



Deep learning of phase transitions for quantum spin chains from correlation aspects

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(Received 9 February 2023; accepted 13 June 2023; published 29 June 2023)

Using machine learning (ML) to recognize different phases of matter and to infer the entire phase diagram has proven to be an effective tool given a large dataset. In our previous proposals, we have successfully explored phase transitions for topological phases of matter at low dimensions either in a supervised or an unsupervised learning protocol with the assistance of quantum-information-related quantities. In this work, we adopt our previous ML procedures to study quantum phase transitions of magnetism systems such as the XY and XXZ spin chains by using spin-spin correlation functions as the input data. We find that our proposed approach not only maps out the phase diagrams with accurate phase boundaries, but also indicates some features that have not been observed in the field of machine learning before. In particular, we define so-called relevant correlation functions to some corresponding phases that can always distinguish between those and their neighbors. Based on the unsupervised learning protocol we proposed [Phys. Rev. B **104**, 165108 (2021)], the reduced latent representations of the inputs combined with the clustering algorithm show the connectedness or disconnectedness between neighboring clusters (phases) just corresponding to the continuous or disrupt quantum phase transition, respectively. This property reminds us of the behavior of order parameters. Moreover, in the silhouette analysis we show that the ferromagnetic states in the XXZ model with various anisotropy parameters correspond to almost the same silhouette value, while the critical or antiferromagnetic states behave quite differently. The analysis further indicates that the minima of silhouette values are close to the phase-transition points, showing strong positive correlation. These results again justify the usefulness of our proposed ML procedures, and they move us a step further toward understanding the relation between ML and quantum phase transitions from correlation function aspects.

DOI: [10.1103/PhysRevB.107.214451](https://doi.org/10.1103/PhysRevB.107.214451)

I. INTRODUCTION

Quantum phase transitions (QPTs) have intrigued people for several decades [1]. Different from classical phase transitions accessed by varying temperatures, QPTs are driven by altering a nonthermal, physical parameter at zero temperature. While Ginzburg-Landau theory [2] is often employed to describe phase transitions, predicting QPTs in a one-dimensional (1D) quantum system with continuous symmetry and sufficient short-range interactions has some challenges. This is because the presence of a local order parameter in such a system would violate the Mermin-Wagner theorem [3], and

thus effective alternatives are sought. Computing correlation functions is just one of the alternatives to detect the long-range orders of the quantum phases and predict QPTs.

Several numerical techniques, such as exact diagonalization [4], quantum Monte Carlo simulations [5], and the density matrix renormalization group (DMRG) [6,7], can be used to compute correlations and ground-state wave functions. However, these methods are often computationally heavy and have limitations. This makes it difficult to map out the entire phase diagram in the parameter space using these methods. Recently, machine learning (ML) has gained significant attention not only in computer science, but also in physics for its ability to reveal hidden structures of correlations, entangled quantities, and complex wave functions. Moreover, ML is becoming a powerful tool for scientific researchers, as it is completely data-driven. For instance, given a set of data, a neural network (NN) can be trained to identify patterns or relate to condensed representations (such as class labels) for the data. The trained model can then predict unseen data points. This advantage has attracted the interest of the physics community in using ML to determine the phase boundaries between different phases of matter, including quantum phase transitions [8–45].

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There are two main approaches to using ML to classify phases of matter. The first approach is supervised learning, where the training data are labeled with known regimes [9–26]. This way is more accurate at identifying phase boundaries, but it requires prior knowledge of the system, such as the number of phases in a particular parameter range. The second approach is unsupervised learning, which does not require any prior knowledge or labeling and instead learns from the training data itself [8,27–45]. While this approach is more difficult and demanding, it is a natural option when exploring a parameter space for scientific discovery without prior knowledge.

In our previous works, we proposed a protocol for locating phase boundaries using machine learning, with either supervised [24,25] or unsupervised learning [8]. In particular, under unsupervised learning, we fed input data into an autoencoder [46–48] to extract effective features of data, and then we applied principal component analysis (PCA) [49,50] to determine the necessary feature dimensions. We next used the K -means clustering algorithm [51,52] followed by silhouette analysis [53,54] to determine the total number of phases without prior knowledge. Finally, we used supervised learning to improve the precision of the phase boundaries by taking the most confident points in silhouette analysis as labeled training seeds. Our method was successful in finding topological phase boundaries using quantum-information-related quantities as the input data.

As mentioned before, correlation functions are often natural quantities to detect long-range orders in QPTs. However, they are usually not computationally “cheap,” with hidden structures, and they can be inaccurate near critical regimes. Therefore, in this study, we employ the ML approach for identifying QPTs, assisted by using correlation functions as the input data type instead of quantum-information-related quantities. We benchmark our approach on two classic 1D magnetism systems, namely the XY and XXZ models. The correlation functions of the 1D XY model can be calculated by fermionization of the spin system [55,56], whereas those of the XXZ model can be calculated by DMRG [6,7,57].

In addition to showing our proposed ML protocol to be effective for detecting QPTs, a few essential observations are highlighted as follows. First, there are two types of phase transitions: first-order (disrupt) and second-order (continuous). It will be interesting to determine if the proposed protocol of ML can distinguish these two. In the XY model, there is a second-order phase transition, while in the XXZ model, both phase transitions exist. In unsupervised learning, the reduced latent representations of the input data after silhouette analysis show huge differences between the two types of phase transitions, unveiling an important signature to distinguish between them when using ML.

Second, one would like to know how the precision of the correlation functions influences the accuracy of the predicted phase transition points (TPs). As for the XY model, since all the numerical calculations can be done with great precision, the predicted phase boundaries are of the order of the statistical error for ML, suggesting that precise phase boundaries can be achieved. On the other hand, for the XXZ model, the accuracies of the correlation functions may fluctuate as a function of the anisotropy of the model in the z -direction with

some fixed truncation basis. Therefore, the accurate positions of the predicted phase boundaries also depend on whether they are first-order or second-order phase transitions. For the former case, the accuracy is not influenced much, while for the latter case, due to the slow gap opening, the predicted results could deviate more. It turns out that to achieve better accuracy, more delicate treatments should be made when training our machines.

The final observation concerns the relevance of the correlation functions in the corresponding phases. We find that if a correlation function is relevant in a certain phase, it can naturally be used to determine the phase boundary between one with the other. On the other hand, without any relevance of the correlation function in a phase, it could easily fail to distinguish between the phases of matter unless the machine could find other patterns to recognize them.

In this paper, we first introduce the XY and XXZ models and their spin-spin correlation functions. Then we show the procedures and the results of ML under supervision for recognizing different phases. This is used to show the effectiveness of taking correlations as the input data, and it can be compared with the later unsupervised method. In the next section, the protocol and the results of unsupervised learning are discussed. We conclude with several important discussions about the accuracies of the predicted phase boundaries and the signatures of the first-order and second-order phase transitions in the ML approach. Moreover, we also discuss why the relevance of the correlation functions for the corresponding phases is essential to make the ML approach effective.

II. XY AND XXZ MODELS

A. XY model

The Hamiltonian of the XY model reads

$$H_{XY} = -\frac{1}{2} \sum_{j=1}^N [(1 + \gamma)\sigma_j^x \sigma_{j+1}^x + (1 - \gamma)\sigma_j^y \sigma_{j+1}^y] - \frac{h}{2} \sum_{j=1}^N \sigma_j^z, \quad (1)$$

describing a chain of N spin-1/2's interacting ferromagnetically with their nearest neighbors. Here σ_i^a with $a = x, y, z$ at site i are Pauli matrices, obeying the usual commutation relations, $[\sigma_i^a, \sigma_j^b] = 2i\delta_{ij}\epsilon^{abc}\sigma_i^c$. The Hamiltonian is symmetric under the mapping $\gamma \rightarrow -\gamma$ or $h \rightarrow -h$, therefore one can only consider the cases in which $\gamma \geq 0$ and $h \geq 0$ without loss of generality. For $\gamma = 1$, one obtains the 1D transverse field Ising model. In our study, we stress the cases with stronger spin-spin interaction along the x -direction, and we consider only the cases with $0 \leq \gamma \leq 1$.

The solution of the XY model in one dimension has been derived for a long time since Lieb, Schultz, and Mattis found the exact solution through the Jordan-Wigner transformation [55]. With the definition $\sigma_j^+ = \frac{1}{2}(\sigma_j^x + i\sigma_j^y)$ and $\sigma_j^- = \frac{1}{2}(\sigma_j^x - i\sigma_j^y)$, the Jordan-Wigner transformation in terms of

spinless Fermion operators c_j and c_j^\dagger is defined as follows:

$$\begin{aligned}\sigma_j^- &= \exp\left(-i\pi \sum_{i=1}^{j-1} c_i^\dagger c_i\right) c_j, \\ \sigma_j^+ &= c_j^\dagger \exp\left(i\pi \sum_{i=1}^{j-1} c_i^\dagger c_i\right).\end{aligned}\quad (2)$$

The Hamiltonian is then transformed to the form

$$H_{XY} = -\left[\sum_{j=1}^N (c_j^\dagger c_{j+1} + \gamma c_j^\dagger c_{j+1}^\dagger + \text{H.c.}) + hc_j^\dagger c_j\right] + \frac{Nh}{2}.\quad (3)$$

Under the periodic boundary ($c_j = c_{N+j}$) condition, the Hamiltonian can be further Fourier transformed into

$$\begin{aligned}H_{XY} &= -\sum_k 2(\cos k + h/2)c_k^\dagger c_k \\ &\quad - i\gamma \sin k (c_k^\dagger c_{-k}^\dagger + c_k c_{-k}) + \frac{N}{2}h,\end{aligned}\quad (4)$$

where the lattice constant is set to 1. The system is decomposed into ‘‘noninteracting’’ (diagonalizable) momentum subspaces, and thus the correlation functions of interest can be calculated within the noninteracting subspaces.

