Quantum Singular Value Decomposition of Correlation Matrix and Holography in One-Dimensional Heisenberg Model

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We present singular value decomposition of spin correlation matrix defined from the ground state of one-dimensional antiferromagnetic quantum Heisenberg model. We find that the decomposition creates a data set that coincides with various domain excitations from classical antiferromagnetic state. We determine the scaling relation for the singular value as a function of the domain size. The nature of the singular value decomposition is thus to reconstruct all possible information about appropriate basis and corresponding weight of the ground-state wavefunction. We discuss implication of the present results in terms of the previous snapshot analysis for classical ferromagnetic spin models and various holographic issues.

1. Introduction

Singular value decomposition (SVD) is a powerful tool for principle component analysis (PCA). Historically, SVD has been applied to wide area beyond simple data analysis. For example, in condensed matter physics, SVD is a core algorithm of density matrix renormalization group (DMRG), which provides us with a systematic way of doing quantum simulation on interacting one-dimensional (1D) lattice models. In DMRG calculation, automatic truncation of unimportant states makes it possible to precisely treat hundreds of lattice sites, and it has been shown that the truncation is closely related to how precise we treat quantum entanglement inherent in our target quantum models.

Recently, a quantum version of SVD attracts much attention because of development of quantum computer technology. In data science community, an important request is that people can carry out standard (classical) SVD for massive data efficiently by high performance quantum computer. The algorithm to realize it is sometimes called quantum SVD. Similarly, quantum speed up of neural network and machine learning is called quantum neural network and quantum machine learning. Even in classical problems, there are many NP hard problems, and thus this strategy arises from current data science and social application quite naturally.

In contrast, our strategy in condensed matter physics side is to apply PCA to quantum data directly in order to extract essential information of our target quantum many-body systems. This is because the Hilbert spaces of our target models are exponentially large and only limited simulations are possible even if we use super-parallel computers. In that sense the real efficient quantum PCA is necessary in condensed matter physics side. Many trials based on tensor-network variational optimization for the ground state are milestones toward the ultimate success of those simulations.

We simply imagine that the first component of the best PCA for the ground state represents a macroscopic state and in special cases the state would be an ordered state in the classical limit. Then, the higher-order components of PCA systematically include quantum fluctuation with various length scales. Even if the strong quantum fluctuation breaks this picture, it is still meaningful to consider how the weights of the higher-order components dominate. This imagination may be too naive, since there are some cases, like topological order, that have no classical correspondence. However, we cannot throw this imagination away, because the viewpoint of order and various-scale fluctuations and their control are quite natural for human recognition and renormalization group. Unfortunately, the algorithms of DMRG and tensor-network methods do not follow this consideration. In these methods, it is very hard to treat entanglement throughout the superblock (whole system) directly, when we propose realistic numerical algorithms. What we can do everytime is sequential optimization of local parts of the whole wavefunction. For the realization of desired quantum PCA, it is worth mentioning to find a quantity that reflects nonlocal entanglement throughout the system.

A SVD analysis of classical spin models has been performed previously by one of the present authors (HM). In this analysis, a spin snapshot created by Monte Carlo simulation was regarded as a matrix. In particular, the snapshot at the critical point was decomposed into a set of patterns with different cluster...
sizes. Due to the nature of definition of SVD, the SVD spectrum for the snapshot data represents Höld conjugate of two-point spin correlator. Then, we can pick up a critical exponent from one snapshot near the critical point, and need not to treat whole information of partition function. Therefore, the length-scale decomposition mechanism and its close relationship to renormalization group theory seem to fit with the present purpose. Unfortunately, in quantum spin models, the superposition of states makes it useless to introduce a definite spin pattern. If we overcome this difficulty, we can extend this unique method to various quantum systems.

In an alternative context, the success for constructing quantum version of the abovementioned SVD analysis also give us a milestone for deeply understanding holographic principle.20–23 The principle states equivalence between quantum field theory and classical theory on curved background, and our strategy of PCA seems to match this principle quite well. If the direct application of SVD to quantum systems is possible, we can examine more about holography in terms of SVD.

