Learning Quantum Phases by Visualization

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Identifying quantum phases of interacting many-body systems is key to understand the emergent phenomena in condensed matter physics. However, such tasks are often extremely challenging due to the exponentially large dimensionality of the associated Hilbert space. Conventional practices usually require the order parameters to specify the quantum states. In this work, we propose a different strategy to access quantum phases by visualization based on the distribution of ground states in Hilbert space. By mapping the quantum states in Hilbert space onto a two-dimensional feature space using an unsupervised nonlinear dimensionality reduction method, the quantum states can be explicitly visualized, from which distinct phases can be easily specified and the phase transition point can be well identified. Our scheme is benchmarked on the phases of several strongly correlated spin systems, including gapped, critical, and topological phases. As our strategy directly learns the quantum phases and phase transitions from the distributions of the quantum states, it does not depend on priori knowledge of order parameters or any other specific physical properties of the quantum systems. This work indicates a highly perceptual route to identify quantum phases and phase transitions particularly in the complex systems of condensed matter by visualization through learning.

I. INTRODUCTION

Studying quantum phases and phase transitions in many-body systems belongs to the most challenging topics in contemporary physics. The characterization of quantum phases within Landau paradigm [1, 2] often requires certain prior knowledge of the order parameters. For the phases beyond the Landau paradigm [3, 4], the main challenge is how to find proper “order parameters” that might be nonlocal or could not be represented by any observables to characterize the quantum phases [5–7].

While the common approaches usually rely on the priori knowledge and human wisdom, machine learning (ML) provides an alternative way to solve the given problem by training a ML model based on certain relevant data. For instance, the artificial neural network is capable of identifying the quantum phases by learning certain given states [8–13] or extracting physical concepts from the observed data [14].

In this work, we propose a different route to access the physical information of quantum phases of many-body systems by probing the ground state (GS) manifolds distributed in Hilbert space (denoted as $\mathcal{H}$). However, it is extremely difficult to probe the GS distributions in $\mathcal{H}$ since the dimensionality of $\mathcal{H}$ space spanned by quantum many-body states is exponentially large. To overcome this difficulty, we apply the unsupervised nonlinear dimensionality reduction (DR) scheme [15–17] known as $t$-distributed stochastic neighbor embedding ($t$-SNE) [18, 19] to map the quantum many-body states from $\mathcal{H}$ to a two-dimensional (2D) feature space (denoted as $\mathcal{R}^2$). Such a DR map is optimized by maximizing the similarity between the GS distributions in $\mathcal{H}$ and in $\mathcal{R}^2$ stochastically. In other words, the GS distributions in $\mathcal{H}$ are optimally demonstrated by those in $\mathcal{R}^2$. By simply viewing the distribution in $\mathcal{R}^2$ by naked eyes or employing

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classical algorithms such as $k$-means [20], we show that the ground states can be readily classified to the correct phases and the critical points can be reliably determined. Our proposal is benchmarked on the one-dimensional (1D) quantum lattice models, where we visualize that the quantum states in various phases (including gapped, critical, and topological phases) cluster into different patterns in $\mathbb{R}^2$, and the phase transitions can be directly specified. Different from the conventional approaches in many-body physics where one usually focuses on the order parameters, entanglements and so on of the states, our work paves a new way by viewing quantum phases from the mutual distances of the states therein, which we expect to be closely associated with the fundamental information of the GS manifold. This present proposal works well not only for quantum data like quantum states but also for classical data like image classification.

II. QUANTUM PHASE VISUALIZATION

Consider a quantum Hamiltonian $\hat{H}(\alpha)$ with $\alpha$ a physical parameter (e.g., a coupling constant or magnetic field), where we suppose a phase transition occurs at $\alpha = \alpha_c$. When $\alpha$ changes continuously, the GS’s (denoted as $|\psi^{\alpha}\rangle$) form a manifold in the Hilbert space $\mathcal{H}$. To proceed, we sample $N$ states by taking different values of $\alpha$. These quantum states are distributed within the manifold.

