Entanglement patterns and generalized correlation functions in quantum many body systems

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We define a generalized, entanglement-based correlation function related to the mutual information of two localized, typically single-site, subsystems of a larger many-body system. The two-site mutual information is defined in terms of the von Neumann entropy of the single-site and two-site density matrices, which, in turn, can be written in terms of expectation values of transition operators between localized states. It can be used to map out entanglement patterns between the subsystems, i.e., sites, of the system. Defining generalized correlation functions as two-point correlation functions of transition operators, we find that the long-distance decay of the mutual information follows the square of that of the most slowly decaying generalized correlation function. We show how the generalized correlation functions are related to conventional correlation functions for spin and fermion lattice models. We explore the behavior of the mutual information, the generalized correlation functions, and their relation for the general spin-1/2 Heisenberg model and for SU(n) Hubbard models with n = 2, 3, 4, and 5, demonstrating the principles on known phases of the spin and SU(2) Hubbard models and obtaining results characterizing the dimerized, trimerized, and quadrimerized phases in the SU(3), SU(4), and SU(5) Hubbard models, respectively. In addition, we extend the picture of the two-site mutual information and the corresponding generalized correlation functions to the n-site case.

I. INTRODUCTION

Phases of many-body systems are often characterized in terms of the long-distance behavior of spatial correlation functions. In particular, the decay of a correlation function to a finite value at long distance is characteristic of an ordered phase, exponential decay indicates a gapped or disordered phase, and power-law decay characterizes the entanglement between subsystems A and B. A number of quantitative measures of entanglement can be extracted from the eigenvalue spectrum and B. A number of quantitative measures of entanglement can be extracted from the eigenvalue spectrum.

The full description of a quantum mechanical system can be given in a pure state by the wavefunction $|\Psi\rangle$ or in a mixed state by the density matrix $\rho$. For a bipartite system in a pure state, information on the entanglement of the two parts of the system is encoded in the reduced density matrix of one subsystem,

$$\rho_A = \text{Tr}_B |\Psi\rangle \langle \Psi|,$$  

where we label the subsystem of interest A and the other subsystem B and Tr$_B$ means carrying out the trace over subsystem B. The eigenvalue spectrum of $\rho_A$ completely characterizes the entanglement between subsystems A and B. A number of quantitative measures of entanglement can be extracted from the eigenvalue spectrum.

The most commonly used measure is the von Neumann entropy $s_A$, which is given in a pure state by the wavefunction $|\Psi\rangle$, or in a mixed state by the density matrix $\rho$,

$$s_A = -\text{Tr} \rho_A \ln \rho_A;$$  

and in a mixed state by the density matrix $\rho$,

$$s_A = -\sum_{\alpha} w_{\alpha} \ln w_{\alpha}.$$

The Hilbert space of a finite many-body quantum system is formed by taking the tensor product of simple building-block systems, which we will denote as “sites”; here we generally take the sites to be local “finite Hilbert spaces” on a regular lattice. In Eq. (2), subsystem A can be formed, in general, from an arbitrary subset of the total set of sites. While the usual practice is to take one, two, or more neighboring sites, it can also be useful to form it from sites that are not adjacent on the lattice.

The number of sites included and where they are located on the lattice can be tailored to obtain specific information on the distribution of entanglement on the lattice, which can then be used to characterize the physical nature of the quantum phase of the system. For example, the scaling behavior of the von Neumann entropy of a contiguous block of sites with the number of sites has been used to study the quantum phases of one-dimensional systems. For systems with local interactions, this “block entropy” diverges logarithmically with block size for critical systems, but saturates for gapped systems, and it has more complex behavior when non-local interactions are present.
The scaling behavior of the entropy of particular subsystems such as the single-site, the nearest-neighbor two-site, and the block entropy as a function of microscopic control parameters can be used to detect and characterize many classes of quantum phase transitions.\textsuperscript{5, 14, 17–22} However, since topological states cannot be described by local order parameters, quantum phase transitions to such states must be detected by alternative means.\textsuperscript{21–28} For example, for two-dimensional systems with topological order such as the Heisenberg model on a kagome lattice, deviations of the block entropy from area-law scaling can be used to determine the topological order parameter.\textsuperscript{29, 31} In addition, a gap in the entanglement spectrum can be used to characterize topological order.\textsuperscript{23}

In the cases discussed above, the entanglement is measured between two subsystems of a bipartite partition of the total system. Thus, it characterizes all the correlations of quantum origin when the total system is in a pure state. While the dependence of these subsystem entropies on size and placement on the lattice can yield some information on spatial properties, they do not contain specific information on the entanglement between sites. In the present paper, we will consider correlations between two sites. Since two sites are embedded in a larger system, they are, in general, in a mixed state, leading to a more complicated picture of the origin of the correlations. The correlations can be of classical or of quantum origin; moreover, there are quantum correlations which are not due to entanglement.\textsuperscript{32}

A useful quantity to numerically characterize all kinds of correlations between pairs of sites is the mutual information

\[ I_{ij} = s_i + s_j - s_{ij}, \] (4)

calculated between two generally placed sites, \(i\) and \(j\). Here \(s_i\) is the von Neumann entropy, Eq. (2), for a subsystem \(A\) chosen to be the single site \(i\), and \(s_{ij}\) is the entropy for \(A\) chosen to consist of sites \(i\) and \(j\). The mutual information \(I_{ij}\) describes the correlation between the two selected subsystems, sites \(i\) and \(j\), embedded in a larger system. When studied for all pairs \(i\) and \(j\), it yields a weighted graph of the overall correlation of both classical and quantum origin in the lattice. The mutual information defined in this way has been used previously to study correlation between neighboring sites in spin and fermionic chains with local interactions\textsuperscript{34} and in quantum chemical problems in order to optimize the network structure\textsuperscript{35, 36} as well as to study molecular bonding properties in various transition metal complexes.\textsuperscript{16, 37–39} Our purpose here is to study its connection to conventional two-point correlation functions in quantum lattice models.

As we will discuss below, matrix elements of the two-site density matrix can be expressed in terms of expectation values of transition operators. These matrix elements have the form of generalized correlation functions and contain, by definition, all two-site correlations. Thus, there is no need for \textit{a priori} knowledge about the nature of the ordering in the system, i.e., no need to explicitly construct particular physical correlation functions. The two-site mutual information consists of a weighted average—in terms of the von Neumann entropy—of generalized correlation functions and, in fact, measures the strength of the entanglement bond between sites \(i, j\). However, it does not explicitly tell us what physical process is responsible for the entanglement in the system. Such information is contained, however, in the generalized correlation functions that make up the two-site density matrix from which the two-site mutual information is formed. The task, then, is to relate the generalized correlation functions to physically motivated correlation functions such as spin-spin, density-density, electron-hole, or pairing correlation functions.

Taking into account the amount and structure of entanglement is very important in developing numerical algorithms. For example, the structure of the variational matrix-product state (MPS) constructed in the density-matrix renormalization group (DMRG)\textsuperscript{40} is best suited to represent a one-dimensional short-range entanglement structure; thus the DMRG is highly effective for systems where such a structure is present.\textsuperscript{41–44} Although more general MPS-based algorithms can overcome some of the restrictions of the DMRG, such as the lack of translational invariance,\textsuperscript{55} all MPSs can only efficiently approximate a state with one-dimensional entanglement structure.

This limitation can be overcome by generalizing MPSs to tensor network states (TNS), a set of methods that promises to be substantially more efficient in higher dimensions and for systems with non-local interactions.\textsuperscript{51–54} Related methods have been used in numerical mathematics to approximate high-dimensional tensor spaces using low-rank tensor factorization methods.\textsuperscript{55} Since the computational cost of all of these methods is determined by the rank of the matrices and tensors,\textsuperscript{56} it is crucial to obtain as much knowledge as possible about the entanglement structure of the system under study and to incorporate this knowledge in the matrix or tensor structure of the state used to simulate the system.

In this paper, we present the general formulation of the two-site density matrix in terms of generalized correlation functions and show how the two-site mutual information can be related to the most important correlation functions. The paper is organized as follows. In Sec. \textbf{II} we describe the theoretical background. In Sec. \textbf{III} we demonstrate our approach on the one-dimensional, spin-1/2, anisotropic Heisenberg model with nearest and next-nearest neighbor interactions. In Sec. \textbf{IV} we present the spatial entanglement pattern for the SU(\(n\)) Hubbard model at various commensurate fillings and, based on the generalized correlation functions, identify the underlying relevant physical processes. Finally, Sec. \textbf{V} contains our conclusions.
II. THE ONE- AND TWO-SITE DENSITY MATRIX

A. Calculation of the one- and two-site density matrices

The \(N\)-site wave function can be written in terms of the single-site \(q\)-dimensional basis as

\[
|\psi\rangle = \sum_{\alpha_1,\ldots,\alpha_N} C_{\alpha_1,\ldots,\alpha_N} |\alpha_1\rangle \cdots |\alpha_N\rangle ,
\]

where the \(\alpha_j\) denote single-site basis states and the set of coefficients \(C_{\alpha_1,\ldots,\alpha_N}\) can be viewed as an \(N\)-th order tensor. The two-site reduced density matrix, \(\rho_{ij}\), can be calculated by taking the trace of \(|\psi\rangle \langle \psi|\) over all local bases except for \(\alpha_i\) and \(\alpha_j\), the bases of sites \(i\) and \(j\), i.e.,

\[
\rho_{ij}([\alpha_i',\alpha_j'],[\alpha_i,\alpha_j]) = \sum_{\alpha_1',\ldots,\alpha_{i-1}',\alpha_i',\alpha_{i+1}',\ldots,\alpha_N} C_{\alpha_1',\ldots,\alpha_{i-1}',\alpha_i',\alpha_{i+1}',\alpha_{i+2}',\ldots,\alpha_N}
\times C_{\alpha_1,\ldots,\alpha_{i-1}',\alpha_i',\ldots,\alpha_N} .
\]

Matrix elements of the single-site density matrix \(\rho_i(\alpha_i',\alpha_i)\) are calculated similarly, except that only \(\alpha_i\) is excluded in the trace. The dimension of \(C\) grows exponentially with system size \(N\); thus, such full tensor representations of the wave function are only possible for small system sizes.

