Construct order parameter from the spectra of mutual information

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In this paper, we try to establish a connection between a quantum information concept, i.e. the mutual information, and the conventional order parameter in condensed matter physics. We show that a non-vanishing mutual information at a long distance means the existence of long-range order. By analyzing the entanglement spectra of the reduced density matrix that are used to calculate the mutual information, we show how to find the local order operator used to identify various phases with long-rang order.

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I. INTRODUCTION

At absolute zero temperature, a quantum many-body system may undergo a phase transition as the system’s parameter varies across a critical point[1]. Except for some unconventional phase transitions, continuous quantum phase transitions can be well characterized in the framework of the Landau’s symmetry-breaking theory. In the Landau’s theory, the concept of the order parameter plays a central role. To characterize a given ordered phase, people usually introduce an order parameter which is nonzero in the symmetry-breaking phase, but vanishes in the other phases. In the recent years, much attention has been paid to using quantum information approaches to investigate quantum phase transitions. A typical example is the role of entanglement in quantum critical phenomena[3–8]. Since the quantum phase transitions occur at the absolute zero temperature, they are purely driven by quantum fluctuations. People believe that the quantum entanglement, as a kind of quantum correlation, should play a very important role in the quantum phase transitions. This point has been proven to be true in the later hundreds of works on the issue (for a review, see[3] and the references therein). The entanglement manifests interesting properties, such as scaling singularity, or maximum[5, 6] etc, in various quantum phase transitions.

However, it seems to us that, besides its interesting behavior around the critical point, the entanglement actually cannot tell us much information about the corresponding phase itself. That is, while the entanglement helps us to witness the quantum phase transition, a non-trivial question is how can we learn the corresponding order parameter of the ordered phases from the behavior of the entanglement. This question leads to the main motivation of the present work. We will show that the non-vanishing mutual information[2] at a long distance not only means the existence of long-range order, but also can tell us the potential order parameter if we analyze the entanglement spectra of the corresponding reduced density matrices. A possible scheme to construct the order parameter will be discussed in detail.

On the other hand, the order parameter plays a very important role in condensed matter physics. In order to study the ground-state properties of a quantum many-body system, people usually assume a special order parameter in various methods. For instance, in the dynamic mean-field theory, a suitable local order parameter usually is assumed at the very beginning. However, such an order parameter strongly depends on the physical intuition of the investigator. That means, if the guessed order parameter is wrong, then all analysis based on the assumption of the order parameter are not physical or even wrong. Therefore, a scheme that can tell us how to find an appropriate order parameter is instructive for many condensed matter theorists in their studies.

The paper is organized as follows. In Sec. II, we firstly discuss the relation between the existence of long-range order and the non-vanishing behavior of the mutual information. In Sec. III, we propose a possible scheme to find the local order operators by analyzing the entanglement spectra of the mutual information. Three simple applications are given in the same section. Finally, we give a discussion and a brief summary in section IV.