To visualize the distribution of certain given GS’s $\{ |\psi^{\alpha}\rangle \}$, we invoke the recipe of t-SNE and map the states to the vectors $\{ y^{\alpha} \}$ living in a two-dimensional feature space $\mathbb{R}^2$, i.e., $|\psi^{\alpha}\rangle \rightarrow y^{\alpha}$ with $y^{\alpha} = [y_1^{\alpha}, y_2^{\alpha}]$ a two-component vector and $f$ a nonlinear map from $\mathcal{H}$ to $\mathbb{R}^2$ (Fig. 1). To be specific, we start from $N$ given states $\{ |\psi^{\alpha}\rangle \}$ and define the joint probability distributions $\{ P(D_{\alpha,\alpha'}^{\mathcal{H}}) \}$ based on the distances $D_{\alpha,\alpha'}^{\mathcal{H}}$ between any two of the states $|\psi^{\alpha}\rangle$ and $|\psi^{\alpha'}\rangle$. Then, we randomly initialize $N$ vectors $\{ y^{\alpha} \}$ in $\mathbb{R}^2$ and define the joint probability distributions $\{ P(D_{\alpha,\alpha'}^{\mathcal{R}}) \}$ based on the distances $D_{\alpha,\alpha'}^{\mathcal{R}}$ between any two of the $\{ y^{\alpha} \}$. Note that the measure of distance in each space can be chosen flexibly. We choose the negative logarithmic fidelity (NLF) [21, 22]

$$D_{\alpha,\alpha'}^{\mathcal{H}} = -\log(|\langle \psi^{\alpha}|\psi^{\alpha'}\rangle|)$$

(1)

to measure the distance between two GS’s in $\mathcal{H}$.

To capture the distribution of $\{ |\psi^{\alpha}\rangle \}$ by that of $\{ y^{\alpha} \}$, we directly optimize $\{ y^{\alpha} \}$ so that the difference between two probability distributions $\{ P(D_{\alpha,\alpha'}^{\mathcal{H}}) \}$ and $\{ P(D_{\alpha,\alpha'}^{\mathcal{R}}) \}$ (averaging over all possible pairs) is minimized. The DR map is left implicit. Consequently, the converged vectors $\{ y^{\alpha} \}$ represent the quantum states $\{ |\psi^{\alpha}\rangle \}$ in the 2D feature space of reduced dimensionality. The specific details of visualization of quantum states through t-SNE can be found in Methods.

III. METHODS

The central idea of our scheme is to visualize the quantum states by reducing the dimensionality of the exponentially large Hilbert space spanned by the quantum states to two using the t-SNE. The t-SNE is a nonlinear DR method that has been widely used in machine learning to visualize high-dimensional data [19]. Given the data in a high-dimensional space (e.g., the GS’s $\{ |\psi^{\alpha}\rangle \}$ in the Hilbert space $\mathcal{H}$), one can define the joint probability for each pair of the data $(|\psi^{\alpha}\rangle$ and $|\psi^{\alpha'}\rangle)$ as

$$P(D_{\alpha,\alpha'}^{\mathcal{H}}) = \frac{P(\alpha|\alpha')+P(\alpha'|\alpha)}{2N}$$

(2)

where $N$ is the number of states and the conditional probability is defined by the distances as

$$P(\alpha|\alpha') = \frac{\exp[-(D_{\alpha,\alpha'}^{\mathcal{H}})^2/2\sigma_\alpha^2]}{\sum_{\beta\neq\alpha}\exp[-(D_{\alpha,\beta}^{\mathcal{H}})^2/2\sigma_\alpha^2]}$$

(3)

with $\{ \sigma_\alpha \}$ the hyper-parameters in t-SNE. One usually does not directly control $\{ \sigma_\alpha \}$ but define a quantity named as perplexity $P$. Given $P$, one can perform the binary search to determine $\{ \sigma_\alpha \}$ that satisfy

$$\log_2 P = -\sum_{\alpha'} P(\alpha'|\alpha) \log_2 P(\alpha|\alpha')$$

(4)

The perplexity controls how non-locally that one state is related to others in the joint probability distributions. Previous works show that the t-SNE is fairly robust to the changes of the perplexity [23]. More results are provided in the Appendix B to show the robustness of phase visualization with different perplexities.

