Designing Quantum Algorithms for State Preparation and Thermal Field Theory

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1 Introduction

Quantum computing has great potential in guiding the future of precise theory calculations needed for particle and nuclear physics. To date, lattice QCD has proved to be a reliable way of performing non-perturbative Quantum Field Theory computations for certain problems, but not all; Lattice QCD computation, usually carried out as a MCMC with real positive probability on the Euclidean space-time, faces several profound and fundamental difficulties, such as the sign problem, that are relevant for thermodynamics with finite particle density (chemical potential), or particle scattering, which are, in general, closely related to features of locally Minkowski space-time.

We are interested in pursuing necessary theoretical and computational developments towards future quantum computing applications for quantum field theory. An area of particular interest is how to efficiently prepare the quantum state of interesting field theories.

We also wish to have a fruitful relationship with quantum computer device design so that we could rapidly become aware about the near-future availability of specific quantum computing resources, and will be able to provide input about design and potential device application from a theoretical perspective, the Co-design concepts of the emerging center C^2QA. Exploiting specific patterns of connectivity of qubits in quantum devices is something that is critical for feasible development during the NISQ era, and is something that we plan to take seriously. We are also interested in other applications beyound quantum field theories where the state preparation techniques we develop could be used, *e.g.* Quantum Machine Learning[1, 2].

2 Adiabatic and Variational state preparation

We propose to study ground state preparation in 1+1 dimension QED, the Schwinger model with an external electric field, a system which has a sign problem. The ground state of the interacting theory is prepared by an adiabatic time-evolution starting from the ground state of the free theory. We provide a method to assess the systematic error caused by a potentially imperfect adiabatic process. This study will show that the adiabatic process requires an unfeasibly large circuit length unrealistic for near terms digital quantum computer simulation.

To circumvent this difficulty, we turn to variational methods like QAOA [3], and more specifically VQCS [4], which allow us to stay at circuit depths realizable on NISQ devices.

3 Parallel simulator of Quantum Computation

Before large scale quantum computation device will emerge, the simulation of quantum circuits on classical supercomputers is very useful for testing ideas and developing algorithms. Building on high-performance computing infrastructure originating in lattice QCD, we are currently designing a parallel (MPI, openMP, SIMD, and SIMT parallelism) quantum computing simulator with flexible state representation, allowing us to explore both dense state and state compression schemes. The system is based on `https://github.com/lehner/gpt` and will include ideas from `https://github.com/daknuett/pyqcs`.

4 Effective representations of states and operators

To propose near future quantum simulation of field theory, it is vital to be able to prepare relevant states with limited number of qubits and circuit depth. Ground states of some low dimensional systems are known to be economically represented by *tensor network states* such as matrix product state (MPS) [5], projected entangled pair state (PEPS) [6], and multi-scale entanglement renormalization ansatz (MERA) [7]. We will

map these states to quantum circuit representations in order to use them as ansatzs for efficient variational state preparation methods.

Specifically, the tensor network structures could point the way towards novel quantum circuits for state preparation on quantum computers, perhaps with very wide but very shallow quantum circuits. If the "key" gate element of a tree-like circuit could be learned variationally to prepare the ground state of scale invariant theories from an initial product state, then this classically trained "key" gate could potentially be implemented on a quantum computer to perform ground state preparations outside of the reach of classical simulation.

While the usefulness of tensor network states has been established in 1+1 dimensional theories and some 2+1 dimensional theories, their applicability in higher-dimensional systems are still limited. For the ultimate purpose of scalable state preparation in a higher dimensional systems, the higher-dimensional tensor network techniques will also be pursued.

Simulating gauge theories is one of the most challenging tasks for simulation, classical or quantum, due to the infinite number degrees of freedom, such as those of gauge degrees of freedom. Exploring their representations on qubits with use of regularization techniques such as quantum link model [8, 9] and gauge group decimation [10, 11] could open up the potential quantum simulation of gauge theories.

5 State preparation for Thermal Field Theory and phase transition

Calculating the density matrix of a thermodynamic ensemble or the corresponding thermal observables is a difficult task for quantum computing. These calculations involve a sum over the entire Hilbert space of the Boltzmann weights $Z(\beta,\mu) = \sum_n \langle n| \exp(-\beta\hat{H}+\mu\hat{N})|n\rangle$ Specifically, in digital Quantum computing, which consists of unitary operations, the implementation of non-unitary operators like the one required for the Boltzmann weights becomes difficult. See for example the projection measurement method implemented in [12] where the quantum advantage is lost. There are several ideas to realize the thermal mixed states in terms of pure states, including Thermal Pure Quantum (TPQ) states [13], or Thermofield Double (TFD) states [14]. In the context of these approaches we will investigate the implementation of non-unitary operators.

For chaotic system case, ETH(Eigenstate thermalization Hypothesis) can be applicable. This may permit the usage of ensemble average values in place of values specific an element of the ensemble provided that certain conditions are met, if only simple operators are considered. Eigenstate thermalization also implies the existence of certain chaotic and quantum error correcting properties [15], and so known properties of such systems could also be leveraged.

6 Entanglement Dynamics of Scattering

Quantum computing for high energy scattering process [16] is also an important topic. Previous works on single particle digitization have been written [17], and will be further pursued. Scattering processes that conserve certain quantum numbers do not reach the whole Hilbert space [18] and thus should not be thought of as universal quantum computers, as one cannot go from a state of one quantum number to a state of a different quantum number. Moreover, input states for scattering tend to be product states of fixed quantum numbers, and not entangled states of multiple quantum numbers (e.g. a superposition of a spin 1 and a spin -1 state). This question deserves more systematic investigation, in particular to develop a theory of entanglement dynamics in scattering, with an eye towards leveraging these entanglement dynamics, possibly in the form of entangled input for particle colliders, to generate otherwise suppressed processes. In addition, the physics of entanglement itself [19] is another important target for us.

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