The essential spin-spin correlation functions we considered here are defined as

$$\rho_{aa}(m) = \langle \Psi_0 | \sigma_0^a \sigma_m^a | \Psi_0 \rangle,\quad (5)$$

where $a = x, y, z$, and Ψ_0 is the ground state of the XY model (1). Note that ρ_{aa} depends only on the relative distance, $r_m - r_0$, between the sites 0 and m due to the translational invariant property. Using Jordan-Wigner transformation, Lieb, Schultz, and Mattis [55] showed that $\rho_{xx}(m)$ can be transformed to the Toeplitz determinant

$$\rho_{xx}(m) = \begin{vmatrix} G_{-1} & G_{-2} & \cdots & G_{-m} \\ G_0 & G_{-1} & \cdots & G_{-m+1} \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ G_{m-2} & G_{m-3} & \cdots & G_{-1} \end{vmatrix},\quad (6)$$

where $G_{l-n} = \langle \Psi_0 | B_l A_n | \Psi_0 \rangle$ with the definitions $A_n = c_n^\dagger + c_n$ and $B_l = c_l^\dagger + c_l$. While $\rho_{yy}(m)$ has the same structure as $\rho_{xx}(m)$,

$$\rho_{yy}(m) = \begin{vmatrix} G_1 & G_0 & \cdots & G_{-m+2} \\ G_2 & G_1 & \cdots & G_{-m+3} \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ G_m & G_{m-1} & \cdots & G_1 \end{vmatrix},\quad (7)$$

$\rho_{zz}(m)$ has a much simpler form,

$$\rho_{zz}(m) = \begin{vmatrix} G_0 & G_m \\ G_{-m} & G_0 \end{vmatrix},\quad (8)$$

due to the fact that spin-1/2 $S_i^z = \frac{1}{2}\sigma_i^z$ is a local operator unlike S_i^x or S_i^y . Through the properties of the ground state

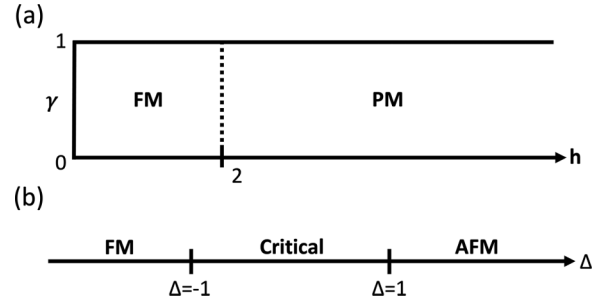


FIG. 1. (a) Phase diagram of the 1D XY model. For $h < 2$, the system is in the ferromagnetic (FM) state, whereas in the case of $h > 2$, the system is paramagnetic. (b) Phase diagram of the 1D XXZ model. In the case of $\Delta > 1$, the system is in the antiferromagnetic (AFM) state, while for $\Delta < -1$, it is FM. In between ($-1 < \Delta < 1$), it is in the gapless critical state.

$|\Psi_0\rangle$ and the advantage from the periodic boundary condition, the correlation function G_{l-n} can be calculated by

$$G_{l-n} = \frac{1}{\pi} \int_0^\pi dk \frac{\gamma \sin k \sin kR - (\cos k + h/2) \cos kR}{\sqrt{(\cos k + h/2)^2 + \gamma^2 \sin^2 k}},\quad (9)$$

where $R = r_l - r_n$, indicating the distance between sites l and n . Interested readers are referred to Appendix A for more details.

According to the Mermin-Wagner theorem [3], continuous symmetry breaking does not occur spontaneously in 1D quantum systems at zero temperature. In other words, no local order parameter can gain any finite expectation value for such systems. However, the phase transitions can still occur and be observed by using appropriate correlation functions. For instance, in Fig. 1(a), the phase diagram is shown for the XY model, and the spin-spin correlation functions for the XY model are shown in Fig. 2. When $h < 2$, the system is in an ordered phase, whose correlation ρ_{xx} asymptotically approaches a constant as $m \rightarrow \infty$. This property represents the long-range order of a ferromagnetic (FM) phase. On the other hand, when $h > 2$, a disordered phase is observed due to the asymptotic

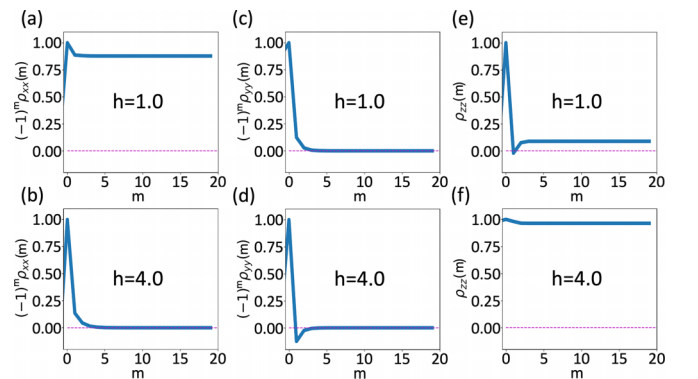


FIG. 2. Spin-spin correlation functions for the XY model with various h . (a) $(-1)^m \rho_{xx}(m)$ for $h = 1.0$. (b) $(-1)^m \rho_{xx}(m)$ for $h = 4$. (c) $(-1)^m \rho_{yy}(m)$ for $h = 1.0$. (d) $(-1)^m \rho_{yy}(m)$ for $h = 4$. (e) ρ_{zz} for $h = 1$. (f) ρ_{zz} for $h = 4$. For all subfigures, $\gamma = 0.5$. One can see that ρ_{xx} is a relevant correlation function in the ferromagnetic phase, whereas ρ_{zz} is relevant in the paramagnetic phase.

behavior $\rho_{xx} \rightarrow 0$ and $\rho_{zz} \rightarrow 1$. Additionally, these properties indicate that the disordered phase is actually paramagnetic (PM). Note that all three correlation functions ρ_{xx} , ρ_{yy} , and ρ_{zz} behave quite differently in FM and PM phases. Therefore, they can serve as good candidates for the input data format of deep learning machines to distinguish different quantum phases.

B. XXZ model

The 1D XXZ model with zero magnetic field, which served as the simplest model for explaining strongly correlated systems, has been “the” model to investigate the magnetism and physics of some other related 1D interacting fermion systems since Heisenberg proposed the XXX model [58] and Bethe gave the first solution by using the Bethe ansatz [59]. The Hamiltonian of XXZ model has the following form:

$$H_{XXZ} = \sum_j S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z, \quad (10)$$

where $S^a = \sigma^a/2$. Its phase diagram is shown in Fig. 1(b). For $\Delta < -1$ the system is in the FM state, while for $\Delta > 1$ it becomes AFM. In between, i.e., in the case in which $-1 < \Delta < 1$, it is in the XY phase (critical regime) due to the fact that its corresponding correlation length is divergent. Note that for $\Delta = 1$ the model corresponds to the AFM Heisenberg model (XXX model), whereas for $\Delta = -1$ it is the FM Heisenberg model.

The XXZ model is a quantum integrable model, which means that they can be solved by using the Bethe ansatz (BA) [59]. However, it has always been a hard topic to obtain spin-spin correlation functions with BA. For instance, to calculate $\langle S_0^+ S_m^- \rangle$, it involves several complicated multidimensional integrals with the highest dimension equal to $2m + 1$ in the complex plane. In other words, for $m \geq 2$ it becomes numerically difficult to calculate the spin-spin correlations [60].

The correlation functions for the critical phase, where $-1 < \Delta < 1$, can be calculated via the bosonization approach [61], which only considers the linear energy spectra near two Fermi points, and it maps the Hamiltonian into an effective bosonic model (Luttinger liquid) parametrized by the group velocity and Luttinger parameters [61]. The outcome is that in the thermodynamic limit, where the correlation length of the system is infinite, the spatial correlations decay algebraically with powers determined by the Luttinger parameters and behave like a (quasi)-long-range order. However, this method only works in the massless Luttinger regime. For the other massive phases, e.g., FM and AFM, Luttinger liquid analysis fails. For our purpose, we need to calculate correlations in all regimes, and hence some other alternative methods must be adopted.

We overcome the issue mentioned above by leveraging a numerical method called density-matrix renormalization group (DMRG), which was developed by White [6,57]. The low-energy spectrum, the correlations, and other useful physics properties of 1D systems can be calculated efficiently by DMRG due to the low bipartite entanglement of 1D systems. In particular, the calculations can be quick and precise with very low truncation errors. Figures 3(a), 3(b) and 3(c)

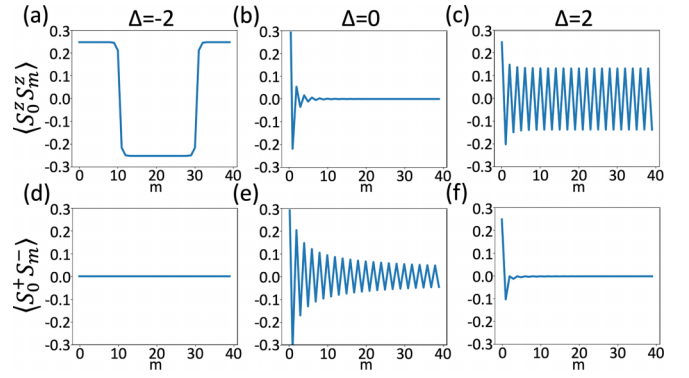


FIG. 3. Spin-spin correlation functions for the XXZ model with various Δ . Parts (a), (b), and (c) are $\langle S_0^z S_m^z \rangle$ for $\Delta = -2$ (FM), $\Delta = 0$ (critical), and $\Delta = 2$ (AFM), respectively. Parts (d), (e), and (f) are $\langle S_0^+ S_m^- \rangle$ for $\Delta = -2$ (FM), $\Delta = 0$ (critical), and $\Delta = 2$ (AFM), respectively. We can see that $\langle S_0^z S_m^z \rangle$ is relevant in the AF and FM phases, while $\langle S_0^+ S_m^- \rangle$ is only relevant in the critical phase.

show $\langle S_0^z S_m^z \rangle$ for $\Delta \leq -1$, $-1 < \Delta \leq 1$, and $\Delta > 1$, respectively, using a specific algorithm called iDMRG with the length of the unit cell $L_{UC} = 40$ and the bond dimension $m_b = 100$ [62], enforcing $U(1)$ symmetry in the $S_z = 0$ sector. The iDMRG algorithm produces Matrix Product State wave functions that are infinite in size, and translationally invariant under shifts of the 40-site unit cell. The large unit cell allows the system to partially phase-separate in the ferromagnetic region, as shown in Fig. 3(a), whereas in the critical phase the wave function will be translationally invariant under a two-site shift [which is the minimum possible translational invariance allowed by the $U(1)$ symmetry for spin-1/2 systems]. One can see that for Fig. 3(a) the correlations develop some plateaus at the values $1/4$ and $-1/4$, showing FM property with total magnetization equal to zero due to the $U(1)$ symmetry. In the critical regime, $-1 < \Delta \leq 1$, $\langle S_0^z S_m^z \rangle$ quickly decays to zero as a function of the distance, which indicates that there is no long-range order at all, as shown in Fig. 3(b). For the AFM ($\Delta > 1$), $\langle S_0^z S_m^z \rangle$ has a zigzag curve, which represents the AFM long-range order, i.e., $(-1)^m \langle S_0^z S_m^z \rangle$ decays to a constant, as shown in Fig. 3(c). Therefore, $S_0^z S_m^z$ can be viewed as a relevant operator for the FM and AFM phases, whereas for the critical phase it is irrelevant.