Motivated by quantum SVD and the previous works, we focus on the quantum correlation matrix of the 1D Heisenberg model, and analyze it by SVD. We will find that the SVD of the correlation matrix can reconstruct all possible information of the basis and the weight of the ground-state wavefunction. The decomposition naturally creates a hierarchy of data set that coincides with various domain excitations from the classical antiferromagnetic spin state. Therefore, instead of considering local entanglement, we can define PCA that starts with the macroscopic order and systematically introduces correlation. It is thus necessary to introduce the SVD of the correlation matrix for desired quantum PCA. We discuss implication of the present results in viewpoint of the previous snapshot analysis for classical spin models and various holographic issues such as exact holographic map, wavelet optimization of MERA network, and inverse Mellin transformation.

The outline of this paper is as follows. In the next section we define our model, physical quantity we are going to focus on, and SVD method. In the third section, we perform detailed analysis based on exact diagonalization form small clusters and numerical optimization based on matrix product state (MPS) for larger systems. In Sec.4, we discuss implications of the present results. In the final section, various aspects associated with the present results are discussed, and we summarize our work. We also comment on future perspectives.

2. Model and Method

Let us start with the antiferromagnetic Heisenberg Hamiltonian in spatially one dimension:

\[
H = J \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1}.
\]

Here \( \vec{S} \) is quantum spin operator, \( \vec{S} = \frac{1}{2} \vec{\sigma} \) with Pauli matrices \( \vec{\sigma} \), \( N \) is the number of lattice sites, and we assume the periodic boundary condition, \( \vec{S}_{N+1} = \vec{S}_1 \). The ground state of this Hamiltonian is represented as \( |\psi\rangle \).

In this paper, we calculate a set of all possible two-point spin correlators at zero temperature

\[
S_{ij} = \langle \psi | S_i^z S_j^z | \psi \rangle = \frac{1}{3} \langle \psi | \vec{S}_i \cdot \vec{S}_j | \psi \rangle,
\]
and construct the following correlation matrix

\[
S = \begin{pmatrix}
S_{11} & S_{12} & \cdots & S_{1N} \\
S_{21} & S_{22} & \cdots & S_{2N} \\
\vdots & \vdots & \ddots & \vdots \\
S_{N1} & S_{N2} & \cdots & S_{NN}
\end{pmatrix}.
\]

We apply SVD to this matrix. We will find that this process can be viewed as a quantum version of snapshot SVD performed previously by one of the present authors.14–17 Unfortunately, the evaluation of all entries is not easy in general. However, once we obtain those values, the SVD is very easily done even for large \( N \) cases. In this paper, we focus on the analysis of functionality of the SVD decomposition of \( S \). In the previous work for classical models,14–19 we considered a particular spin pattern generated by Monte Carlo method, and regarded it as a matrix. In the quantum case, however, it is impossible to define a particular spin pattern due to quantum superposition. Instead of using snapshots, we introduce the abovementioned correlation matrix to treat all possible quantum correlation.

Note that this type of correlator matrix was previously used for evaluation of entanglement Hamiltonian for free fermions.24,25 Furthermore, the correlation matrix is also considered for definition of space-time metric in the exact holographic mapping.26,27 Thus, the correlation matrix is a key quantity to consider entanglement and holography. In these previous works, SVD was not examined yet, even though SVD is a key method to extract essential information of our target system. Therefore, we would like to clarify the functionality of SVD to quantum correlation matrix.

The SVD of the correlation matrix is defined by

\[
S_{ij} = \sum_{n=1}^{N} U_{in} \sqrt{\lambda_n} V_{jn},
\]

where \( \sqrt{\lambda_n} \) are singular values and \( U_{in} \) and \( V_{jn} \) are column unitary matrices. Because of the symmetry \( S_{ij} = S_{ji} \), we find \( U_{in} = V_{jn} \). These conditions show that SVD is equivalent to the matrix diagonalization in the present case and \( \sqrt{\lambda_n} \) is the eigenvalue of the matrix \( S \). For this reason, we obtain the following identity

\[
\sum_{n=1}^{N} \sqrt{\lambda_n} = trS = tr\Lambda = \frac{N}{4},
\]
where $\Lambda$ is the diagonal matrix with $\Lambda_{nn} = \sqrt{\Lambda_{nn}}$.