Fortunately, the \(N\)th-order tensor \(C\) can, in many cases, be efficiently factorized into a product of matrices,

\[
C_{\alpha_1,\ldots,\alpha_N} = A_{\alpha_1} \cdots A_{\alpha_N} ,
\]

leading to a MPS representation of the wave function, where the \(A_{\alpha_i}\) are \(M\times M\) matrices in general. For systems with open boundary conditions, \(A_{\alpha_i}\) and \(A_{\alpha_N}\) are row and column vectors, respectively. In the MPS representation, the calculation of \(\rho_{ij}\) by means of Eq. (6) corresponds to the contraction of the network over all states except those at sites \(i\) and \(j\), as depicted in Fig. 1 for a chain with \(N = 8\) sites.

![Fig. 1.](image)

FIG. 1. Contraction of the MPS network to calculate the two-site reduced density matrix for a chain with \(N = 8\).

In the MPS-based two-site DMRG method, the system is divided into four subsystems, and \(|\psi\rangle\) is formed from the tensor products of the corresponding Hilbert spaces as

\[
|\psi\rangle = \sum_{\alpha_1,\alpha_{i+1},\alpha_{i+2},\alpha_r} C_{\alpha_1,\alpha_{i+1},\alpha_{i+2},\alpha_r} |\phi^{(l)}_{\alpha_1}\rangle |\alpha_{i+1}\rangle |\alpha_{i+2}\rangle |\phi^{(r)}_{\alpha_r}\rangle .
\]

Here \(|\phi^{(l)}_{\alpha_1}\rangle\) and \(|\phi^{(r)}_{\alpha_r}\rangle\) denote the \(M\)-dimensional basis of a renormalized \(l\)-site or \(r\)-site block, respectively, where \(l + 2 + r = N\). As the DMRG procedure is carried out, operators needed to represent the Hamiltonian of a given model or to carry out measurements are iteratively transformed into the multi-site block basis. For a given partitioning, expectation values can be calculated within this basis. If the transformation matrices \(O\), which have dimension \(M \times (M \cdot q)\), are also stored, the MPS wave function can be formed by identifying \(O[q]\langle M, M\rangle \equiv A_{\alpha_1}(M, M)\). Calculating the one- and two-site reduced density matrices is also possible, as worked out for spin-1/2 fermion models in Refs. 35,38, but is less straightforward because the DMRG wave function is represented in terms of multi-site renormalized block basis states.

B. Expression in terms of generalized correlation functions

The trace in Eq. (8), as carried out over the MPS wave function given by Eq. (8), can be decomposed into a sum of projection operators related to the bases described by the free variables \(\alpha_i\) and \(\alpha_j\). That is, the matrix representation of the one-site reduced density matrix \(\langle \alpha_i' | \rho_i | \alpha_i \rangle\) can be constructed from operators describing transitions between the single-site basis states \(|\alpha_i\rangle\), and the two-site density matrix \(\langle \alpha_i' \alpha_j' | \rho_{ij} | \alpha_i \alpha_j \rangle\) can be constructed from operators describing transitions between two-site basis states \(|\alpha_i \alpha_j\rangle\). This is a generalization of the procedure introduced in the DMRG context for spin-1/2 fermion models in Refs. 35,38. In the following, we refer to expectation values of pairs of state-transition operators as generalized correlation functions in order to distinguish them from conventional correlation functions, i.e., those based on physically motivated operators such as local spin or density operators.

For a \(q\)-dimensional local Hilbert space, we can represent transitions between the basis states using \(q^2\) possible transition operators \(T^{(m)}\) with \(m = 1 \cdots q^2\). The structure of the \(q \times q\) operators \(T^{(m)}\) is simple: each operator contains only a single non-vanishing element with the value one at matrix position \(\alpha', \alpha\), where \(|\alpha\rangle\) is the initial state and \(|\alpha'\rangle\) is the final state; explicitly, \((T^{(m)})_{\alpha',\alpha} = \delta_{\alpha + q(\alpha - 1),m}\). It thus acts like a transition matrix from state \(|\alpha\rangle\) to \(|\alpha'\rangle\), i.e., \(T^{(m)}\) transforms the state \(|\alpha\rangle\) with \(\alpha = (m - 1)(\text{mod } q)\) into state \(|\alpha'\rangle\) with \(\alpha' = [(m - 1)/q] + 1\), \(T^{(m)}|\alpha\rangle = |\alpha'\rangle\), where \([x]\) denotes the floor function, the integral part of \(x\). These operators can be extended to operate on the complete Hilbert space consisting of \(N\) local Hilbert spaces labeled...
by $i = 1, \ldots, N$ as
\[
T_i^{(m)} = \bigotimes_{j=1}^{i-1} \mathbb{1} \otimes T_i^{(m)} \otimes \bigotimes_{j=i+1}^{N} \mathbb{1},
\]
where the operators on the right-hand side act on the appropriate local single-site basis, and $\mathbb{1}$ is the identity operator on the local basis. For the many-electron wave function, the matrix elements of the one and two-site reduced density matrices can be expressed in terms of expectation values of products of $T_i^{(m)}$ operators acting on specific sites. When the individual local states are completely distinguished by abelian quantum numbers, the one-site density matrix is diagonal and has the form
\[
\rho = \rho_{ij} \delta_{ij},
\]
where $\rho_{ij}$ are the initial and final states, respectively, on spatial site $i$. Thus, reduced density matrices can be expressed in terms of expectation values of two-site operator products. The two-site reduced density matrix $\rho_{ij}$ has non-zero matrix elements only between two-site states possessing the same quantum numbers because $\rho_{ij}$ does not change the quantum numbers of the two sites (i.e., $\rho_{ij}$ is block-diagonal in the two-site product basis), reducing the number of matrix elements that need be calculated. The symmetry properties of $\rho_{ij}$ further reduce the number of expectation values to be determined.

Once the two-site reduced density matrix $\rho_{ij}$ is constructed, $s_{ij}$ can be determined from its eigenvalues $w_{ij, \alpha}$ using Eq. (3), and the mutual information can be calculated using Eq. (11). An important feature of this method is that one can also analyze the sources of entanglement encoded in $I_{ij}$ by studying the behavior of the matrix elements of $\rho_{ij}$. We term the expectation values $(T_i^{(m)} T_j^{(n)}) = \langle \Psi | T_i^{(m)} T_j^{(n)} | \Psi \rangle$ generalized correlation functions. As we will see below, they can be used to identify the relevant physical processes that lead to the generation of the entanglement.

It is important to take into account that when $\rho_{ij}$ is calculated, the system is decomposed into three subsystems, so that the usual definitions of entanglement, which assume a bipartite division, must be extended. For a tripartite system, the wave function can be written
\[
|\Psi\rangle = \sum_{\alpha, \alpha', \beta} C_{\alpha, \alpha', \beta} |\alpha_i, \alpha_j, \beta\rangle,
\]
where $\alpha_i$ and $\alpha_j$ label the bases of the sites $i$ and $j$, and $\beta$ labels the basis of the environment, which is composed of the remaining sites. A given generalized correlation function describes the transition from a particular initial state to a particular final state. It can be expressed in terms of the coefficients of the corresponding wave function in the tripartite basis as
\[
\langle T_i^{(m)} T_j^{(n)} \rangle = \sum_{\alpha_i, \alpha_j, \beta} \sum_{\alpha_i', \alpha_j', \beta'} C_{\alpha_i', \alpha_j', \beta'}^{*} C_{\alpha_i, \alpha_j, \beta} \langle \alpha_i' \alpha_j' \beta' | T_i^{(m)} T_j^{(n)} | \alpha_i, \alpha_j, \beta \rangle = \sum_{\beta} C_{l(m), l(n), \beta}^{*} C_{r(m), r(n), \beta},
\]
where $r(m) = (m-1)(mod q)$ and $l(m) = \lfloor (m-1)/q \rfloor + 1$. A given generalized correlation function measures the expectation value of the resonance amplitude between the initial and final states within a particular environment. Thus, its value depends on the amplitude of the coefficients of the two states. For example, it can be used to characterize the singlet valence bond between sites with spin-1/2 degrees of freedom.

In general, $\langle T_i^{(m)} T_j^{(n)} \rangle$ contains both connected and disconnected contributions between subsystems $i$ and $j$. Therefore, it can, in general, scale to a finite value as the distance $l = |i - j|$ is increased. Note that this can occur even if the many-body state is not characterized by long-range order, i.e., even if the physical correlation function go to zero for large $l$. In order to circumvent this behavior, we generally study the connected part of the generalized correlation functions,
\[
\langle T_i^{(m)} T_j^{(n)} \rangle_C = \langle T_i^{(m)} T_j^{(n)} \rangle - \langle T_i^{(m)} \rangle \langle T_j^{(n)} \rangle,
\]
where the disconnected part, given by the product of the expectation values of the local transition operators, is subtracted out. Note that the mutual information is formulated in such a way, Eq. (4), that the disconnected parts of the general correlation functions do not contribute. However, there is no way to express $I_{ij}$ directly as a function of the connected parts of the generalized correlation functions.

The spatial behavior of the correlation functions depends essentially on the type of intermediate states for which the matrix elements of $T_i^{(m)}$ and $T_j^{(n)}$ are finite between these states and the ground state. Different $T_i^{(m)}$ operators may transfer the ground state to the same intermediate state and, therefore, different generalized correlation functions may have similar properties. Therefore, we can classify the generalized correlation functions according to their type of decay. This behavior will also be investigated in detail in the following sections.

