A discriminating string order parameter for topological phases of gapped SU(N) spin chains

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I. INTRODUCTION

For a long time, the classification of distinct phases of matter was synonymous with Landau’s theory of symmetry breaking. The latter applies to systems where the symmetry of the Hamiltonian is spontaneously broken in the ground state, such as ferromagnets at sufficiently low temperature. Different phases can be distinguished in terms of order parameters which correspond to expectation values of local observables, e.g. the magnetization. Another hallmark of the theory is the existence of massless Goldstone modes if continuous symmetries are broken.

Landau’s paradigm was challenged with the advent of gapped physical systems in which distinct phases exist even though the ground state (or the ground states) preserves the same symmetries as the Hamiltonian. Such systems are characterized by topological order, a term that was originally coined for fractional quantum Hall systems. Since topological orders are usually related to discrete invariants, they enjoy protection against continuous deformations of the system. It might happen that protection against deformations is not solely due to topology but that it rather appears in conjunction with a symmetry which has to be preserved. In this case one speaks about symmetry protected topological orders.

The Haldane phase of SO(3) invariant antiferromagnetic spin chains based on $S = 1$ is one of the first and best understood examples of a non-trivial symmetry protected topological phase. For the interactions it is custom to choose a specific deformation of the Heisenberg Hamiltonian as a representative. The resulting model is commonly referred to as the AKLT chain. While the exact ground state for the Heisenberg Hamiltonian is not known, the AKLT chain provides a convenient laboratory which allows to establish several important properties of the Haldane phase with full mathematical rigor. In particular, the ground states of the AKLT Hamiltonian are known explicitly, both for periodic and for open boundary conditions. Moreover, it could be proven that the chain has a mass gap and that ground state correlation functions of local observables decay exponentially.

The evidence for the identification of the Haldane phase as a non-trivial topological phase of matter can be summarized as follows. First of all, open boundary conditions imply the existence of massless edge modes. The system thus exhibits a bulk-boundary correspondence which is widely regarded as a typical characteristic of non-trivial topological phases. It was later understood that the topological nature is due to symmetry fractionalization which allows the edge modes to carry a discrete $Z_2$-valued topological quantum number. Secondly, all these features can also be observed in a characteristic entanglement spectrum which provides a virtual realization of edges even in the presence of periodic boundary conditions. Finally, and most importantly for our present paper, there exists a non-local string order parameter sensitive to a kind of diluted anti-ferromagnetic order, which allows to distinguish the topologically trivial from the topologically non-trivial phase.

Various extensions of the AKLT setup to higher rank groups and supersymmetric systems have been considered, see e.g. Ref. 3, 8–11. Other generalizations include $q$-deformations of the symmetry group which can be used to describe anisotropic spin chains. In all these examples the matrix product (or valence bond) state formalism plays a crucial role. The latter has also proven extremely useful in connection with the classification of symmetry protected topological phases in general one-dimensional spin systems. Indeed, by now it is well known that topological phases can be distinguished based on the properties of (virtual) boundary modes that arise when the system is considered with open boundary conditions or when parts of the system are traced out. Matrix product states are relevant in this context since their boundary and entanglement properties are almost trivial to access. Also, there is a natural way to associate a so-called parent Hamiltonian to each matrix product state which, in turn, is realized as the ground state of the former.

The classification results just mentioned yield the number of potential topological phases and an explicit way...
of constructing a representative Hamiltonian for each of them. However, given an arbitrary physical system, i.e. a Hilbert space, a Hamiltonian and a symmetry, no universal recipe how to recover its topological class is known at present. Since all topological properties are encoded in the ground state wave functions, this is first of all due to the lack of knowledge of the latter. But even if the ground states are known exactly or approximately through a numerical calculation, the definition of a quantity which can be calculated efficiently and which can discriminate between all different topological phases is still an open problem. The degeneracy of massless edge modes might serve as a first indication but it still leaves ambiguities. Even access to the full entanglement spectrum (including the energy and all additional quantum numbers) might not be sufficient as long as the contributions from the two edges cannot clearly be separated from each other.