We can estimate mathematical properties of eigenvalues of this correlation matrix. When some kind of long-range order emerges at low temperature (there is no order in 1D case), the off-diagonal components $S$ have finite values of the same order of the diagonal parts. Then the first eigenvalue becomes dominant. On the other hand, only the diagonal components are important at high temperature due to exponential decay of correlation. The quantum criticality is an exceptional case, and we need more careful analysis. The quantum criticality occurs at zero temperature limit in the 1D Heisenberg model. Then, the correlator shows algebraic decay. In this case, there still exist various magnitudes of eigenvalues, although the first eigenvalue starts to dominate the other eigenvalues.

In the following, we first try to examine a small system exactly, and then perform numerical simulation based on MPS for larger systems. We may find analytical representation of SVD even for general cases, since the asymptotic behavior of the correlation function is given by $S_{ij} \propto |i-j|^{-1}$. Algebraic properties of the Hilbert matrix may help us to resolve this problem, but in the present stage this is an interesting future work.

3. Result

3.1 Preliminary: Exact analysis for 4-site ring

Let us first consider the 4-site case in which we can obtain the exact eigenstates. The ground state for $S_{\text{tot}} = 0$ is a resonant state of spin singlet pair:

$$
|\psi\rangle = \frac{1}{\sqrt{12}} \left( -|\uparrow\downarrow\downarrow\downarrow\rangle + 2|\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle \right) 
-|\downarrow\uparrow\uparrow\downarrow\rangle + 2|\uparrow\downarrow\uparrow\downarrow\rangle - |\downarrow\uparrow\downarrow\downarrow\rangle )
+ \frac{1}{\sqrt{12}} \left( |\uparrow\downarrow\downarrow\downarrow\rangle + 2|\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle \right)_{34}
+ \frac{1}{\sqrt{12}} \left( |\uparrow\downarrow\downarrow\downarrow\rangle + 2|\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle \right)_{23}. \quad (6)
$$

Before going into evaluation of quantum correlation matrix, we summarize the entanglement properties of this state, and point out some disadvantage of using DMRG and multiscale entanglement renormalization ansatz (MERA).) To define entanglement, we need to divide whole system into two (subsystem and environment), and there are different patterns of spatial division. We call site 1 (2) as A (B). The partial density matrix for subsystem $A \otimes B$ is defined by

$$
\rho_{A \otimes B} = tr_{B}(\psi \langle \psi |)
= \frac{1}{12} |\uparrow\uparrow\rangle \langle \uparrow\uparrow| + \frac{1}{12} |\downarrow\downarrow\rangle \langle \downarrow\downarrow| 
+ \frac{5}{12} |\uparrow\downarrow\rangle \langle \uparrow\downarrow| + \frac{5}{12} |\downarrow\uparrow\rangle \langle \downarrow\uparrow|,
$$

and the entanglement entropy is evaluated as

$$
S_{A \otimes B} = -tr_{A \otimes B}(\rho_{A \otimes B} \log \rho_{A \otimes B}) = 2 \log 2 - \frac{1}{2} \log 3. \quad (8)
$$

Similarly, we calculate the partial density matrix for single site $A$

$$
\rho_{A} = tr_{B}(\psi \langle \psi |) = \frac{1}{2} |\uparrow\rangle \langle \uparrow| + \frac{1}{2} |\downarrow\rangle \langle \downarrow| \quad (10)
$$
and the entanglement entropy is evaluated as

$$
S_{A} = -tr_{A}(\rho_{A} \log \rho_{A}) = \log 2. \quad (11)
$$

We also obtain

$$
S_{B} = -tr_{B}(\rho_{B} \log \rho_{B}) = \log 2, \quad (12)
$$
where $\rho_{B} = tr_{A}(\psi \langle \psi |)$. The mutual information is also given by