II. NON-VANISHING MUTUAL INFORMATION AND LONG-RANGE ORDER

Let us consider a general quantum many-body system described by the Hamiltonian $H = \sum_i h_i$, where $h_i$ is the local Hamiltonian. $h_i$ can be the kinetic energy, interaction, etc. To learn the potential long-range correlations existing in the system’s ground state $|\Psi\rangle$, we focus on two small blocks, $i$ and $j$, separated by a distance $|i – j|$. Without loss of generality, we assume that the block has a minimum size with which the block can capture the potential long-range correlation existing in the system, and the distance $|i – j|$ is comparable to the system’s size. The reduced density matrix of the block $i$ can be...
expressed as
\[
\langle \mu' | \rho_i | \mu \rangle = \text{tr}(a_{i\mu'} a^\dagger_{i\mu}),
\] (1)
where $\rho = |\Psi\rangle \langle \Psi|$, \text{tr} is used to trace out all other degrees of freedom of the system except for the block $i$, $a_{i\mu}$ is the annihilation operator for the state $|\mu\rangle$ localized at the block $i$. The operators $a_{i\mu}$s satisfy the commutation (or anti-commutation) relation for bosonic (or fermionic) states. Similarly, we can define the reduced density matrix of the two blocks $i$ and $j$
\[
\langle \mu' | \rho_{i\setminus j} | \mu \rangle = \text{tr}(a_{i\mu'} a^\dagger_{j\mu} a_{i\mu} a^\dagger_{j\mu}).
\] (2)
The reduced density matrices are positive semidefinite and can be normalized as
\[
\text{tr}(\rho_{i}) = \text{tr}(\rho_{j}) = \text{tr}(\rho_{i\setminus j}) = 1. \tag{3}
\]
So if we diagonalize these matrices
\[
\rho_{i} = \sum_{\mu} p_{\mu} |\varphi_{\mu}\rangle \langle \varphi_{\mu}|,
\] (4)
\[
\rho_{j} = \sum_{\nu} p_{\nu} |\varphi_{\nu}\rangle \langle \varphi_{\nu}|,
\] (5)
\[
\rho_{i\setminus j} = \sum_{\mu, \nu} q_{\mu, \nu} |\phi_{\mu, \nu}\rangle \langle \phi_{\mu, \nu}|,
\] (6)
for a given reduced density matrix, say $\rho_{i}$, the diagonal elements \{\{p_{\mu}\}\} then have a probability interpretation in the corresponding eigenstate space. The von-Neumann entropy
\[
S = -\sum_{\mu} p_{\mu} \log_{2} p_{\mu} \tag{7}
\]
measures the entanglement between the block $i$ and the rest of the system.

To study the correlation between the block $i$ and $j$, we introduce the mutual information
\[
S(i|j) = S(\rho_{i}) + S(\rho_{j}) - S(\rho_{i\setminus j}). \tag{8}
\]
In the quantum information science, the mutual information measures the total correlation between the two blocks. It has also been used to study quantum critical phenomena in recent years\cite{7, 8}. For the completeness of the work, we show that the non-vanishing behavior of the mutual information at a long distance leads to the existence of long-range order, as discussed in Ref. 8. For this purpose, we express the mutual information as
\[
S(i|j) = \text{tr}(\rho_{i\setminus j} \log_{2} \rho_{i\setminus j}) - \text{tr}(\rho_{i\setminus j} \log_{2} \rho_{i} \otimes \rho_{j}). \tag{9}
\]
Then
\[
S(i|j) = \sum_{\mu, \nu} q_{\mu, \nu} \log_{2} q_{\mu, \nu}
- \sum_{\mu, \nu} \langle \phi_{i\mu, j\nu} | \rho_{i\setminus j} \log_{2} (\rho_{i} \otimes \rho_{j}) | \phi_{i\mu, j\nu} \rangle, \tag{10}
\]
in the basis of $|\phi_{\mu\nu}\rangle$. Insert the identity
\[
\sum_{\mu, \nu} |\varphi_{\mu\nu}\rangle \langle \varphi_{\mu\nu}| = 1,
\]
The mutual information becomes
\[
S(i|j) = \sum_{\mu, \nu} q_{\mu, \nu} \log_{2} q_{\mu, \nu} - \sum_{\mu, \nu} P_{\mu', \nu', \mu} q_{\mu, \nu} \log_{2} (p_{\mu} p_{\nu}), \tag{11}
\]
with
\[
P_{\mu' \nu', \mu} = \langle \phi_{i\mu, j\nu} | \varphi_{i\nu', j\nu'} \rangle \langle \varphi_{i\mu, j\nu'} | \phi_{i\mu, j\nu} \rangle \tag{12}
\]
which satisfies
\[
P_{\mu' \nu', \mu} > 0, \sum_{\mu' \nu'} P_{\mu' \nu', \mu} = 1, \sum_{\mu' \nu'} P_{\mu' \nu', \mu} = 1. \tag{13}
\]
Eq. 11 can be rewritten as
\[
S(i|j) = \sum_{\mu, \nu} q_{\mu, \nu} \left( \log_{2} q_{\mu, \nu} - \sum_{\mu' \nu'} P_{\mu' \nu', \mu} \log_{2} (p_{\mu} p_{\nu}) \right). \tag{14}
\]
Now we divide the problem into the following two cases.