For this reason, the most promising route to a complete characterization of topological phases seems to be the definition of suitable non-local order parameters. Important progress in this direction has recently been achieved in Ref. 20 and 22 (see also Ref. 23 and 24). While these approaches seem to be sufficiently general to embrace continuous symmetry groups as well, the concrete implementations have mainly been concerned with discrete symmetries so far and do not cover the case of \( PSU(N) \).

In the present paper we will follow an alternative route and use it for the characterization of anti-ferromagnetic spin chains with \( PSU(N) \) symmetry. As has been shown in Ref. 21 there are \( N \) distinct topological phases which can be realized in such chains. These \( N \) phases correspond to the \( N \) different ways, the center \( Z_N \) of the group \( SU(N) \) can be realized on possible boundary spins. Just as in the \( SO(3) = SU(2)/Z_2 \) AKLT chain before, the situation can be understood as a fractionalization of the physical symmetry \( PSU(N) = SU(N)/Z_N \) in a setup with open boundary conditions. Our main result is an explicit expression for a string order parameter for \( SU(N) \) spin chains which can easily be evaluated once the ground state is known, see Eq. (13). In contrast to earlier approaches it is essential that our string order parameter is a matrix valued quantity. Instead of extracting the information about the topological phase from the absolute value of the matrix entries we will rather infer it from relative complex phases between off-diagonal matrix elements. It will be proven that the order parameter defined in this way is quantized and that it is sensitive to the representation class of boundary spins with respect to the action of \( Z_N \). The string order parameter thus allows to extract a discrete topological invariant which permits to discriminate all \( N \) distinct phases of \( PSU(N) \) spin chains. It is important to note that the topological invariant will only change when the system undergoes a discontinuity. For this reason it may be used as a good (numerical) measure for the identification of topological quantum phase transitions.

In order to check the validity and applicability of our analytical results we study the phase transition between two topologically non-trivial phases of an \( PSU(3) \) spin chain. Each of the two phases exhibits a subtle breaking of inversion symmetry through the spontaneous occurrence of boundary modes. For this reason the Hamiltonian cannot be written as a polynomial in the invariant scalar product \( \hat{S}_1 \cdot \hat{S}_2 \) but rather requires the use of higher order Casimir operators. To our knowledge this is the first time that such Casimir operators are employed systematically in the formulation of spin chains. We then continue with a numerical investigation of the topological order using DMRG. The quantization of the topological order and its discontinuity at the phase transition, see Figure 4, provide a clear confirmation of our analytical predictions.

Even though spin chains based on higher rank groups like \( SU(N) \) are unlikely to be found in real materials, there is a chance that the corresponding Hamiltonians can be engineered artificially using ultracold atoms in optical lattices. Also, special points in the moduli space of spin chains and spin ladders might exhibit an enhanced symmetry. This for instance happens for \( SO(3) \) spin chains which are known to possess an \( SU(3) \) symmetric point for a certain choice of the couplings. It should be noted that string order parameters have also been suggested for other systems, e.g. 1D Haldane Bose insulators. Since the latter has been observed in experimental measurement it seems natural that a similar experimental verification should be possible for \( PSU(N) \) spin chains and the string order parameter obtained from Eq. (13).

The paper is organized as follows. In Section II we start with a concise definition of the physical setup under consideration and we introduce a few of the concepts that turned out to be useful in the classification of topological phases: Matrix product states and projective representations. Afterwards we provide a thorough discussion of the representation theory of \( su(N) \) and review the origin of the \( N \) distinct phases of \( PSU(N) \) spin chains. Section III contains the main result of our paper. We introduce a string order parameter and evaluate it in the thermodynamic limit. In a series of arguments we show that the string order parameter includes discrete topological information and we identify the latter with the parameter specifying the topological phase of the spin chain. Finally, Section IV is devoted to the numerical study of a family of \( PSU(3) \) symmetric spin chains which interpolates between two topologically non-trivial phases. The toy model provides a clear confirmation of our analytical results. Some more technical parts of the proofs and a brief introduction into Casimir operators of \( su(3) \) have been moved to the Appendices.

II. PRELIMINARIES

In this Section we introduce the notation and the structures that are used in the main part of our text. We start with a description of the physical setup and a brief out-
line of the matrix product state formalism. The latter is used to motivate the existence of \( N \) different phases of \( PSU(N) \) spin chains. We then review some essential aspects concerning the representation theory of the Lie algebra \( su(N) \).