$$
I_{M} = S_{A} + S_{B} - S_{A \otimes B} = \frac{1}{2} \log 3. \quad (13)
$$

These entropy values characterize the formation of fluctuation of singlet pairs represented in Eq. (7). In particular, the leading term of the magnitude of $S_{A \otimes B}, 2 \log 2$, represents two singlets (the second term in Eq. (7)) which are cut by partial truncation of environmental degrees of freedom, $\Lambda \otimes B$. The mutual information represents net quantum correlation between $A$ and $B$ embedded into whole 4 site ring. The viewpoint from these entropy values seems to be very nice. On the other hand, when we look at the eigenstates of partial density matrix $\rho_{A \otimes B}$, the situation changes. We easily find that the triplet eigenstates for the eigenvalue 1/12 are $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, and $|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle / \sqrt{2}$, and the singlet eigenstate for the eigenvalue 9/12 is $|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle / \sqrt{2}$. The leading component is singlet, but this singlet is located inside of partial system. The nonlocal entanglement across the boundary must be represented by complex combination of triplet states. They are very asymmetric. Thus, the two terms in Eq. (7) are not equally treated by a simple SVD for the wavefunction approximation. In DMRG calculation, this asymmetric is a reason for worse numerical convergence in periodic boundary condition. In the MERA tensor network, this asymmetric nature is somehow relaxed by the introduction of disentangler tensors. However, this relaxation is imperfect. For the ground state $|\psi\rangle = \sum_{s_{1},...s_{4}} \psi^{s_{1}...s_{4}} |s_{1}...s_{4}\rangle$, the MERA corresponds decomposition of the coefficient $\psi^{s_{1}...s_{4}}$ by a set of functional tensors:

$$
\psi^{s_{1}...s_{4}} = \sum_{a,b} \sum_{\alpha,\beta,\gamma,\delta} T^{ab}_{\alpha\beta} W_{a}^{\alpha\beta} U^{\beta\gamma} W_{b}^{\beta\gamma} U^{\gamma\delta} W_{c}^{\gamma\delta}. \quad (14)
$$

In this representation, the two types of singlet pairs in Eq. (7) is still treated asymmetrically. To relax this asymmetry, we need to introduce extra tensor dimension, or combination of different types of networks that are con-
sistent with all terms in Eq. (7).

To automatically find correct information of the wave-function by overcoming the abovementioned weak points, it is efficient for us to introduce SVD of quantum correlation matrix. In the present approach, the asymmetric treatment of singlet pairs does not occur, and the successful quantum PCA is possible as we will see later.

On the basis of the abovementioned facts, we analyze the correlation matrix which can be evaluated as

$$
\lambda S = \sqrt{\lambda_1} v_{1n},
$$

(17)

where the singular values are given by

$$
\lambda_1 = \frac{2}{3}, \quad \lambda_2 = \sqrt{\lambda_3} = \frac{1}{6}, \quad \lambda_4 = 0,
$$

(18)

and we confirm \( \sqrt{\lambda_1 + \lambda_2 + \lambda_3} = 4/4 = 1 \). All non-zero components of SVD are

$$
S^{(1)} = \frac{1}{6} \left( \begin{array}{cccc} 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \end{array} \right),
$$

(19)

$$
S^{(2)} = \frac{1}{12} \left( \begin{array}{cccc} 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right),
$$

(20)

and

$$
S^{(3)} = \frac{1}{12} \left( \begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 \end{array} \right).
$$

(21)

We find that the first principle component, \( S^{(1)} \), clearly represents the Néel order, the classical limit of our ground state. This is a simple product state without entanglement. The higher-order components, \( S^{(2)} \) and \( S^{(3)} \), represent some magnetic excitation from the Néel order. Note that the second and the third components share the same singular value.

