Unsupervised machine learning on classification of quantum phases

Hsuan-Yu Wu[1], Kwai-Kong Ng[1]

[1]Department of Applied physics, Tunghai University, Taichung, Taiwan

Abstract

Recently, an algorithm [1] has been developed to apply video compression methods to the imaginary time direction of data generated by quantum Monte Carlo (QMC) simulations, followed by quantum phase classification tasks performed by a convolutional neural network (CNN). This method was originally used for supervised learning. The present study further extends the method to unsupervised learning, attempting to distinguish different quantum phases of unknown ground state phases of quantum systems and identify corresponding quantum phase transition parameters. This method can also be applied to some thermal phase transitions to determine the critical temperatures for different phases.

Method

- Consider training data with a window boundary. If the data belongs to the same phase, it cannot be distinguished, otherwise, it can be distinguished.

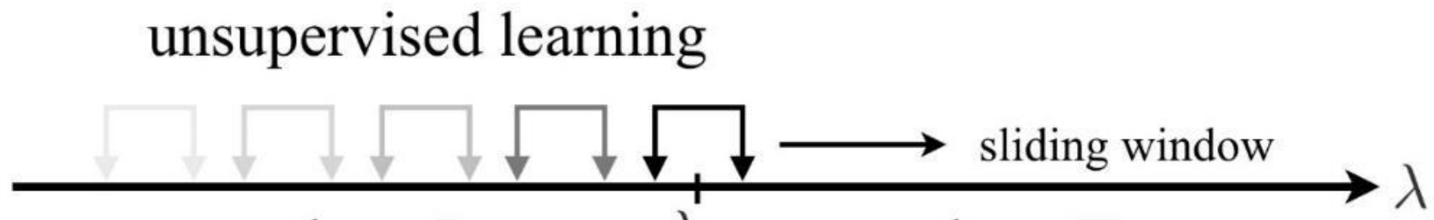

Fig1. Illustration of the operation process[2]

- The method of extracting data involves applying video compression to the imaginary time direction of data generated by quantum Monte Carlo (QMC) simulations and then using a convolutional neural network (CNN) to perform classification.

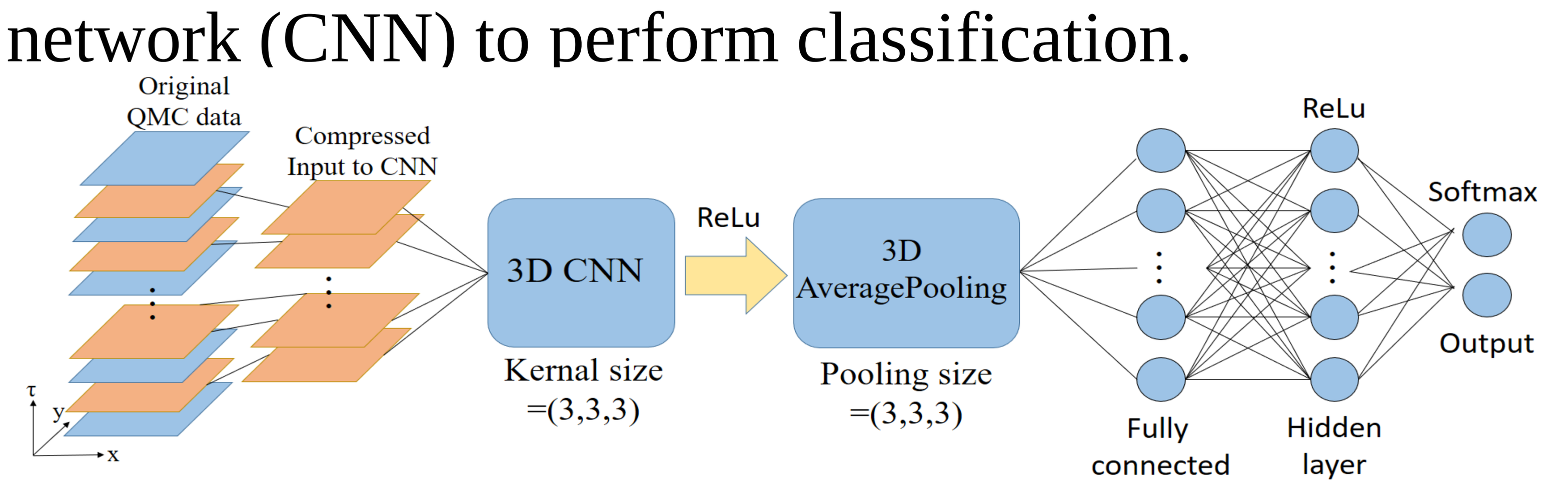

Fig2. The number of kernels is 32, the number of hidden layer neurons is 512, the loss function is binary cross-entropy, the optimizer used is Adam, and L2 regularization with a parameter of 0.08 is added.