A. Physical setup

Throughout this paper we are considering spin chains which are characterized by the following data. The spins reside at sites \( k \) on a circular chain with periodic boundary conditions, the index running over the set \( k = 1, \ldots, L \). It will be assumed that the length of the chain is large but finite. The spins are described by operators \( \vec{S}_k \) which take values in the Lie algebra \( su(N) \) and which act on on-site Hilbert spaces \( \mathcal{H}_k \). The total Hilbert space \( \mathcal{H} = \bigotimes_k \mathcal{H}_k \) is the product of all on-site Hilbert spaces. For simplicity we will assume that all Hilbert spaces \( \mathcal{H}_k \) are irreducible representations of \( su(N) \) since otherwise the system would admit a natural interpretation as a spin ladder instead of a spin chain. Finally, the dynamics of the system is described by a local Hamiltonian \( H \) which commutes with the total spin \( \vec{S} = \sum_k \vec{S}_k \). It can thus be written in terms of Casimir operators of \( su(N) \). The simplest Hamiltonians can be expressed as a function of \( \vec{S}_k \cdot \vec{S}_l \) (corresponding to the quadratic Casimir) where the dot denotes an invariant scalar product. More complicated Hamiltonians, e.g. involving many-body interactions or breaking the permutation symmetry between the two sites, can be defined using higher order Casimir operators. An example of this type will be discussed in Section IV.

Actually, the precise form of the Hamiltonian is not particularly important for the purpose of this paper since we will almost exclusively be concerned with properties of states. To be precise, our attention rests on the ground state \( |\phi\rangle \) of the system which will always be assumed to be a non-degenerate finitely correlated state (non-degenerate at least in a system with periodic boundary conditions). Moreover, there should exist a gap to the first excited state, thus implying exponential decay of local correlation functions. Both properties, the uniqueness and the gap, should persist in the thermodynamic limit.

The simplest way to realize an anti-ferromagnetic spin chain is as follows. The on-site Hilbert spaces are alternating between a space \( \mathcal{V} \) and its dual \( \mathcal{V}^* \). The total Hilbert space is given by \( \mathcal{H} = (\mathcal{V} \otimes \mathcal{V}^*)^L/2 \) and the spin dynamics is described by the translation invariant Heisenberg Hamiltonian

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

with nearest neighbor interactions. The coupling constant \( J \) is assumed to be positive, thereby favoring anti-parallel spin alignment. For the symmetry group \( SU(2) \) and \( \mathcal{V} \) being the \( S = 1/2 \) representation, the Hamiltonian \( [1] \) arises naturally from the electronic Hubbard model at half filling. However, with regard to the study of topological phases, the Heisenberg model is not ideal in many respects. First of all, apart from the overall normalization there are no free parameters in the Hamiltonian so it can only serve as a representative of one physical phase. Also, besides the fact that the ground state is not known exactly, the absence or presence of a gap has not been fully established. The absence of a gap is known for certain representations \( \mathcal{V} \). For other representations, the existence of a gap can be proven in the limit of “large spin” using a mapping to a \( \sigma \)-model with a topological \( \Theta \)-term. More recently, the question of the Haldane gap has been revisited in Ref. 8 [21 and 34].

In order to realize different topological phases while retaining full analytic control over the ground state of the system, it is useful to consider modifications of the Heisenberg Hamiltonian which are obtained by generalizing the AKLT construction. These Hamiltonians arise as “parent Hamiltonians” of specific matrix product states (MPS) since all our considerations take place on the level of ground states we will refrain from giving detailed expressions for the Hamiltonians. The only exception is a specific family of Hamiltonians with \( su(3) \) symmetry which will be the subject of Section IV and which interpolates between two Hamiltonians associated with different topological phases. It will be used to abandon the idealized environment of MPS parent Hamiltonians and to provide a numerical check of our ideas in a more realistic scenario.