To map $\{ |\psi^{\alpha}\rangle \}$ onto $\{ y^{\alpha} \}$ in $\mathbb{R}^2$, one can randomly initialize $\{ y^{\alpha} \}$ and define the joint probabilities $\{ P(D_{\alpha,\alpha'}^{\mathcal{R}}) \}$ as the Student $t$-distribution [19]

$$P(D_{\alpha,\alpha'}^{\mathcal{R}}) = \frac{[1+(D_{\alpha,\alpha'}^{\mathcal{R}})^2]^{-1}}{\sum_{\beta\neq\alpha}[1+(D_{\alpha,\beta}^{\mathcal{R}})^2]^{-1}}$$

(5)

where the measure of the distances in $\mathbb{R}^2$ is chosen to be the Euclidean distances $D_{\alpha,\alpha'}^{\mathcal{R}} = |y^{\alpha} - y^{\alpha'}|$. To capture $\{ |\psi^{\alpha}\rangle \}$ by $\{ y^{\alpha} \}$, the strategy of t-SNE is to optimize $\{ y^{\alpha} \}$ by minimizing the Kullback-Leibler (KL) divergence [24] between $\{ P(D_{\alpha,\alpha'}^{\mathcal{H}}) \}$ and $\{ P(D_{\alpha,\alpha'}^{\mathcal{R}}) \}$.

The KL divergence is defined as

$$\text{KL}(\mathcal{H}, \mathbb{R}^2) = \sum_{\alpha\alpha'} P(D_{\alpha,\alpha'}^{\mathcal{H}}) \log \frac{P(D_{\alpha,\alpha'}^{\mathcal{H}})}{P(D_{\alpha,\alpha'}^{\mathcal{R}})}.$$ 

(6)

The gradients by varying $y^{\alpha}$ are given by

$$\frac{\delta\text{KL}(\mathcal{H}, \mathbb{R}^2)}{\delta y^{\alpha}} = 4 \sum_{\alpha'} \frac{(P(D_{\alpha,\alpha'}^{\mathcal{H}}) - P(D_{\alpha,\alpha'}^{\mathcal{R}})) (y^{\alpha} - y^{\alpha'})}{1+(D_{\alpha,\alpha'}^{\mathcal{R}})^2}.$$ 

(7)

One may use a gradient-descent approach to minimize $\text{KL}(\mathcal{H}, \mathbb{R}^2)$. The converged $y^{\alpha}$ are considered as the embedding of $\psi^{\alpha}$ in $\mathbb{R}^2$ where the mutual distances among $\{ |\psi^{\alpha}\rangle \} \in \mathcal{H}$ are optimally retained by $y^{\alpha}$.
IV. RESULTS

We firstly examine our proposal on the 1D transverse field Ising model (TFIM) [25], where the Hamiltonian reads $H(h_x) = \sum_i \hat{S}_i^z \hat{S}_{i+1}^z - h_x \sum_i \hat{S}_i^x$, where $\hat{S}_i^z$ and $\hat{S}_i^x$ stand for the z- and x-component spin operators, respectively, and $h_x$ is the transverse field. It has been rigorously shown that a Landau-type quantum phase transition occurs at the critical field $h_{x_c} = 0.5$, which separates the antiferromagnetic (AFM) and polarized ferromagnetic (FM) phases. We employ the density matrix renormalization group (DMRG) [26] to calculate the GS’s for different transverse fields in the form of matrix product states (MPS) [27–30]. The visualizations of quantum phases of the 1D TFIM using three distinct schemes (i.e., t-SNE, PCA and t-SNE with NLF) are presented in Fig. 2.

In Fig. 2 a, we choose the distance between two GS’s as the Euclidean distance $D_{\alpha,\alpha'} = ||\psi_{\alpha} - \psi_{\alpha'}||$ for comparison, where the vector $\psi_{\alpha}$ is simply formed by all the variational parameters in the corresponding MPS (i.e. all tensor elements). The t-SNE is used to reduce the dimensionality from $N$ to 2 with $N$ the total number of tensor elements in the MPS. We adopt the canonical form [31] to fix the gauge degrees of freedom of the MPS. It is known that MPS can give an efficient parametrization of the exponentially-large number of GS’s of the Hamiltonian under study, where $N$ scales only linearly with the system size [32]. However, our results show that the states after DR are mixed up in $R^2$. It suggests that such a parametrization may not reflect well the quantum state distribution in $\mathcal{H}$.

In Fig. 2 b, we pick the bipartite entanglement spectra (ES) $s^\alpha$ of the GS’s as the input data, which is $\chi$-dimensional with $\chi$ the dimension cut-off in DMRG. Then these ES are mapped onto $R^2$ by means of principal component analysis (PCA) [33]. Different from the t-SNE, the PCA uses a linear transformation for DR and obtains the two components in $R^2$ that optimally retain the covariances of the data in $\mathcal{H}$. The states from the two phases form a 1D stream in $R^2$ with a break corresponding to the region near the transition point. Our results by PCA are consistent with those on the Kitaev chain [12]. As indicated in Fig. 2 b, it is not easy to identify the critical point from the distribution of ES with reduced dimensionality by PCA.