Case I: For any matrix element in $\rho_{i\setminus j}$, if we can always find $\langle a_{i\mu'}^\dagger a_{i\mu}^\dagger a_{j\nu'}^\dagger a_{j\nu} \rangle = \langle a_{i\mu'}^\dagger a_{i\mu} \rangle \langle a_{j\nu'}^\dagger a_{j\nu} \rangle$ such that $\rho_{i\setminus j} = \rho_{i} \otimes \rho_{j}$, then $P_{\mu' \nu', \mu}$ is a unit matrix and we have $S(i|j) = 0$. In this case, any linear superposition of $a_{i\mu} a_{i\nu}$ is not correlated, so the system does not have any long-range order.

Case II: If there exist some elements that $\langle a_{i\mu'}^\dagger a_{i\mu}^\dagger a_{j\nu'}^\dagger a_{j\nu} \rangle \neq \langle a_{i\mu'}^\dagger a_{i\mu} \rangle \langle a_{j\nu'}^\dagger a_{j\nu} \rangle$, then $P_{\mu' \nu', \mu}$ is not correlated, so the system does not have any long-range order.

Case II: If there exist some elements that $\langle a_{i\mu'}^\dagger a_{i\mu}^\dagger a_{j\nu'}^\dagger a_{j\nu} \rangle \neq \langle a_{i\mu'}^\dagger a_{i\mu} \rangle \langle a_{j\nu'}^\dagger a_{j\nu} \rangle$, then $P_{\mu' \nu', \mu}$ is not correlated, so the system does not have any long-range order.

Eq. 12 is no longer a unit matrix. Since the log function is concave,
\[
\sum_{\mu', \nu'} P_{\mu' \nu', \mu} \log_{2} (p_{\mu} p_{\nu}) < \log_{2} \left( \sum_{\mu', \nu'} P_{\mu' \nu', \mu} p_{\mu} p_{\nu} \right),
\]
we have
\[
S(i|j) \geq \sum_{\mu, \nu} q_{\mu, \nu} \log_{2} Q_{\mu, \nu}
- \frac{1}{\ln 2} \sum_{\mu, \nu} q_{\mu, \nu} (1 - Q_{\mu, \nu}) = 0, \tag{15}
\]
where
\[
Q_{\mu, \nu} = \frac{q_{\mu, \nu}}{\sum_{\mu', \nu'} P_{\mu' \nu', \mu} p_{\mu} p_{\nu}}.
\]
So the mutual information is non-vanishing
\[
S(i|j) > 0. \tag{16}
\]
In this case, $\rho_{i\setminus j} \neq \rho_{i} \otimes \rho_{j}$. Actually, $S(i|j) > 0$ is the sufficient and necessary condition for the existence of the correlation between two blocks. That is, if and only if $S(i|j) > 0$, we can find matrix elements satisfying
\[
\langle a_{i\mu}^\dagger a_{i\mu'} a_{j\nu'}^\dagger a_{j\nu} \rangle \neq \langle a_{i\mu}^\dagger a_{i\mu} \rangle \langle a_{j\nu'}^\dagger a_{j\nu} \rangle. \tag{17}
\]
Then \( \langle a^\dagger_{i\mu} a_{j\nu} \rangle \) plays a role of local order operator at site \( i \). Nevertheless, there are usually many terms satisfying the above inequality, the operator \( \langle a^\dagger_{i\mu} a_{j\nu} \rangle \) is not a good candidate for long-range order parameter.

To find a good candidate of the order parameter, we need to analyze spectra of the mutual information. To proceed, we would like to mention some properties of the mutual information:

i) If the rank of \( \rho_i \) is 1, then there is no correlation between \( \rho_i \) and \( \rho_j \).

Prove: If the rank of \( \rho_i \) is 1, then \( \rho_i \) is a pure state and \( S(\rho_i) = 0 \). Since \( S(i|j) = S(\rho_i) + S(\rho_j) - S(\rho_{i,j}) \) is non-negative, so \( S(i|j) = 0 \). There is no correlation between the blocks \( i \) and \( j \).

ii) If the rank of \( \rho_i \) is \( \xi \), for any \( \mu > \xi \), the operator \( a^\dagger_{i\mu} a_{i\mu} \) does not correlated.

