Neural Network and Monte Carlo studies of the Berezinskii–Kosterlitz–Thouless (BKT) phase transition for the two-dimensional (2D) classical XY model on the honeycomb lattice

Fu-Jiun Jiang

Department of Physics, National Taiwan Normal University, 88, Sec.4, Ting-Chou Rd., Taipei 116, Taiwan

INTRODUCTION

Recently, the techniques of Machine Learning (ML) have become popular in investigating many-body system. For instance, Neural Network (NN) has been employed to uncover the critical phenomena of several physical models successfully. In this study, we use a extremely simple supervised NN, namely a multilayer perceptron (MLP) to explore the Berezinskii–Kosterlitz–Thouless (BKT) phase transition of the two-dimensional (2D) classical XY model on the honeycomb lattice. Apart from this, traditional Monte Carlo calculations are conducted for this model as well.

MICROSCOPIC MODELS

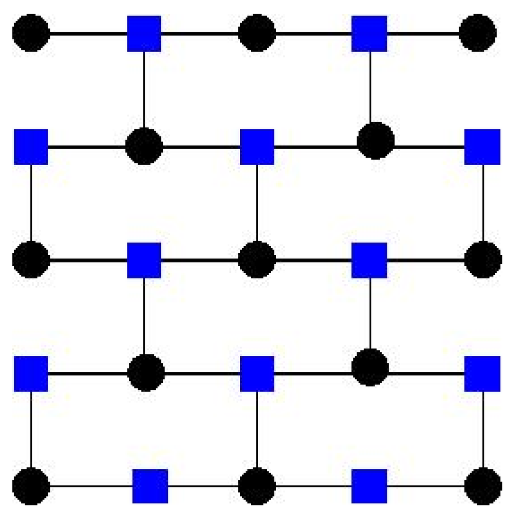

Fig. 1: The periodic 4 by 4 honeycomb lattice implemented in this study.

The Hamiltonian of the two-dimensional (2D) classical XY model on the honeycomb lattice is expressed as

$$H = -\sum_{\langle ij \rangle} \vec{e}_i \cdot \vec{e}_j, \qquad (1)$$

where $\langle ij \rangle$ refers to the nearest neighbor sites i and j, and $\vec{e}_i$ is a vector at site i with $\vec{e}_i \in S^2$. In other words, each XY spin $\vec{e}_i$ can be represented as $\vec{e}_i = (\cos\theta_i, \sin\theta_i)$ with $0 \le \theta_i < 2\pi$.

Fig. 1 demonstrates the periodic honeycomb lattice implemented in this investigation.

The employed MLP

The employed MLP here is consist of one input layer, one hidden layer of 512 neurons, and one output layer. The pictorial representation of the considered NN is depicted in fig. 2.

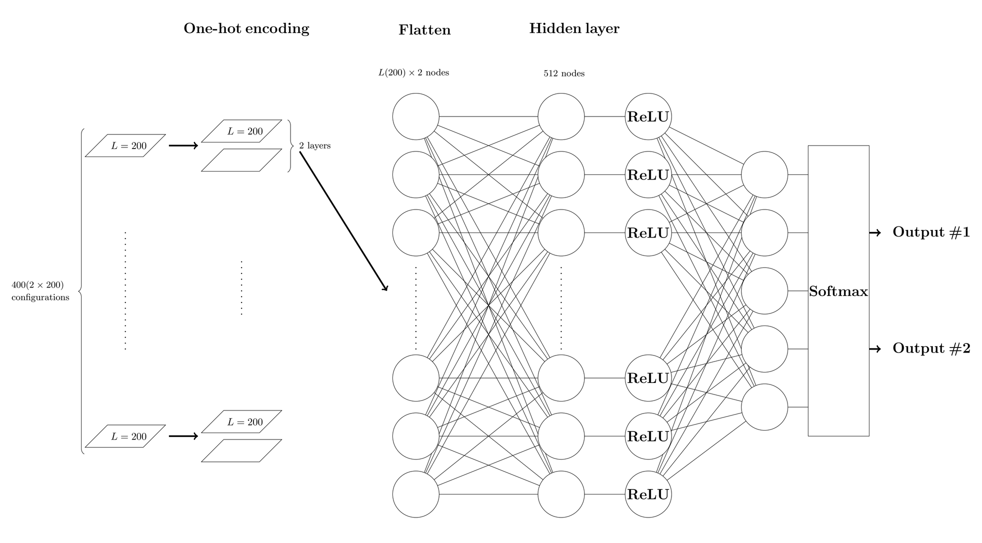

Fig. 2: The MLP used in this investigation.