B. Matrix product states and topological phases

Let the vectors \( |i_k\rangle \) denote an orthonormal basis of the on-site Hilbert spaces \( \mathcal{H}_k \). Using an iterated Schmidt decomposition, any state \( |\phi\rangle \) of a periodic spin chain of length \( L \) can be written as

\[
|\phi\rangle = \sum_{i_1 \ldots i_L} \text{tr}(A^{[1]}_{i_1} \cdots A^{[L]}_{i_L}) |i_1 \cdots i_L\rangle ,
\]

with a certain set of matrices \( A^{[k]} \) carrying three different indices, one physical and two auxiliary ones. Such a state is known as a matrix product state. To be precise, one has to distinguish different types of MPS depending on the behavior of the system in the thermodynamic limit \( L \to \infty \). If one wishes to describe the ground state of a critical system, the size of the matrices \( A^{[k]} \) will grow beyond any limit. In our current paper we are only interested in gapped systems and hence we will assume that the dimension of the matrices \( A^{[k]} \) (and their nature) stabilizes for sufficiently large values of \( L \). The resulting infinite volume states are known as finitely correlated states [12]. Even though we are eventually interested in the thermodynamic limit, an accurate description of the physics of the system can be obtained by working with...
finite but large $L$ for this class of states. In the presence of a finite gap, there are exponential corrections to expectation values which quickly die away if $L$ is sufficiently large.

The structure $[\mathfrak{g}]$ arises naturally if one associates two auxiliary spaces $\mathcal{H}_{(k,L)}$ and $\mathcal{H}_{(k,R)}$ to each physical site $k$ such that $\mathcal{H}_{(k,R)} = \mathcal{H}_{(k+1,L)}$. This guarantees the existence of a maximally entangled state $|k\rangle = \sum_q |q⟩|q⟩ \in \mathcal{H}_{(k,L)} \otimes \mathcal{H}_{(k+1,L)}$ where $|q⟩$ refers to an orthonormal basis of $\mathcal{H}_{(k,R)}$. The state $|φ⟩$ is the image of the tensor product $|I⟩ = |I_1⟩ \otimes \cdots \otimes |I_{L-1}⟩$ of completely entangled pairs under the map $A = A^{[1]} \otimes \cdots \otimes A^{[L]}$. The application of the map $A$ to the product of completely entangled pairs $|I⟩$ effectively converts the tensor product into a matrix product.

In the spin chains we are interested in, the physical Hilbert spaces $\mathcal{H}_k$ carry a unitary representation of $SU(N)$. Moreover, the ground state $|φ⟩$ should be invariant under the action of $SU(N)$. These two properties imply the existence of additional structures which are realized on the data of an MPS. Let $R^{[k]}$ denote the representation of $SU(N)$ on the space $\mathcal{H}_k$. According to Ref. 21, this on-site symmetry lifts to the auxiliary level

$$R^{[k]}(g) \cdot A^{[k]} = D^{[k]}(g)A^{[k]}D^{[k+1]}(g)^{-1}, \quad (3)$$

thereby promoting $\mathcal{H}_{(k,L)}$ and $\mathcal{H}_{(k,R)}$ to representations of $SU(N)$. In other words, the homomorphisms $A^{[k]}$ should be equivariant projections from $\mathcal{H}_{(k,L)} \otimes \mathcal{H}_{(k,R)}$ to $\mathcal{H}_k$, i.e. they should commute with the action of $SU(N)$.

In fact, a careful inspection of relation (2) shows that the physical Hilbert space $\mathcal{H}_k$ and the associated auxiliary spaces $\mathcal{H}_{(k,L/R)}$ enter the discussion on a different footing. To understand this, we need to let us consider a moment where $D^{[k]} = D^{[k+1]}$ and that the auxiliary spaces form an irreducible representation of $SU(N)$. In view of Schur’s Lemma, the right hand side of Eq. 3 and hence also the left hand side is invariant in this case if $g$ is chosen to be in the center $Z_N$ of the symmetry group $SU(N)$. In other words, $R^{[k]}$ descents to a representation of the quotient group $PSU(N) = SU(N)/Z_N$ where no such requirement exists for the matrix $D^{[k]}$. The latter only needs to implement a projective representation of $PSU(N)$.

$$D(g_1)D(g_2) = ω(g_1,g_2)D(g_1g_2) \quad (4)$$

with $g_1,g_2 \in PSU(N)$ and $ω(g_1,g_2) \in U(1)$, i.e. a representation up to phase factors. It is known that the projective representations of $PSU(N)$ fall into $N$ different classes when considered modulo obvious equivalences (see e.g. Ref. 21).

