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Digital Quantum Simulation for Energy Spectroscopy of Schwinger Model

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We discuss a method to efficiently compute energy spectra in quantum field theories by digital quantum simulation. We utilize a quantum algorithm called coherent imaging spectroscopy which quenches the ground state with a perturbation oscillating periodically in time for various frequencies and then reads off excited energy levels from values of frequencies having loss of the vacuum-to-vacuum probability by the quench. We demonstrate this method in the Schwinger model which is the (1+1)-dimensional quantum electrodynamics with a topological term. In particular, the ground state of the Schwinger model on lattice is prepared by adiabatic state preparation and then we apply various types of quenches to the approximate ground state via Suzuki-Trotter time evolution. We benchmark the types of quenches and argue their (dis)advantages especially in the context of studying quantum field theories. We also estimate the computational complexity to obtain physically reasonable results which likely implies efficiency of the method in the early fault-tolerant quantum computer era.

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1. Introduction

Recently, technology on quantum computers rapidly advances and there has been growing attention in theoretical physics including high energy physics (e.g. [1–3]). One of the most important applications to high energy physics is the digital quantum simulation of quantum field theories because it provides it is naturally implemented in the operator formalism of quantum field theory and potentially a good solution to the infamous sign problem in the conventional Monte Carlo approach (e.g. [4–6]). Instead we typically pay the price of dealing with a huge Hilbert space but it may be overcome by quantum computers in future. It motivates us to extend and demonstrate the utility of digital quantum simulation in the context of quantum field theory.

Here we discuss a method to study energy spectroscopy of quantum field theories by digital quantum simulation. Inspired by the experimental method called coherent imaging spectroscopy [7], we consider a quantum algorithm to compute excited energies in lattice field theories. The main idea is to quench the ground state with a perturbation oscillating periodically in time for various frequencies and then read off excited energy levels from values of frequencies having loss of the vacuum-to-vacuum probability following the quench. We demonstrate our method in the Schwinger model which is the $(1+1)$-dimensional quantum electrodynamics with non-trivial topological angle θ [8, 9]. The Schwinger model is a well-known good test ground for quantum simulations of field theories in the high energy physics context [10–29]. Since the Schwinger model can have the non-trivial topological term i.e. the θ-term, it is naively hard to study the Schwinger model with not small θ by conventional Monte Carlo approach due the sign problem.[1] Thus, it is worth to study its physics by the quantum simulation which is not easily captured by the conventional approach.

2. The lattice Schwinger model in operator formalism

To put the theory on quantum computer, we consider the lattice Schwinger model in operator formalism and map it to a spin system. The Lagrangian density of the Schwinger model is

$$\mathcal{L}_0 = \frac{1}{2g^2}F_{01}^2 + \frac{\theta}{2\pi}F_{01} + \overline{\psi}i\gamma^\mu\left(\partial_\mu + iA_\mu\right)\psi - m\overline{\psi}\psi\,, \tag{1}$$

where m, g, and θ are the mass of the electron, the gauge coupling and the topological angle, respectively. The field ψ is the two-component Dirac spinor associated with the electron while F_{01} denotes the field strength of the gauge field A_μ. Here, rather than Eq. (1), we work in another physically equivalent Lagrangian obtained by the chiral transformation $\psi \to e^{i\theta\gamma_5/2}\psi$ as in [15, 32]:

$$\mathcal{L} = \frac{1}{2g^2}F_{01}^2 + \overline{\psi}i\gamma^\mu\left(\partial_\mu + iA_\mu\right)\psi - m\overline{\psi}e^{i\theta\gamma^5}\psi\,. \tag{2}$$

Note that the θ-term is canceled by the chiral rotation due to the transformation of the path integral measure closely related to the chiral anomaly [33].

Now we put the theory on a one-dimensional spatial lattice with open boundary condition. In the temporal gauge, the Hamiltonian of the lattice Schwinger model with the staggered fermion is

[1] One can circumvent the sign problem for the Euclidean path integral if we map it to the bosonized theory, which is the massive scalar field theory with the trigonometric potential [30, 31].