The magnitude R of the NN output vectors is considered as the quantity to examine the targeted phase transition. In particular, theoretically the largest and smallest values of R are given by 1 and $1/\sqrt{2}$, respectively. Hence for a given linear system size L, the temperature T where the associated curve of R intersects with $\frac{1+1/\sqrt{2}}{2}$ is treated as the pseudo-critical temperature corresponding to that L.

THE NUMERICAL RESULTS

The MLP employed in this study is a pre-trained MLP. In other words, no training is performed here. Moreover, the MLP was trained using only two-type of artificially made ferromagnet-like configurations, not the real configurations.

The needed spin configurations used for the NN predictions are generated using the cluster-type Wolff algorithm. All these produced configurations are considered for the NN predictions.

The R as functions of T for $L = 64$ and $L = 128$ are shown as the left and the right panels of fig. 3. The horizontal lines are $\frac{1+1/\sqrt{2}}{2}$.

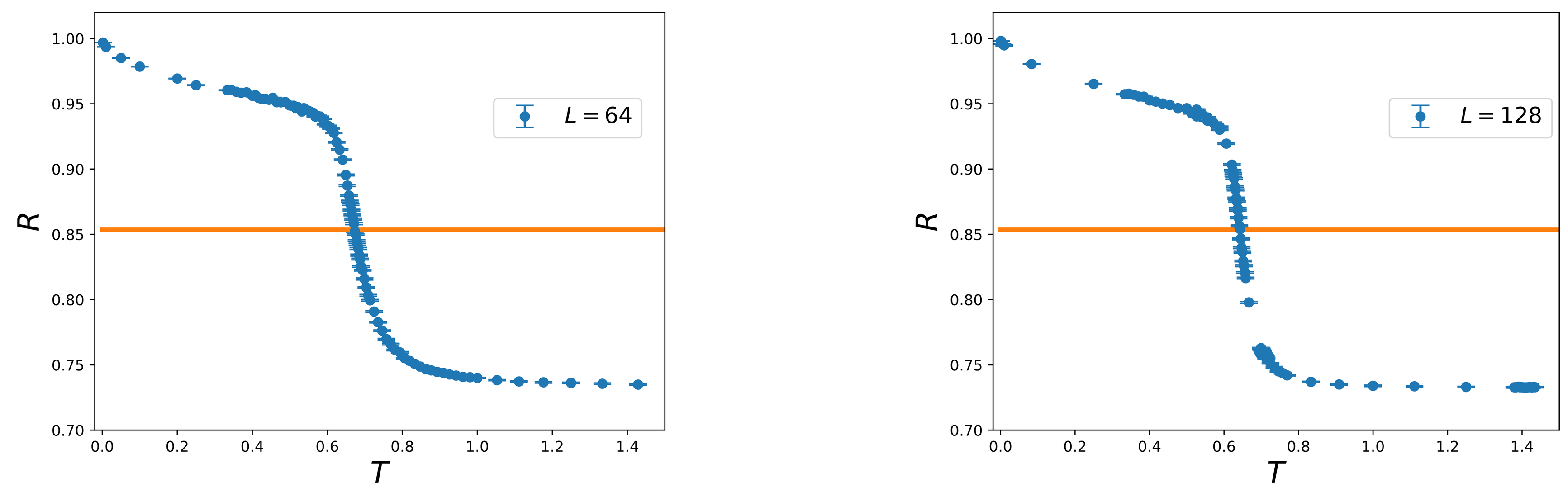

Fig. 3: R as functions of T for $L = 64$ (left) and $L = 128$ (right).