- We use an extended hard-core boson Hamiltonian on a triangular lattice, as shown below.

$$H = -t \sum_{\langle ij \rangle} (b_i^\dagger b_j + \text{H.c.}) + V \sum_{\langle ij \rangle} n_i n_j + \mu \sum_i n_i,$$

Results

- **Quantum transition**

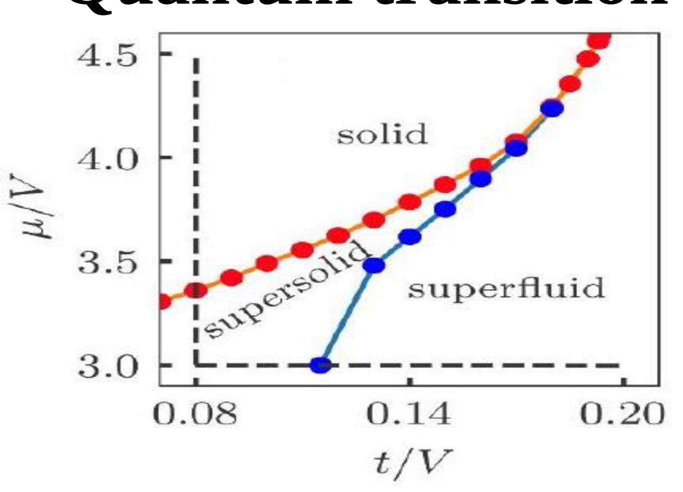

Fig3. Distribution of solid, supersolid, and superfluid states at T=0.01 in Quantum transition.[1]

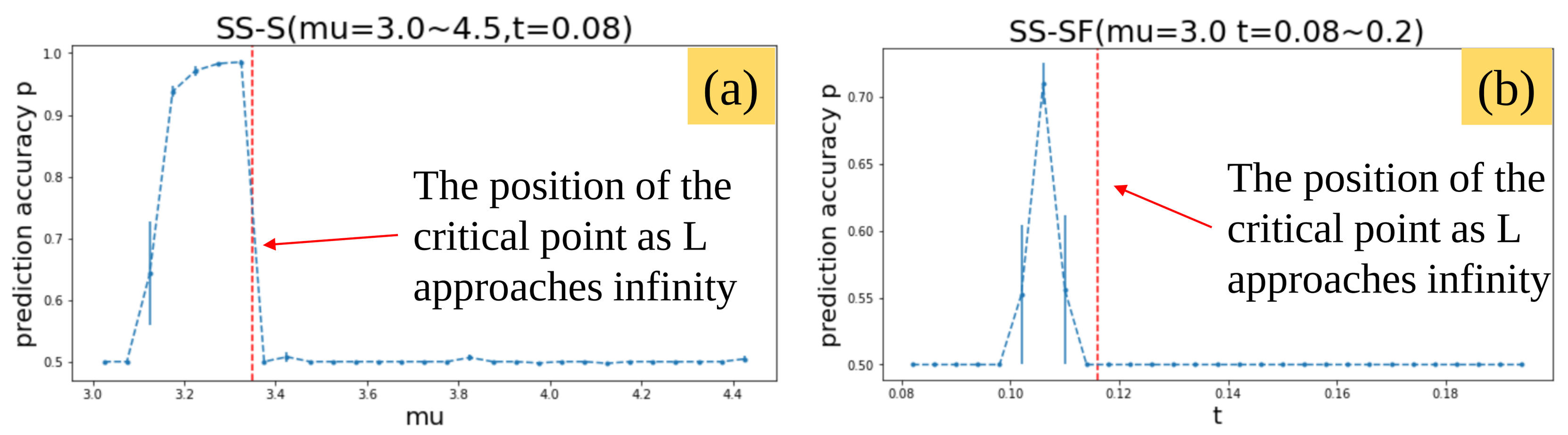

Fig4. Quantum transitions from (a) supersolid to solid and (b) supersolid to superfluid at L=18, with intervals of 0.05 and 0.004, respectively.