C. Example: spin-1/2 case

As an example, we first consider a spin-1/2 model. The local Hilbert space is two-dimensional and is spanned by the spin-up basis state $|\uparrow\rangle$ and the spin-down basis state $|\downarrow\rangle$. The action of the four possible $T^{(m)}$ is summarized in Table I (for $m = 1 \ldots 4$). Their representations as standard one-site operators are given as

\[ T_i^{(1)} = -S_i^- + \frac{1}{2} \mathbb{1}, \quad T_i^{(2)} = S_i^-, \]
\[ T_i^{(3)} = S_i^+, \quad T_i^{(4)} = S_i^+ + \frac{1}{2} \mathbb{1}. \]  

Using these definitions, we can express the physical correlation functions, $G_{ij}$, directly in terms of the generalized correlation functions,

\[ G_{ij}^{xx} = \langle S_i^x S_j^x \rangle = \frac{1}{4} \left( \langle T_i^{(2)} T_j^{(3)} \rangle + \langle T_i^{(3)} T_j^{(2)} \rangle \right), \]
\[ G_{ij}^{yy} = \langle S_i^y S_j^y \rangle = \frac{1}{4} \left( \langle T_i^{(2)} T_j^{(3)} \rangle + \langle T_i^{(3)} T_j^{(2)} \rangle - \langle T_i^{(3)} T_j^{(3)} \rangle \right), \]
\[ G_{ij}^{zz} = \langle S_i^z S_j^z \rangle = \frac{1}{4} \left( \langle T_i^{(1)} T_j^{(4)} \rangle + \langle T_i^{(4)} T_j^{(1)} \rangle \right) - \langle T_i^{(1)} T_j^{(1)} \rangle - \langle T_i^{(4)} T_j^{(4)} \rangle. \]  

For the most general spin Hamiltonian, all generalized correlation functions might be different. In the rest of the paper, we will consider the XXZ Heisenberg model in which $\langle T_i^{(2)} T_j^{(2)} \rangle = \langle T_i^{(3)} T_j^{(3)} \rangle = 0$ and $\langle T_i^{(2)} T_j^{(3)} \rangle = \langle T_i^{(3)} T_j^{(2)} \rangle$. In addition, due to up-down symmetry $\langle T_i^{(1)} T_j^{(1)} \rangle$, $\langle T_i^{(4)} T_j^{(4)} \rangle$ are not independent and they are related to $\langle S_i^z \rangle$ and $\langle S_j^z \rangle$. On the other hand, as was mentioned earlier, the matrix elements of $\rho_{ij}$ can be expressed in terms of the same generalized correlation functions. The non-vanishing matrix elements are shown for the XXZ model in Table II where, for easier readability, the notation $m/n$ is used for $\langle T_i^{(m)} T_j^{(n)} \rangle$.

| $\rho_{ij}$ | $|\downarrow\rangle_i |\downarrow\rangle_j$ | $|\downarrow\rangle_i |\uparrow\rangle_j$ | $|\uparrow\rangle_i |\downarrow\rangle_j$ | $|\uparrow\rangle_i |\uparrow\rangle_j$ |
|------------|------------------|------------------|------------------|------------------|
| $|\downarrow\rangle_i |\downarrow\rangle_j$ | $1/1$ | $1/4$ | $2/3$ | $3/2$ |
| $|\downarrow\rangle_i |\uparrow\rangle_j$ | $1/4$ | $4/1$ | $1/4$ | $4/1$ |
| $|\uparrow\rangle_i |\downarrow\rangle_j$ | $1/4$ | $4/1$ | $1/4$ | $4/1$ |
| $|\uparrow\rangle_i |\uparrow\rangle_j$ | $1/4$ | $4/1$ | $1/4$ | $4/1$ |

TABLE II. Block-diagonal form of the two-site reduced density matrix expressed in terms of generalized correlation functions. Here $m/n$ denotes $\langle \Psi | T_i^{(m)} T_j^{(n)} | \Psi \rangle$.

The eigenvalues of the two-site density matrix $\omega^{(\alpha)}$ ($\alpha = 1, \ldots, 4^2$) can easily be calculated. Two of the eigenvalues are determined by the $1 \times 1$ blocks given by $\langle T_i^{(1)} T_j^{(1)} \rangle$ and $\langle T_i^{(4)} T_j^{(4)} \rangle$ and can be expressed as

\[ \omega_{ij}^{(1)} = \frac{1}{4} - \frac{1}{2} \langle S_i^+ S_j^- \rangle + \frac{1}{2} \langle S_i^- S_j^+ \rangle, \]
\[ \omega_{ij}^{(2)} = \frac{1}{4} + \frac{1}{2} \langle S_i^+ S_j^- \rangle + \frac{1}{2} \langle S_i^- S_j^+ \rangle. \]  

Here we consider specifically the $S_i^z = \sum_i S_i^z = 0$ sector for which $\langle S_i^z \rangle = 0$; the expressions above can then be simplified to

\[ \omega_{ij}^{(1)} = \omega_{ij}^{(2)} = 1/4 + \langle S_i^z S_j^z \rangle. \]  

In order to obtain the two other eigenvalues, the $2 \times 2$
In general, the eigenvalues scale to a constant value as a function of the distance \( l = |i - j| \). For example, when sites \( i \) and \( j \) are uncorrelated, both \( \langle S_i^z S_j^z \rangle \) and \( \langle S_i^+ S_j^- \rangle \) vanish, and \( \omega_{ij}^{(0)} = 1/4 \) for all \( \alpha \). This means that the two-site subsystem is in a maximally mixed state, and all \( q^2 \) states are equally probable. As a consequence, \( I_{ij} = 0 \) since \( s_{ij}(2) = \ln 4 \) and \( s_{ij}(1) = s_j(1) = \ln 2 \).

In contrast, for the ferromagnetic ground state, an example of an ordered state, \( \langle S_i^z S_j^z \rangle = 1/4, \langle S_i^+ S_j^- \rangle = 1/2, \) and \( \langle S_i^+ S_j^- \rangle = 0 \); thus, \( \omega_{ij}^{(0)} = 1 \) and \( \omega_{ij}^{(0)} = 0 \) for \( \alpha = 1, 2, 3 \). Since the two-site subsystem is in a pure state, it is fully separable from the rest of the system. The correlation between sites \( i \) and \( j \), as given by the mutual information \( I_{ij} \), is also zero, since \( s_i(1) = s_j(1) = 0 \). The decay rate for a given eigenvalue, however, can depend on more than one correlation function. Therefore, in order to determine the exponent of the decay of the eigenvalues in the \( l \to \infty \) limit, one has to analyze all the generalized correlation functions that comprise a particular eigenvalue.

The asymptotic behaviour of the mutual information can also be determined in terms of the asymptotic behavior of the generalized correlation functions. When the expectation values of the generalized correlation functions become small for large distance \( l = |i - j| \), the von Neumann entropy for two sites, \( s_{ij}(2) = -\sum_\alpha \omega_{ij}^{(0)} \ln \omega_{ij}^{(0)} \), can be series-expanded using \( \ln (1 + x) \approx x - \frac{x^2}{2} \), when \( x \ll 1 \). In order to determine the leading terms in \( s_{ij}(2) \), we keep the second-order terms in the series expansion and obtain

\[
\ln \omega^{(1)} = \ln \left( \frac{1}{4} \left( 1 + 4 \langle S_i^z S_j^z \rangle \right) \right) \\
\approx \ln \frac{1}{4} + 4 \langle S_i^z S_j^z \rangle - 8 \langle S_i^z S_j^z \rangle^2
\]  

and

\[
\ln \omega^{(3)} = \ln \left( \frac{1}{4} \left( 1 - 4 \langle S_i^z S_j^z \rangle + 4 \langle S_i^+ S_j^- \rangle \right) \right) \\
\approx \ln \frac{1}{4} - 4 \left( \langle S_i^z S_j^z \rangle + \langle S_i^+ S_j^- \rangle \right) \\
- 8 \left( \langle S_i^z S_j^z \rangle + \langle S_i^+ S_j^- \rangle \right)^2.
\]

Inserting these expressions into \( s_{ij} \), we obtain, to leading order,

\[
s_{ij} \approx \ln 4 - 8 \langle S_i^z S_j^z \rangle^2 - 4 \langle S_i^+ S_j^- \rangle^2
\]  

for large \( l = |i - j| \). Since \( s_i = \ln(2) \) is a constant, it follows from Eqs. (14) and (23) that \( I_{ij} \) decays as the square of the slowest decaying correlation function.

This analysis can be extended to higher spin values and to models with more than one quantum number. For example, for a spin-one model, the two-site density matrix contains 19 different generalized two-site correlation functions. For a spin-1/2 fermionic model, 36 different two-site general correlation functions have to be calculated; they are given explicitly in Ref. but are also summarized in Sec. For fermions with larger numbers of flavors, this number increases significantly. To indicate how this occurs, we summarize the number of nonzero matrix elements in the reduced two-site density matrix, i.e., the number of operator combinations to be calculated, in Table III for the models studied in the present work. Note that the number of non-vanishing independent correlation functions to be calculated can be reduced by taking into account up-down or left-right symmetries.

| Model           | \( q \) | \( N_{\text{ops}} \) |
|-----------------|--------|-------------------|
| S=1/2 spin      | 2      | 6                 |
| S=1 spin        | 3      | 19                |
| 2-flavor fermion| 4      | 36                |
| 3-flavor fermion| 8      | 216               |
| 4-flavor fermion| 16     | 1296              |
| 5-flavor fermion| 32     | 7776              |

TABLE III. Number of nonzero matrix elements of the two-site reduced density matrix for \( S \)-spin bosonic and \( S \)-flavor fermion systems with local Hilbert space dimension \( q \).

We note that the procedure outlined can be extended to obtain the \( n \)-site reduced density matrix. However, the structure of correlations as well as that of the entanglement becomes much more complicated if more than two sites are involved, and, accordingly, the relevant measures of correlations and their interpretations are not well-understood. Nevertheless, the correlation in the respective subsystems can be characterized by generalizations of the two-site mutual information. For example, the three-site correlation can be defined as a Venn-diagram-based three-site generalization of the two-site mutual information,

\[
I_{ijk}^{(3)} = S(\rho_i) + S(\rho_j) + S(\rho_k) - S(\rho_{ij}) - S(\rho_{jk}) - S(\rho_{ik}) - S(\rho_{ijk}).
\]

The three-site reduced density matrix \( \rho_{ijk} \) can be expressed in straightforward way; Table IV gives its definition for the spin-1/2 case.