Prove: If

\[
\rho_i|\varphi_{i\mu}\rangle = 0,
\]  

Then

\[
\langle a^\dagger_{i\mu} a_{i\mu} \rangle = 0. 
\]  

The correlation function becomes

\[
\langle a^\dagger_{i\mu} a_{i\nu} a^\dagger_{j\nu} a_{j\mu} \rangle = \sum_{\mu', \nu'} \langle a^\dagger_{i\mu} a_{i\nu} | \varphi_{i\mu'} \varphi_{j\nu'} \rangle \langle \varphi_{i\mu'} \varphi_{j\nu'} | a^\dagger_{j\mu} a_{j\nu} \rangle = 0. 
\]  

iii) For \( \mu \neq \nu \), \( \langle a^\dagger_{i\mu} a_{i\nu} \rangle = \langle a^\dagger_{i\nu} a_{i\mu} \rangle = 0. \) If \( \langle a^\dagger_{i\mu} a_{i\nu} a^\dagger_{j\nu} a_{j\mu} \rangle \neq 0 \), \( a^\dagger_{i\mu} a_{i\nu} + a^\dagger_{i\nu} a_{i\mu} \) is a good candidate of the order parameter.

These three properties will be used in the next section to construct local order operator.

### III. CONSTRUCT LOCAL ORDER OPERATOR

In this section, we show how to construct the potential local order parameter from the spectra of the reduced density matrices. We have show that the long-range order exists if and only if the mutual information does not vanish at long distance. However, the mutual information can not tell us directly which kind of order exists in the phase. To find the potential order parameter, we need to look into the spectra of the mutual information.

At the beginning, we need to decide the minimum size of the two correlated blocks. If the block size is too large, even if the mutual information does not vanish, the final order parameter obtained might be too complicated to be well understood. On the other hand, if the block size is too small, the corresponding mutual information might not be able to find the order parameter. For instance, in the spin dimer or trimer ordered phase, the mutual information between two single spins usually decays exponentially because the spin-spin correlation function decays exponentially too. Therefore, to decide an appropriate block size is important. For this purpose, we can start from a relatively large block size. In this case, it is easier to witness if there exist long-range order in the system. Then we reduce the size of the blocks step by step until find the minimum size of the correlated blocks. Once the minimum block size is decided, we continue to find the potential order parameters from the mutual information of the two blocks.

**Diagonal long-range order**: Usually, there are two kinds of long-range order. One is the diagonal long-range order, the another is the off-diagonal long-range order. Whether the order is diagonal or off-diagonal depends on the basis used to define the reduced density matrices. Without loss of generality, we use the eigenstates \( |\varphi_{i\mu}\rangle \) of \( \rho_i \) to define the local modes. Then the set \( \{p_{\mu}\} \) is the probability distribution of these modes.

We now consider the first case of diagonal long-range order. In this case, if we express the combined block \( \rho_{i,j} \) in the basis \( |\varphi_{i\mu}\varphi_{j\nu}\rangle \), we can find that there exist some diagonal elements \( q_{\mu\nu} \neq p_{\mu} p_{\nu} \). We have shown that if the rank of \( \rho_i \) is \( \xi \), for any \( \mu > \xi \), the operator \( a^\dagger_{i\mu} a_{i\mu} \) does not correlated. Therefore, the potential order operator can be constructed as a superposition of nonzero diagonal elements of \( \rho_i \)

\[
O_i = \sum_{\mu \leq \xi} w_{\mu} a^\dagger_{i\mu} a_{i\mu}.
\]  

Clearly, the definition still makes the order parameter not unique especially if the rank of \( \rho_i \) is large. To have an explicit form, we can apply various conditions on the set of coefficient \( \{w_{\mu}\} \).

The first condition can be the traceless condition, i.e.,

\[
\sum_{\mu \leq \xi} w_{\mu} p_{\mu} = 0,
\]  

which makes

\[
\text{tr} (O_i) = 0.
\]  

A special case is that the rank of \( \rho_i \) is 1, then the traceless condition will not leads to any order parameter. With the above condition, we need only to calculate the function \( \langle O_i O_j \rangle \) for the correlation function.

The second condition can be the normalization condition. That is the maximum value in the set \( \{w_{\mu}\} \) is 1. This condition defines a maximum amplitude of the correlation function \( \langle O_i O_j \rangle \).