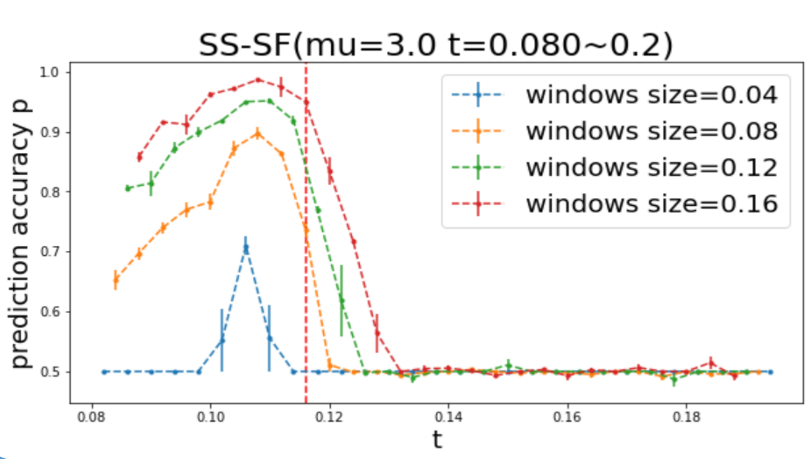

Fig 5. The variations in the results of window sizes in the results of Figure 4 (b).

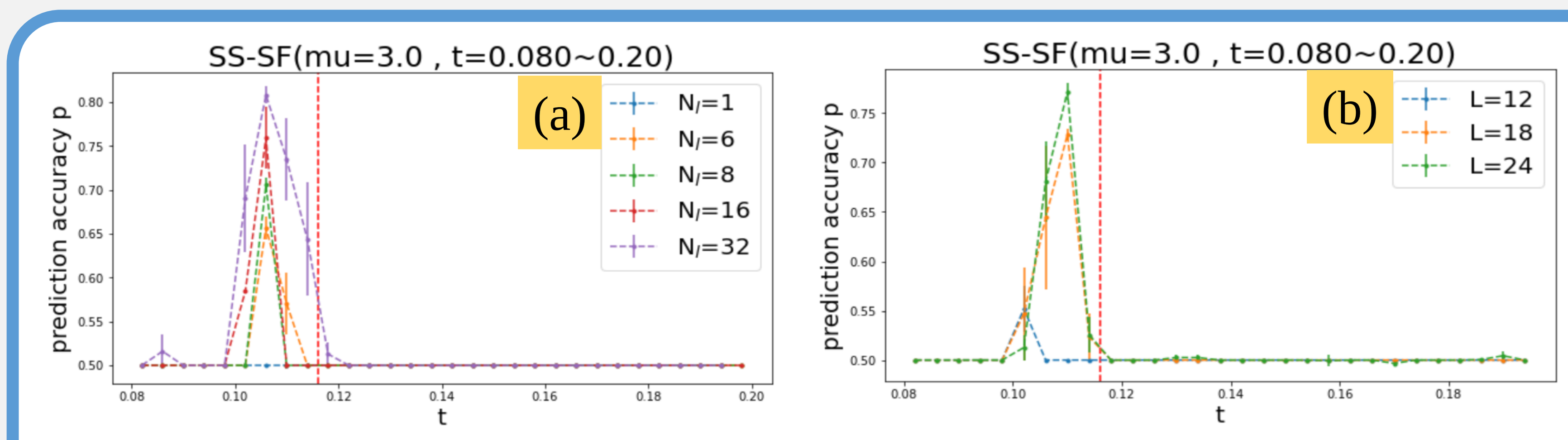

Fig 6. The variations in the results of (a) imaginary time layer N_l, and (b) lattice size L in the results of Figure 4 (b).