On the other hand, the behaviors of $\langle S_0^+ S_m^- \rangle$ are shown in Figs. 3(d), 3(e) and 3(f). From the figures one can see that $\langle S_0^+ S_m^- \rangle$ decays to zero for both FM and AFM phases, while for the critical phase it shows the XX long-range order similar to the XY model for $\gamma = 1$. Therefore, contrary to $S_0^z S_m^z$, $S_0^+ S_m^-$ can be viewed as a relevant operator for the critical phase, whereas for both FM and AFM it is irrelevant. The relevance of the correlation operators is very important for the outcomes of the deep learning process, as we will discuss later in the paper.

III. SUPERVISED LEARNING

A. Data preparation

In previous studies [8,24,25], we used quantum-information-related quantities, such as Majorana correlation

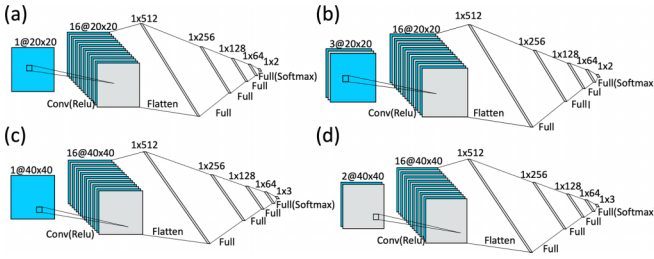


FIG. 4. The schematic illustrations of the convolutional neural networks for various input data: (a) ρ_{xx} , ρ_{yy} , or ρ_{zz} ; (b) ρ_{xx} , ρ_{yy} , and ρ_{zz} all together; (c) $\langle S_0^z S_m^z \rangle$ or $\langle S_0^+ S_m^- \rangle$; (d) both $\langle S_0^z S_m^z \rangle$ and $\langle S_0^+ S_m^- \rangle$.

matrices (MCMs), block correlation matrices (BCMs), one-particle entanglement spectra (OPES), or one-particle entanglement eigenvectors (OPEEs) as input data for deep-learning processes. The whole data construction of the entanglement-related data is based on the calculations of the fermion-fermion correlation functions, and thus we take here the spin-spin correlation functions of the XY and XXZ models in analogy with those of fermion models.

For the XY model, we prepare each of $\rho_{xx}(r_j - r_i)$, $\rho_{yy}(r_j - r_i)$, and $\rho_{zz}(r_j - r_i)$ as an $m_s \times m_s$ matrix, where $r_i, r_j = 0, 1, \dots, m_s - 1$, by calculating G_{l-n} and the Toeplitz determinant for each entry. The subsystem length, $m_s = \max |r_j - r_i| + 1$, is set to be less than 40, and the precision of the integrals is 10^{-16} by using Romberg integrals.

On the other hand, for the XXZ model, we use the iDMRG algorithm with matrix product states (Matrix Product Toolkit by McColluch [63]) to compute correlation functions, $\langle S_i^\alpha S_j^{\alpha'} \rangle$, where $\alpha, \alpha' = z, +, -$. We take the length of the unit cell $L_{UC} = 40$ and the bond dimension $m_b = 100$. For the ground-state calculation, its energy is compared with the result of the Bethe ansatz, and the precision is distributed within the range of 10^{-12} – 10^{-4} . For the critical phase, the accuracy is relatively lower, whereas for the gapped phases (FM and AFM) the precision is much higher.

B. Deep-learning processes

The usage of different types of neural network architectures to recover phase transitions often depends on data types and their characteristics. For instance, matrices or tensors can be naturally viewed as single- or multichannel 2D “images,” and then a convolutional neural network (CNN) would be an efficient candidate for the pattern recognition in the “images” due to its inductive priors, such as translational invariance and spatial locality. Here, the matrices based on the spin-spin correlation functions just belong to these kinds of data types.

In the XY model, there are three essential correlation functions: ρ_{xx} , ρ_{yy} , and ρ_{zz} . One can choose one of them as the input data or put all of them into the machines with model architectures shown in Figs. 4(a) and 4(b), respectively. In situation (a), each “image” contains information of an $m_s \times m_s$ matrix, whereas in (b), the input data are “images” of dimension, $3 \times m_s \times m_s$. “3” indicates the dimension along which all ρ_{xx} , ρ_{yy} , and ρ_{zz} are stacked together. On the other hand, for the XXZ model, there are two important correlations: $\langle S_0^z S_m^z \rangle$ and $\langle S_0^+ S_m^- \rangle$. They can also be put into the machines

individually or all together, as shown in Figs. 4(c) and 4(d). In this paper, we choose $m_s = 20$ for the XY model and $m_s = 40$ for the XXZ model.

The basic neural networks designed for the phase recognition task are shown in Fig. 4. By using Keras in the TENSORFLOW package [64], all NNs begin with a convolutional layer containing 16 kernels (filters) of the size 3×3 and ReLU activation functions, and then they connect to four fully connected ReLU activated layers with 512, 256, 128, and 64 neurons, respectively. Finally, they are followed by an output dense layer with two (XY) or three (XXZ) neurons plus a softmax function. The output of each neuron can now be interpreted as the probability for each phase with which the input may associate. Note that the zero-padding technique on the input data is used to keep the same input size, and no pooling layers are needed due to the small size of the input data.

In the supervised learning, the labeled training data are needed. In the XY model, we first chose two magnetic fields h individually for the FM and AFM phases, each of which is expanded within a window of size 0.1 in units of h at a constant anisotropy γ to collect labeled data points. In fact, the training points can be either chosen arbitrarily deep inside each phase or via the most confident points with the best silhouette value in the unsupervised learning approach, which will be explained in the next section. For the XXZ model, six training points are first chosen and then expand in the same manner. Here, we purposely took two points for each phase for the sake of good precision at the inference stage. Moreover, we found that there is a more natural way to take these points by using unsupervised learning, as we will discuss later. By setting the train-validation split ratio as 0.2, we adopt the ADAM optimization [65] for training at a learning rate 10^{-4} with categorical cross entropy as the loss function. Once the loss is converged after training, at the inference stage we fix whole parameters in the trained model and feed with new data for prediction. The rapid drop for the “probability” output of the NN indicates that the trained model recognizes the phase transition from one phase to the other as a function of the input spin-spin correlation functions.

C. Supervised results

1. XY model

For the supervised learning of an XY model, we choose regions around two magnetic fields h as training points. For each region, 1000 ρ_{xx} , ρ_{yy} , and ρ_{zz} are calculated according to Eqs. (6), (7), (8), and (9). Those correlation functions are based on a thermodynamic system, where the system size is infinite, with a periodic boundary condition.

After training, our trained model can distinguish different phases for a given dataset and locate the phase boundaries by inputting a set of unseen data points along the magnetic field h . In the XY model, 20 000 testing data points are collected uniformly from $h = 1$ to 10. By feeding ρ_{xx} , ρ_{yy} , and ρ_{zz} all together, the results are shown in Fig. 5(a). Typically training after 40 epochs, both training and validation losses drop to 10^{-6} , indicating that the trained model becomes reliable, as shown in Fig. 5(b). The probability of the neuron output for predicting the FM phase drops from 1 to 0 at

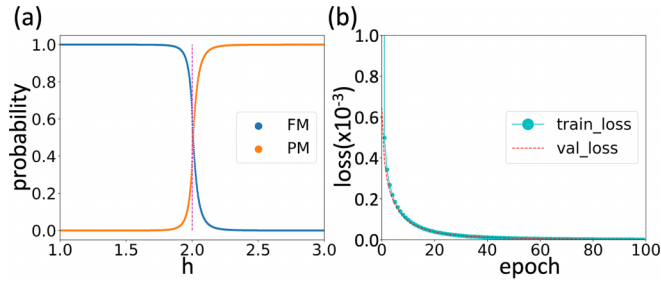


FIG. 5. (a) Each neuron output of the final softmax layer corresponding to the probability of each phase as a function of h with $\gamma = 0.5$ by feeding ρ_{xx} , ρ_{yy} , and ρ_{zz} all together into the machine. Although the training set from the correlation functions is far beyond the h region shown here, the trained CNN can still recognize a quantum phase transition near $h = 2$. The dashed line indicates the theoretical phase-transition point. (b) The validation loss follows the trend of the training loss well, suggesting no overfitting happened.

$h = 2$, while the other output for predicting the PM phase rises from 0 to 1. These two curves cross each other at $h_c = 1.94, 1.95, 1.95, 1.95$ for $m_s = 5, 10, 15, 20$, respectively, as listed in Table I. The predicted critical points are around 1.95. The results for different m_s are not changing too much due to the small sizes of the correlation functions. They are all within the statistical errors.

In Fig. 6 we show the predicted critical points by inputting the three correlation functions individually. The corresponding CNN architecture is shown in Fig. 4(a). In the case of $m_s = 20$, h_c are 1.95, 1.95, and 1.92 with standard deviations 0.01, 0.01, and 0.02 for the training data of ρ_{xx} , ρ_{yy} , and ρ_{zz} , respectively. We can see that the results are almost the same as those by inputting the three correlation functions all together. Therefore, we can confirm that ρ_{xx} , ρ_{yy} , and ρ_{zz} all contain the important information to locate the critical points.

In Table I the critical points found by inputting the correlations with difference size m are shown. Essentially there exists no significant difference of the precision among them. In other words, since DL can be viewed as a statistical model building, within the statistical errors one can use small-sized correlation functions to find the critical points with good precision.

2. XXZ model

For the supervised learning of the XXZ model, we take two anisotropies, i.e., Δ values, for each phase as training point centers, and thus there are six in total. Around each Δ , 1000 $\langle S_0^z S_m^z \rangle$ and $\langle S_0^+ S_m^- \rangle$ are calculated by MPS Toolkit of iDMRG [63].

TABLE I. Predicted critical points by training spin-spin correlation functions of different sizes $m_s = 5, 10, 15, 20$ for the XY model.

	$\rho_{xx}, \rho_{yy}, \rho_{zz}$	ρ_{xx}	ρ_{yy}	ρ_{zz}
$m_s = 5$	1.94	1.96	1.96	1.90
$m_s = 10$	1.95	1.96	1.96	1.91
$m_s = 15$	1.95	1.96	1.96	1.91
$m_s = 20$	1.95	1.95	1.95	1.92

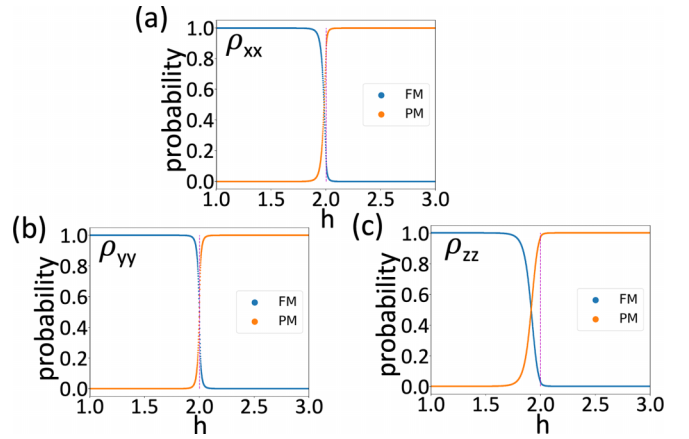


FIG. 6. Results of supervised learning of the XY model by feeding (a) ρ_{xx} , (b) ρ_{yy} , or (c) ρ_{zz} individually. The predictions are close to the exact value $h = 2$.