**D. Efficient calculation of the two-site density matrix**

In general, two-site operators in the DMRG method cannot be calculated accurately as a product of two one-site operators if sites \( i \) and \( j \) belong to the same DMRG
block, i.e.,

$$\langle \Psi | OT_i T_j O^\dagger | \Psi \rangle \neq \langle \Psi | OT_i O^\dagger | \Psi \rangle \langle \Psi | OT_j O^\dagger | \Psi \rangle,$$  \hspace{1cm} (25)

where $O$ is the DMRG transformation matrix. This is due to the truncation of the Hilbert space, so that $OO^\dagger \neq 1$. Therefore, all operators that have the form of two-site correlation functions must be renormalized and stored independently. These operators, however, can be calculated independently once the DMRG wave function is available so that the procedure can be parallelized very efficiently. The computational speedup scales roughly linearly with the number of correlation functions calculated. This well-known optimization has been implemented in our DMRG code for some time now. We transform the operators for the final basis for a given superblock configuration (i.e., for a given left and right partitioning of the lattice) using the transformation matrices obtained in previous iteration steps as

$$O_{l,l-1} \cdots O_{3,2} O_{2,1} T_i T_j O_{1,2}^\dagger O_{3,2}^\dagger \cdots O_{l,l-1}, i, j \in \text{Block}_l$$

$$O_{r,r-1} \cdots O_{3,2} O_{2,1} T_i T_j O_{1,2}^\dagger O_{3,2}^\dagger \cdots O_{r,r-1}, i, j \in \text{Block}_r$$

$$O_{l,l-1} \cdots O_{3,2} O_{2,1} T_j O_{1,2}^\dagger O_{3,2}^\dagger \cdots O_{l,l-1}, i \in \text{Block}_l$$

$$O_{r,r-1} \cdots O_{3,2} O_{2,1} T_j O_{1,2}^\dagger O_{3,2}^\dagger \cdots O_{r,r-1}, j \in \text{Block}_r.$$

Here $O$ is an $m' \times (m \cdot q)$ matrix, where $m'$ is determined using the dynamic block-state selection procedure\cite{56,57} with a predefined accuracy threshold $\chi$, and $l + 2 + r = N$ for the two-site DMRG. To illustrate the computational demands required, it took four days on 100 CPUs in parallel to calculate the 8000 correlation functions for the SU(5) Hubbard model with $N = 90$ lattice sites (our largest system size) using $M = 512$ block states.

### III. FRUSTRATED OR ANISOTROPIC SPIN-1/2 HEISENBERG CHAIN

In this section, we treat the spin-1/2 Heisenberg chain with additional frustration or anisotropy in order to investigate the properties of the generalized correlation functions and the two-site mutual information. The general Hamiltonian has the form

$$H = \sum_i J_1 \left[ \frac{1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + \Delta S_i^z S_{i+1}^z \right]$$

$$+ \sum_i J_2 \left[ \frac{1}{2} (S_i^+ S_{i+2}^- + S_i^- S_{i+2}^+) + \Delta S_i^z S_{i+2}^z \right], \hspace{1cm} (26)$$

where $S_i^+$ and $S_i^-$ are the spin raising and lowering operators, respectively, and $S_i^z$ is the $z$ component of the spin. Here $J_1$ and $J_2$ denote the strength of the nearest and next-nearest-neighbor couplings, respectively, and $\Delta$ parameterizes the anisotropy. We set $J_1 = 1$ without loss of generality. The geometry of the coupling terms of the frustrated Heisenberg chain is depicted in Fig. 2. For

$$\Delta = 1,$$

the phase diagram of the model as a function of $J_2/J_1$ is well-known\cite{59}. For $J_2 < 0.241$ the model is critical and behaves as a pure Heisenberg chain, while for $J_2 > 0.241$ a spin gap opens and the ground state is dimerized. At the Majumdar-Gosh point\cite{60} $J_2 = 0.5$, the model is exactly solvable. For larger $J_2$, the characteristic wave vector of the spin correlations moves continuously from $k = \pi/2$ to $\pi$, and the ground state is characterized by incommensurate oscillations\cite{61,62}.

### A. Entanglement pattern for finite systems

The elements of the two-site mutual information $I_{ij}$ give a map of the entanglement structure, which can be depicted graphically. In the remainder of the paper, all results shown are for finite systems with open boundary conditions. We start with the pure Heisenberg case, $J_2 = 0$; in Fig. 3 we display a density plot of $I_{ij}$. It can be seen that $I_{ij}$ scales to zero slowly with increasing distance $l = |i-j|$, i.e., sites are entangled with each other over a long range. Note that the two-site entropy $s_{ij}(2)$ scales to a finite value, ln $4$, for large $l$ and that the single-site entropy $s_i = \ln 2$, cancelling each other out in $I_{ij}$ for large $l$. The long-range entanglement structure is a consequence of the fact that the model at this point is critical, falling into the universality class of the Wess-Zumino-Witten model with central charge $c = 1$.

In contrast, at $J_2 = 0.5$, $I_{ij}$ is zero for all $l = |i-j| \geq 1$, except on alternating nearest-neighbor bonds, i.e., $i$ odd and $j = i + 1$, as can be seen in the graphical bond-strength plot in Fig. 4. Zero $I_{ij}$ values correspond to $s_{ij}(2) = \ln 4$, while nonzero values correspond to $s_{i,i+1}(2) = 0$, with $s_i = \ln 2$. This means that every other pair of nearest-neighboring sites form a maximally entangled pair and that each such pair is completely dis-
consider the critical exponents $\nu_a$ of the correlation functions $(S_i^a S_j^a) \sim |i - j|^{-\nu_a}$ with $a \in \{x, y, z\}$. The values of these critical exponents have a known dependence on $\Delta$,

$$\nu_x = \nu_y = 1/\nu_z = 1 - \arccos(\Delta)/\beta. \quad (27)$$

As discussed in Sec. II C the generalized correlation functions $(T_i^{(m)} T_j^{(n)})$ can be expressed directly in terms of the spin-spin correlation functions $(S_i^a S_j^a)$ and $(S_i^+ S_j^-)$, so that the $\nu_a$ in Eq. (27), should directly determine the behavior of $(T_i^{(m)} T_j^{(n)})$.

In general, the two-site correlation functions fall into groups characterized by the type of decay and, for algebraic decay, the value of the exponent, which we will denote by $\nu_{gk}$, where $k$ labels the group number. For example, the XXZ Heisenberg chain, Eq. (24) implies that there will be algebraic decay that falls into two groups in general, $\nu_x = \nu_y$, and $\nu_z = 1/\nu_x$, which coalesce into one group for $\Delta = 1$. In Fig. 5(a), we have plotted the connected part $(T_i^{(m)} T_j^{(n)})_C$ of the two independent generalized two-site correlation functions used to construct the two-site reduced density matrix (see Table II) as well as $I_{ij}$ itself as a function of $j$ for $i = 1$ for $\Delta = 1$ and various system sizes on a log-log scale. For the

**B. Scaling of the mutual information**

In order to further analyze the properties of $I_{ij}$, we consider first the $J_2 = 0$ case and vary $\Delta$ in Hamiltonian 24, i.e., take the interaction to be nearest-neighbor only, but with XXZ anisotropy. The ground state of the system is critical for $-1 < \Delta < 1$, and it has ferromagnetic and antiferromagnetic order for $\Delta \leq -1$ and $\Delta > 1$, respectively. In order to characterize the behavior, we entangled from the rest of the system. The ground state is a simple product state built from such singlet bonds, as is directly evident in Fig. 4.

**FIG. 3.** (Color online) Logarithmic density plot of the magnitude of the components of the two-site mutual information $I_{ij}$ for the isotropic spin-1/2 Heisenberg chain for $J_2 = 0$ on a 16-site chain.

**FIG. 4.** (Color online) Graphical representation of the magnitude of the components of the two-site mutual information for the isotropic frustrated spin-1/2 Heisenberg chain for $J_2 = 0.5$ on a $N = 32$-site chain. For clarity, the sites of the zigzag ladder are plotted on a circle and labeled by their position.

**FIG. 5.** (Color online) Decay of the connected part $(T_i^{(m)} T_j^{(n)})_C$ of the various two-site general correlation functions used to construct the two-site reduced density matrix for the SU(2) symmetric case, $\Delta = 1$, we find that both independent generalized correlation functions scale to zero algebraically as $l \rightarrow \infty$ with an exponent $\nu_3 = 0.95(3)$, i.e., they do, in fact, fall into a single group. The mutual information $I_{1,1}$ also decays to zero algebraically, $I_{1,1} \sim l^{\nu_3}$.
TABLE V. Characterization of the two-site correlation functions based on their decay type and the value of their exponent for the spin-1/2 anisotropic Heisenberg chain at $\Delta = 0.5$ with $N = 128$ sites. Here $\Delta S$ shows how $T^{(m)}_\nu$ changes the spin quantum number. The corresponding conventional correlation functions as given in Eq. (16) are indicated by $G$. Operator combinations in group 1 correspond to transverse components and in group 2 to the longitudinal component of the spin correlations. The exact critical exponents are $\nu_1 = 0.69(4)$, $\nu_2 = 2/3$, and $\nu_3 = 3/2$.

| Operator combination | Second quantized form | $\Delta S$ | $G$ |
|----------------------|-----------------------|------------|-----|
| $T^{(2/3)}_\nu$ | $S^+_i S^+_j$ | $-1$ | $G^{2x}$, $G^{2y}$ |
| $T^{(3/2)}_\nu$ | $S^+_i S^+_{j+1}$ | $1$ | $G^{2x}$, $G^{2y}$ |

For $\Delta \neq 1$, we summarize the content and behavior of the two groups of correlation functions, corresponding to longitudinal and transverse correlations, in Table V for $\Delta = 0.5$. We obtain $\nu_{g1} = 1.48(3)$ (exact value: $\nu_2 = 3/2$), $\nu_{g2} = 0.69(4)$ (exact value $\nu_2 = \nu_g = 2/3$), and $\nu_3 = 1.39(5)$ (exact value: $\nu_3 = 2 \times n_{g1} = 4/3$).

For $\Delta \neq 1$, we also find that the mutual information decays twice as fast as the slowest decaying correlation function, as can be seen explicitly in Fig. 3b. For a purely XX interaction, $\Delta = 0$, we obtain $\nu_{g1} = 0.52(5)$ for $\langle T^{(2/3)}_\nu \rangle$ (exact value: $\nu_2 = \nu_g = 0.5$), while $\langle T^{(1)}_\nu \rangle$, $\langle T^{(2)}_1 T^{(4)}_1 \rangle$, and $\langle T^{(3)}_1 T^{(4)}_1 \rangle$ decay with an exponent $\nu_{g2} = 2.15(8)$ (exact value: $\nu_2 = 2$). The mutual information decays with the exponent $\nu_3 = 1.07(3) \simeq 2 \times \nu_{g1}$.

