Usage Report for Fiscal Year 2023

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

Under-developed quantum computing promises a new way of directly solving the quantum many-body system on a quantum computer. One of the central issues in this field is the development of suitable quantum algorithms that can efficiently work on quantum devices, especially currently accessible noisy intermediate-scale quantum (NISQ) devices.

The leading quantum algorithm 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

We consider a quantum many-body model named alternating Heisenberg chain (AHC) [1]. Similar to the uniform 1D Heisenberg model, the AHC only includes the spin couplings on the nearest neighbor sites, but the coupling strength on even bonds (denoted as J) and on odd bonds (denoted as J') are not equal. Fixing $J=1$ and Tuning J', two phases are observed in the AHC: a symmetry-protected topological (SPT) phase ($J' < 1$) and a topological trivial dimmer phase ($J' > 1$).

To efficiently obtain the ground state for both two phases in quantum simulation, we constructed a proper PQC by cooperating with the different topological features in these two phases (for more details, see [2]). The circuit depths of this PQC are controlled by the parameter D. Employing this PQC, we perform VQE simulations for the AHC with various J' values and systems sizes using a statevector quantum circuit simulator provided by Qiskit [3]. D is fixed to 1 for testing the feasibility of the shallowest PQC case. For making a comparison, we also perform the exact diagonalization (ED) calculations. These classical simulations have been done on the HOKUSAI supercomputer at RIKEN.

3. Result

The energy deviation of the VQE from the ED calculations for various J' is shown in Fig. 1(a). We find that it is smaller than the energy gap of the system in a finite J' region, indicating the accuracy of the VQE simulation. Meanwhile, we also calculate the wave-function fidelity between these two states and observe consistent results [see Fig. 1(b)].

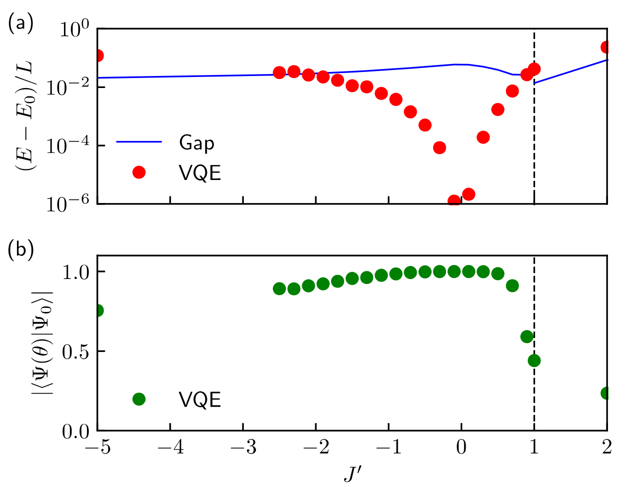

FIG. 1. (a) Energy difference per site and (b) wave-function fidelity F between the ground state of the $L=16$ AHC obtained by ED and the corresponding VQE optimized circuit state with $D=1$. (Adopted from [2].)

4. Conclusion

By extensive VQE simulations and ED calculations, we conclude that even using *D=1* shallow PQC, we can successfully obtain the ground state of the AHC in a region where this model is not exactly solvable. By considering the realizability of this shallow PQC, we propose that an efficient quantum simulation of the AHC can be performed on real NISQ devices by adopting this PQC *Ansatz*.

5. Schedule and prospect for the future

In the future, we plan to apply this PQC construction method to the quantum simulation of 2D SPT phases.

6. Reference

[1] K. Hida, Phys. Rev. B **45**, 2207 (1992)

[2] R.-Y. Sun, T. Shirakawa, and S. Yunoki, Phys. Rev. B **108**, 075127 (2023)

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

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Fiscal Year 2023 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

1. Rong-Yang Sun, Tomonori Shirakawa, and Seiji Yunoki. "Efficient Variational Quantum Circuit Structure for Correlated Topological Phases." Physical Review B 108, 075127 (2023).

[Oral presentation]

1. Rong-Yang Sun, Tomonori Shirakawa, and Seiji Yunoki. "Scalable quantum simulation for topological quantum phases on noisy quantum devices", 34th IUPAP Conference on Computational Physics, August 8, 2023, Kobe, Japan.

2. Rong-Yang Sun, Tomonori Shirakawa, and Seiji Yunoki. "Scalable quantum simulation for topological quantum phases on noisy quantum devices", ExU-YITP Workshop on Condensed Matter Physics and Quantum Information, September 25, 2023, Kyoto, Japan.