As for the XY model, after training the machine can serve as a well-trained model to find out the TPs by feeding a set of unseen data points along Δ . Here, we also take 2000 testing data points to explore phase transitions. By inputting both $\langle S_0^z S_m^z \rangle$ and $\langle S_0^+ S_m^- \rangle$, we show the predicted critical points in Fig. 7(a). Typically after 14 epochs of training, the training and validation losses decrease to less than 10^{-8} as shown in Fig. 7(b). Namely, the trained model has found the optima for finding those critical points. The probability of predicting the FM phase drops from 1 to 0 around the critical point $\Delta_c = -1$, whereas that of predicting the critical phase rises from 0 to 1. A similar situation also happens for the critical point between the critical and AFM phases. The predicted critical points (Δ_c^1, Δ_c^2), which are taken at the crossing points of the probabilities, are $(-1.05, 1.19)$, $(-1.03, 1.19)$, $(-1.05, 1.20)$, and $(-1.03, 1.21)$ for $m_s = 10, 20, 30$, and 40 , respectively, as shown in Table II. The predicted Δ_c^1 are closer to -1 , whereas the differences between the predicted Δ_c^2 and the real critical point 1 are bigger. To understand the situation, we feed $\langle S_0^z S_m^z \rangle$ and $\langle S_0^+ S_m^- \rangle$ separately into machines.

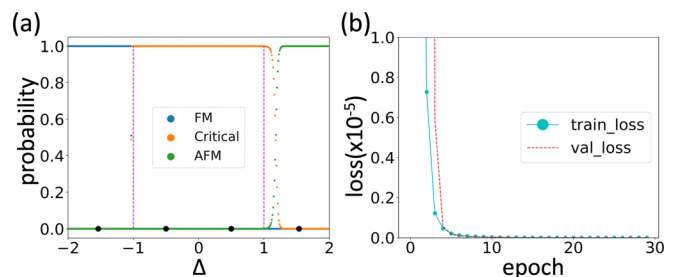


FIG. 7. (a) Neuron output of the final softmax layer corresponding to the probability of each phase as a function of Δ by feeding both $\langle S_0^z S_m^z \rangle$ and $\langle S_0^+ S_m^- \rangle$ into the trained machine. Although the training set from the correlation functions is far beyond the Δ region shown here, the CNN can still recognize quantum phase transitions near $\Delta = -1$ and 1. The dashed lines indicate the theoretical phase-transition points. (b) The validation loss follows the trend of the training loss well, suggesting no overfitting happened.

TABLE II. Predicted critical points by training spin-spin correlation functions of different sizes $m_s = 10, 20, 30, 40$ for the XXZ model.

	$\langle S_0^z S_m^z \rangle, \langle S_0^+ S_m^- \rangle$		$\langle S_0^z S_m^z \rangle$		$\langle S_0^+ S_m^- \rangle$	
	Δ_c^1	Δ_c^2	Δ_c^1	Δ_c^2	Δ_c^1	Δ_c^2
$m_s = 10$	-1.05	1.19	-1.09	1.17	-1.06	1.20
$m_s = 20$	-1.03	1.19	-1.02	1.24	-1.03	1.15
$m_s = 30$	-1.05	1.20	-1.02	1.27	-1.06	1.12
$m_s = 40$	-1.03	1.21	-1.02	1.29	-1.05	1.10

Figure 8 shows the probability of predicting the critical points by feeding the correlation functions $\langle S_0^z S_m^z \rangle$ and $\langle S_0^+ S_m^- \rangle$ separately. One can also see the predicted values in Table II for different subsystem size $m_s = 10, 20, 30, 40$. For the first-order phase transition from the FM phase to the critical one, i.e., $\Delta = -1$, either $\langle S_0^z S_m^z \rangle$ or $\langle S_0^+ S_m^- \rangle$ can predict more precise TPs. However, for the second-order TPs, $\Delta_c = 1$, $\langle S_0^+ S_m^- \rangle$ is getting more and more precise through increasing m_s , whereas the predicted values by feeding $\langle S_0^z S_m^z \rangle$ are not so precise throughout different subsystem sizes.

The aforementioned phenomena can be understood as follows. Near any first-order TPs, the gaps are opened faster, therefore the machine can easily recognize TPs, while near the second-order TPs, the gaps are opened much more slowly, and thus the precision for finding such TPs is poorer from both correlations. However, when going into the AFM phase, $\langle S_0^z S_m^z \rangle$ shows a smaller growth than the decrease of $\langle S_0^+ S_m^- \rangle$ and it results in bigger prediction errors for Δ_c^2 . These results suggest why the predicted critical points Δ_c^2 obtained by inputting two correlation functions together are in between the predicted values obtained by feeding each correlation individually. The more imprecise results obtained by $\langle S_0^z S_m^z \rangle$ weaken the prediction precision when two correlation functions are input spontaneously.

The results for the XXZ model are not as precise as those for the XY model due to the fact that we use numerics (iDMRG) to calculate the correlations for the XXZ model, instead of using analytical expressions as in the XY model. However, the results are still encouraging. In particular, the predicted critical points obtained from $\langle S_0^+ S_m^- \rangle$ are in surprisingly good agreement with the analytical results when $m_s \leq 20$. This shows the advantage and the effectiveness of

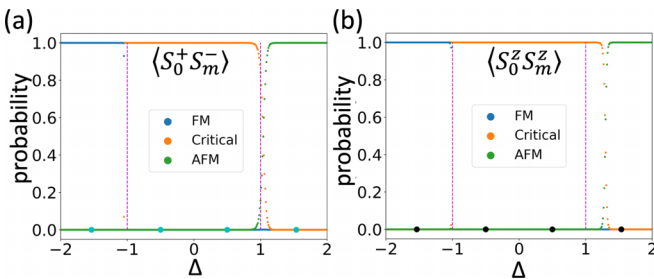


FIG. 8. Results of supervised learning of the XXZ model by feeding (a) $\langle S_0^+ S_m^- \rangle$ and (b) $\langle S_0^z S_m^z \rangle$ separately, with $m_s = 40$. Please refer to Sec. III C for more discussions.

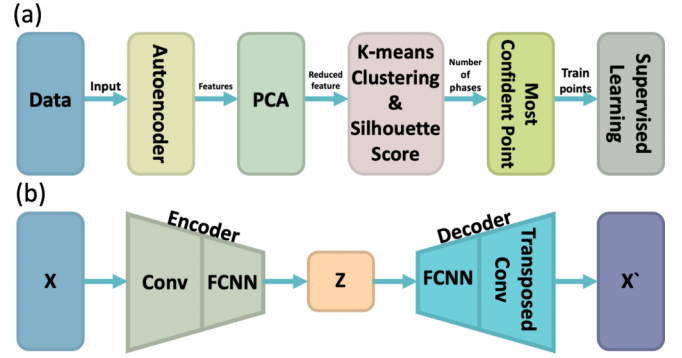


FIG. 9. (a) The proposed working protocol to identify different phases and to finely determine the phase boundaries without prior knowledge. (b) The schematic model architecture of the autoencoder (AE). (Conv denotes convolution module; FCNN denotes fully connected neural network module.)

our approach for searching the patterns in the correlation functions.

IV. UNSUPERVISED LEARNING

A. ML algorithms

One of the ultimate goals in ML is to discover the hidden patterns behind given data without any human intervention or manual labeling. These kinds of ML algorithms are called unsupervised learning. Since one does not need any label tagging in the process of unsupervised learning, it is usually difficult and commonly considered as a kind of holy grail in the science community. In our previous study [8], we already demonstrated a working procedure to obtain the TPs by mainly unsupervised learning, and thus we just introduce our method here in a simpler version.

The proposed working protocol is schematically shown in Fig. 9(a). There are four steps: (i) The input correlation functions are fed into an autoencoder (AE) for unsupervised training in order to extract effective features via dimension reduction. (ii) The necessary feature dimension is determined by principal component analysis (PCA) when 99% of total variance of input features is kept. (iii) The total number of phases is then determined by K -means clustering for the extracted, necessary features, followed by silhouette analysis (SA). (iv) Sharp phase boundaries can be further obtained with the help of supervised learning, which we constructed in the last section. We explain a few key algorithms below.

An AE compresses input data into a more efficient representation in an unsupervised way. It consists of two parts, namely an encoder and a decoder. A typical model architecture of AE is shown in Fig. 9(b). It is made of a convolution layer followed by a linear module composed of fully connected hidden layers. In the decoder, it is arranged in a reversed manner to that of the encoder, except that now the convolution layer is replaced by a transposed convolutional one.

As opposed to AE, PCA is a linear method to reduce the dimension and to visualize the data. To do that, PCA uses an orthogonal and linear transformation of the input features to a sorted set of new variables by their variance.

Once the extracted features are obtained from the input data, the K -means algorithm is taken as a clustering algorithm without any supervision. Given the number of clusters n , K -means is used to find out the best cluster formation such that the variance within each cluster is minimized.

However, in order to use K -means to find out the best cluster formation, one still has to provide the number of clusters n . To find out n automatically, we employ SA. For a give set of clusters, SA assigns a value, called the Silhouette value $s(x)$, which is bounded between $+1$ and -1 , to each data point within a cluster. $s(x)$ can be interpreted as a measure of how alike x is to its own cluster (cohesion) compared to the other one (separation). One computes s -score, namely the mean of $s(x)$, as a function of the number of clusters n after K -means clustering, and then we take the best n as the one giving the maximum s -score.

Once the best choice for n is given, the data point with the highest silhouette value within the same cluster can serve as the most confident point to build a “labeled” training set to train a supervised neural network. It can improve the precision of the predicted critical points originally obtained in an unsupervised learning over the parameter space.

B. Unsupervised results

1. XY model

We first prepare the input image dataset of correlation functions by generating 10 001 ρ_{xx} , ρ_{yy} , and ρ_{zz} with the same method described in the supervised learning at evenly divided magnetic field h from 0 to 10, with subsystem size $m_s = 20$ of an infinite chain with periodic boundary conditions. We feed the three correlation functions all together or separately. In Fig. 10 we show the results by feeding three correlation functions at the same time, while Figs. 11–13 show the results by inputting ρ_{xx} , ρ_{yy} , and ρ_{zz} , respectively, into the machine.