Note that in order to obtain more accurate values for the critical exponents, we would have to carry out an accurate finite-size scaling, probably including non-leading effects such as logarithmic corrections. When the U(1) symmetry is broken, for example, by switching on a magnetic field, the operators split up into a larger number of groups, as $T^{(2/3)}_\nu \neq T^{(4)}_1 T^{(4)}_1$ and $T^{(3/2)}_\nu \neq T^{(4)}_1 T^{(4)}_1$. In higher spin sectors, we find the same relationship, but additional oscillations appear in the decay of the correlation functions, and $\langle S^+_i S^+_{j+1} \rangle$ scales to finite value due to the finite value of $S^+_i$.

Table 1 illustrates a similar analysis for finite values of $J_2$ for $\Delta = 1$ and in the 0.241 < $J_2$, the isotropic frustrated chain, in which the system is gapped due to the emergence of a bond-ordered ground state. We find that all two-site correlation functions as well as $I_1 l$ decay exponentially with $l$. We find that the decay length of $I_1 l$ is half of the longest correlation length obtained for the two-site generalized correlation functions, i.e., $I_1 l$ decays as the square of the most slowly decaying correlation function, in accordance with the behavior found in the critical cases.

IV. SU(n) HUBBARD MODEL

In this section, we apply our method to the SU(n) symmetric Hubbard model for $n = 2, 3, 4, 5$ for commensurate fillings $f = p/q$, where $p$ and $q$ are relatively prime. The SU(n) Hubbard model has the Hamiltonian

$$\mathcal{H} = -t \sum_{i=1}^{N} \sum_{\sigma=1}^{n} (c^{\dagger}_{i \sigma} c_{i+1, \sigma} + c^{\dagger}_{i+1, \sigma} c_{i, \sigma}) + \frac{U}{2} \sum_{i=1}^{N} \sum_{\sigma, \sigma'} \delta_{n_i, \sigma} n_{i, \sigma'},$$

(28)

where $N$ is the number of sites in the chain. The operator $c^{\dagger}_{i \sigma}$ creates (annihilates) an electron at site $i$ with spin $\sigma$, where the spin index is allowed to take on $n$ different values. Here $n_{i, \sigma}$ denotes the particle-number operator, $t$ the hopping integral between nearest-neighbor sites, and $U$ the strength of the on-site Coulomb repulsion. For consistency, the spin (or, for $n > 2$, flavor) index of the operators will be indicated by a subscript index running from 1 to $n$, even for the SU(2) case. In what follows, we will take $t$ as the unit of energy.

By studying the length-dependence of the entropy of finite blocks of long chains, some of us showed in a previous work that the system has drastically different behavior depending on whether $q > n$, $q = n$, or $q < n$. In addition, by taking the Fourier transform of the oscillatory behavior of the block entropy, we were able to determine the position of soft modes in the excitation spectrum when the model is critical and the spatial inhomogeneity of the ground state when the system is gapped.

When $q > n$, the umklapp processes are irrelevant, and the model is equivalent to an $n$-component Luttinger liquid with central charge $c = n$. When $q = n$, the charge and spin modes are decoupled, and the umklapp processes open a charge gap for finite $U_c > 0$, while the spin modes remain gapless and the central charge $c = n - 1$. The value of $U_c$ is still a subject of debate, but it is known that the translational symmetry is not broken in the ground state for any $n$.

On the other hand, when $q < n$, the charge and spin modes are coupled, the umklapp processes open gaps in all excitation branches, and a spatially non-uniform ground state develops. Bond-ordered dimerized, trimer-
ized, or tetramerized phases can be found as the filling is varied. These known results are summarized in Table VI and a schematic plot of the spatial inhomogeneity of the ground state determined using dimerization entropy is shown in Fig. 6 for various fillings and \( n \) values.

| \( q = n \) | \( n \) | \( n-1 \) | \( \cos(n-1) \) | \( 2\pi p/n \) |
| \( q < n \) | \( n \neq 2 \) | \( \cos \) | \( 2\pi p/q \) |
| \( q > n \) | \( n \) | \( \cos(n-1) \) | \( 2\pi p/q \) |

TABLE VI. Central charge \( c \) and type of phase, as characterized by the number of soft modes in the charge and spin sectors (CxSy), for the \( p/q \)-filled SU\((n)\) Hubbard model.

A. The half-filled SU(2) Hubbard model

We first treat the simplest and best understood case, the SU(2) Hubbard model at half filling. For convenience, we use the standard notation \( \uparrow \) and \( \downarrow \) for the \( \sigma = \{1, 2\} \) spin states. For a spin-1/2 fermionic model, single-electron basis states can be empty, occupied with a single spin-down or spin-up electron, or doubly occupied. These states we denote as \( | \downarrow \rangle \), \( | \downarrow \rangle \), \( | \uparrow \rangle \), and \( | \uparrow \rangle \), respectively. Since the local basis is four-dimensional, 16 possible transition operators \( T_i^{(m)} \) as displayed in Table VII arise. They can be written explicitly in terms of local fermion creation \( c_{i\sigma}^\dagger \), annihilation \( c_{i\sigma} \) and density \( n_{i,\sigma} \) operators as

\[
T^{(1)} = (1 - n_{\uparrow})(1 - n_{\downarrow}), \quad T^{(2)} = (1 - n_{\uparrow})c_{\uparrow}^\dagger c_{\downarrow},
\]

\[
T^{(3)} = c_{\uparrow}(1 - n_{\downarrow}), \quad T^{(4)} = -c_{\downarrow}c_{\uparrow},
\]

\[
T^{(5)} = (1 - n_{\uparrow})c_{\downarrow}^\dagger, \quad T^{(6)} = (1 - n_{\uparrow})n_{\downarrow},
\]

\[
T^{(7)} = -c_{\uparrow}c_{\downarrow}^\dagger, \quad T^{(8)} = c_{\downarrow}n_{\downarrow},
\]

\[
T^{(9)} = c_{\uparrow}^\dagger(1 - n_{\downarrow}), \quad T^{(10)} = c_{\downarrow}^\dagger c_{\downarrow},
\]

\[
T^{(11)} = n_{\uparrow}(1 - n_{\downarrow}), \quad T^{(12)} = -n_{\uparrow}c_{\downarrow},
\]

\[
T^{(13)} = c_{\uparrow}^\dagger c_{\downarrow}, \quad T^{(14)} = c_{\downarrow}n_{\downarrow},
\]

\[
T^{(15)} = -n_{\uparrow}c_{\downarrow}^\dagger, \quad T^{(16)} = n_{\uparrow}n_{\downarrow}.
\]

Following the procedure outlined in Sec. II A the non-vanishing matrix elements of the two-site density matrix \( \rho_{ij} \) are given in Table VIII. Note that the two-site density matrix is block-diagonal in the particle number \( N_c \) and in the \( z \) component of the spin \( S_z \). The block-diagonal structure is evident, and the values of \( m \) and \( n \) appropriate for each matrix element are displayed.

| \( | \downarrow \rangle \) | \( | \downarrow \rangle \) | \( | \uparrow \rangle \) | \( | \uparrow \rangle \) | \( | \uparrow \rangle \) | \( | \uparrow \rangle \) |
| \( T^{(1)} \) | \( T^{(2)} \) | \( T^{(3)} \) | \( T^{(4)} \) | \( T^{(5)} \) | \( T^{(6)} \) |
| \( T^{(7)} \) | \( T^{(8)} \) | \( T^{(9)} \) | \( T^{(10)} \) | \( T^{(11)} \) | \( T^{(12)} \) |
| \( T^{(13)} \) | \( T^{(14)} \) | \( T^{(15)} \) | \( T^{(16)} \) |

TABLE VII. Single-site operators describing transitions between single-site basis states for a \( S = 1/2 \) spin system.

We analyze the decay properties of the various generalized correlation functions that appear in the operator decomposition of the reduced two-site density matrix, as given in Eq. 29 and Table VIII, and the two-site mutual information. Their behavior is displayed for \( U = 0 \) and \( U = 10 \) in Figs. 7 and 8. The exact critical exponents of conventional correlation functions, which have the form \( G_{ii+i+1} = \langle A_i A_{i+i+1} \rangle \sim l^{-\nu_c} \), where \( A \) is a single-site spin, density, fermion-creation, or pair-creation operator (see Table IX), are known from the effective conformal field theory and are related to the behavior of finite-size corrections to the ground state. They are determined by the operator content of \( A \), namely, by the number of creation and annihilation operators for up- or down-spin particles on the two branches (left and right) of the dispersion relation. The exponents depend in a relatively simple manner on four parameters, i.e., on how the operator \( A \) changes the number of electrons, \( \Delta N_c \), the spin, \( \Delta S_z \), and on the value of charge current \( J_z \) and spin current \( J_\sigma \). In general, the exponents depend on \( U \), and are known exactly in the limiting cases. They are summarized in Table IX for both the half-filled and the non-half-filled systems. At half filling, a metal-insulator transition takes place at \( U = 0 \), leading to different behavior for
for the operator decomposition of the reduced two-site density matrix and the mutual information on a log-log scale for the SU(2) Hubbard model at half filling and $U = 0$, calculated on a 128-site chain. The mutual information is indicated by blue diamonds, and the straight lines are the results of our fits.

$U = 0$ and $U > 0$. For the non-half-filled case, the prefactor of the leading term, which determines the critical exponent of the correlation function, may vanish in the $U \to \infty$ limit. Therefore, the $U = \infty$ case must be treated separately. For example, for finite but large $U$, $\nu_G_{nn} = 3/2$, whereas $\nu_G_{nn} = 2$ for $U = \infty$.