In terms of Fourier analysis, the principle component \( S^{(1)} \) has periodicity characterized by the wave number \( k_1 = \pi \) with the lattice constant \( a = 1 \). The second components are degenerate, and for both of them the wave number can be defined as \( k_2 = \pi/2 \). From these data, we may imagine close relationship between \( k_n \) and \( \lambda_n \). We would like to know much clearer physical meaning of this wave number. The wave number is related to the size of the antiferromagnetic domain. To see this feature we redefine the wavefunction as

$$
\langle \psi \rangle = \langle \psi \rangle_1 + \langle \psi \rangle_2,
$$

(22)

$$
\langle \psi \rangle_1 = \frac{1}{\sqrt{3}} (|↓↑↓↓⟩ + |↑↓↑↓⟩ + |↓↓↑↑⟩ + |↑↑↓↓⟩ + |↓↓↑↑⟩ + |↑↑↓↓⟩).
$$

(23)

The first component is nothing but the sum of classical antiferromagnetic spin configurations. Due to the periodic boundary condition, the second component \( \langle \psi \rangle_2 \) represents some combination of one domain excitation (two domain walls) from the classical antiferromagnetic state. Let us introduce matrices \( S_n \) with \( n = 1, 2 \) whose entries are defined by

$$
(S_n)_{ij} = \langle \psi_n | S_i S_j^{\dagger} | \psi_n \rangle.
$$

(25)

Then we find

$$
S_1 = S^{(1)},
$$

(26)

$$
S_2 = 4 \left( S^{(2)} + S^{(3)} \right).
$$

(27)

Therefore, the SVD component for the quantum correlation matrix is nothing but the quantity that reflects precise information of the ground-state wavefunction.

3.2 Numerical results

To examine the nature of quantum correlation matrix for larger systems, we perform numerical calculation based on MPS optimization of the ground state on lattice with \( N = 64 \) under the periodic boundary condition. We assume the form of MPS as

$$
|\psi\rangle = \sum_{s_1 = \uparrow, \downarrow} \cdots \sum_{s_N = \uparrow, \downarrow} \text{tr}(A_1^{s_1} \cdots A_N^{s_N}) |s_1 \cdots s_N\rangle,
$$

(28)

and optimize it so that the variational energy, \( E = \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle \), is minimized. For the minimization, we solved the generalized eigenvalue problem \( H_{\text{eff}} |A\rangle = EN_{\text{eff}} |A\rangle \) for the vector \( |A\rangle \) that is defined by one-dimensional arrangement of each matrix. Here, the dimension of each matrix \( A_x^i \), \( \chi_i \) is taken to be up to \( \chi = 10 \). Starting from random matrices, we repeat optimization of all matrices sequentially by 40 times. The energy eigenvalue almost converges by much smaller number of iterations (typically 2 times), but we need many iterations for convergence of the singular value spectrum. We also perform exact diagonalization calculation for \( N = 12 \) in order to confirm reliability of the MPS calculation (not shown here).

Figure 1 shows the matrix element of the ground-
state quantum correlation matrix. The intensity is strong near the diagonal area, but we can still find finite amount of intensity away from the diagonal line. This is related to algebraic decay of spin correlation at quantum critical point. Because of the periodic boundary condition, we find somehow strong intensity near the upper right and lower left regions.

Figure 2 shows the squared singular value spectrum. We find that the spectral data are basically doubly degenerate except for the largest and the smallest singular values, $\lambda_1$ and $\lambda_{64}$. The degeneracy is a consequence of translation of identical spin patterns as we have already discussed in the previous subsection. Only the smallest singular value $\lambda_{N=64}$ is negligible numerically, and that is consistent with Eq. (18) in which we have $\lambda_{N=4} = 0$. The envelope of the spectrum seems to show power-law decay, and this would be originated from power-law correlation of each entry in $S$ due to quantum criticality. We will discuss this point later.

To understand the origin of the degeneracy, we show

Figure 3. SVD components from $S^{(1)}$ to $S^{(13)}$. The data have been normalized for better presentation.
some of characteristic SVD components, $S^{(n)}$, after normalization in Fig. 3. These data are composed of modulated antiferromagnetic patterns (blue and red dots are mixed in each cluster). We find that $S^{(1)}$ for the largest singular value actually represent the perfect classical Néel order and each degenerate components with $n \geq 2$ represent domain excitations from the classical Néel order (Note that the domain boundaries are smeared out). The size of ordered area inside of single domain, $L_n$, is clearly characterized by

$$L_n = \frac{N}{n},$$

(29)