Following the ML protocol described in ML algorithms, we first have to train a neural network to encode our input data to effective representations in the latent space. To discover the minimum dimension d_z of the latent space, a series of AEs with the same model architecture is trained except for the number of hidden neurons in the middlemost layer n_{mid} from 2 to 10. For each n_{mid} , the necessary dimension of the converged latent representation to keep at least 99% variance of them by PCA is recorded. For doing the statistical analysis, we repeat the same training procedures 100 times with the same initial weight distribution. In this way, the minimum dimension d_z is decided if such a number becomes indispensable (dominant) in the discrete distribution of d_z when n_{mid} increases.

To obtain the best number of clusters n , we utilize SA through the K -means algorithm. In the following calculations, we already fixed $n_{\text{mid}} = d_z = 2$ (fed data: three correlations, ρ_{xx} , ρ_{yy}) or $n_{\text{mid}} = d_z = 3$ (ρ_{zz}) hidden neurons in the middlemost layers as suggested by (a) of Figs. 10–13, respectively. In (b) of those four figures, the mean silhouette values achieve the highest one when $n = 2$, suggesting that there are two different phases (clusters) for the XY model.

In (c) of Figs. 10–13, we show the projection of latent representations into a 2D space spanned by the first two principal components (features). These plots show us how the system could be separated into two clusters (phases). The feature

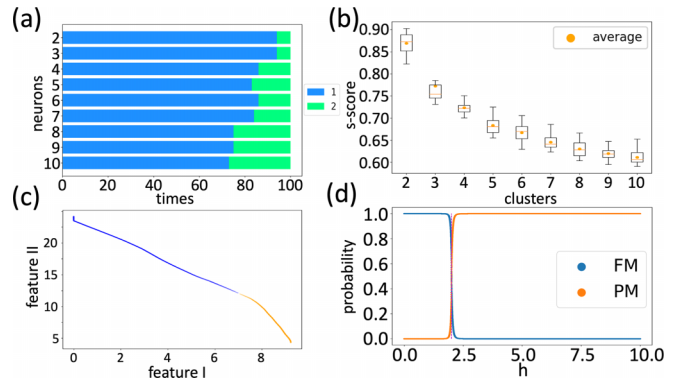


FIG. 10. AE results for the combined spin-spin correlation functions (ρ_{xx} , ρ_{yy} , ρ_{zz}) of the XY model as the input data. (a) The discrete distribution of the necessary number of neurons d_z for a given n_{mid} of neurons in the middlemost layer (2 to 10 along the y axis). Results from 100 independently trained AEs are statistically calculated: The length of every color bar is proportional to the number of times that d_z occurred within 100 models. Different colors in the legend represent different d_z . (b) The box plot of the s -scores as a function of n clustering (via K -means method). (c) Latent representations projected to a subspace spanned by the first two principal components (feature map). Each color indicates its corresponding cluster (phase). (d) The neuron output (phase diagram) as a function of h with $m_s = 20$, $\gamma = 0.5$ for the 1D XY model from a trained CNN by supervised learning in the last step of the ML protocol. The dashed line indicates the theoretical phase-transition boundary.

plot is a continuous curve, which characterizes a second-order phase transition. We will see the differences of such feature plots between the first- and the second-order phase transition in the next subsection.

By going through the aforementioned recipe, the TPs are statistically found at the mean values 2.03, 1.97, 1.98, and 2.09 with the standard deviations 0.03, 0.02, 0.02, and 0.14 for Figs. 10–13, respectively, after collecting clustering results from 100 sets of latent representations via different trained AEs.

The silhouette values of the XY model are drawn in Fig. 14. One can see that the minima of silhouette values almost lie on the TPs. This suggests that SA can serve as a good indicator for phase transitions. To find more accurate TPs, we first take

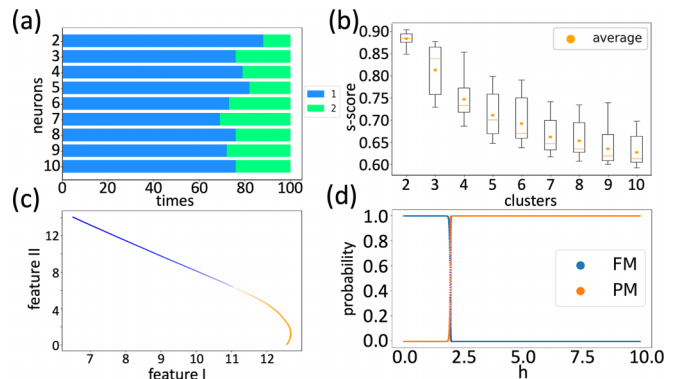


FIG. 11. Same as Fig. 10, except that here, ρ_{xx} function is taken as the input data.

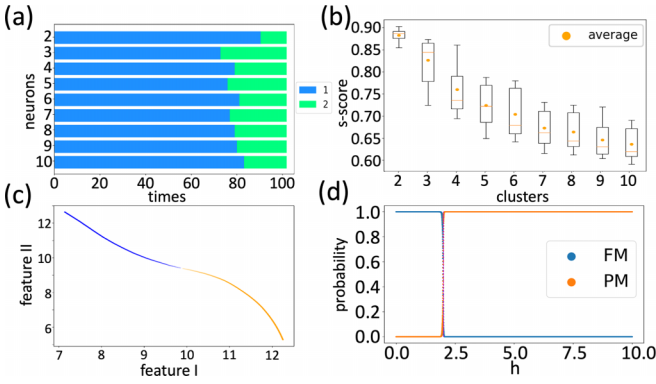


FIG. 12. Same as Fig. 10, except that here, ρ_{yy} function is taken as the input data.

two representative points, which obtain the highest s -score in each cluster. We call them the most confident points (MCPs). In our case, they are (0.89, 6.31), (0.85, 6.15), (0.85, 6.13), and (0.87, 6.34) for the input data as the combined three correlations, ρ_{xx} , ρ_{yy} , and ρ_{zz} , respectively. For each phase, we expand symmetrically around the MCP by a window of 0.1 to get 1000 points with equal spacing. These 2000 data points form our training dataset with labels, and the original 10 001 ones become our test dataset (without labels). By further training CNN models with these labeled datasets, the PTs found become sharper at mean values, 1.95, 1.95, 1.95, and 1.92 with smaller standard deviation, 0.03, 0.01, 0.01, and 0.02, as shown in Figs. 10–13, respectively, at the testing stage.

2. XXZ model

For the XXZ model, we prepare the input “images” by generating 20 001 $\langle S_0^+ S_m^- \rangle$ and $\langle S_0^z S_m^z \rangle$ by iDMRG at evenly divided Δ from -10 to 10 . In unsupervised learning we choose the subsystem size $m_s = 40$. Similar to the case of the XY model, we input both correlation functions $\langle S_0^+ S_m^- \rangle$ and $\langle S_0^z S_m^z \rangle$ together or separately. In Fig. 15 we show the results by feeding both correlation functions, whereas in Figs. 16 and 17 the results by inputting $\langle S_0^+ S_m^- \rangle$ and $\langle S_0^z S_m^z \rangle$, respectively, into machines are shown.

Similar to the XY model, we first train a neural network to encode our data of correlation functions to the latent rep-

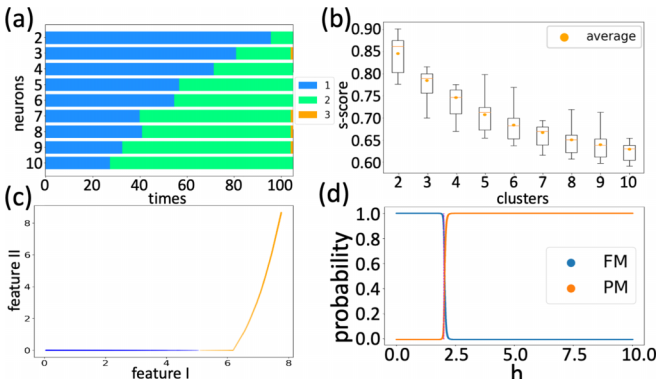


FIG. 13. Same as Fig. 10, except that here, ρ_{zz} function is taken as the input data.

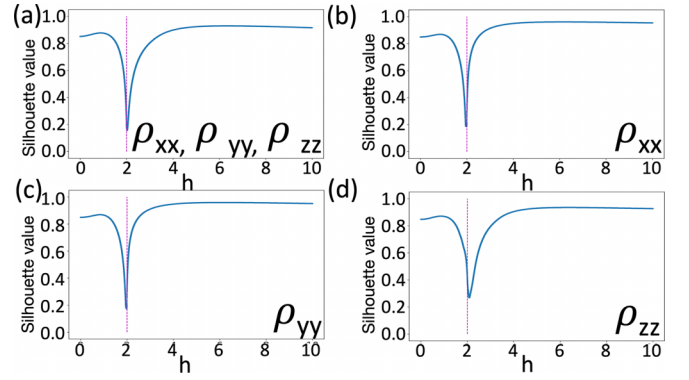


FIG. 14. Silhouette values as a function of h for $\gamma = 0.5$ and $m = 20$ with (a) ρ_{xx} , ρ_{yy} , and ρ_{zz} all together; (b) ρ_{xx} ; (c) ρ_{yy} ; and (d) ρ_{zz} as the input data. Notice that the minima of silhouette values are close to the phase-transition point $h = 2$.

resentation. We determine the minimal dimension d_z of the latent space as follows. First, we train 100 AEs with the same model architecture for each given number of hidden neurons in the middlemost layer (n_{mid} , from 2 to 10). In (a) of Figs. 15–17, we then compute the discrete distribution of d_z , i.e., the necessary dimensions of the latent representations to keep at least 99% variance of all encoded representation

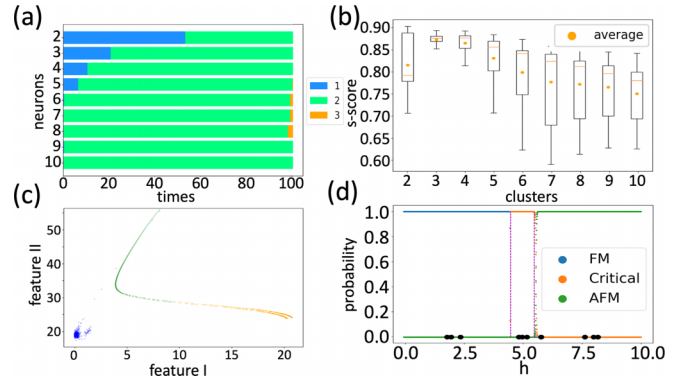


FIG. 15. AE results for both spin-spin correlation functions ($\langle S_0^+ S_m^- \rangle$ and $\langle S_0^z S_m^z \rangle$) of the XXZ model as the input data. (a) The discrete distribution of the necessary number of neurons d_z for a given n_{mid} of neurons in the middlemost layer (2 to 10 along y axis). Results from 100 independently trained AEs with both correlation functions are statistically calculated: The length of every color bar is proportional to the number of times that d_z occurred within 100 models. Different colors in the legend represent different d_z . (b) The box plot of the s -scores as a function of n clustering (via K -means method). (c) Latent representations projected to a subspace spanned by the first two principal components (feature map). Each color indicates its corresponding cluster (phase). It is obvious that for the first-order phase transition, the two clusters are disconnected, whereas for the second-order phase transition, they are continuously connected. (d) The neuron output (phase diagram) as a function of Δ for the 1D XXZ model from a trained CNN by supervised learning in the last step of the ML protocol. We choose 10 seeds (gray dots) as our labeled training data. The dashed lines indicate the theoretical phase-transition boundaries. Please see the main text and discussions for more details.