Usually, the above two conditions are enough to decide the form the order parameter. In case that there are still some degrees of freedom in \( \{w_{\mu}\} \), one may fix the residue degrees of freedom by considering the other related physical properties of the ground state.

Once the order parameter is obtained, the correlation function becomes

\[
\langle O_i O_j \rangle = \sum_{\mu' \nu'} \langle O_i | \varphi_{i\mu'} \varphi_{j\nu'} \rangle \langle \varphi_{i\mu'} \varphi_{j\nu'} | O_j \rangle.
\]
expressed as nonzero off-diagonal elements in $\rho$. Range order exists if the combined block pair parameter, the first step is to find all possible indices of the off-diagonal long-range order. To find the order relation function is the exact form of the order parameter, the next step is to determine the set $\{w_\mu\}$ with suitable conditions.

iv) If the reduced density matrix of the combined block $\rho_{i;j}$ is not diagonal in the basis of $\rho_i \otimes \rho_j$, define the off-diagonal order parameter

$$O_i = \sum_{(\mu, \nu)} \left( w_{\mu\nu} a_{i\mu}^{\dagger} a_{i\nu} + w_{\mu\nu}^{*} a_{i\nu}^{\dagger} a_{i\mu} \right),$$

where the pairs $\langle \mu, \nu \rangle$ can be determined from nonzero off-diagonal elements in $\rho_{i;j}$. Determine the set $\{w_\mu\}$ with suitable conditions.

v) Calculate the correlation function $\langle O_i O_j \rangle$ as a function of $i-j$ to determine the mode of the order parameter.

A. Application I: Ferromagnetic long-range order

As a simple application, we take a spin chain with ferromagnetic long-range order as an example. We consider such a state,

$$|\Psi\rangle = \frac{1}{\sqrt{2}} (|↑↑\cdots↑↑\rangle + |↓↓\cdots↓↓\rangle).$$

For this state, we can find the minimum block size with which the mutual information does not vanish is 1. The reduced density matrix of a single spin is

$$\rho_i = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

in the basis of $\{|↑\rangle, |↓\rangle\}$. For any two spins at site $i$ and $j$, the reduced density matrix $\rho_{i;j}$

$$\rho_{i;j} = \begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2 \end{pmatrix},$$

in the basis of $\{|↑↑\rangle, |↓↓\rangle, |↑↓\rangle, |↓↑\rangle\}$. Therefore,

$$S(\rho_i) = 1,$$

and

$$S(\rho_{i;j}) = 1.$$

The mutual information between any two spins becomes

$$S(i|j) = S(\rho_i) + S(\rho_j) - S(\rho_{i;j}) = 1.$$
we have
\[ w_1 = -w_2. \] (38)

Let \( w_1 = 1 \), we find a traceless operator for the local site
\[ O_i = a_i^\dagger a_i - a_i^\dagger a_i, \] (39)

which actually is the Jordan–Schwinger representation of the \( z \)-component of Pauli matrix \( \sigma_i^z \).

Having found the order parameter, the next step is to determine the mode of the corresponding correlation function. From the two-site reduced density matrix \( \rho_{i\cup j} \), we have
\[ \langle a_j^\dagger a_i a_i a_j \rangle = \frac{1}{2}, \] (40)
\[ \langle a_j^\dagger a_i a_i a_j \rangle = \frac{1}{2}, \] (41)

which is independent of the distance between \( i \) and \( j \). Therefore, the correlation function is
\[ \langle \sigma_i^z \sigma_j^z \rangle - \langle \sigma_i^z \rangle \langle \sigma_j^z \rangle = 1. \] (42)

So in this case, the order parameter is \( \sigma^z \) with mode 0. For a comparison, we consider another state with antiferromagnetic long-range order,
\[ |\Psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow \cdots \uparrow\downarrow \rangle + |\downarrow\uparrow \cdots \downarrow\uparrow \rangle). \]

In a similar way, we can find that the order parameter is \( \sigma^z \). Nevertheless, we notice that for even \( |i - j| \)
\[ \rho_{i\cup j} = \begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2 \end{pmatrix}, \] (43)

while for odd \( |i - j| \)
\[ \rho_{i\cup j} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \] (44)

So the correlation function becomes
\[ \langle \sigma_i^z \sigma_j^z \rangle = 1, \text{ for even } |i - j| \] (45)
\[ \langle \sigma_i^z \sigma_j^z \rangle = -1, \text{ for odd } |i - j|. \] (46)

In this case, the order parameter is still \( \sigma^z \), however, the mode becomes \( \pi \).