Fig. 2 c demonstrates the results using our proposal, in which the t-SNE is applied to reduce nonlinearly the dimensionality based on the NLF’s [Eq. (1)] between any two GS’s in $\mathcal{H}$. It is obvious that the states inside the AFM and FM phases cluster, and the distribution in $R^2$ exhibits an “hourglass” pattern formed by two oval regions. The critical point between the AFM and FM phases can be easily identified by naked eyes (or by unsupervised learning methods; see Appendix A) where the two ovals touch each other. This result indicates that the NLF is a more proper choice for measuring the distance between two GS’s in reducing the dimensionality of the GS’s by t-SNE. The convergence and robustness against small noises of the t-SNE with NLF for the visualization of quantum states and phase transitions as well as for the classical data are presented in Appendix C.
To further demonstrate the “hourglass” pattern and the identification of phase transitions by our proposal, we turn to the spin-1 antiferromagnetic Heisenberg uniform chain in a magnetic field \( h_z \), where the Hamiltonian reads
\[
\hat{H}(h_z) = \sum_i \sum_{x,y,z} \hat{S}_i^x \hat{S}_{i+1}^x - h_z \sum_i \hat{S}_i^z.
\]
For \( h_z < h_c \) with the transition point \( h_c \approx 0.414 \), the system is in a topological phase known as Haldane phase [34–36] with non-trivial boundary excitations and long-range string orders [37–39]. For \( h_z > h_c \), the spin gap is closed by the magnetic filed, and the system enters a topologically trivial magnetic (TTM) phase. As shown in Fig. 3, an “hourglass”-like distribution emerges, where the Haldane phase and TTM phase are obviously separated.

The touching point of the two oval clusters appears at \( h_z = 0.42 \) (note \( h_z \) is discretized with the interval \( \delta h = 0.01 \)), indicating the critical magnetic field. The estimated critical field by the touching point is slightly higher than expected, possibly due to the finite-size effects that tend to increase the gap (here we take the system size \( L = 128 \) in DMRG).

Fig. 3 b shows the parttern formed by the GS’s of the spin-1 Heisenberg AFM model on zigzag chain with nearest neighboring (NN) and next-nearest neighboring (NNN) couplings \( \hat{H}(J_1, J_2) = \sum_i \sum_{x,y,z} (J_1 \hat{S}_i^x \hat{S}_{i+1}^x + J_2 \hat{S}_i^x \hat{S}_{i+2}^x) \), where \( J_1 \) and \( J_2 \) denotes the strength of the NN and NNN couplings, respectively. Such a system is frustrated [40] as there is a competition between two kinds of resonating valence bond configurations, of which both possess non-trivial topological properties. A quantum phase transition occurs at \( (J_2/J_1)_{c} \approx 0.744 \) [41, 42], where the system is in the Haldane phase and the NNN Haldane phase on two sides of the critical point. Again, an “hourglass” pattern emerges, where the two phases cluster in two oval areas. The touching point with \( J_2/J_1 = 0.745 \) (the interval of the discretization step \( \delta(J_2/J_1) = 0.005 \)) accurately identifies the transition point.

Determining the critical points of more than two phases is challenging with the existing machine-learning-based methods as confusion [12]. We consider the 1D spin-\( \frac{1}{2} \) anisotropic XXZ model \( \hat{H} = \sum_i (\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y) + \Delta \sum_i \hat{S}_i^z \hat{S}_{i+1}^z \) with \( \Delta \) representing the magnetic anisotropy. This system possesses three phases, say the FM (\( \Delta < -1 \)), XY (\( -1 < \Delta < 1 \)), and AFM phases (\( \Delta > 1 \)) [43].

Fig. 4 a shows the visualiztion of the quantum phases of this model in the space spanned by feature 1, feature 2, and the anisotropy parameter \( \Delta \). The expected transition points \( \Delta = -1 \) and \( \Delta = 1 \) are indicated by two semitransparent planes. While the states in the FM or AFM phase cluster within the two oval regions of \( R^2 \) [see Fig. 4 b], the states in the XY phase form a 1D stream. The phase transition points can be accurately identified as the end points of this stream, which touch on the \( \Delta = 1 \) and \( -1 \) planes, respectively.