The extracted pseudo-critical temperatures $T_{BKT}(L)$ from the NN outputs as a function of $1/L$ is depicted in the left panel of fig. 4.

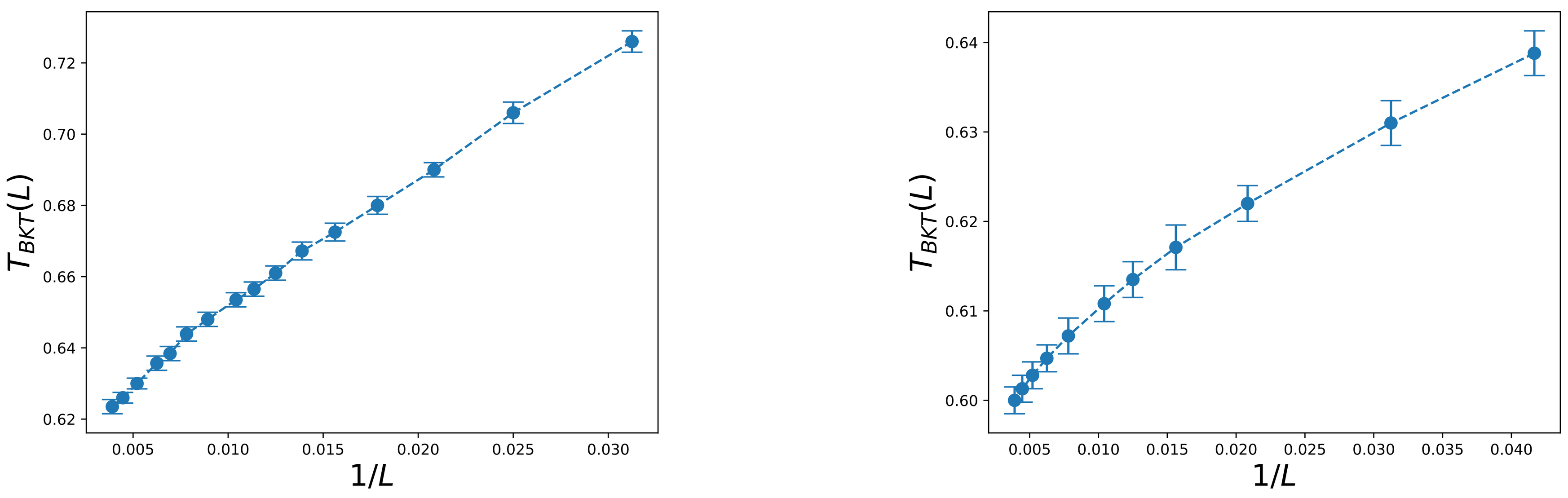

Fig. 4: $T_{BKT}(L)$ as functions of $1/L$. The outcomes of the left and the right panels are from NN and helicity modulus, respectively. The horizontal lines are $\frac{1+1/\sqrt{2}}{2}$.

A fit of the data in the left panel fig. 4 leads to $T_{BKT,c} = 0.572(3)$ which deviates significantly from the well-known approximation $T_{BKT,c} = 1/\sqrt{2}$.

In our Monte Carlo simulations, we compute the pseudo-critical temperatures for each considered L from the quantity helicity modulus. The extracted pseudo-critical temperatures $T_{BKT}(L)$ from the helicity modulus as a function of $1/L$ are depicted in the right panel of fig. 4.

With a fit of the data in the right panel of fig. 4 to the expected finite-size scaling ansatz, we arrive at $T_{BKT,c} = 0.576(4)$ which agree well with that determined from the NN method.

CONCLUSION

In this study, we investigate the BKT phase transition of the 2D classical XY model on the honeycomb lattice using both the NN and Monte Carlo methods. The critical temperature $T_{BKT,c}$ obtained from the NN and MC approaches are given by 0.572(3) and 0.576(4), respectively. The values of $T_{BKT,c}$ computed by two completely different ways agree quantitatively with each other. Our results deviate in a non-negligible manner with the well-known approximation $1/\sqrt{2}$. The outcome of $1/\sqrt{2}$ is calculated with an approximated action S. Hence the mentioned deviation is anticipated.

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