**B. Application II: Dimer order**

Now let us consider a uniformly weighted superposition of the two nearest-neighbor valence bond state,
\[ |\psi_1\rangle = [1, 2][3, 4] \cdots [L - 1, L] \]
\[ |\psi_2\rangle = [L, 1][2, 3] \cdots [L - 2, L - 1] \] (47)

where
\[ [i, j] = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle_j - |\downarrow\uparrow\rangle_j). \]
The inner product \( \langle \psi_2 | \psi_1 \rangle \) decays exponentially with the system size, so the state we consider can be written as
\[ |\Psi\rangle = \frac{1}{\sqrt{2}} (|\psi_1 \rangle + |\psi_2 \rangle). \] (48)

The state is the ground state of the Majumdar-Ghosh model [10]. For a single spin, the reduced density matrix is
\[ \rho_i = \begin{pmatrix} 1/4 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 \\ 0 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 1/4 \end{pmatrix}. \] (49)

For two spins separated by a long distance
\[ \rho_{i\cup j} = \begin{pmatrix} 1/8 & 0 & 0 & 0 \\ 0 & 3/8 & -1/4 & 0 \\ 0 & -1/4 & 3/8 & 0 \\ 0 & 0 & 0 & 1/8 \end{pmatrix}. \] (50)

Therefore \( \rho_{i\cup j} = \rho_i \otimes \rho_j \), the \( S(i|j) = 0 \). There is no long-range spin-spin correlation. The results mean that the block including only one spin is too small to find the long-range correlation. So we let the block include two neighboring spins. The reduced density matrix of two spins at site \( i \) and \( i + 1 \) is
\[ \rho_i = \begin{pmatrix} 1/8 & 0 & 0 & 0 \\ 0 & 3/8 & -1/4 & 0 \\ 0 & -1/4 & 3/8 & 0 \\ 0 & 0 & 0 & 1/8 \end{pmatrix}. \] (51)

The matrix can be diagonalized as
\[ \rho_i = \frac{5}{8} |\varphi_{i,0}\rangle \langle \varphi_{i,0}| + \frac{1}{8} |\varphi_{i,1}\rangle \langle \varphi_{i,1}| \]
\[ + \frac{1}{8} |\varphi_{i,2}\rangle \langle \varphi_{i,2}| + \frac{1}{8} |\varphi_{i,3}\rangle \langle \varphi_{i,3}| \] (52)

where
\[ |\varphi_{i,0}\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle_i - |\downarrow\uparrow\rangle_i), \] (53)
\[ |\varphi_{i,1}\rangle = |\uparrow\rangle_i \downarrow\rangle_i, \] (54)
\[ |\varphi_{i,2}\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle_i + |\downarrow\uparrow\rangle_i) \] (55)
\[ |\varphi_{i,3}\rangle = |\downarrow\rangle_i \downarrow\rangle_i. \] (56)

are spin singlet state and spin triplet states respectively. Then the entropy
\[ S(\rho_i) = 3 - \frac{5}{8} \log_2 5. \]

For any two pairs of spin, if the distance \( |i - j| \) between them is even, the density matrix is of dim \( 16 \times 16 \). In the
basis of spin singlet and spin triplet states, the reduced density matrix \( \rho_{\alpha \beta} \) is diagonal

\[
\rho_{\alpha \beta} = \frac{1}{2} |\varphi_{\alpha,0} \varphi_{\beta,0} \rangle \langle \varphi_{\alpha,0} \varphi_{\beta,0} | + \frac{1}{32} I.
\]  

(57)

The entropy is

\[
S(\rho_{\alpha \beta}) = 5 - \frac{17}{32} \log_2 17.
\]

The mutual information between the two blocks can be evaluated as

\[
S(i|j) \simeq 0.269.
\]