We can express the conventional correlation functions as linear combinations of the generalized correlation functions. For example, using the definitions of single-site transition operators as given in Eq. (29) and noting that

$$c_\uparrow = c_\uparrow (\mathbb{1} - n_\uparrow) + c_\downarrow n_\uparrow = \mathcal{T}^{(5)} - \mathcal{T}^{(15)},$$

$$c_\downarrow = c_\uparrow (\mathbb{1} - n_\downarrow) + c_\downarrow n_\downarrow = \mathcal{T}^{(9)} - \mathcal{T}^{(14)},$$

$$c_\uparrow = c_\uparrow (\mathbb{1} - n_\uparrow) + c_\downarrow n_\uparrow = \mathcal{T}^{(2)} - \mathcal{T}^{(12)},$$

$$c_\downarrow = c_\uparrow (\mathbb{1} - n_\downarrow) + c_\downarrow n_\downarrow = \mathcal{T}^{(3)} - \mathcal{T}^{(8)},$$

$$n_\uparrow = n_\uparrow (\mathbb{1} - n_\uparrow) + n_\downarrow n_\uparrow = \mathcal{T}^{(6)} - \mathcal{T}^{(16)},$$

$$n_\downarrow = n_\downarrow (\mathbb{1} - n_\downarrow) + n_\uparrow n_\downarrow = \mathcal{T}^{(11)} - \mathcal{T}^{(16)},$$

$$S^z = \frac{1}{2} (n_\uparrow - n_\downarrow) = \frac{1}{2} (n_\uparrow (\mathbb{1} - n_\downarrow) - n_\downarrow (\mathbb{1} - n_\uparrow)) = \frac{1}{2} (\mathcal{T}^{(11)} - \mathcal{T}^{(6)}),$$

TABLE VIII. The two-site reduced density matrix $\rho_{ij}$ for SU(2) fermions expressed in terms of single-site operators, $\mathcal{T}_i^{(m)}$ with $m = 1 \cdots 16$. For better readability only the operator number indices, $m$, are shown; thus, $m/n$ corresponds to $(\mathcal{T}_i^{(m)})_{j}^{(n)}$. Here $N_z$ and $S^z$ denote the particle-number and $z$ spin component quantum numbers of the two sites.

| $\rho_{ij}$ | $N_z = 0$, $S^z = 0$ | $N_z = 1$, $S^z = \frac{1}{2}$ | $N_z = 2$, $S^z = -\frac{1}{2}$ | $N_z = 1$, $S^z = \frac{3}{2}$ | $N_z = 2$, $S^z = -\frac{3}{2}$ | $N_z = 3$, $S^z = \frac{3}{2}$ | $N_z = 3$, $S^z = -\frac{3}{2}$ | $N_z = 4$, $S^z = 0$ |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| $\rho_0$ | $-$ | $-$ | $-$ | $-$ | $-$ | $-$ | $-$ | $-$ |
| $\rho_1$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ |
| $\rho_2$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ |
| $\rho_3$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ | $\frac{1}{2} \uparrow \downarrow$ |

TABLE IX. Conventional correlation functions and corresponding exact values of the critical exponents, where $n = n_1 + n_2, S^z = (n_1 - n_2)/2$ and $S^+ = c_\uparrow^\dagger c_\downarrow^\dagger$ with $\sigma \in \{1, 2\} \equiv \{\downarrow, \uparrow\}$ and $W = 4t$ is the bandwidth.
the conventional correlation functions can be written as

\[ G_{n,n} = \langle T_i^{(6)} T_j^{(6)} \rangle + 2 \langle T_i^{(6)} T_j^{(16)} \rangle + 2 \langle T_i^{(11)} T_j^{(6)} \rangle + 2 \langle T_i^{(11)} T_j^{(11)} \rangle + 2 \langle T_i^{(11)} T_j^{(16)} \rangle + 2 \langle T_i^{(16)} T_j^{(6)} \rangle + 2 \langle T_i^{(16)} T_j^{(11)} \rangle + 4 \langle T_i^{(16)} T_j^{(16)} \rangle, \]

\[ G^{zz} = \frac{1}{4} (\langle T_i^{(11)} T_j^{(11)} \rangle + \langle T_i^{(6)} T_j^{(6)} \rangle - \langle T_i^{(6)} T_j^{(11)} \rangle - \langle T_i^{(11)} T_j^{(6)} \rangle), \]

\[ G^{(+,-)} = \langle T_i^{(7)} T_j^{(10)} \rangle, \]

\[ G_{c\uparrow c\downarrow} = \langle T_i^{(5)} T_j^{(2)} \rangle - \langle T_i^{(5)} T_j^{(12)} \rangle - \langle T_i^{(15)} T_j^{(2)} \rangle + \langle T_i^{(15)} T_j^{(12)} \rangle, \]

\[ G_{c\uparrow c\uparrow} = \langle T_i^{(9)} T_j^{(3)} \rangle + \langle T_i^{(9)} T_j^{(8)} \rangle + \langle T_i^{(14)} T_j^{(3)} \rangle + \langle T_i^{(14)} T_j^{(8)} \rangle, \]

\[ G_{p^{(0)}} = \langle T_i^{(13)} T_j^{(4)} \rangle. \]

Note that for \( G_{c\downarrow c\downarrow} \) and \( G_{c\uparrow c\downarrow} \) the contribution of the fermionic phase factor should be included explicitly via \( T_i^{(m)} = \langle T_i^{(m)} \rangle \exp(i\pi \sum_{i=1}^{n} n_i) \). For \( U = 0 \), all generalized correlation functions and thus the mutual information decay algebraically due to soft modes at \( k = 0 \) and \( k = 2k_F \) in both the spin and charge sectors. These soft modes lead to a \( 2k_F \) oscillation in the leading terms. Grouping the operators according to their decay type and increasing value of the exponent (see Table X), we identify three groups. The correlation functions with the slowest algebraic decay are those in group 1. They are composed of operators describing single-particle transfer processes weighted by the occupation number of the spin-up and down-particle in various ways. Specifically, these generalized correlation functions have the form \( \langle A_i B_j A_i' B_j' \rangle \), where, for example, \( A \equiv c_{\uparrow} \) and \( B \) and \( B' \in \{n_2, 1 - n_2\} \). The corresponding single-site transition operators change the number of electrons by \( \Delta N_c = \pm 1 \) and the spin by \( \Delta S^z = \pm 1/2 \), and we obtain the exponent \( \nu_{G1} \sim 0.98(4) \). Operators in the generalized correlation functions falling into group 2 describe density-like correlations, \( \Delta N_c = 0 \), \( \Delta S^z = 0 \), and decay algebraically with an exponent \( \nu_{G2} \sim 3.89(6) \). The generalized correlation functions have the form \( \langle A_i B_j A_i' B_j' \rangle \) with \( A_i, A_i', B_j, B_j' \in \{n_1, n_2, (1 - n_1), (1 - n_2)\} \), and the corresponding single-site transition operators are related to basis states with odd numbers of particles. Operators falling into group 3 describe spin-, density-, and pair-like correlations \( \Delta N_c \in \{0, \pm 2\} \), \( \Delta S^z \in \{\pm 1, 0\} \), and decay algebraically with an exponent \( \nu_{G3} \sim 1.93(5) \). The corresponding single-site transition operators are related to basis states with even numbers of particles.

We now consider the physical correlation functions, in particular, the equal-time single and two-particle Green

\[
\begin{array}{c|c|c|c}
(m/n) & \text{Second quantized form} & \Delta N_c & \Delta S^z & G \\
\hline
(12/15) & [\pi_{n1} \pi_{n2}] \downarrow [\pi_{n1} \pi_{n2}^\dagger] \uparrow & -1 & 0.5 & G_{c\downarrow c\uparrow}^{(1)} \\
(2/15) & [\pi_{n1} \pi_{n2}] \downarrow [\pi_{n1} \pi_{n2}^\dagger] \downarrow & -1 & 0.5 & G_{c\uparrow c\downarrow}^{(1)} \\
(2/5) & [\pi_{n1} \pi_{n2}] \downarrow [\pi_{n1} \pi_{n2}^\dagger] \downarrow & -1 & 0.5 & G_{c\uparrow c\downarrow}^{(1)} \\
(3/14) & [\pi_{n1} \pi_{n2}] \downarrow [\pi_{n1} \pi_{n2}^\dagger] \downarrow & -1 & 0.5 & G_{c\uparrow c\downarrow}^{(1)} \\
(5/12) & [\pi_{n1} \pi_{n2}] \downarrow [\pi_{n1} \pi_{n2}^\dagger] \downarrow & 1 & -0.5 & G_{c\downarrow c\uparrow}^{(1)} \\
(9/8) & [\pi_{n1} \pi_{n2}] \uparrow [\pi_{n1} \pi_{n2}^\dagger] \downarrow & -1 & 0.5 & G_{c\downarrow c\uparrow}^{(1)} \\
(9/8) & [\pi_{n1} \pi_{n2}] \downarrow [\pi_{n1} \pi_{n2}^\dagger] \downarrow & -1 & 0.5 & G_{c\downarrow c\uparrow}^{(1)} \\
(11/11) & [\pi_{n1} \pi_{n2}] \downarrow [\pi_{n1} \pi_{n2}^\dagger] \uparrow & 0 & 0 & G_{mn}^{(1)} \\
(1/16) & [\pi_{n1} \pi_{n2}] \downarrow [\pi_{n1} \pi_{n2}^\dagger] \uparrow & 0 & 0 & G_{mn}^{(1)} \\
(1/1) & \{\pi_{n1} \pi_{n2}\} \downarrow \{\pi_{n1} \pi_{n2}\} \uparrow & 0 & 0 & G_{mn}^{(1)} \\
(1/14) & \{\pi_{n1} \pi_{n2}\} \downarrow \{\pi_{n1} \pi_{n2}\} \uparrow & 0 & 0 & G_{mn}^{(1)} \\
(1/3) & \{\pi_{n1} \pi_{n2}\} \downarrow \{\pi_{n1} \pi_{n2}\} \uparrow & 0 & 0 & G_{mn}^{(1)} \\
(6/11) & \{\pi_{n1} \pi_{n2}\} \downarrow \{\pi_{n1} \pi_{n2}\} \uparrow & 0 & 0 & G_{mn}^{(1)} \\
(6/6) & \{\pi_{n1} \pi_{n2}\} \downarrow \{\pi_{n1} \pi_{n2}\} \uparrow & 0 & 0 & G_{mn}^{(1)} \\
(7/10) & \{\pi_{n1} \pi_{n2}\} \downarrow \{\pi_{n1} \pi_{n2}\} \uparrow & 0 & 0 & G_{mn}^{(1)} \\
(7/10) & \{\pi_{n1} \pi_{n2}\} \downarrow \{\pi_{n1} \pi_{n2}\} \uparrow & 0 & 0 & G_{mn}^{(1)} \\
(11/16) & [\pi_{n1} \pi_{n2}] \downarrow [\pi_{n1} \pi_{n2}^\dagger] \uparrow & 0 & 0 & G_{mn}^{(1)} \\
(1/14) & \{\pi_{n1} \pi_{n2}\} \downarrow \{\pi_{n1} \pi_{n2}\} \uparrow & 0 & 0 & G_{mn}^{(1)} \\
(1/6) & \{\pi_{n1} \pi_{n2}\} \downarrow \{\pi_{n1} \pi_{n2}\} \uparrow & 0 & 0 & G_{mn}^{(1)} \\
(6/16) & \{\pi_{n1} \pi_{n2}\} \downarrow \{\pi_{n1} \pi_{n2}\} \uparrow & 0 & 0 & G_{mn}^{(1)} \\
(6/16) & \{\pi_{n1} \pi_{n2}\} \downarrow \{\pi_{n1} \pi_{n2}\} \uparrow & 0 & 0 & G_{mn}^{(1)} \\
\end{array}
\]

Table X. Similar to Table IX but for the half-filled SU(2) Hubbard model at \( U = 0 \). Generalized correlation functions \( \langle T_i^{(m)} T_j^{(m)} \rangle \) are denoted as \( (m/n) \), and only the \( m \leq n \) components are shown. Here \( \Delta N_c \) and \( \Delta S \) indicate how \( T_i^{(m)} \) changes the charge and spin quantum numbers, respectively. The corresponding conventional correlation functions, \( G \), are listed in the last column.