for $n = 1$ and even $n$ values. Now we take $N = 64$, and then need to assume $n < 32 = N/2$ in order to keep $L_n \geq 2$ which is the minimum size of antiferromagnetic domain. When this condition is not satisfied, we can not create antiferromagnetic domains. Because of this fact, smaller singular value components ($n \geq 32$) behave quite differently. Figure 4 shows such tendency. In this case also, we find periodic nature of the correlation, but each cluster shows ferromagnetic correlation, not antiferromagnetic. These data represent high energy components. Except for $S^{(64)}$, we notice that the total magnetic moment is zero, since the ferromagnetic domains with different signs exist. As for $S^{(64)}$, the bulk ferromagnetic basis state still exists, but this contribution vanishes due to the fact that $\lambda_{64} = 0$. Thus the condition $S^z_{\text{tot}} = 0$ is kept successfully.

Figure 5 shows the scaling plot for $\lambda_n$. This scaling corresponds to the envelope of $\lambda_n$ as a function of $n$ in order to fit $\lambda_1, \lambda_2, \lambda_4, \ldots$. For $n < N/2$ (antiferromagnetic correlation remains), we find

$$\lambda_n \propto \frac{1}{n} e^{-n/N}.$$  

(30)

This form is quite similar to the Ornstein-Zernike for-
mula for the two-point correlator away from the critical point, if we regard $n$ and $N$ as a length scale associated with magnetic domain formation and the correlation length $\xi$, respectively. Note that each SVD component has a particular length scale $L_n$, but the abovementioned correlation length is the whole system size, not $L_n$. Combining Eq. (29) with Eq. (30), we obtain

$$\lambda_n \propto L_n e^{-1/L_n}. \quad (31)$$

This is direct relationship between the SVD spectrum and domain size. When the domain size is very large, Eq. (31) leads to $\lambda_n \propto L_n$.

### 4. Discussion

Let us consider the numerical results. As we have already discussed in the preliminary exact analysis, the present SVD can extract information of many-body wavefunction from the correlation data. This is a non-trivial result, since the information of the wavefunction is usually smeared out after the calculation of the correlation function. Here, the wavefunction is decomposed into basis states with different energy scales which are characterized by the domain sizes of the number of the domain boundary. Then, the index of SVD behaves like a length scale, and this feature is essentially the same as that in the previous work for the classical ferromagnetic Ising model on 2D square lattice.$^{14-19}$ Therefore, the present approach can be viewed as a quantum version of snapshot SVD.

The present SVD decomposition clearly has the feature of holographic transformation in the sense that the quantum state is reconstructed from a set of classical states. In the theory of exact holographic map,$^{26,27}$ the space-time metric in the classical side of the holography is defined from the two-point correlation function in the quantum side. We are very much interested in the relationship between this map and the present result. To precisely examine the relationship, we need to examine how to redefine the metric from the present result. This is a future work to be resolved.

Among related previous works, we imagine that the wavelet optimization of MERA network may also be related to the present decomposition.$^{28,29}$ To compare these methods, we have performed Haal wavelet transformation of $S$. However, the wavelet patterns are not similar to the present result except for the principle component. This is because the wavelet transformation for $S$ corresponds to the coarse graining for distribution of spin correlation (the wavelet optimization of MERA corresponds to the coarse-graining in the real space).

Furthermore, we can analytically represent the holographic nature of SVD by the inverse Mellin transformation with slight modification from the classical case.$^{30}$ Let us assume the following form in the asymptotic region, $|i-j| \gg 1$:

$$U_{in} V_{jn} \sim \sqrt{e^{-|i-j|/L_n}/|i-j|}, \quad (32)$$

which represents that the SVD component has information about two-point correlator with finite correlation length (domain size) $L_n$. Since the exponential decay factor becomes dominant in the asymptotic region, this form can be roughly decomposed into the product between $U_{in}$ and $V_{jn}(= U_{jn})$. The abovementioned form has also exchange symmetry between site indices $i$ and $j$, and this fact also supports the reliability of Eq. (32). We can show that this assumption leads to the correct asymptotic form of $S_{ij} \sim |i-j|^{-1}$ for $|i-j| \gg 1$. Actually, we evaluate $S_{ij}$ as