The nonzero value of the mutual information between two spin pairs means that we can find the potential order parameter in their spectra. For this purpose, we define it as

\[
O_i = w_0 |\varphi_{i,0} \rangle \langle \varphi_{i,0} | + w_1 |\varphi_{i,1} \rangle \langle \varphi_{i,1} | + w_2 |\varphi_{i,2} \rangle \langle \varphi_{i,2} | + w_3 |\varphi_{i,3} \rangle \langle \varphi_{i,3} |.
\]  

(58)

Due to the symmetry among the three states \( \{|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle\} \), we let \( w_1 = w_2 = w_3 \). Then the traceless condition becomes

\[
\frac{5}{8} w_0 + \frac{3}{8} w_1 = 0.
\]  

(59)

Upon the normalization condition, we let \( w_0 = -1 \), we have

\[
O_i = - |\varphi_{i,0} \rangle \langle \varphi_{i,0} | + \frac{5}{3} |\varphi_{i,1} \rangle \langle \varphi_{i,1} | + \frac{5}{3} |\varphi_{i,2} \rangle \langle \varphi_{i,2} | + \frac{5}{3} |\varphi_{i,3} \rangle \langle \varphi_{i,3} |.
\]  

(60)

In terms of spin operators, the order parameter can be expressed as

\[
O_i = 1 + \frac{2}{3} \sigma_i \cdot \sigma_{i+1}.
\]  

(61)

The correlation function then can be calculated as

\[
\langle O_i O_j \rangle = \frac{5}{8} \quad \text{for even } |i - j|.
\]  

(62)

\[
\langle O_i O_j \rangle = \frac{1}{2} \quad \text{for odd } |i - j|.
\]  

(63)

The mode of the order parameter is therefore \( \pi \).

Traditionally, people use the operator \( \sigma_i \cdot \sigma_{i+1} \) to describe the spin dimer order. Except for a difference in a constant, the order parameter Eq. (61) obtained via our scheme is exactly the same as the traditional order parameter.

C. Application III: Diagonal versus off-diagonal long-range correlation

To see the off-diagonal long-range correlation, we take the ground state of the one-dimensional antiferromagnetic Heisenberg model as an example. The model Hamiltonian reads

\[
H = \sum_{j=1}^{N} (S_{j}^x S_{j+1}^x + S_{j}^y S_{j+1}^y + S_{j}^z S_{j+1}^z),
\]  

(64)

where \( S_{j}^x, S_{j}^y \) and \( S_{j}^z \) are spin-1/2 operators at site \( j \). The model has a global SU(2) symmetry, and can be exactly solved by the Bethe-ansatz method [12]. From the Bethe-ansatz solution, the energy spectra of the system, its ground state properties, and the thermodynamics of the system have been studied explicitly. Moreover, for the Heisenberg model, the function \( \langle S_j S_{j+r} \rangle \) now can be calculated by using the generation function method [13]. However, it is not our motivation to readdress all these interesting issues. Instead, to illustrate our scheme, let us forget all of the known results at the beginning.

Now suppose we do not know any information of long-range correlation existing in the ground state of the system, we can only calculate the ground state via numerical methods such as exact diagonalization and density-matrix renormalization group [14]. With this state, we find that the reduced density matrix of a single site is

\[
\rho_i = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}
\]

(65)

so the entropy \( S(\rho_i) = 1 \). For two separated spins, the reduced density matrix has the form

\[
\rho_{\alpha \beta} = \begin{pmatrix} u & 0 & 0 \\ 0 & w & z \\ 0 & 0 & u \end{pmatrix}
\]  

(66)

with \( 2u + 2w = 1, w \neq u, and z \neq 0 \). For instance, if \( |j-i| = 5 \), we have \( u \simeq 0.219, w \simeq 0.281, and z \simeq 0.062 [12] \), then \( S(\rho_{\alpha \beta}) \simeq 1.969 \). The mutual information becomes 0.031. Differ from the usual long-range order for which the mutual information tends to a constant as the distance between two blocks tends to infinite, we find the mutual information here decays algebraically and becomes zero finally. However, such a correlation still has a divergent correlation length, so it still differs also from the disordered state for which the correlation length is finite. To distinguish the correlation from disorder and long-range order, we call such a correlation as long-range correlation instead of long-range order.

