Quantum-Inspired explainable-AI

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Introduction

Many modern quantum materials such as the magic angle graphene heterostructures, high-temperature superconductors, etc, are becoming the cornerstone for the continuous prosperity of human society. However, to understand these quantum materials such that one could design and eventually manufacture better ones, we would rely on large-scale quantum many-body simulations to compute their properties at the first place, but these computations, including quantum Monte Carlo, tensor-networks and neural-networks usually come with heavy computation complexities.

Here, we report our recent progress on the combination of machine learning techniques and quantum manybody simulations (mainly quantum Monte Carlo), as well as the progress of recent numerical studies of the strongly correlated phenomenon in quantum manybody systems.

Methodology development

- **Generative neural network**

Monte Carlo methods are widely used in numerically studying problems in statistic and quantum manybody physics. For the critical systems (or phase transition problem), the update scheme of Markov chain Monte Carlo methods will typically suffer from the so-called critical slowing phenomenon, rendering the long autocorrelation time and low simulation efficiency. To tackle such a problem, we develop a generative neural network (c.f. Fig 1) to generate configurations with the distribution similar as the underlying Hamiltonian [1].

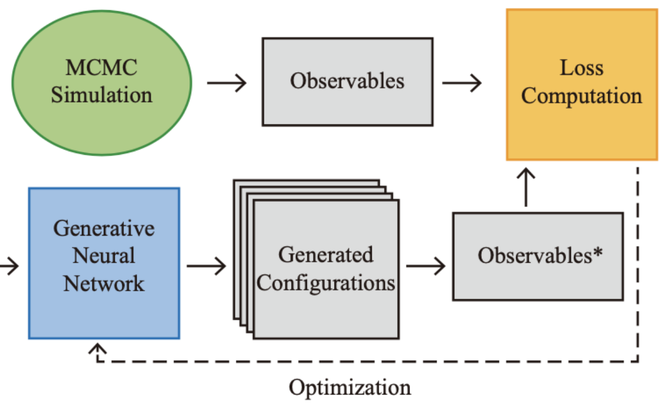

Fig 1: Workflow of generative neural network.

We test the method in two typical problems in quantum manybody physics, that is, the 2D square-lattice Ising model $H = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j$ and the Hubbard model defined in 2D honeycomb lattice $H = -t\sum_{\langle i,j\rangle,\sigma}(c^\dagger_{i,\sigma}c_{j,\sigma} + h.c.) + U\sum_i(n_{i,\uparrow} - 1/2)(n_{i,\downarrow} - 1/2)$, with the following neural network structure,.

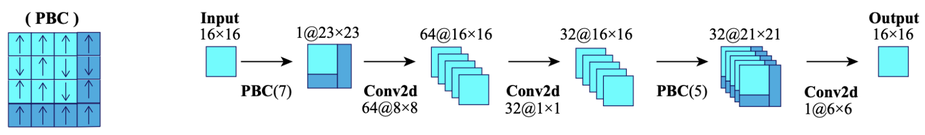

Fig 2: Neural network for training 2D square-lattice Ising model.

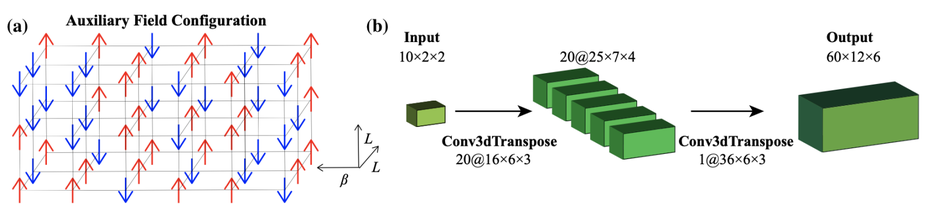

Fig 3: Neural network for training 2D honeycomb-lattice Hubbard model.

- **Performance**

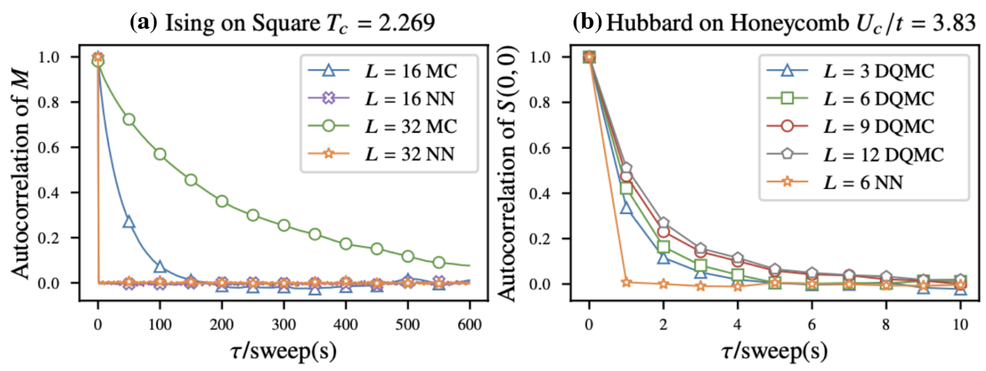

Fig 4: Autocorrelation comparison between different methods in (a) 2D Ising model, and (b) Hubbard model.

