point for further optimization. More precisely, we solve the $N = 4$ with $M = 3$ layers of the QAOA algorithm including in the layers a modified or "blocked" Hamiltonian, H^B. The "blocked" Hamiltonian has the same structure of Eqs. åq:hamiltonian but with only the 1-qubit terms and the 2-qubit ones that connect sites 0 and 1 (the first block) and the terms that connect qubits 2 and 3 (the second block). In this way the four sites are split into two non-interacting blocks

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 $M = 3$ steps, meaning with 2 steps performed with the "blocked" Hamiltonian and 1 step with the exact Hamiltonian, for the same parameters as in Table 1. The results for the $N = 4$ are obtained after parameter optimization, the results for $N = 6, 8, 10$ have been computed using the same optimal parameters for $N = 4$. The number of qubits in parentheses represents the amount of CNOT gates required if optimal custom gates are used.

and this modified Hamiltonian can thus be implemented in a single 2-qubit gate. The complete QAOA trial wave function then reads

$$|\psi_3^B(\vec{\gamma},\vec{\beta})\rangle = e^{-i\beta_3 H_0} e^{-i\gamma_3 H} e^{-i\beta_2 H_0} e^{-i\gamma_2 H^B} e^{-i\beta_1 H_0} e^{-i\gamma_1 H^B} |\psi_0\rangle \ . \tag{13}$$

The $M = 3$ layers allow correction for any possible "error" from the blocked Hamiltonian adding a layer with the exact Hamiltonian H. The key difference between this ansatz and the $M = 3$ equivalent from Eq. 9 is that the operator $e^{-i\gamma_n H^B}$ can be implemented more effectively as a single gate, greatly reducing the length of the algorithm.

To scale the system to a larger lattice, one can use the same values for $\vec{\beta}, \vec{\gamma}$ as found for a smaller system as a starting guess for the minimizer: this greatly simplifies the variational problem. In Table 2 we can see that the optimal parameters for the blocked $N = 4$ system give very good results for the ground state of systems up to $N = 10$, without the need to solve any variational problem at that size.

5. Summary and Outlook

We found that it is possible to efficiently prepare the ground state of the 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 quickly becomes prohibitively large for current quantum hardware. Better adiabatic time discretizations can help improve convergence in fewer steps. QAOA on the other hand requires considerably fewer 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 plan to test these algorithms on real quantum hardware and to apply these findings as a starting point for further studies such as implementing the Rodeo algorithm [20] to obtain the spectrum of the theory.

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