V. DISCUSSION AND CONCLUSION

Our results show that the states in the XY phase, which are critical and can be described by the conformal field theory with central charge \( c = 1 \), form a 1D stream in \( R^2 \). In contrast, the non-critical phases (the FM/AFM and gapped topological phases) exhibit oval clusters. To explain the cause of different patterns of the distributions given by the critical and non-critical phases,
we propose the following intuitive arguments. As the distance of two states (in both $\mathcal{H}$ and $\mathcal{R}^2$) is positively associated with the difference of their physical quantities (e.g., magnetizations, correlations, entanglement spectrum, etc.), the states within each phase should cluster because they share similar physics and thus should have small distances between each other.

The physics of the states within the gapped phase are almost identical. The distances among the states within each phase are insignificant. Even the energy levels do cross due to finite-size effects or numerical errors, the differences of the physics for these states should be minor. Therefore, the quantum states are expected to cluster in a small region in $\mathcal{R}^2$. The situations for the gapless but non-critical phases are similar. Take the polarized phase in TFIM as an example. For different $h_x$’s with $h_x > 0.5$, the distances among the states are more minor than the distances between the states in different phases. In the vicinity of the critical point, the gap gradually closes, and the energy levels become dense, implying that the physical properties change more drastically as the physical parameter alters. Consequently, the distances between the quantum states with different parameters become more significant in this region than those within the non-critical phases.

When two non-critical phases are separated by a critical phase instead of a critical point, the distances of the states within the critical phase should be more significant than those within the non-critical phases. This leads to the distribution of the GS’s of XXZ model (Fig. 4) in the critical phase forms a 1D stream in $\mathcal{R}^2$.

In summary, we propose a scheme to visualize quantum phases and to identify phase transition points via machine learning. The key idea is to map the quantum states in the Hilbert space $\mathcal{H}$ where the state distribution is difficult to access, onto the 2D feature space $\mathcal{R}^2$ by the nonlinear DR method $t$-SNE, where the negative logarithmic fidelity is adopted to measure the distances between different quantum states. It is found that the distribution in $\mathcal{R}^2$ exhibits different patterns for distinct phases, from which the phase transition points can be readily identified. The success of this proposal is demonstrated on a few of 1D quantum many-body models, including those with the conventional phases within Landau paradigm, the topological phases with nonlocal orders, and the critical phase described by CFT. This present strategy for visualization through learning works well not only for the quantum data but also for the classical data.

While our scheme of visualizing quantum phases via learning are flexible and general, more rigorous and robust relations between the distributions in $\mathcal{R}^2$ and the physical properties of the quantum phases (e.g., criticality and topology) space are to be established. As a nonlinear DR method, the $t$-SNE works as a “black box” which guarantees the minimization of the KL-divergence in a variational sense (see Methods), but it is unknown how to interpret it, for instance, what the two features ($y_1$ and $y_2$ in $\mathcal{R}^2$) stand for. This would motivate people to seek for the DR methods with higher interpretability, which would assist us to unveil more novel properties of quantum many-body systems by this visualization scheme.

Our proposal can be easily generalized to $\mathcal{R}^d$ for $d \geq 3$. It can also be readily applied to interacting fermions. Other DR methods, e.g., the manifold learning algorithms [17] and those based on the probabilistic graphical models [44], can be utilized in the present proposal in order to gain better performance and higher interpretability. Towards this direction, it might eventually become possible to characterize quantum phases from the patterns of the GS manifolds via learning.

**FIG. 4.** (Color online) **Visualization for the quantum phases that including critical phase.** a The three dimensional visualization of the distinct phases in the 1D anisotropic XXZ antiferromagnetic (AFM) Heisenberg model with anisotropy $\Delta$. In addition to the two dimensions of features $y_1$ and $y_2$ of $\mathcal{R}^2$, $\Delta$ is also plotted as the third dimension for a better visualization. Two expected transition points at $\Delta = -1$ and 1 are indicated by two semitransparent planes to assist visualization. b The visualization of a in feature space $\mathcal{R}^2$. Three phases (AFM, XY and FM) are clearly visualized with different patterns in the 3D or 2D space. There are 400 ground states calculated by discretizing $\Delta$ with an interval 0.01. We take the system size $L = 120$, the dimension cut-off of DMRG $\chi = 160$, iteration steps in $t$-SNE $n_{iter} = 5000$ with the perplexity $P = 24$. The distances among the states within the gapped phase are almost identical. The distances among the states within each phase are more minor.
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Appendix A: IDENTIFYING THE VISUALIZED QUANTUM PHASES BY K-MEANS

After mapping the ground states to the two-dimensional feature space $\mathcal{R}^2$, we show that different quantum phases can be distinguished simply by naked eyes from how the quantum states are distributed in $\mathcal{R}^2$. Below, we show that one may use $k$-means algorithm [20] to classify the states based on the distributions in $\mathcal{R}^2$.