**FIG. 8.** (Color online) Correlation functions as in Fig. 7 but measured relative to the middle of the chain and for \( U = 10 \), with (a) the two groups of exponentially decaying functions plotted on a semi-logarithmic scale and (b) the two groups of algebraically decaying correlation functions plotted on a log-log scale, both as a function of distance \( l \). The straight lines are the results of our fits.
functions. According to Eq. (37), $G_{nn}$ can be expressed as a linear combination of generalized correlation functions from group 2 and group 3: therefore, the smallest $\nu$ of these two groups determine $\nu_{G_{nn}} \simeq 1.92(5)$, which is in agreement with the analytic result given in Table XI. According to Eqs. (38) and (39), $G^{zz}$ and $G^{+-}$ are composed of generalized correlation functions from group 3 only; we obtain $\nu_{G^{zz}} = \nu_{G^{+-}} \simeq 1.92(5)$, which is also consistent with the analytic result given in Table XI. According to Eq. (40), $G^{c_{\sigma}c_{\sigma}}$ is composed of generalized correlation functions from group 1 only; we obtain $\nu_{G^{c_{\sigma}c_{\sigma}}} \simeq 0.98(4)$, reproducing the analytic result given in Table XI. According to Eq. (41), $G^{(0)}_{c_{\sigma}}$ is composed of generalized correlation functions from group 3 only; we obtain with $\nu_{G^{(0)}_{c_{\sigma}}} = 1.92(6)$, in agreement with the analytic result given in Table XI. We have again confirmed that the mutual information decays twice as rapidly as the most slowly decaying correlation function, one which corresponds to one-particle transfer processes, and decays with the exponent $\nu_{I} = 1.95(4)$. This means that the quasi-long-range entanglement in the metallic case is due to one-particle-like hopping, as expected.

For $U = 10$, it is known from the analytic picture that the charge modes are gapped, while the spin modes are gapless. Thus, the correlation functions that couple to the charge mode are expected to decay exponentially, while those that couple to the spin mode are expected to decay algebraically. Classifying the correlation functions according to the type of decay and the value of the correlation length or the exponents as described above, we find two groups of exponentially decaying and two groups of algebraically decaying correlation functions, as summarized in Table XI. We find that the mutual information again decays twice as fast as the slowest algebraically decaying correlation functions; we obtain an exponent $\nu_{I} = 1.95(5) \simeq 2 \times 0.98(3)$. The most slowly decaying correlation functions ($\nu_{G_{f1}} = 0.98(3)$) are in group 1 and correspond to spin-flip excitations, $\Delta N_c = 0, \Delta S^c \in \{\pm 1, 0\}$, as is to be expected from the spin-density-like nature of the ground state. The

| Group-1(algebraic), $\nu_{G_{c_{\sigma}c_{\sigma}}} = 1.12(3)$ |
|------------------|-------------------------------|
| (12/15), (15/12), (5/12), (12/5), (3/14), (14/3), (8/14), (14/8), (2/15), (15/2), (8/9), (9/8), (9/2), (5/2), (3/9), (9/3) |

| Group-2(algebraic), $\nu_{G^{zz}} = 1.48(4)$ |
|------------------|-------------------------------|
| (7/10), (10/7), (1/11), (11/1), (6/11), (11/6), (1/6), (6/1), (1/11), (1/6), (6/1) |

| Group-3(algebraic), $\nu_{G^{+-}} = 2.47(4)$ |
|------------------|-------------------------------|
| (11/16), (16/11), (1/16), (16/1), (6/16), (16/6), (16/16) |

| Mutual information(algebraic), $\nu_{I} = 2.19$ |
|------------------|-------------------------------|
| (4/13), (13/4) |

TABLE XII. Similar to Table XI but for the quarter-filled SU(2) Hubbard model at $U = 10$. The corresponding single-site transition operators are summarized in Eq. (29). The generalized correlation functions ($\langle T^{(m)}_{i} T^{(n)}_{j} \rangle$) are denoted as $(m/n)$. Three groups with exponents $\nu_{G_{f1}} = 1.12(3)$, $\nu_{G_{f2}} = 1.48(4)$, and $\nu_{G_{f3}} = 2.47(4)$. Applying Eqs. (37)–(41), we obtain the corresponding exponents of the conventional correlation functions, $\nu_{G^{c_{\sigma}c_{\sigma}}} = 1.12(3)$, $\nu_{G^{c_{\sigma}c_{\sigma}}} = 1.48(4)$, and $\nu_{G^{(0)}_{c_{\sigma}}} \nu \simeq 2.47(4)$, again in agreement with the analytic results given in Table XI. The mutual information decays algebraically with an exponent $\nu_{I} = 2.19(4)$, indicating that the long-range entanglement is due to the one-particle hopping term.

![FIG. 9. (Color online) Finite-size scaling of the single-particle ($\Delta_{\text{band}}$) and pair ($\Delta_{\text{pair}}$) gap for the half-filled SU(2) Hubbard model at (a) $U = 0$ and (b) $U = 10$, illustrating that $2 \times \Delta_{\text{band}}(N) = \Delta_{\text{pair}}(N)$ for all $N$ and for $U = 0$ in the thermodynamic limit for $U = 10$, respectively.](image-url)
B. High-spin SU(n ≥ 3) Hubbard models

Next we consider high spin models, i.e., n ≥ 3 at half filling, f = 1/2, for large Coulomb interaction, U = 10. For half filling and finite U values, it has been shown using bosonization that the ground state is dimerized for even values of n [22]. The same scenario has also been shown numerically to occur for odd n values [23]. For n = 3 and q < n, only the half-filled case occurs; therefore, we investigate the behavior of the entanglement bonds only for n = 4 and n = 5. The entanglement pattern for a finite n = 4 chain of length N = 24 is shown in Fig. 10(a), finite-size scaling of the leading entanglement bonds in Fig. 10(b), and the resulting entanglement bonds in the thermodynamic limit in Fig. 10(c). It can be clearly seen that the strong and weak bonds alternate between nearest-neighbor pairs, as is expected for a dimerized phase.

![Diagram](image)

**FIG. 10.** (Color online) (a) Graphical representation of the components of the two-site mutual information for the SU(4) Hubbard model at half filling for N = 24 lattice sites. (b) Finite-size scaling of the leading entanglement bonds. (c) Entanglement pattern in the thermodynamic limit, with the width of the lines indicating the strength of the entanglement bonds. Entanglement bonds $I_{N/2,N/2-1}$, $I_{N/2,N/2-1}$, $I_{N/2,N/2-1,N/2-2}$, $I_{N/2+1,N/2+2}$, $I_{N/2+1,N/2+2}$, $I_{N/2,N/2-1}$ are denoted by the symbols ×, ◊, □, ○, and ◻, respectively.

Since the spin and charge modes are coupled and both modes are gapped, all generalized correlation functions decay exponentially, $G_{i+i'} = \langle A_i B_{i+i'} \rangle \sim \exp(-l/\xi)$ with $\xi$ the decay length, as can be seen in Fig. 11. We

![Diagram](image)

**FIG. 11.** (Color online) Similar to Fig. 8 but for the SU(4) Hubbard model at $f = 1/2$ filling and $U = 10$ calculated for a chain with $N = 60$ sites.

| $\xi$ | group number | $\Delta N_e$ | $\Delta S_e$ | Representative operator combination: $(T^{(m)}_n T^{(n)}_m)$ |
|-------|--------------|--------------|---------------|-------------------------------------------------|
| 2.32(4) | g1          | 0            | $±(3,±2,±1)$ | $(c_1 c_2 n_{34} n_{34}) (c_1 c_2 n_{34} n_{34})$ |
|       | g2          | 0            | 0             | $(n_1 n_2 (1-n_3) n_{4}) (n_1 n_2 (1-n_3) n_{4})$ |
| 1.92(3) | g3          | 0            | $±(4,±2,0)$   | $(c_1 c_2 c_3 c_4) (c_1 c_2 c_3 c_4)$ |
|       | g4          | 0            | 0             | $(n_1 n_2 n_{34} n_{34}) (n_1 n_2 n_{34} n_{34})$ |
| 1.25(4) | g5          | $±1$         | $±3,±2,±1$    | $(c_1 n_2 n_{34}) (c_1 n_2 n_{34})$ |
| 0.88(6) | g6          | $±1$         | $±3,±2,±1$    | $(c_1 c_2 c_3 n_{4}) (c_1 c_2 c_3 n_{4})$ |
| 0.61(8) | g7          | $±2$         | $±3,±2,±1$    | $(c_1 n_2 n_{34}) (c_1 n_2 n_{34})$ |
| 0.46(5) | g8          | $±2$         | $±3,±2,±1$    | $(c_1 c_2 c_3 n_{4}) (c_1 c_2 c_3 n_{4})$ |
| 0.36(7) | g9          | $±3$         | $±3,±2,±1$    | $(c_1 c_2 c_3 n_{4}) (c_1 c_2 c_3 n_{4})$ |
| 0.22(7) | g10         | $±4$         | 0             | $(c_1 c_2 c_3 n_{4}) (c_1 c_2 c_3 n_{4})$ |
| 0.16(4) | g11         | 1            | 1             | Mutual Information |