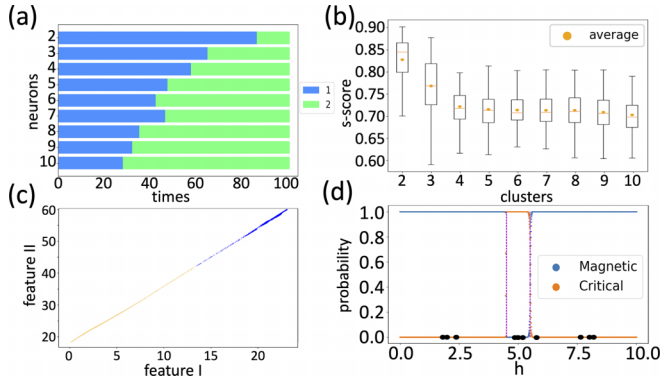


FIG. 16. Same as Fig. 15, except that here, $\langle S_0^+ S_m^- \rangle$ is taken as the input data. Moreover, in (b), since $\langle S_0^+ S_m^- \rangle$ is not relevant in the FM and AFM phases, i.e., they cannot distinguish FM from AFM, they show only two clusters (critical and magnetic phases); in (c), unlike the input data with $\langle S_0^z S_m^z \rangle$, there exists no signature of the first-order phase transition if we only feed $\langle S_0^+ S_m^- \rangle$ into the machine, therefore the two clusters are continuously connected. Please see the main text and discussions for more details.

vectors for each n_{mid} by PCA. d_z is finally suggested to be 3 for the input data using both correlation functions in Fig. 15, 2 for those using $\langle S_0^+ S_m^- \rangle$ in Fig. 16, and 4 for those using $\langle S_0^z S_m^z \rangle$ in Fig. 17 as the input data.

After d_z is obtained, the latent representation of all input data from previously trained AEs is taken with $n_{\text{mid}} = d_z$, and then SA is done to estimate the optimal number of clusters n via K -means. The results are shown in (b) of Figs. 15–17, which specify that the mean s -score reaches the highest one when $n = 3$ in Figs. 15 and 17; however, for the input data as $\langle S_0^+ S_m^- \rangle$, $n = 2$ in Fig. 16. This difference suggests that using $\langle S_0^z S_m^z \rangle$ as input data is possible to find the correct number of clusters (phases), whereas using $\langle S_0^+ S_m^- \rangle$ can only recognize two clusters (phases) because they confuse FM and AFM phases.

By projecting the multidimensional latent representations into a 2D space spanned by the first two principal components (features), we have (c) of Figs. 15–17. We first investigate

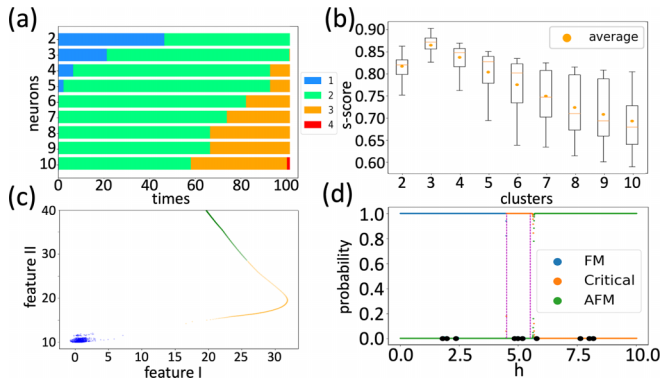


FIG. 17. Same as Fig. 15, except that here, $\langle S_0^z S_m^z \rangle$ is taken as the input data. Moreover, in (b), it is obvious that for the first-order phase transition, the two clusters are disconnected, whereas for the second-order phase transition, they are continuously connected. Please see the main text and discussions for more details.

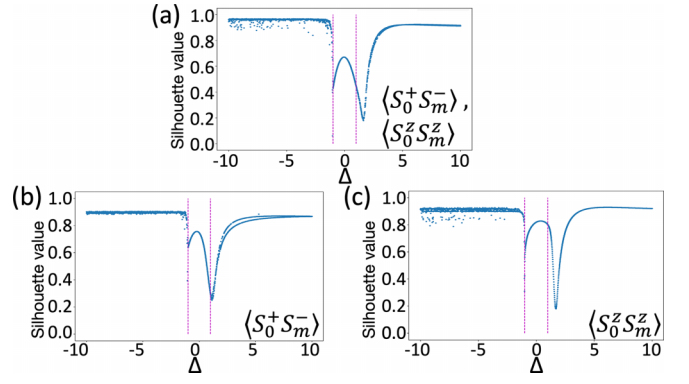


FIG. 18. Silhouette values as a function of Δ for $m_s = 40$ with the input data as (a) both $\langle S_0^+ S_m^- \rangle$ and $\langle S_0^z S_m^z \rangle$, (b) $\langle S_0^+ S_m^- \rangle$, and (c) $\langle S_0^z S_m^z \rangle$. Some signatures are shown here: silhouette values for the FM phase are almost the same, which means they all can be the most confident points. For the first-order phase transition, the minima of silhouette values mostly lie around the critical point $\Delta = -1$, whereas for the second-order phase transition, they have some deviations from the critical point $\Delta = 1$ except in the case in which the input data are $\langle S_0^+ S_m^- \rangle$.

Fig. 15(c) for the input data as both correlation functions. The plot suggests how the system could be divided into three clusters. Moreover, the points with blue, which represent the FM phase, are discontinuously separated from the other clusters. Such discontinuity is a signature of the first-order phase transition at $\Delta_c = -1$. On the other hand, the green and orange lines are connected continuously, which represent a second-order phase transition at $\Delta_c = 1$. The same phenomena can also be seen in Fig. 17, whose data originate from $\langle S_0^z S_m^z \rangle$ correlations.

However, for Fig. 16 it looks quite different. In this figure, $\langle S_0^+ S_m^- \rangle$ correlations are used as input data, and they cannot distinguish between FM and AFM phases. Therefore, the latent representation does not have the signature of a first-order phase transition. The two curves are continuously connected.

Figures 18(a), 18(b) and 18(c) show silhouette values of training data from both correlations $\langle S_0^+ S_m^- \rangle$ and $\langle S_0^z S_m^z \rangle$, respectively. There are two minima of silhouette values. On the left-hand side of the figures, the minima are -1.04 , -1.05 , and -1.01 in Figs. 18(a), 18(b) and 18(c), respectively, which lie almost at the critical points. However, those on the right-hand side behave quite differently, where the minima lie at $\Delta = 1.41$, 1.12 , and 1.70 in Figs. 18(a), 18(b) and 18(c), respectively. For input data as $\langle S_0^+ S_m^- \rangle$, the minimum is close to the critical point 1, while for those as $\langle S_0^z S_m^z \rangle$ the minimum lies away from the TP. The reason for the latter case is due to the slow gap opening phenomenon for the second-order phase transition, which means the correlation length is long near the critical point. When both correlation functions are stacked as input data, we obtain the median among the three minima shown in Figs. 18(a), 18(b) and 18(c). As far as the maxima of silhouette values are concerned, they are 6.08, 5.25, and 6.30 for the AFM phase in Figs. 15–17, whereas for the FM phase, silhouette values remain almost constant, and the point of maximal silhouette value changes for every new training, which means that almost every point represents the most confident one. Finally, the maxima of silhouette values

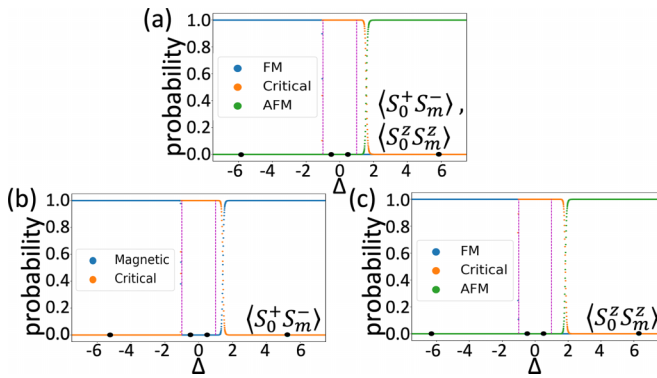


FIG. 19. Supervised learning results with only four training seeds (gray dots) without the seeds related to the cutoff precision of iDMRG when the input data originate from (a) both $\langle S_0^+ S_m^- \rangle$ and $\langle S_0^z S_m^z \rangle$, (b) $\langle S_0^+ S_m^- \rangle$, and (c) $\langle S_0^z S_m^z \rangle$. For the first-order phase transition, the critical points remain intact, while for the second-order phase transition the results are worse than those with the extra training seeds related to the cutoff precision.

for the critical phase always occur at $\Delta = 0$ no matter what kind of input data we feed.

The TPs found by the input data as both correlation functions $\langle S_0^+ S_m^- \rangle$ and $\langle S_0^z S_m^z \rangle$ are at the mean values $(-1.03, 1.61)$, $(-1.04, 1.19)$, and $(-1.01, 1.68)$ with the standard deviations $(0.14, 0.20)$, $(0.01, 0.29)$, and $(0.00, 0.09)$, respectively, after collecting clustering results from 100 sets of latent representations via different trained AEs. For the first-order phase transitions $\Delta_c = -1$, the predicted values are very precise with small standard deviations. However, for the second-order phase transition $\Delta_c = 1$, the predicted results are imprecise with larger standard deviations. To make the predictions more precise, we further train a CNN classifier via supervised learning to predict all the TPs. To prepare the labeled data, we choose ten seeds in the following way: For the AFM phase, three seeds (5.25, 6.08, 6.30) are chosen from the most confident points of SA in Figs. 18(a), 18(b) and 19(c) (see Sec. V for more details). Instead, we choose the mirror reflecting points against 0, $(-5.25, -6.08, -6.30)$, as three seeds for the FM phase since each point in the FM phase has almost the same silhouette value and thus each can be chosen deliberately as the most confident point. For the critical phase, we also choose three seeds $(-0.21, 0.00, 0.38)$, which are the most confident points of SA in Figs. 18(a), 18(b) and 18(c). Finally, an additional seed is chosen at 1.54, which indicates the iDMRG cutoff point. We will have a detailed explanation for these choices in Sec. V. For each seed, we expand symmetrically around it by a window width $\Delta = 0.1$ to obtain 1000 points with equal spacing. These 10 000 labeled data points then form our training dataset, while the original 20 001 ones become our test dataset (no labels). As shown in (d) of Figs. 15–17, the phase boundaries obtained by the CNN classifier are at mean values $(-1.03, 1.19)$, $(-1.05, 1.02)$, and $(-1.02, 1.28)$ with standard deviations $(0.01, 0.03)$, $(0.01, 0.06)$, and $(0.01, 0.02)$. For the first-order phase transition, the predicted values and standard deviations are similar to the case in which no further supervision is applied. However, for the second-order phase transition, the predicted values become more precise with smaller standard deviations.