Since \( w \neq u \), according to our scheme, we can find that, as discussed in the subsection III(A), the operator with diagonal long-range correlation is just \( \sigma_i^x = a_i^+ a_{i+1} - a_i^+ a_{i+2} \).

However, from the expression (66), we notice the off-diagonal element \( z \) is nonzero too. So we predict that there exist some kinds of off-diagonal long-range correlation. The potential operator can be defined as

\[
O_i = w a_i^+ a_{i+1} + w^* a_i^+ a_{i+1} + x (a_i^+ a_{i+2} + a_i^+ a_{i+1}) + y (a_i^+ a_{i+2} - a_i^+ a_{i+1})
\]

\[
= x O_i^x - y O_i^y.
\]  

(67)
Due to the exchange symmetry between $i$ and $j$, one can prove that $\langle O_x^i O_x^j \rangle = 0$. From the expression (66), we have

$$\langle a_{i1}^\dagger a_{i2} a_{j1}^\dagger a_{j2} \rangle = 0, \quad (68)$$
$$\langle a_{i1}^\dagger a_{i2} a_{j2}^\dagger a_{j1} \rangle = z, \quad (69)$$
$$\langle a_{i1}^\dagger a_{i2} a_{j2}^\dagger a_{j1} \rangle = z, \quad (70)$$
$$\langle a_{i2}^\dagger a_{i1} a_{j1}^\dagger a_{j2} \rangle = 0, \quad (71)$$

These equalities hold true if $\langle O_x^i O_x^j \rangle = \langle O_y^i O_y^j \rangle$. Therefore, both $O_x^i$ and $O_y^j$ (or their linear combination) can be regarded as the operator which has off-diagonal long-range correlation. From Eq. (67), we can see that $O_x^i$ and $O_y^j$ are the Jordan–Schwinger representation of the $x$ and $y$ components of Pauli matrices $\sigma_x^i$ and $\sigma_y^j$, respectively. A careful scrutiny may find that $u = w = z$, this equality which can be verified numerically means that $\langle \sigma_x^i \sigma_x^j \rangle = \langle \sigma_y^i \sigma_y^j \rangle$.

Having obtained the operators for diagonal and off-diagonal long-range correlation, we can find the mode of these operators by calculating the corresponding correlation functions. Take the $\langle \sigma_x^i \sigma_x^j \rangle$ as the example, we have $\langle \sigma_x^i \sigma_x^{i+1} \rangle = -0.59084$, $\langle \sigma_x^i \sigma_x^{i+2} \rangle = 0.242716$, $\langle \sigma_x^i \sigma_x^{i+3} \rangle = -0.200992$, $\langle \sigma_x^i \sigma_x^{i+4} \rangle = 0.138610$, therefore the mode of the correlation function $\langle \sigma_x^i \sigma_x^{i+r} \rangle$ is $\pi$. In the same way, the mode of the operators $\sigma_y^i$ and $\sigma_y^j$ are $\pi$ too.

Up to now, we have obtained the desired operators with antiferromagnetic long-range correlations. This kind of correlation is consistent with the definition of the Hamiltonian. The coefficient of each interaction term in the Hamiltonian is positive. The three terms $S_x^i S_x^{i+1}, S_y^i S_y^{i+1}, S_z^i S_z^{i+1}$ favor to form antiferromagnetic order in the ground state. From our analysis, we have $\langle \sigma_x^i \sigma_x^j \rangle = \langle \sigma_y^i \sigma_y^j \rangle = \langle \sigma_z^i \sigma_z^j \rangle$. The result can be explained from the global SU(2) symmetry of the Hamiltonian.

IV. SUMMARY

In summary, we have shown that the non-vanishing behavior of the mutual information at a long-range distance means the existence of long-range order. While the mutual information is operator-independent, we could still find the potential diagonal or off-diagonal order parameter from its spectra. A possible scheme to construct the order parameter was provided. Our scheme, as shown by also three simple examples, can not only find the diagonal order parameter, but also the off-diagonal order parameter. To find a correct order parameter is very important in various studies in the condensed matter physics, our scheme is therefore instructive for many condensed matter theorists to explore new physics in unknown quantum many-body systems.

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