$K$-means method is an unsupervised learning algorithm and can be used to implement classification tasks. For a set of samples $\{\mathbf{y}^{\alpha}\}$, $k$-means partitions them into $K$ clusters $\{\mathcal{S}^k\}$ with $k = 1, \ldots, K$. The center of each cluster (denoted as $\mathbf{m}^k$; also called the centroids) can be defined by the samples therein as

$$\mathbf{m}^k = \frac{1}{N^k} \sum_{\mathbf{y}^{\alpha} \in \mathcal{S}^k} \mathbf{y}^{\alpha}, \quad (A1)$$

where $N^k$ is the number of samples in $\mathcal{S}^k$.

To classify $\{\mathbf{y}^{\alpha}\}$, one performs the following two steps iteratively. The first step is to assign the samples to the $K$ clusters according to the given $\{\mathbf{m}^k\}$, where any sample in a given cluster should possess the smallest Euclidean distance to the center of this cluster than to other centers. It means that the samples are divided into $K$ sets $\{\mathcal{S}^k\}$ by satisfying

$$\mathcal{S}^k = \{\mathbf{y}^{\alpha} : \|\mathbf{y}^{\alpha} - \mathbf{m}^k\| \leq \|\mathbf{y}^{\alpha} - \mathbf{m}^j\| \quad \forall j\}, \quad (A2)$$

where $\|\mathbf{y}^{\alpha} - \mathbf{m}^k\|$ represents the Euclid distance between the sample $\mathbf{y}^{\alpha}$ and the center $\mathbf{m}^k$, and $j$ goes over all centers. The second step is to update $\{\mathbf{m}^k\}$ based on the present $\{\mathcal{S}^k\}$ according to Eq. (A1). These two steps are executed iteratively until $\{\mathbf{m}^k\}$ converges.

We apply $k$-means to categorize the ground states of spin-1 antiferromagnetic Heisenberg chain into two phases ($K = 2$) after mapping those states onto $\mathcal{R}^2$ space by $t$-SNE. In Fig. A1, the numbers represent the ground states with reduced dimensionality $\{\mathbf{y}^{\alpha}\}$ in different magnetic fields $\alpha$, and the two stars represent the centers $\{\mathbf{m}^k\}$. The states divided into two clusters are marked by different colors. To begin with, one first randomly initializes the positions of the centers, with which the states are divided into two clusters according to Eq. (A2). After four steps of iterations, $\{\mathbf{m}^k\}$ converges, and the states in different phases are successfully divided to the two clusters. Fig. A1 shows how the centers converge by making use of

$$D(n_{it}) = \sum_{k} \|\mathbf{m}^k(n_{it}) - \mathbf{m}^k(n_{it} - 1)\|, \quad (A3)$$

with $\{\mathbf{m}^k(t)\}$ the centers after $t$ iterations. We find that $D(t)$ decreases almost to 0 for $n_{it} = 4$.

Though $K$ is previously known in the above example, it can also be determined automatically when one does not know how many clusters that the samples should be divided into. We refer to the silhouette coefficient (SC) [45] and Calinski-Harabasz index (CHI) [46] for this purpose. The $SC$ is defined as

$$SC = \frac{1}{J} \sum_{\alpha=1}^{J} \frac{D_{in}^\alpha - D_{out}^\alpha}{\max(D_{in}^{\alpha}, D_{out}^{\alpha})}, \quad (A4a)$$

$$D_{in}^{\alpha} = \frac{1}{N_{k(\alpha)} - 1} \sum_{\mathbf{y}^{\alpha'} \notin \mathcal{S}^{k(\alpha)}} \|\mathbf{y}^{\alpha'} - \mathbf{y}^{\alpha}\|, \quad (A4b)$$

$$D_{out}^{\alpha} = \frac{1}{N - N_{k(\alpha)}} \sum_{\mathbf{y}^{\alpha'} \notin \mathcal{S}^{k(\alpha)}} \|\mathbf{y}^{\alpha'} - \mathbf{y}^{\alpha}\|, \quad (A4c)$$

where $k(\alpha)$ represents the cluster that the $\alpha$-th data point belongs to, $D_{in}^\alpha$ ($D_{out}^\alpha$) is the average distance of sample $j$ to others in (not in) the same cluster. The value of $SC$ ranges from -1 to 1. The optimal $K$ is chosen so that $SC \rightarrow 1$ [45].