Analogous considerations apply if the assumption $D^{[k]} = D^{[k+1]}$ fails. By choosing suitable representations of $SU(N)$ on the auxiliary spaces, one can realize any symmetry group $SU(N)/Γ$ on the physical Hilbert spaces $\mathcal{H}_k$, where $Γ \subset Z_N$ is an arbitrary subgroup of the center of $SU(N)$. It can be shown that the group $SU(N)/Γ$ has $|Γ|$ distinct classes of projective representations.

In a series of papers, the projective class of the representation of the physical symmetry on the auxiliary spaces has been identified as a topological invariant of 1D gapped spin chains. In other words, the projective class arising in the MPS representation of the respective ground states remains invariant upon deformation of the Hamiltonian. For the symmetry group $PSU(N)$, the previous argument predicts exactly $N$ distinct topological phases. For a general treatise on 1D spin systems with continuous on-site symmetries we refer the interested reader to Ref. 21.

The different topological phases of a spin chain with a given symmetry can all be realized explicitly by defining suitable parent Hamiltonians. More precisely, for each MPS $|φ⟩$ of the form $[\mathfrak{g}]$ there exists a local Hamiltonian with the following two properties: The state $|φ⟩$ is the unique ground state of the Hamiltonian and there exists a gap. When considered with open boundary conditions, this construction will lead to gapless edge modes which transform according to the projective representations $B_L = \mathcal{H}_{(1,L)}$ and $B_R = \mathcal{H}_{(L,R)}$. Even though the energy of boundary states will receive corrections and the degeneracy with the ground state might get lost upon deformation of the Hamiltonian, they will remain stable until the mass gap closes in the bulk. Intuitively, the correlation length will diverge at the phase transition, thus allowing the two boundaries modes of the spin chain to interact with each other and to disappear.

C. The Lie algebra $su(N)$ and its representations

For a more detailed discussion of $SU(N)$ spin chains and a concise formulation of our result we need to review the representation theory of the Lie algebra $su(N)$ (see e.g. Ref. 35 and 39). The latter is the Lie algebra $\mathfrak{g}$ of traceless $N \times N$ matrices and it is generated (as a vector space) by the matrices $E^{ab}$ with $a \neq b$ and by $H^a = E^{aa} - E^{a+1,a-1}$. Here $E^{ab}$ denotes the elementary matrix $(E^{ab})_{cd} = δ_{ac}δ_{bd}$ with a single non-zero entry in row $a$ and column $b$. The diagonal matrices $H^a$ generate the Cartan subalgebra $\mathfrak{h}$ of $su(N)$. The other generators $E^{ab}$ are called positive or negative roots, depending on whether $a < b$ or $a > b$. As a consequence, the Lie algebra $su(N)$ admits a triangular decomposition $\mathfrak{g} = \mathfrak{g}_+ \oplus \mathfrak{h} \oplus \mathfrak{g}_-$ into positive roots $\mathfrak{g}_+$, negative roots $\mathfrak{g}_-$ and the Cartan subalgebra $\mathfrak{h}$. As a Lie algebra, $su(n)$ is generated by the positive and negative simple roots $E^{ab}$ with $|a - b| = 1$.

All finite dimensional representations $V$ of $su(N)$ are so-called weight representations in which all generators $H^a$ are represented by diagonal matrices $ρ_V(H^a)$. By abuse of notation we will simply omit to write the map $ρ_V$ in case it is clear that we are acting on a representation.
If $\mu \in \mathfrak{h}^*$ one says that a vector $v \in V$ has weight $\mu$ provided that
\[ H^a v = \mu(H^a)v =: \mu_a v \quad (5) \]
The different eigenvalues $\mu_a$ can be assembled into a tuple $\mu = (\mu_1, \ldots, \mu_{N-1})$ of Dynkin labels and should be regarded as physical charges characterizing the state $v$. A convenient basis for the space $\mathfrak{h}^*$ is given by the fundamental weights $\omega_i$ which are dual to the Cartan generators in the sense that $\omega_i(H^a) = \delta_{ai}^0$. A weight can thus also be written as $\mu = \sum_a \mu_a \omega_a$. Any representation space $V$ can be split into distinct eigenspaces with regard to the action of the generators $H^a$. This leads to the weight space decomposition
\[ V = \bigoplus_{\mu \in \mathfrak{h}^*} V_\mu \quad (6) \]
In a finite dimensional representation all weights $\mu$ are necessarily integral, i.e. $\mu_a \in \mathbb{Z}$. The set of all weights forms the weight lattice $P$ which is an abelian group under addition.