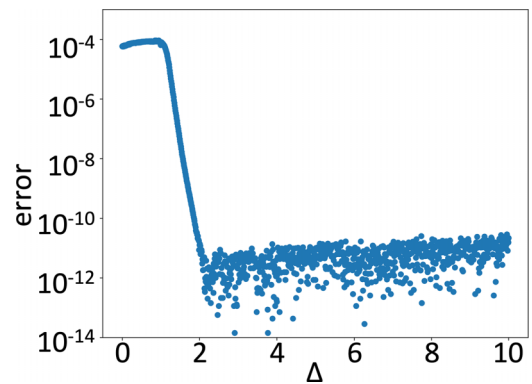


FIG. 20. The errors of the ground states of the XXZ model with various positive Δ compared with the exact solution of the Bethe ansatz.

V. DISCUSSION AND CONCLUSION

The proposed ML method of feeding the spin-spin correlation functions to predict the magnetic quantum phase transition points has shown its advantage with (supervised learning) or without (unsupervised learning) prior knowledge on the phases of matter. However, there are still several issues we would like to mention here.

(i) In the supervised learning, we only used one training point (seed) in each phase for the XY model to obtain precise phase-transition points; however, for the XXZ model, we need two points. To show the necessity of using six training points, in Figs. 19(b) and 19(c) we show the trained results of the input data as $\langle S_0^+ S_m^- \rangle$ and $\langle S_0^z S_m^z \rangle$, respectively, by using four training points, i.e., one for the AFM phase, one for the FM phase, and two for the critical phase for the sake of symmetry. The predicted phase-transition points are at the mean values of $(-1.06, 1.27)$ and $(-1.03, 1.76)$ with the standard deviations $(0.01, 0.09)$ and $(0.01, 0.08)$ for the input data as $\langle S_0^+ S_m^- \rangle$ and $\langle S_0^z S_m^z \rangle$, respectively. The predicted TPs are on the same level as those of six training points for the first-order phase-transition point at $\Delta_c = -1$, however they are less precise for the second-order phase transition at $\Delta_c = 1$.

The basic reason behind this difference can be understood as follows. For the XY model, we can adjust the accuracy uniformly down to 10^{-16} by using Romberg integrations; however, for the XXZ model, the precision controlling is much more difficult. Figure 20 shows the errors of the ground-state energy by using iDMRG with the number of the bond dimension $m_b = 100$ compared with the exact solutions of the Bethe ansatz from $\Delta = 0$ to 10. In the critical regime, the errors are about 10^{-4} , and then it drops quickly to 10^{-12} from $\Delta = 1$ to 2. In other words, the training data that we calculate around the most confident point in SA have precision up to 10^{-12} ; however, around the critical points the errors increase to 10^{-4} . It turns out that the information around the most confident point cannot sufficiently represent that around the critical point. Therefore, we need an extra training point (seed) near the second-order phase-transition point. After the calculation, we found that $\Delta = 1.536$ is just the point with a cutoff precision, 10^{-8} , which can then be an appropriate extra seed around the critical TP. We have to check that the cutoff

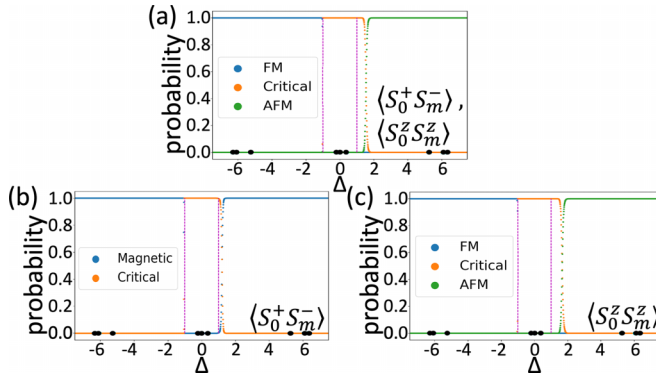


FIG. 21. In the last step of the unsupervised learning working protocol, we use supervised learning to improve the precision of the predicted critical points. Here we show the supervised learning results with only nine training seeds (gray dots), including the most confident points of the three datasets using different correlation functions as the inputs, respectively. Note that the extra seed related to the numerical cutoff precision is not included. For the first-order phase transition, the critical points remain intact, while for the second-order phase transition the results are worse than those by using nine training seeds plus the extra seed corresponding to the numerical cutoff precision (a total of 10 seeds).

point we obtained is on the right-hand side of the minimum within silhouette values around $\Delta_c = 1$ in Fig. 18(a), because SA provides a suggestion where the approximated critical point could be. And this is precisely the case we encountered here. If it lies on the left-hand side of the minimum, however, we should decrease our cutoff precision instead.

In unsupervised learning, we establish a way of finding training points (seeds) for the XXZ model. For the AFM and the critical phases, we choose the three most confident points according to silhouette values in the cases when the input data are both correlations, $\langle S_0^+ S_m^- \rangle$ and $\langle S_0^z S_m^z \rangle$, respectively. In the FM phase, we choose the mirror reflecting points of those in the AFM phase. In Fig. 21 we show the training results of supervised learning using nine training seeds. The TPs we obtain are at the mean values, $(-1.03, 1.54)$, $(-1.05, 1.18)$, and $(-1.02, 1.72)$, with the standard derivations $(0.01, 0.09)$, $(0.02, 0.11)$, and $(0.01, 0.08)$ corresponding to Figs. 21(a), 21(b) and 21(c), respectively. For easy comparison, the results with both 10 and 9 training seeds are listed in Table III. We can see that the results for the second-order phase transitions are worse than those where we add an extra seed representing the cutoff property, whereas for the first-order phase transition the results remain mostly unchanged. This suggests that we truly need the cutoff point to be a reference to fix the precision of the predicted phase boundary.

TABLE III. Comparison of the predicted critical points obtained by using 9 and 10 training seeds.

	$\langle S_0^z S_m^z \rangle, \langle S_0^+ S_m^- \rangle$		$\langle S_0^z S_m^z \rangle$		$\langle S_0^+ S_m^- \rangle$	
	Δ_c^1	Δ_c^2	Δ_c^1	Δ_c^2	Δ_c^1	Δ_c^2
9 seeds	-1.03	1.54	-1.02	1.72	-1.05	1.18
10 seeds	-1.03	1.19	-1.02	1.28	-1.05	1.02

(ii) For the XY model, $\rho_{xx}(m)$ for $m \approx \infty$ is significantly large in the PM phase, and so is $\rho_{zz}(m)$ in the FM phase. They are defined as relevant correlations for the corresponding phases. Similarly, for the XXZ model, $\langle S_0^+ S_m^- \rangle$ is relevant in the critical phase only, whereas $\langle S_0^z S_m^z \rangle$ is relevant in both the FM and AFM phases.

To distinguish whether correlations are relevant or irrelevant has its advantages. The relevant correlations can be used to find the phase boundaries between their corresponding phases and their neighbored phases. For instance, since $\rho_{xx}(m)$ is relevant for the PM phase, it can easily be used to find the TP between PM and FM. Likewise $\rho_{zz}(m)$ can also be used to find the phase boundary.

In contrast to the XY model, for the XXZ model the situation is more complicated. In unsupervised learning, $\langle S_0^+ S_m^- \rangle$ can find two phase boundaries: one is between the AFM and critical phases, and the other is between the critical and FM phases. However, by the clustering algorithm, they can only be grouped to two clusters. This is because the $\langle S_0^+ S_m^- \rangle$ is only relevant for the critical phase, but irrelevant in both FM and AFM phases. Therefore, the machine cannot distinguish the behaviors between the FM and AFM phases and can only differentiate the critical phase from the magnetic one.

On the other hand, there exist three clusters when $\langle S_0^z S_m^z \rangle$ correlations are used as input data. The reason is obvious: though $\langle S_0^z S_m^z \rangle$ are relevant for both FM and AFM phases, their behaviors are totally different. Therefore, the machine is not confused between them. As a result, three phases are distinguished out of the training model, i.e., two relevant phases and one irrelevant phase.

Before further discussing the XXZ model, one interesting point is worth mentioning here. Though $\rho_{yy}(m)$ is irrelevant for both PM and FM phases, by using this kind of input data it can still find the phase boundary. The reason is that the machine finds the different pattern of the correlations: In the PM phase, $\rho_{yy}(m)$ has a positive-negative oscillation for small m , while in the FM phase it remains positive. Therefore, even though the correlations are irrelevant, they could sometimes be used to distinguish the phases if the correlation patterns are different.

(iii) In the XXZ model there exist both first- and second-order phase transitions. This fact allows us to investigate the differences of the training processes and their outcomes.

First of all, the biggest difference lies in the feature maps (2D latent representation). In Fig. 17(c), where the correlation functions $\langle S_0^z S_m^z \rangle$ are used as input data, the blue dots represent the points in the FM phase. It is obvious that those points are separated from the other orange (critical phase) and green (AFM phase) lines, which are continuously connected (in principle). That means that the first-order phase transition from the FM to the critical phase is characterized by two discontinuous clusters, whereas the second-order phase transition features two continuous lines. This is analogous to the behavior of order parameters in higher dimensions. In higher dimension (quantum criticality in dimensions higher than two, or classical criticality in dimensions higher than three), the local order parameter changes discontinuously across the first-order critical point while continuously across the second-order one. However, in one dimension, there exists no symmetry breaking according to the Mermin-Wagner

theorem, and thus the local order parameters are all zero in all phases. One can use the correlation functions instead of the local order parameters to find the phase-transition points. By using the unsupervised (deep) learning, it is first found in this paper that the cluster points of the feature maps (2D latent representation) represent the same characteristic as the local order parameters if the relevant correlation functions are used as input data. This is highly interesting and deserves further investigations in the near future.