In these two cases, we compare the autocorrelation time with the ones of traditional Markov chain Monte Carlo method, and find the new-proposed method does shorten the autocorrelation while still reproduce the correct magnetization distribution and observables.

Microscopic understanding of twisted bilayer graphene

- **Effective Model**

The research field of twisted bilayer graphene has recently quickly thrived since the discovery of correlated insulator and unconventional superconductivity in experiments. In our previous work [2], we demonstrated a quantum anomalous Hall state can emerge from a pure interaction model [c.f. Fig 5 (a,b)] in agreement with the experimental observation.

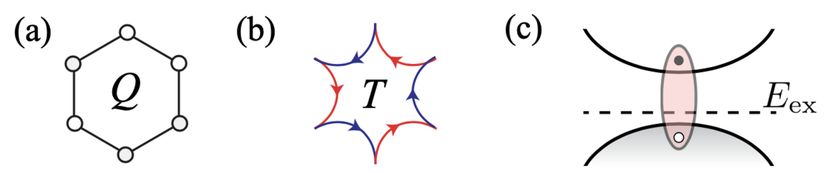

Fig 5: The effecitve model with (a) cluster charge Q and (b) assisted hopping T terms. (c) illustrates the formation of exciton bound state.

- **Exciton proliferation**

We study the finite-T properties of the model and identitfy the excitonic bound state with significantly lower energy than the mean-field gap, which renders a intermediate-T exciton proliferation regime [c.f. Fig 6] [3].

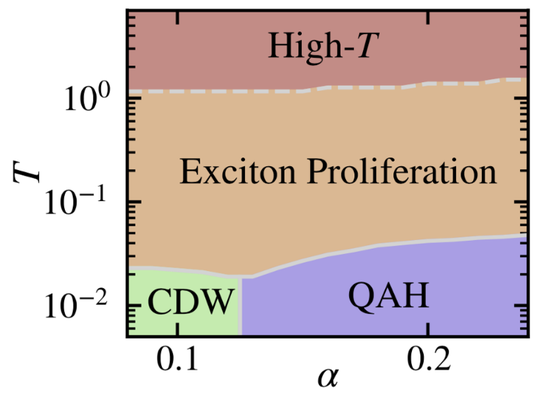

Fig 6: The finite-temperature phase diagram of TBG model.

Accurate entanglement measurement

- **Nonequilibrium algorithm**

We have improved the nonequilibrium algorithm put forward by J. D'Emidio and put forward a new more-parallelized one. The new algorithm [4], as shown in Fig 7, takes advantages of the fact that a nonequilibrium process can be further split into many small processes, then each CPU can execute only part of the calculation, thus greatly improving the computing speed.

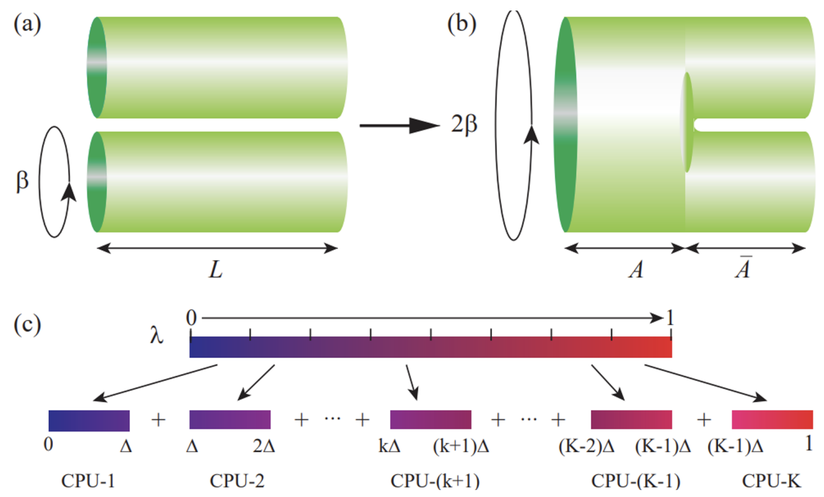

Fig 7: The schematic diagram of the QMC configurations and the nonequilibrium increment method.

With this new method, we measured the second Rényi entropy separately at the 3D O(3) QCP and the DQCP. We find that the logarithmic corrections to the area law shows the fundamental difference of DQCP with the normal QCP.

References

[1] Hongyu Lu, Chuhao Li, Bin-Bin Chen, Wei Li, Yang Qi, and Zi Yang Meng.
Network-initialized monte carlo based on generative neural networks.
Chinese Physics Letters, 39(5):050701, 2022.

[2] Bin-Bin Chen, Yuan Da Liao, Ziyu Chen, Oskar Vafek, Jian Kang, Wei Li, and Zi Yang Meng.
Realization of topological mott insulator in a twisted bilayer graphene lattice model.
Nature Communications, 12(1):5480, 2021.

[3] Xiyue Lin, Bin-Bin Chen, Wei Li, Zi Yang Meng, and Tao Shi.
Exciton proliferation and fate of the topological mott insulator in a twisted bilayer graphene lattice model.
Phys. Rev. Lett., 128:157201, Apr 2022.

[4] Jiarui Zhao, Yan-Cheng Wang, Zheng Yan, Meng Cheng, and Zi Yang Meng.
Scaling of entanglement entropy at deconfined quantum criticality.
Phys. Rev. Lett., 128:010601, Jan 2022.