**TABLE XIII.** Categorization of the generalized correlation functions for the half-filled SU(4) Hubbard model at $U = 10$. We
of the eight parameters. The possible values of $\Delta N_c$ and $\Delta S^c$ corresponding to the eight different groups are given in Table XIV. In general, the single-site transition operators, $T_i^{(m)}$, can contain $r$ fermion operators and $4 - r$ density-like operators with $r = 0, \ldots, 4$. In addition, the $r$ fermion operators are constructed from various combinations of creation and annihilation operators with different spin values. Some representative operator combinations are listed in the last column of Table XIV. It is clear that the largest decay length corresponds to those generalized correlation functions where $A_i$ does not change the particle number, i.e., $\Delta N_c = 0$. These are the slowest decaying correlation functions and are collected in groups 1 and 2. Group 2 also includes single-site transition operators with $r = 0$ fermion operators, and they are related to components of spin- and density-like conventional correlation functions. In the subsequent groups, as the single-site transition operator adds more and more particles to the system, the corresponding decay length decreases. The fastest decaying correlation functions correspond to $\Delta N_c = 4$, which is the maximum value. In addition to the strong $\Delta N_c$ dependence, the decay length also depends on $\Delta S^c$ because the related single-site transition operators describe different spin-flip processes. Single-site transition operators in group 3, 5, 7, and 8 contain $r = 1, 2, 3$, and 4 fermionic creation operators and $4 - r$ density-like operators, respectively. Their corresponding decay length drops systematically by a factor of two within our numerical error. A similar tendency is observed for groups 2, 4, and 6. It is worth reiterating that the decay length of the slowest decaying generalized correlation function also decays exponentially with a decay length $\xi_i = 1.16 = \varepsilon_{1i}/2$. Therefore, it has half of the longest decay length of the slowest decaying generalized correlation function.

In order to further elucidate the origin of the behavior of the decay lengths of the different groups, we have calculated the band gaps formed by adding particles with different flavors as well as by adding particles with the same flavor. In both cases, the scaled gaps become equal in the thermodynamic limit, indicating that the level structure in the energy spectrum is uniformly spaced. A similar structure has been found in the spin sector as well. This behavior is shown for the one-half-filled SU(4) Hubbard model in Fig. 12. The fact that higher excitation gaps are integer multiples of the one-particle gap holds already for the finite chain with $N = 60$ lattice sites for which the decay lengths of the generalized correlation functions have been determined. These decay lengths are sometimes but not always integer multiples of each other. In addition, the observed trend for groups 3, 5, 7, and 8 and for groups 2, 4, and 6 is not linear. This can be understood by the fact that when band gaps are determined, the particles are added to the overall system. Thus, they are delocalized along the whole chain, whereas, for single-site transition operators with increasing $\Delta N_c$, more and more particles are added to a single-site subsystem. Higher excitations are possible in the latter case, so the decay length can decrease faster than the band gaps for the same $\Delta N_c$ values.

In summary, the slowest decaying generalized correlation functions belong to group 1, which have a decay length of $\varepsilon_{1i} = 2.32$. The two-site mutual information also decays exponentially with a decay length $\xi_i = 1.16 = \varepsilon_{1i}/2$. Therefore, it has half of the longest decay length of the slowest decaying generalized correlation function.

A similar analysis for $f = 1/3$, i.e., the one-third-filled case, is presented in Fig. 13. Note that highly entangled three-site units are connected by a single entanglement bond. The strengths of the extrapolated values of the entanglement bonds show that next-nearest-neighbor entanglement is also important within the three-site entangled units. In addition, the entanglement map has left-right symmetry with respect to the mid-point of the three-site unit. The characterization of the correlation functions is summarized in Table XIV and finite-size scaling of the relevant energy gaps is shown in Fig. 13. The scaled gaps become equal again in the thermodynamic limit, indicating an equidistant level structure in the energy spectrum of both the charge and spin sectors. According to Fig. 14, the decay length of the slowest decaying correlation function is $\xi_{1i} = 6.18(5)$, for which $\Delta N_c = 0$ and $\Delta S^c = 0$. The decay length of the two-site mutual information is $\xi_i = 3.02(4) = \varepsilon_{1i}/2$.

We consider the case of higher flavor number, $n = 5$, in order to study even more extended spatial entanglement patterns. For $f = 1/4$, i.e., the quarter-filled case, a quadrimerized phase occurs, as can be seen in Fig. 14. The highly entangled four-site units are connected by single entanglement bonds. The strengths of

![FIG. 12.](image-url) (Color online) Finite-size scaling of the band gaps related to adding (a) one, two, three, or four particles to the system and (b) the spin gap for the half-filled SU(4) Hubbard model at $U = 10$. The energy gap of an excited state measured with respect to the ground state is labeled by $\Delta\Delta N_1, \Delta N_2, \Delta N_3, \Delta N_4$, where $\Delta N_x$ shows the change in the number of particles with spin $\sigma$. Note that highly entangled three-site units are connected by a single entanglement bond. The strengths of the extrapolated values of the entanglement bonds show that next-nearest-neighbor entanglement is also important within the three-site entangled units. In addition, the entanglement map has left-right symmetry with respect to the mid-point of the three-site unit. The characterization of the correlation functions is summarized in Table XIV and finite-size scaling of the relevant energy gaps is shown in Fig. 13. The scaled gaps become equal again in the thermodynamic limit, indicating an equidistant level structure in the energy spectrum of both the charge and spin sectors. According to Fig. 14, the decay length of the slowest decaying correlation function is $\xi_{1i} = 6.18(5)$, for which $\Delta N_c = 0$ and $\Delta S^c = 0$. The decay length of the two-site mutual information is $\xi_i = 3.02(4) = \varepsilon_{1i}/2$.

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FIG. 13. (Color online) Similar to Fig. 10 but for the SU(4) Hubbard model at one-third-filling. The entanglement bonds $I_{N/2,N/2-1}$, $I_{N/2,N/2+1}$, $I_{N/2-1,N/2+3}$, $I_{N/2-2,N/2-3}$ are denoted by the symbols $\times$, $\Diamond$, $\Box$, and $\circ$, respectively.

FIG. 14. (Color online) Similar to Fig. 12 but for the one-third-filled SU(4) Hubbard model at $U = 10$.

The extrapolated values of the entanglement bonds indicate that next-nearest neighbor entanglement is present within the four-site structure. In addition, second- and third-nearest-neighbor entanglement bonds also acquire finite strengths in the thermodynamic limit.

V. CONCLUSION

In this paper, we have formulated a method to characterize entanglement patterns in correlated systems. The measure that we use is the two-site mutual information, which is formed from the von Neumann entropy of the two-site and one-site density matrices. We have shown that, in general, the reduced density matrix of an $n$-site subsystem can be expressed in terms of $n$-site generalized correlation functions, which can be related to all $n$-site correlation functions based on site-local operators. The mutual information can be generalized to the $n$-site case. The major part of this work, in particular, the numerical
symmetric generalized Hubbard model. For the half- and quarter-filled $n = 2$ case, we classify the generalized correlation functions into groups according to type of decay (algebraic or exponential) and rapidity of decay (value of exponent and correlation length, respectively). The classification is consistent with the known excitation spectra at these points. We find that the two-site mutual information again decays as the square of the most slowly decaying correlation functions at long distances.

For higher spin models, i.e., $n \geq 3$ at half filling for large Coulomb interaction, we have confirmed the expected entanglement pattern of the dimerized ground state in which strong and weak bonds between nearest-neighbor pairs alternate on successive bonds. For $n \geq 4$ at one-third-filling, highly entangled three-site units are connected by a single entanglement bond. Within such three-site units, next-nearest-neighbor entanglement is also important. For even higher numbers of flavors, $n \geq 5$ and at one-third-filling, we have again found three-site units with similar properties. On the other hand, at quarter filling, we have found highly entangled four-site units which are connected by single entanglement bonds. Within such entangled four-site units, second and third nearest-neighbor entanglement bonds also acquire finite strength in the thermodynamic limit.

Therefore, based on our numerical results, we conclude that for $f = 1/q$-filling and $q < n$, units of highly entangled $q$-site units are connected by single entanglement bonds in the ground state and within such entangled $q$-site units, first-, second-, and up to $q − 1$-neighbor entanglement bonds also acquire finite strength in the thermodynamic limit. In addition, due to gaps in all excitation branches, all generalized correlation functions, together with the two-site mutual information, decay exponentially. Based on the decay length, they fall into several groups. We have found that their decay lengths depend on how the corresponding single-site transition operator changes the number of particles and the spin, consistent with the picture obtained from conformal field theory. The two-site mutual information again decays as the square of the most slowly decaying correlation functions; these correlation functions can also be used to identify the elementary excitation gap.

We remark that our method can easily be incorporated into a wide class of matrix-product-state- and tensor-network-state-based methods, of which the the density-matrix renormalization group (DMRG) method is just one example. In particular, the method can be applied to higher-dimensional lattices to provide the basis for an optimization procedure to order matrix-product states and to construct efficient network topologies for tensor-network-state approaches. Extension of the present work to study three-body entanglement is part of our planned future work.

FIG. 16. (Color online) Similar to Fig. 10 but for the SU(5) Hubbard model at quarter-filling. Entanglement bonds $I_{N/2,N/2−1}$, $I_{N/2−1,N/2}$, $I_{N/2−2,N/2−1}$, $I_{N/2−3,N/2−2}$ are shown by symbols $\times$, $\circ$, $\square$, $\star$, $\circ$, $\star$, $\circ$, $+$, respectively.

calculations, concentrate on the two-site case.

For the $S = 1/2$ Heisenberg model, we have shown explicitly how the generalized correlation functions are constructed and have shown that the dominant long-distance behavior of the mutual information follows the square of the most slowly decaying correlation function, which decays algebraically as the inverse of the distance. The addition of a next-nearest-neighbor frustrating exchange to the isotropic model leads to the opening of a spin gap and exponentially decaying correlation functions. For this case, we have found that the dimer-product ground state at the exactly solvable Majumdar-Gosh point is reflected directly in the entanglement pattern of the mutual information. For the anisotropic Heisenberg model without frustration, both the generalized and the physical correlation functions can be divided into two groups that decay algebraically with different exponents. These exponents can be understood in terms of the known exact values for the transverse and longitudinal components of the spin correlations.

Finally, in Sec. LV we have applied the methods described previously to the one-dimensional SU($n$)-
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