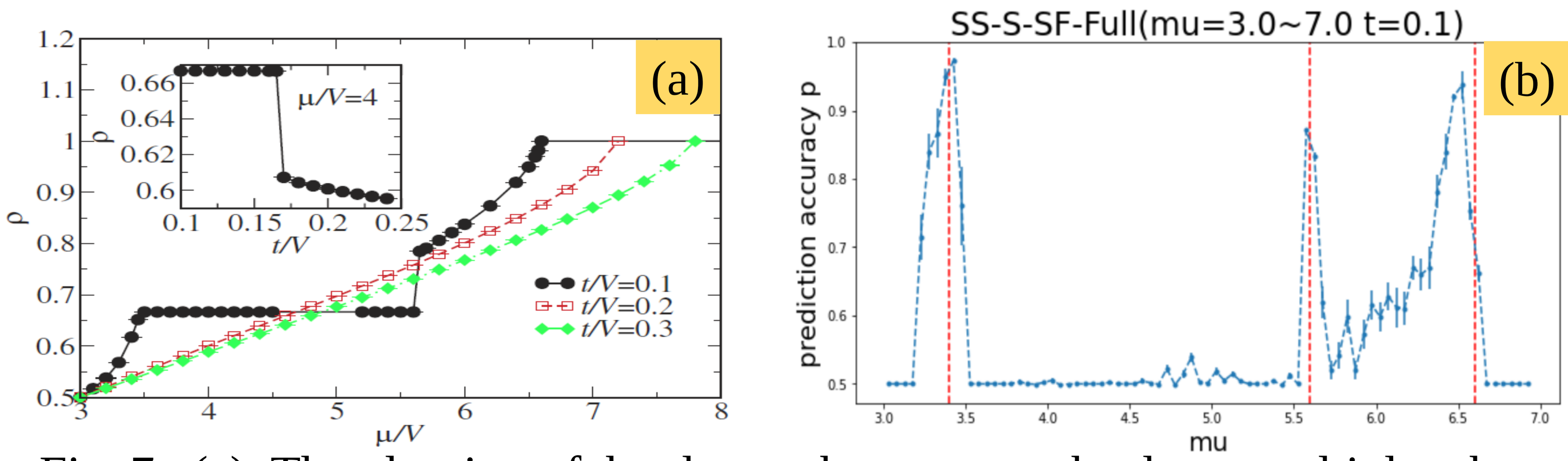

Fig 7. (a) The density of hard-core bosons graph along multiple phase transition paths[3], (b) where our model predicts the results. Here, L=18 with an interval of 0.1.

- **Thermal transition**

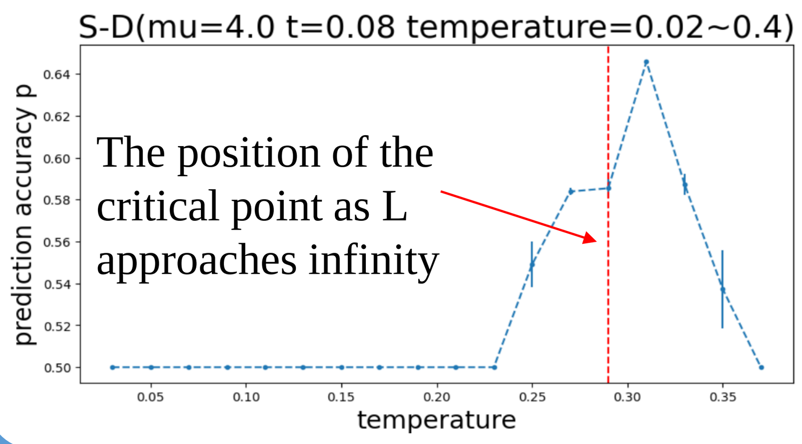

Fig 8. The thermal transition of solid at L=18, with intervals of 0.02.

Conclusion

- Without the need to pre-inform relevant state information, our method has been proven to be able to roughly capture the location of the critical point of quantum transition.
- By introducing imaginary time, our model can better capture the characteristics of the critical point.
- By changing the window size, we can better determine the approximate range of the critical point based on the width of the peak.
- In the future, it may be attempted to use extrapolation methods to search for the critical point as L approaches infinity.

References

[1] Xiao-Yu Dong, Frank Pollmann and Xue-Feng Zhang, Physical Review B **99**, 121104(R) (2019)

[2] Peter Broecker, Fakher F. Assaad, and Simon Trebst, arXiv:1707.00663v1

[3] Stefan Wessel and Matthias Troyer, PRL 95, 127205 (2005)

[4] D.-R. Tan and F.-J. Jiang, Physical Review B **102**, 224434 (2020)