The $CHI$ is defined as [46]:

$$CHI = \frac{\text{Trace}(B)}{(K - 1)} / \frac{\text{Trace}(W)}{(J - K)}, \quad (A5a)$$

$$\text{Trace}(B) = \sum_{k=1}^{K} N^k \|\mathbf{m}^k - \mathbf{m}^0\|^2, \quad (A5b)$$

$$\text{Trace}(W) = \sum_{k=1}^{K} \sum_{\mathbf{y}^{\alpha} \in \mathcal{S}^{k(\alpha)}} \|\mathbf{y}^{\alpha} - \mathbf{m}^k\|^2. \quad (A5c)$$

$B$ is the between-cluster scatter matrix and $W$ is the within-cluster scatter matrix; $\mathbf{m}^0$ is the centroid of the whole dataset. The optimal $K$ is chosen so that $CHI$ reaches its maximum. [46].

For the grounds states of the spin $S=1$ antiferromagnetic Heisenberg uniform chain and zigzag chain. Fig. A2 shows the $SC$ and $CHI$ calculated from the distribution of the ground states in $\mathcal{R}^2$. One can see that the optimal number of clusters should be $K = 2$, consistent with the fact that there are two phases for each system. In this way, one does not need priori knowledge about either the properties of the original states or the number of phases.
Appendix B: Convergence and robustness of $t$-SNE for quantum phase visualization

Fig. A3 show in $t$-SNE, how the distribution in $R^2$ of the ground states of the transverse field Ising model converges. Remind that for $N$ given states $|\psi^\alpha\rangle$ in the Hilbert space $\mathcal{H}$, the $t$-SNE directly optimizes $y^\alpha$ in $R^2$ that are the $N$ corresponding low-dimensional vectors after reducing the dimensionality. Initially, $y^\alpha$ are randomly determined. In Fig. A3 a-e show the $y^\alpha$ after $n_{it}$ iterations with $n_{it} = 250, 300, 350, 400, 500$, respectively. One can see that after $n_{it} \approx 400$ iterations, the distribution converges, where the two quantum phases are clearly visualized. The KL divergence, which indicates the difference between the distributions of the samples in $\mathcal{H}$ and $R^2$, decays with $n_{it}$ as shown in Fig. A3 f. A GIF was provided in another file to animatedly show how the states cluster in $R^2$ as the iteration time increases [47].

From the previous works in machine learning, it is known that the visualization by $t$-SNE is robust to the perplexity $P$. Fig. A4 shows that the ground states of the transverse field Ising model (TFIM) by $t$-SNE with different perplexities form similar hourglass-like patterns. The difference of these patterns is to what extent the hourglass extends in the two-dimensional plane. This is consistent with the fact that the perplexity controls how nonlocally one state is correlated to others from the joint probability distribution. More specifically, as the dimensionality is reduced, the distribution in $R^2$ may not respect the mutual relations among the states in $\mathcal{H}$. For instance, it is possible that one has $||y^1 - y^2|| < ||y^1 - y^3||$ in $\mathcal{H}$ but $||y^1 - y^2|| > ||y^1 - y^3||$ in $R^2$. A small perplexity means that the distribution in $R^2$ should in prior satisfy the mutual relations of distances for those with small distances. Consequently in the visualization with small $P$, different clusters tend to separate apart mutually. This leads to a “thinner” hourglass than those with
larger perplexities. Note that in practice, the perplexity is usually smaller than the number of samples [19].

We also investigate the visualization of quantum phases under noises. The noisy quantum states are defined by

$$|\Psi^\alpha_\delta\rangle = \sqrt{1-\delta}|\Psi^\alpha\rangle + \sqrt{\delta}|\Psi_{\text{random}}\rangle. \quad \text{(A1)}$$

where $|\Psi^\alpha\rangle$ is the ground state in the transverse magnetic field $\alpha$, and $\delta$ is a small constant that controls the strength of the noise. $|\Psi_{\text{random}}\rangle$ is a random matrix product state (MPS) whose bond dimensions are identical to those of the ground states. All elements of the tensors in $|\Psi_{\text{random}}\rangle$ are generated randomly by the Gaussian distribution $N(0,1)$.