$$S_{ij} = \sum_{n=1}^{N} U_{in} \sqrt{\lambda_n} V_{jn}$$

$$\propto \sum_{n=1}^{N} \sqrt{e^{-n/N}} \sqrt{e^{-|i-j|/L_n}/|i-j|}$$

$$\sim \int_{1}^{N} dn \frac{e^{-n|i-j|/2N}}{(n|i-j|)^{1/2}}, \quad (33)$$

where the factor $e^{-n/L_n}$ is important for convergence of the sum and the factor $e^{-n/N}$ does not play a role on the abovementioned evaluation for $|i-j| \gg 1$ (Note that the factor $e^{-n/N}$ is necessary for the convergence of $\sum_n \lambda_n$). By changing the integration parameter as $x = n|i-j|/2N$, we obtain

$$S_{ij} \propto \sqrt{2N} \int_{|i-j|/2N}^{\infty} dx \frac{e^{-x}}{x^{1/2}} \propto \frac{1}{|i-j|}, \quad (34)$$

where the integral can be approximated to the gamma function $\Gamma(1/2) = \int_{0}^{\infty} e^{-x} x^{-1/2} dx = \sqrt{\pi}$ in the asymptotic region.

### 5. Summary and Future Perspective

We presented SVD of correlation matrix of 1D antiferromagnetic quantum Heisenberg model. We found that the decomposition naturally creates a hierarchy of data set that coincides with the ground and various excited states in the classical 1D antiferromagnetic model. We think that the SVD analysis for the correlation matrix gives us a very natural way of a quantum PCA and overcomes disadvantage of treating local entanglement. The present SVD method is also closely related to holographic transformation. The classical limit of the ground state is the principle component, but at the same time the domain excitations play important roles in the residual singular values. We have obtained important relationships associated with domain size, the scaling of SVD spectrum, and reconstruction formula of the two-point correlator.
The presence of a successful method for selectively observing basis states of a quantum wavefunction may also be suggestive for the study of weak value, weak measurement, and related topics associated with quantum measurement that does not break quantum superposition.\cite{31,32,33}

To examine holographic principle more deeply, it is important to examine the nature of the black hole in the classical side. For this purpose, it is necessary to examine finite-temperature effects in the quantum side. Fortunately, the present method can be simply extended to finite temperature cases. We introduce the correlation matrix at inverse temperature $\beta$

$$S_{ij}(\beta) = \frac{1}{Z} \text{tr} \left( e^{-\beta H} S_i^z S_j^z \right) = \frac{1}{Z} \sum_n e^{-\beta E_n} \langle n | S_i^z S_j^z | n \rangle,$$

(35)

where $H | n \rangle = E_n | n \rangle$ and $Z = \text{tr} \left( e^{-\beta H} \right) = \sum_n e^{-\beta E_n}$. In terms of holography, the finite-temperature effect can be mapped onto the existence of a black hole in the classical gravity side, and the existence is characterized by the information loss of lower-energy states. An interesting question is how the SVD for finite-temperature quantum correlation matrix picks us information of the black hole. Even if we introduce finite temperature effect, we expect that the basis states represented by Figs. 3 and 4 are still kept. This is because the abovementioned definition still contains information of the ground state examined in this study. Thus, the finite-temperature effect should be reflected to the decrease in the larger singular value spectrum. Actually, we have obtained such tendency by the preliminary calculation based on the numerically exact diagonalization for $N = 12$. More precise numerical result will be presented elsewhere. In the condensed matter physics side, the information of the Unruh effect and world-line entanglement is extracted from SVD analysis of quantum Monte Carlo data for the XXZ chain.\cite{34}

Whether the present result is related to this work is an interesting question.

The approach presented in this paper can be applicable to any quantum many-body models, some of which may not have clear order parameters. Thus, this flexibility would lead to generic approach for construction of quantum PCA. We also hope that the present analysis opens a new door to have deeper understanding for entanglement and holographic principle. There are still many open issues to be resolved.

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