given by [34, 35]

$$H = J\sum_{n=0}^{N-2} L_n^2 - i\sum_{n=0}^{N-2}\left(w-(-1)^n\frac{m}{2}\sin\theta\right)\left[\chi_n^\dagger U_n\chi_{n+1} - \text{h.c.}\right] + m\cos\theta\sum_{n=0}^{N-1}(-1)^n\chi_n^\dagger\chi_n\,, \tag{3}$$

where N is the number of lattice sites. The parameters are defined in terms of the lattice spacing a and coupling constant g as

$$J = \frac{g^2a}{2}, \quad w = \frac{1}{2a}, \tag{4}$$

where we measure all the dimensionful quantities in the unit of g. The lattice fields satisfy the canonical commutation relations

$$[U_n, L_m] = i\delta_{mn}U_n, \quad \{\chi_n^\dagger, \chi_m\} = \delta_{mn}, \quad \{\chi_n, \chi_m\} = 0, \tag{5}$$

and physical states have to satisfy the lattice version of the Gauss law:

$$L_n - L_{n-1} = \chi_n^\dagger\chi_n - \frac{1-(-1)^n}{2}. \tag{6}$$

Solving the Gauss law and applying the Jordan-Wigner transformation [36]:

$$\chi_n = \left(\prod_{\ell<n} -iZ_\ell\right)\frac{X_n - iY_n}{2}, \tag{7}$$

with the Pauli spins (X_n, Y_n, Z_n) at site n, the lattice Hamiltonian is reduced to the following spin Hamiltonian

$$H = H_{ZZ} + H_{XX} + H_{YY} + H_Z, \tag{8}$$

where

$$\begin{aligned}
H_{ZZ} &= \frac{J}{2}\sum_{n=1}^{N-2}\sum_{0\le k<\ell\le n} Z_kZ_\ell = \frac{J}{2}\sum_{n=1}^{N-2}\sum_{k<n}(N-n-1)Z_kZ_n\,,\\
H_{XX} &= \frac{1}{2}\sum_{n=0}^{N-2}\left\{w-(-1)^n\frac{m}{2}\sin\theta\right\}X_nX_{n+1}\,,\\
H_{YY} &= \frac{1}{2}\sum_{n=0}^{N-2}\left\{w-(-1)^n\frac{m}{2}\sin\theta\right\}Y_nY_{n+1}\,,\\
H_Z &= \frac{m\cos\theta}{2}\sum_{n=0}^{N-1}(-1)^nZ_n + \frac{J}{2}\sum_{n=0}^{N-2}\text{mod}(n+1,2)\sum_{\ell=0}^{n}Z_\ell\,.
\end{aligned} \tag{9}$$

This is the qubit description of the lattice Schwinger model.

3. Simulation method for energy spectroscopy

Let us first outline our simulation method for the energy spectroscopy of the lattice field theory. The key idea is to quench the ground state of the theory by a periodic time dependent perturbation with a particular frequency ω and measure the survival probability of the ground state after the quench. If the value of ω is close to the energy difference between those of the excited states and the ground state, then there should be a transition to the excited state from the ground state and the survival probability of the ground state should be small at some time. If not, then the survival probability should not become small at any time. Repeating this process for various values of ω, we can estimate the energy spectrum. More specifically, we have freedom to choose quantum algorithms basically at two parts: how to prepare the ground state and implement the time evolution. Here, for simplicity, we adopt the adiabatic state preparation for the ground state and Suzuki-Trotter approximation for the time evolution [37–39] while we could use different algorithms like variation-based ones, block-encoding and so on, depending on purposes and properties of hardware.

Coming back to the lattice Schwinger model Eq. (8), we prepare the ground state of the spin Hamiltonian by adiabatically changing the initial state which is given by the ground state $|\mathrm{vac}_0\rangle$ of the simpler initial Hamiltonian: $H_0 := H|_{w=0,\theta=0,m_{\mathrm{lat}}=M_0}$ with $M_0 > 0$ as in [15, 17, 19]. Specifically the initial state $|\mathrm{vac}_0\rangle$ is given by

$$|\mathrm{vac}_0\rangle := |1010\cdots101\rangle\,. \tag{10}$$

Changing the coefficients of the Hamiltonian so that each coefficient interpolates the values in the initial Hamiltonian H_0 and the target Hamiltonian Eq. (9), the adiabatic theorem implies that the state after the time evolution is approximately the ground state of the target Hamiltonian Eq. (9) under the assumptions of the theorem.

Next, we introduce a time dependent perturbation by a gauge-invariant operator whose coefficient periodically depends on time with a particular frequency ω. Specifically, we consider the pseudo-chiral condensate $\overline{\psi}\gamma_5\psi$ as a quenching operator. In particular we consider spatially modulated quenches on the lattice given by the following Pauli spin operators

$$\Delta H(t) = \frac{B_p}{2}\sum_{n=0}^{N-2}(-1)^{n+1} f_n \sin(\omega t)\,(X_nX_{n+1} + Y_nY_{n+1})\,, \tag{11}$$

where the coefficient f_n controls the spatial modulation while B_p with the mass dimension one controls the overall strength of the quench. One of standard choices on f_n is simply that of discrete Fourier transformation:

$$f_n^{(k)} := \cos\left(\frac{k\pi n}{N-1}\right) \quad (k = 0, 1, 2, \cdots), \tag{12}$$

where we call the integer k the mode number.

