Usage Report for Fiscal Year 2022

Project Title: Development of quantum algorithms for quantum many-body systems

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1. Background and purpose of the project, relationship of the project with other projects

The investigations of correlated quantum many-body systems are challenged because of the exponentially increased complexity from the high-dimensional Hilbert space. Currently under-developed quantum computing promises a new way of directly solving the quantum many-body system on a quantum computer where the computing capacity is also exponentially increased. One of the central issues in this field is the development of suitable quantum algorithms which can efficiently work on quantum devices, especially accessible noisy intermediate-scale quantum (NISQ) devices.

Since the current quantum devices are far from perfect and have severe restrictions, the corresponding classical simulation is crucial to developing quantum algorithms. Given the quantum nature of the quantum computing system, its classical simulation needs extensive computational resources and should be performed on the supercomputer.

One of the leading quantum algorithms for solving quantum many-body systems on NISQ devices is the variational quantum eigensolver (VQE) where the ground state of the target quantum many-body system is obtained by variationally optimizing a parametrized quantum circuit (PQC) as the *Ansatz* state in a quantum-classical hybrid loop.

2. Specific usage status of the system and calculation method

An important issue in VQE is constructing a suitable PQC for the system which is under investigated. Here, we consider the toric code in an external magnetic field, where the original quantum loop gas (as the ground state of the toric code model and being a topologically ordered state) catches an extra tension for each of the loop which is proportional to the length and the system becomes non exactly solvable. For this system, we design a PQC to describe such weight-adjustable quantum loop gas (dubbed PLGC). The PLGC has the optimal circuit structure which can be evaluated on current NISQ devices.

Employing PLGC, we perform VQE simulations for the toric code model in an external magnetic field with several different system sizes using the exact statevector quantum circuit simulator provided by Qiskit [1] on HOKUSAI supercomputer at RIKEN. In practice, the simultaneous perturbation stochastic approximation (SPSA) classical optimizer is adopted to update the parameters. For comparison, we also perform the exact diagonalization (ED) calculations for the same system using Quspin library [2].

3. Result

The variational energies obtained from VQE and ED for the system with different magnetic field strength are shown in FIG. 1. We find that the VQE energy is excellent agreement with the exact energy obtained by the ED method for all magnetic field strengths on all different clusters considered. To further check the scaling behavior of the energy with the system size, we perform a finite size scaling for the per qubit energy deviation (see the inset of FIG. 1). The infinite size extrapolation confirms that the deviation of VQE energy is consistently smaller than *0.01*. This means that the ground state of the toric code model in an external magnetic field, which is a nonexactly solvable quantum many-body system can be achieved by the VQE calculations with the

PLGC *Ansatz*.

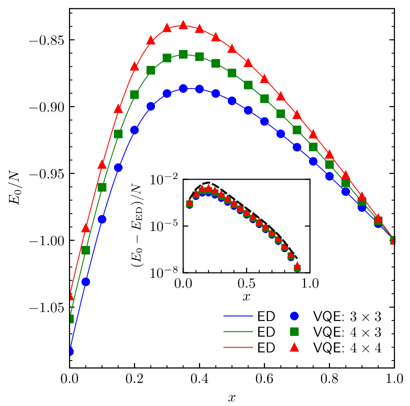

FIG. 1. Ground state energy obtained by the VQE calculations as a function of magnetic field strength (*x = 0* for no field case and *x = 1* for infinite large field case) for the toric code model in an external magnetic field on different clusters with the size *N = 12*, *17*, and *24* (indicated by blue circles, green squares, and red triangles, respectively). The numerically exact ground state energy obtained by the ED method are also plotted by the solid lines with the same colors. The inset show the corresponding energy difference per qubit indicated by the same symbols. The dashed line displays the extrapolated values to *N* goes to infinite by fitting the energy difference for the three different cluster with a second-order polynomial of *1/N*.

4. Conclusion

By extensive VQE simulations and ED calculations, we conclude that the elaborately constructed PLGC *Ansatz* can successfully obtain the ground state of the toric code model in an external magnetic field with any field strength. By considering the realizability of the PLGC, we propose that a useful quantum advantage can be achieved by realizing a scalable VQE calculation using PLGC on the NISQ device.

5. Schedule and prospect for the future

In the future, we plan to extend the PLGC-type circuit construction to include other topological orders, especially to non-Abelian cases.

Reference

[1] Qiskit: https://qiskit.org

[2] Weinberg, Phillip, and Marin Bukov, SciPost Physics **2** 1 003 (2017).

Fiscal Year 2022 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

Rong-Yang Sun, Tomonori Shirakawa, and Seiji Yunoki, "Parametrized quantum circuit for weight-adjustable quantum loop gas", Physical Review B 2023 Jan 25;107(4):L041109/1-4.

[Oral presentation]

Rong-Yang Sun, "Quantum simulation for correlated quantum many-body systems on noisy quantum devices", Workshop: Challenges and opportunities in Lattice QCD simulations and related fields, February 15, 2023, Kobe, Japan.

[Poster presentation]

Rong-Yang Sun, Tomonori Shirakawa, and Seiji Yunoki, "Parametrized quantum circuit for weight-adjustable quantum loop gas", Workshop: Challenges and opportunities in Lattice QCD simulations and related fields, February 15, 2023, Kobe, Japan.