Additionally, we observe that by using supervised learning or unsupervised learning, the first-order phase transition is relatively easier to predict, whereas it is difficult to find the second-order phase transition when correlation functions are used as input data. This is because the gaps in the FM phase are all similarly large with various Δ , and suddenly drop to zero across the phase boundary to the other phase. For the machine, it is easily trained to distinguish between their differences. However, for the second-order phase transition, the gap opens very slowly. Therefore, the correlation functions are all similar across the phase boundary. Especially when the results are not so precise, the machine can be confused very easily, resulting in a large error of the predicted second-order phase boundary. In particular, that is also why we need an extra training seed related to the cutoff point of iDMRG to improve the precision of the predicted second-order TP.

(iv) The silhouette values also reveal some special features for the phase transitions. For instance, in the XXZ model, Fig. 18 shows that the silhouette values of the data in the FM phase are almost the same, i.e., all of them can be the most confident points. On the other hand, for the critical and AFM phases, silhouette values have a wide range of difference.

For the XY model, $h = 2$ is a second-order phase transition from the PM to FM phase, whose behavior, as shown in Fig. 14, is similar to that of the second-order phase transition at $\Delta = 1$ in the XXZ model (see Fig. 18). Therefore, we can infer that for the second-order phase transition, because of the slow gap opening, the silhouette value climbs from a small value to a constant one. This would be in sharp contrast to the case of the first-order phase transition. Since the gap here closes very abruptly, those gapped states in the FM phase would have almost the same silhouette value.

Another interesting feature of SA is that the minima of silhouette values are not far away from the phase-transition points. For the XXZ model, the minimum of the silhouette values near the FM to the critical phase lies almost exactly at the critical point $\Delta = 1$, whereas for the second-order phase transition, the minima, which are at $\Delta = 1.41$, 1.12, and 1.70 in Figs. 18(a), 18(b) and 19(c), respectively, do not lie exactly at the critical points. This also characterizes the difference between the first- and second-order phase transitions.

(v) Finally, we aim to present a rule of thumb for optimizing the utilization of ML in the study of phase transitions. When considering accuracy and the phase space defined by model parameters, it is advised that if the system is anticipated to exhibit only one or two phase transitions influenced by a single relevant model parameter, direct scanning of the phase space using experimental probes or the other numerical methods may yield superior accuracy and efficiency. Conversely, if the system is expected to possess a complex phase diagram resulting from multiple relevant model parameters, conventional

approaches may encounter challenges in analysis, making ML techniques the most advantageous choice.

To conclude, we use spin-spin correlation functions as input data to feed into machines in either a supervised or an unsupervised way of ML to find the phase-transition points of the XY and XXZ models. The results show sharp boundaries and good precision to the exact values. Particularly in the unsupervised learning, the obtained latent representation (feature map) after dimension reduction and silhouette values, which we have proposed in our previous work, provides insightful signatures of first-order and second-order phase transitions. We also show the importance of relevant correlation functions, which can be used as input data to find the phase boundaries between their corresponding phases and the neighbored ones. This concept is quite useful when the systems are more complicated and the phase boundaries have no exact solutions. What we have to do in such systems is to find out their relevant correlation functions and hence use them to find the phase boundaries.

ACKNOWLEDGMENTS

M.-C.C. acknowledges the NSTC support under Contract No. 111-2112-M-005-013 and the Asian Office of Aerospace Research and Development (AOARD) for support under Award No. FA2386-20-1-4049. I.P.M. acknowledges support from the Australian Research Council (ARC) Discovery Project Grant No. DP200103760.

APPENDIX A: CORRELATION MATRICES OF XY MODELS

To obtain ρ_{xx} , ρ_{yy} , and ρ_{zz} we follow Lieb, Schultz, and Mattis [55]. In fact,

$$\rho_{xx}(l-m) = \langle \Psi_0 | (\sigma_l^+ + \sigma_l^-) (\sigma_m^+ + \sigma_m^-) | \Psi_m \rangle. \quad (\text{A1})$$

Through the Jordan-Wigner transformation, Eq. (2), we obtain

$$\rho_{xx}(l-m) = \langle \Psi_0 | (c_l^\dagger - c_l) \exp \left(i\pi \sum_{k=l+1}^{m-1} c_k^\dagger c_k \right) (c_m^\dagger + c_m) | \Psi_0 \rangle. \quad (\text{A2})$$

By using the fact that

$$\exp(i\pi c_k^\dagger c_k) = (c_k^\dagger + c_k)(c_k^\dagger - c_k), \quad (\text{A3})$$

we end up with the equation

$$\rho_{xx}(l-m) = \langle \Psi_0 | B_l A_{l+1} B_{l+1} \cdots A_{m-1} B_{m-1} A_m | \Psi_0 \rangle, \quad (\text{A4})$$

where $A_k = c_k^\dagger + c_k$ and $B_k = c_k^\dagger - c_k$. We hence perform Wick's theorem [66] to obtain ρ_{xx} in Eq. (6).

It is also similar for ρ_{yy} . $\rho_{yy}(l-m)$ has the following form:

$$\rho_{yy}(l-m) = \langle \Psi_0 | (\sigma_l^+ - \sigma_l^-) (\sigma_m^+ - \sigma_m^-) | \Psi_m \rangle, \quad (\text{A5})$$

which can be Jordan-Wigner-transformed to

$$\rho_{yy}(l-m) = (-1)^{l-m} \langle \Psi_0 | A_l B_{l+1} A_{l+1} \cdots B_{m-1} A_{m-1} B_m | \Psi_0 \rangle, \quad (\text{A6})$$

with the help of the equation

$$\exp(i\pi c_k^\dagger c_k) = -(c_k^\dagger - c_k)(c_k^\dagger + c_k). \quad (\text{A7})$$

TABLE IV. Model architecture of AE used for Figs. 10–13. Note that $c = 3$ when using all ρ_{xx} , ρ_{yy} , ρ_{zz} together as the input data, while $c = 1$ when using ρ_{xx} , ρ_{yy} , or ρ_{zz} , respectively, as the input data. Moreover, “features” in the parameters column indicates the number of neurons in the middlemost layer of AE, n_{mid} .

Layer	Parameters	Activation
	Input: $c \times 20 \times 20$	
Conv.	$16 \times 3 \times 3$	ReLU
Linear	$c \times 6400 \times 512$	ReLU
Linear	512×256	ReLU
Linear	256×128	ReLU
Linear	128×64	ReLU
Linear	$64 \times \text{features}$	ReLU
Linear	$\text{features} \times 64$	ReLU
Linear	64×128	ReLU
Linear	128×256	ReLU
Linear	256×512	ReLU
Transposed conv.	$c \times 3 \times 3$	Sigmoid

After we make use of Wick’s theorem, ρ_{yy} is expressed as Eq. (7).

Finally $\rho_{zz}(l - m)$ has the form

$$\rho_{zz} = \langle \Psi_0 | (2\sigma_l^+ \sigma_l^- - 1)(2\sigma_m^+ \sigma_m^- - 1) | \Psi_m \rangle. \quad (\text{A8})$$

To obtain ρ_{zz} , we have to use the identity

$$\begin{aligned} 2\sigma_k^+ \sigma_k^- - 1 &= -(\sigma_k^+ + \sigma_k^-)(\sigma_k^+ - \sigma_k^-) \\ &= -(c_k^\dagger + c_k)(c_k^\dagger - c_k), \end{aligned} \quad (\text{A9})$$

and thus we have

$$\rho_{zz}(l - m) = \langle \Psi_0 | A_l B_l A_m B_m | \Psi_m \rangle. \quad (\text{A10})$$

After we make use of Wick’s theorem, the result becomes Eq. (8).

To calculate G_{l-m} , we have to transform H_{XY} into the momentum space as $H_{XY} - Nh/2 = \sum_k \mathbf{c}_k^\dagger H(k) \mathbf{c}_k$ with the notation $\mathbf{c}_k^\dagger = (c_k, c_{-k}^\dagger)^T$ as the Nambu particle-hole basis and

$$H(k) = \mathbf{R} \cdot \sigma, \quad (\text{A11})$$

where $\mathbf{R} = (0, -\gamma \sin k, \cos k + h/2)^T$ and $\sigma = (\sigma_1, \sigma_2, \sigma_3)^T$ as a vector composed of three Pauli matrices. By using this notation, one can calculate first the correlation function in the momentum space,

$$G(k) \equiv \langle \mathbf{c}_k \mathbf{c}_k^\dagger \rangle, \quad (\text{A12})$$

TABLE V. Model architecture of AE used for Figs. 15–17. Note that $c = 2$ when using both $\langle S_0^z S_m^z \rangle$ and $\langle S_0^+ S_m^- \rangle$ as the input data, while $c = 1$ when using $\langle S_0^z S_m^z \rangle$ or $\langle S_0^+ S_m^- \rangle$, respectively, as the input data. Moreover, “features” in the parameters column indicates the number of neurons in the middlemost layer of AE, n_{mid} .

Layer	Parameters	Activation
	Input: $c \times 40 \times 40$	
Conv.	$16 \times 3 \times 3$	ReLU
Linear	51200×512	ReLU
Linear	512×256	ReLU
Linear	256×128	ReLU
Linear	128×64	ReLU
Linear	$64 \times \text{features}$	ReLU
Linear	$\text{features} \times 64$	ReLU
Linear	64×128	ReLU
Linear	128×256	ReLU
Linear	256×512	ReLU
Transposed conv.	$c \times 3 \times 3$	Sigmoid

where $\langle \dots \rangle$ denotes the expectation values of the ground state, $\langle \Psi_0 | \dots | \Psi_0 \rangle$. After some straightforward algebra, we obtain

$$G(k) = \frac{1}{2} \left(1 + \frac{\mathbf{R} \cdot \sigma}{R} \right), \quad (\text{A13})$$

with the definition $R \equiv |\mathbf{R}| = \sqrt{(\cos k + h/2)^2 + \gamma^2 \sin^2 k}$. Finally, through the relation

$$\begin{aligned} \langle B_l A_m \rangle &= \frac{1}{L} \sum_k e^{-ik(r_l - r_m)} \langle c_k^\dagger c_{-k}^\dagger \rangle \\ &\quad - \langle c_k c_{-k} \rangle - \langle c_k c_k^\dagger \rangle + \langle c_{-k}^\dagger c_{-k} \rangle, \end{aligned} \quad (\text{A14})$$

and using Eq. (A13), we obtain Eq. (9).

APPENDIX B: MODEL ARCHITECTURES

Here we present explicit neural network architectures for our numerical results shown in Secs. IV B and V. In the case of the XY model, for the AE used for Figs. 10–13, the model architecture is given in Table IV.

As for fine-tuning the phase boundaries via supervised learning, additional CNN models are employed with the same architectures shown in Figs. 4(a) and 4(b). On the other hand, in the case of the XXZ model, the architecture of AE used for Figs. 15–17 is given in Table V.

Similarly, CNN models are employed to fine-tune the phase boundaries via supervised learning. They basically have the same architectures shown in Figs. 4(c) and 4(d), except that the number of neurons in the output layer, n , now should be determined by the outcome of K -means clustering analysis.

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