For implementation of the time evolution in the quantum circuit, we adopt the second order Suzuki-Trotter approximation. Namely, the time evolution operator with the Hamiltonian Eq. (9) at each Trotter step Δt_{ST} is decomposed as

$$e^{-i\Delta t_{ST}H} \simeq e^{-i\frac{\Delta t_{ST}}{2}H_{XX}}e^{-i\frac{\Delta t_{ST}}{2}H_{YY}}e^{-i\Delta t_{ST}(H_{ZZ}+H_Z)}e^{-i\frac{\Delta t_{ST}}{2}H_{XX}}e^{-i\frac{\Delta t_{ST}}{2}H_{YY}} + O\left(\frac{1}{M^3}\right), \tag{13}$$

where M is an integer to denote the total number of time steps of the quench. During the quench, we take the coefficient of the Hamiltonian Eq. (9) to be Eq. (11). Finally, we make the measurement of the survival probability of the ground state defined by[2]

$$\left|\langle \mathrm{vac}|\mathcal{T} e^{-i\int dt(H+\Delta H(t))}|\mathrm{vac}\rangle\right|^2 , \tag{14}$$

where the state $|\mathrm{vac}\rangle$ is the ground state of the target Hamiltonian H and the symbol $\mathcal{T}$ stands for the time order product. Technically, the last measurement procedure requires the adiabatic preparation of vacuum on the bra vector $\langle \mathrm{vac}|$ at the end of the quantum circuit for the simulation.

4. Results

4.1 Parameter setup

Before presenting our results, we explain how values of the parameters are set up in our simulation. First note that the simulation involves four different (angular) frequency scales:

- Trotterization frequency $\omega_{ST} := \frac{2\pi}{\Delta t_{ST}}$ from the Suzuki-Trotter approximation.
- Quench frequency ω.
- Resolution $\Delta\omega$ for frequency domain of the quench.
- Frequency domain $\Omega := \frac{2\pi}{T}$ determined by the simulation time scale $T = M\Delta t_{ST}$.

Also, the perturbative theory with respect to B_p suggests a useful (dimensionless) quantity $\gamma := |\langle f\,|\Delta V|\,\mathrm{vac}\rangle|$. where $\Delta H(t) = B_p \Delta V \sin(\omega t)$ and $|f\rangle$ is one of the excited energy eigenstate with the energy different from the ground state energy by E_{dif}. Then the perturbative calculation [40] shows that the transition probability between the ground state and excited state $|f\rangle$ is given by

$$P_{\mathrm{vac}\to f}(t) = \left(\gamma B_p\right)^2 \frac{\sin^2\left[\left(E_{\mathrm{dif}}-\omega\right)t\right]}{\left(E_{\mathrm{dif}}-\omega\right)^2} + O\left(B_p^3\right) . \tag{15}$$

In our simulation, we take B_p to be small and basically setup the parameters based on the following intuitions from the formula: (i) the transition between the states occurs in a short enough simulation time where the perturbation result is approximately valid, (ii) the parameter $\Delta\omega$ to determine the resolution of the quench frequency is sufficiently fine such that the argument inside the sin function in the formula Eq. (15) can be sufficiently small, namely $\Delta\omega\, T < 1$, around the energy gap $\omega \sim E_{\mathrm{dif}}$.

To judge whether or not the transition occurs, we introduce the probability threshold P_{th} ($0 \lesssim P_{\mathrm{th}} < 1$) as follows. When the vacuum survival probability after the quench is smaller than $1 - P_{\mathrm{th}}$, we identify the loss of the ground state and identify the frequency ω of the quench with the energy gap. Therefore we should take the lower bound of estimated the simulation time T larger certain time T_{th} such that $T > T_{\mathrm{th}} = \frac{\sqrt{P_{\mathrm{th}}}}{\gamma B_p}$. The resolution $\Delta\omega$ for the quench frequency should be smaller than resolution of the energy spectrum i. e. differences among neighboring