In Fig. A5, we show the visualizations of $\{|\Psi^\alpha_\delta\rangle\}$ with $\delta = 0, 0.03, 0.05, 0.06, 0.07$ and $0.10$. For $\delta \leq 0.03$, the clusters of the AFM and FM phases are clearly separated, and the boundary of the clusters successfully gives the critical point. By increasing $\delta$ to $\delta > 0.03$, two clusters gradually merge into each other, and it becomes more and more difficult to identify the critical point. These results suggest that our quantum phase visualization scheme is robust against small random noises.

**Appendix C: Visualization of classical data with negative logarithmic fidelity**

Below, we show that our scheme can also be applied to visualize classical data, such as the images in the MNIST [48] and fashion-MNIST [49] datasets. To calculate the negative logarithmic fidelity (NLF) of the classical samples, we firstly map each pixel $x_n^\alpha$ to the Hilbert space by

$$|\phi(x_n^\alpha)\rangle = \cos \frac{\pi x_n^\alpha}{8}|0\rangle + \sin \frac{\pi x_n^\alpha}{8}|1\rangle, \quad \text{(A1)}$$

where $x_n^\alpha$ with $0 \leq x_n \leq 1$ denotes the value of the $n$-th pixel in the $\alpha$-th image, and $\{|i\rangle\}$ ($i = 0, 1$) denote the orthonormal basis in the two-dimensional Hilbert space. Then an image can be mapped to a product state as

$$|\psi^\alpha\rangle = |\phi(x_1^\alpha)\rangle \otimes |\phi(x_2^\alpha)\rangle \otimes \cdots |\phi(x_n^\alpha)\rangle, \quad \text{(A2)}$$

Obviously, $|\psi^\alpha\rangle$ is a state defined in the $2^n$-dimensional Hilbert space with $L$ the total number of pixels in one image. The NLF between two images is defined as

$$D_{\alpha,\alpha'}^H = -\log \left( \langle \psi^\alpha | \psi^{\alpha'} \rangle \right), \quad \text{(A3)}$$

With $D_{\alpha,\alpha'}^H$, the images can be visualized by $t$-SNE by following the same the steps for visualizing the ground states.
FIG. A4. (Color online) Distribution of quantum states in 2D feature space varies with perplexities of t-SNE. Visualization of the grounds states of TFIM by t-SNE with different perplexities $P = 18, 20, 22, 26, 28,$ and $30$. We take the total iteration times in t-SNE $n_{it} = 5000$, the system size $L = 80$, and dimension cut-off in DMRG $\chi = 30$.

FIG. A5. (Color online) Distribution of quantum states in 2D feature space varies with noises. The visualization of the ground states of TFIM under small noise by $t$-SNE with different strengths of noise $\delta = 0, 0.03, 0.05, 0.06, 0.07,$ and $0.10$ in a-f, respectively. We take the perplexity $P = 24$, the total iteration time $n_{it} = 1000$, the system size $L = 80$, and dimension cut-off in DMRG $\chi = 30$. 
The visualizations of the images in MNIST and fashion-MNIST based on NLF are shown in Fig. A6 a and c, respectively. As a comparison, the visualizations using the Euclidean distance $D_{\alpha, \alpha'} = \|x^\alpha - x'^\alpha\|$ in the $t$-SNE are shown in Fig. A6 b and d for MNIST and fashion-MNIST, respectively. Both schemes show similar visualization results, which indicates that our scheme also works well for visualizing classical data.

**FIG. A6.** (Color online) **Visualization of classical datasets by $t$-SNE with NLF and Euclidean distance.**

The visualization of the MNIST dataset and the fashion-MNIST dataset by $t$-SNE with NLF or the Euclidean distance. In a and c, the images are mapped onto the Hilbert space, where the distance of two different images are measured by NLF. In b and d, the distance of two different images are measured by the Euclidean distance in the original feature space. For both MNIST and Fashion-MNIST datasets, we take 1000 images (100 images from each class) as the input of $t$-SNE. We take $P = 16$ and total iteration times $n_{it} = 5000$.

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