Implementation of Finite-Temperature Calculation in TeNeS

Tsuyoshi OKUBO
Institute for Physics of Intelligence, University of Tokyo
7-3-1 Hongo, Bunkyo-ku, Tokyo 133-0033

In quantum many-body problems, such as quantum spin systems and strongly correlated electron systems, the dimension of the Hilbert space increases exponentially with the number of spins or particles, making precise analysis of large systems difficult. The tensor network method, which is one technique to overcome such difficulties, represents quantum states as a network constructed by the contraction of small tensors, thereby reducing the effective degrees of freedom and enabling the computation of large systems. The infinite projected entangled pair state/infinite tensor product states (iPEPS/iTPS) is a tensor network that can directly represent the ground state of an infinitely large system. We are developing a tensor network library TeNeS based on iPEPS/iTPS [1, 2]. TeNeS supports MPI and OpenMP hybrid parallelization, and enables us to calculate the ground states of various two-dimensional lattice models.

This year, through the support of Project for Advancement of Software Usability in Materials Science (PASUMS), we have implemented the finite-temperature calculation in TeNeS. The finite-temperature calculation is essential for the analysis of the physical properties of quantum many-body systems, such as the specific heat, and magnetization. The finite-temperature calculation is performed by the imaginary time evolution of the density matrix represented by the infinite projected entangled pair operator/infinite tensor product operator (iPEPO/iTPO) [3] (See Fig. 1). Such imaginary time evolution for iPEPO/iTPO is algorithmically similar to the ground state calculation based on iPEPS/iTPS, and we can easily implement the finite-temperature calculation in TeNeS.

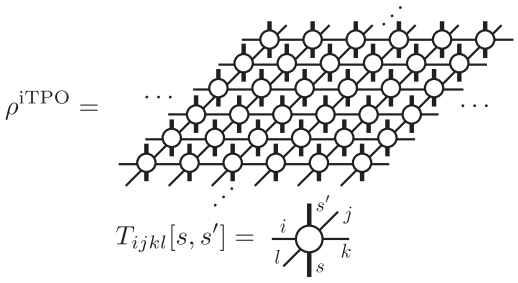

Figure 1: Tensor network diagram of a density matrix ρ represented as an iPEPO/iTPO. Vertical open legs stand for indices of local Hilbert space.

In addition to the finite-temperature calculation, we also implemented the real-time evolution of a pure state using TeNeS. The algorithm of the real-time evolution is essentially the same as the imaginary time evolution. However, usually approximation based on iPEPS/iTPS becomes less accurate for longer time evolution due to the increase of quantum entanglement. Thus, real-time evolution approximated by iPEPS/iTPS is limited to short time evolution.

The finite-temperature calculation and the real-time evolution implemented in TeNeS are useful for the analysis of the physical properties of quantum many-body systems. We hope

that TeNeS can enhance research in the field of quantum many-body systems.

TeNeS was developed with Yuichi Motoyama, Kazuyoshi Yoshimi, Satoshi Morita, Tatsumi Aoyama, Takeo Kato, and Naoki Kawashima.

References

[1] Y. Motoyama, T. Okubo, K. Yoshimi, S. Morita, T. Kato and N. Kawashima, Comput. Phys. Commun. **279**, (2022) 108437.

[2] https://github.com/issp-center-dev/TeNeS

[3] A. Kshetrimayum, M. Rizzi, J. Eisert, and R. Orús, Phys. Rev. Lett. **122**, (2019) 070502.