[2]The authors in [7] adopted the various energy eigenstates $\langle E_n|$ for the basis of the measurement after the quench. This was possible because energy eigenstates were explicitly known in that problem while such information is generally not available. Here we observe only the loss probability of the ground state.

parameters	symbol	value	remark	parameters	symbol	value	remark
the number of qubits	N	11	odd integer	overall strength of the quench	B_p	0.02500	Eq. (11)
lattice spacing	a	0.9000		the inverse lattice constant	w	0.5556	$w = 1/(2a)$
the number of shots	N_s	20000		quench frequency gap	$\Delta\omega$	0.0500	
the number of steps	M	1000		steps for adiabatic preparation	M_{adia}	2500	$M_{\text{adia}}/M = 2.5$
simulation time	T	40.0000		IR frequency cutoff	Ω	0.1571	$\Omega = 2\pi/T$
Trotterization time	Δt_{ST}	0.0400	$\Delta t_{ST} = T/M$	Trotteriztation frequency	ω_{ST}	157.0796	$\omega_{ST} = 2\pi/\Delta t_{ST}$

Table 1: The choice of the simulation parameters except m, θ and f_n. All the dimensionful parameters are in the unit of the gauge coupling g i.e. $g = 1$ pratically.

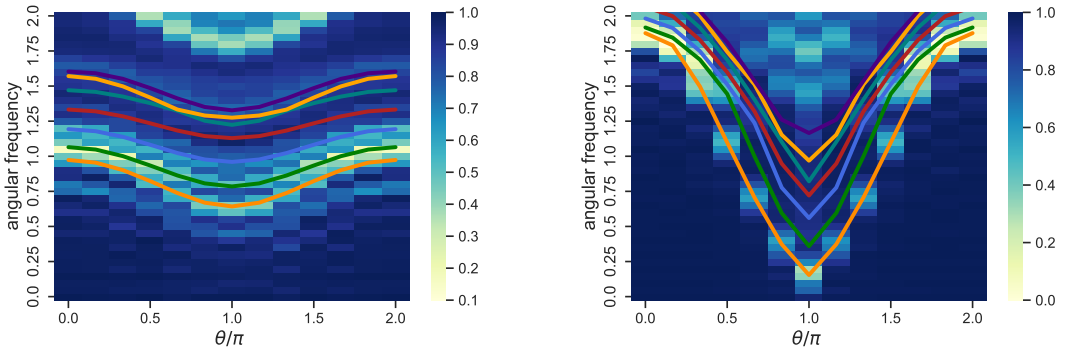
excited energies. To have a reasonable approximation by the Suzuki-Trotter time evolution, the time dependent perturbation should not quickly change in neighboring Trotter steps. More specifically, the order of magnitude of accumulated errors from the second order Suzuki-Trotter approximation scales as $\epsilon_{ST} \sim O\left(M\left(\omega\Delta t_{ST}\right)^3\right) \sim O\left(\omega^3\omega_{ST}^{-2}\Omega^{-1}\right)$. Thus, the reliable simulation requires the accumulative error ϵ_{ST} to be small and we find $\omega_{ST} \gg \Omega^{-\frac{1}{2}}\omega^{\frac{3}{2}}$. Combining the scaling laws above, we find the hierarchy among the frequency scales; $\Delta\omega < \Omega < \omega < \omega_{ST}$. According to the above considerations, we set values of the parameters as in Table 1.

4.2 Simulation results

Let us present our simulation results of the energy spectroscopy. The simulations are implemented using a classical simulator (IBM Qiskit). Figure 1 shows our results obtained by the spatially constant quench ($f_n = 1$) for various values of θ and two values of the mass which are expected to represent different phases. In more detail, the density plots in figure 1 are obtained by computing minima of the vacuum survival probability during the quench for various values of ω and θ. Therefore, in lighter regions of the plots, we interpret that there are transitions from the ground state at some time during the quench. The left panel shows the result for $m = 0.1000$ where the theory is expected to be in the gapped phase for any θ. Indeed the density plot exhibits the first light color region around the first excited energy, which is distant from the ground state energy for all the values of θ. The right panel shows the result for $m = 0.6000$ where the continuum theory at $\theta = \pi$ is expected to have spontaneous symmetry breaking of parity in the infinite volume limit and therefore a small energy gap for large finite volume. We see that the simulation result also implies such small energy gap at $\theta = \pi$.

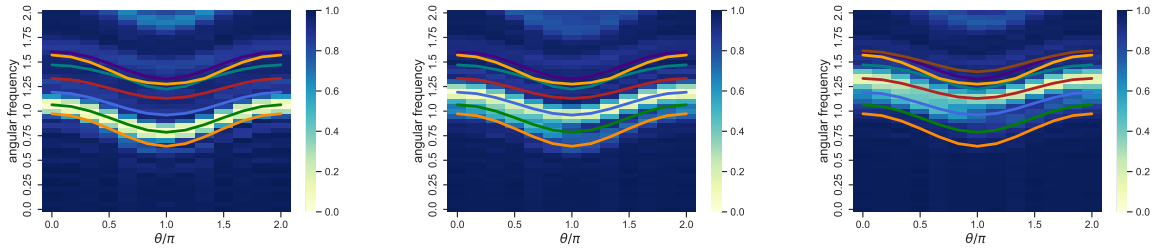
Note also that the plots show dark color regions around some other excited energies. This is consistent if we interpret the excited states as the states with momenta.[3] Namely, when momentum is conserved, the constant quench of the ground state should not have momenta and therefore the transition to such states are prohibited. More precisely, the momentum is not a strictly conserved quantity for open boundary condition but it is approximately conserved for large volume and the plot is interpreted to reflect such approximate conservation. This point is an advantage of our method when we are particularly interested in mass spectra of quantum field theories because we can filter transitions to excited states with momenta. More generally, appropriately choosing types

[3] In the continuum theory for $\theta = 0$, one particle states of the Schwinger boson [8, 9] on an interval of the length L have the energies given by $E_n^2 = M_S^2 + (n\pi/L)^2$ with $M_S = g/\sqrt{\pi}$.



(a) $m = 0.1000$ **(b)** $m = 0.6000$

Figure 1: The density plot for minima of the vacuum survival probability during the quench for various values of the topological angle θ under the pseudo-chiral condensate quench without the spatial modulation ($k = 0$). Solid lines denote the excited energies obtained by the exact diagonalization result using the python library `QuSpin`.



(a) $k = 1$ **(b)** $k = 2$ **(c)** $k = 3$

Figure 2: Similar plots to figure 1 for spatially modulated quenches focusing on the $m = 0.1000$ case. In each panel, the quench operator carries a distinct mode number (a) $k = 1$, (b) $k = 2$, and (c) $k = 3$.

of operators for the quench based on (approximate) quantum numbers, one can mitigate transitions to "unwanted" states depending on contexts. This point is different from other methods like typical variation-based methods to construct excited states one by one starting with the ground state.

Figure 2 shows the results obtained by spatially modulated operators of the quench for the small mass regime ($m = 0.1000$). The mode number k, introduced with the spatial modulation in the form of Eq. (12), labels and distinguish the eigenstates. We see that the plots with different k's have the lighter color regions in different places. We interpret this as transitions to excited states with nonzero momenta and the spatially modulated quench captures excited states with nonzero momenta.

5. Conclusion and Outlook

We discussed a method to efficiently compute energy spectra in quantum field theories by digital quantum simulation. Our results imply that quench-induced state transition of quantum

mechanical system can be used to computer the energy spectra in the lattice gauge theory. We introduced distinct types of gauge-invariant quenches and found that the low-energy excited spectra can be read off from the loss of the vacuum survival probability at specific frequencies close to the excited energies.

One can also estimate computational complexity to obtain reasonable results based on the argument in section 4.1. Let us estimate the number of the controlled-Z (CZ) or CNOT gate given probability threshold $P_{\rm th}$. First, the number of the controlled gates at each Trotter time step quadratically depends on the number of qubits, as seen from the Hamiltonian Eq. (9). Hence, the total number of the controlled gates for $M = T/\Delta t_{ST}$ Trotter steps is given by $\mathcal{N}_{CZ} = O\left(MN^2\right)$. Combined with the argument in section 4.1, this is bounded below as $\mathcal{N}_{CZ} > O\left(\left(\omega\sqrt{P_{\rm th}}/\gamma B_p\right)^{\frac{3}{2}} N^2\right)$, which depends on the energy scale ω and characteristic number γ of the quench.

There are various interesting directions for future work. First, it would be obviously interesting if we implement the simulation on a real quantum device. Another interesting direction is to precisely compare the computational complexity of our method with other approaches to energy spectra of quantum field theories. This is not only for quantum algorithm approaches but also for classical approaches like tensor network, which is another powerful approach to operator formalism of quantum system as it has been nicely demonstrated in the Schwinger model [41–45]. It would be also interesting to apply our method to the two-flavor Schwinger model and compute the mass spectrum of the composite particles which are recently explored by DMRG simulation based on different ideas [46, 47].

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