Let us now turn our attention to finite dimensional irreducible representations. As is well known, the latter are labeled by weights $\lambda$ whose Dynkin labels $\lambda_a$ are all non-negative integers. Such weights are called dominant. The set of dominant weights, denoted by $P^+$, defines the fundamental Weyl chamber of the weight lattice $P$. Within an irreducible representation $\lambda$, the different weights are all related by the application of roots $\alpha$. The latter should be thought of as the charges of the root generators $E^{ab}$ (for $a \neq b$) with respect to the Cartan generators $H^a$. Phrased differently, for each weight $\mu$ in the representation $\lambda$ one has $\lambda - \mu \in Q$ where $Q$ is the root lattice which is generated by the (finite) set of roots $\alpha$.

A distinguished role is played by the adjoint representation in which the Lie algebra is represented on itself (regarded as a vector space) by means of the adjoint map $X \mapsto \text{ad} X = [X, \cdot]$. The non-zero weights of the adjoint representation are precisely the roots $\alpha$. The $N-1$ simple roots have weights $\alpha_a$ which are just the rows of the $su(N)$ Cartan matrix $A_{ab} = 2\delta_{ab} - \delta_{a-b,1}$. For our purposes it will be important that there exists a unique weight $\rho = \frac{1}{2}\sum_{a>0} \alpha = (1, \ldots, 1)$, the so-called Weyl vector, which has a scalar product $(\rho, \alpha_a) = 1$ with each of the simple roots $\alpha_a$. The dual generator $H^\rho \in \mathfrak{h}$ is characterized by the property
\[ \alpha_a(H^\rho) = 1 \quad (7) \]
for all $a = 1, \ldots, N-1$. This generator will play an important role in the definition of the string order parameter in Section III. With the previous choice of simple roots one can find the following explicit expression for the diagonal entries of the matrix $H^\rho = \text{diag}(H^1, \ldots, H^{N-1}) \in \mathfrak{h}$,
\[ H^\rho_a = \frac{N+1}{2} - a \quad (8) \]
Indeed, one can easily check that this defines the unique traceless diagonal matrix with $H^\rho_a - H^\rho_{a+1} = 1$, as required by Eq. (7).

The final ingredient that will be needed below is the Weyl group of $su(N)$. The Weyl group can be regarded as the symmetry of the root system. It consists of rotations and reflections which leave the set of roots invariant and is thus a subgroup of the orthogonal group in $N-1$ dimensions. For $su(N)$, the Weyl group is isomorphic to the symmetric group $S_N$. Under the action of the Weyl group, the weight lattice $P$ may be decomposed into orbits. In our considerations below it will be crucial that each of these orbits has at least one element in the fundamental Weyl chamber of dominant weights $P^+$. In other words, for each weight $\mu \in P$ one can find an element $S \in W$ such that $\mu' = S\mu$ is in the fundamental Weyl chamber, i.e. $\mu' \in P^+$. Note that the element $S$ need not be unique.

In order to derive the explicit action of the Weyl group on a weight it is convenient to switch to an alternative set of elements $\epsilon_i$ ($i = 1, \ldots, N$) which span the dual $\mathfrak{h}^*$ of the Cartan algebra of $su(N)$. Given any $H \in \mathfrak{h}$ they are defined by $\epsilon_i(H) = H_{ij}$. Since $su(N)$ matrices are traceless, these vectors satisfy the constraint $\sum_i \epsilon_i = 0$ which leads to a slight redundancy when weights are expressed in terms of the $\epsilon_i$. However, this disadvantage is compensated by the simple transformation behavior under the action of the Weyl group $W$ which, for $su(N)$, is isomorphic to the symmetric group $S_N$. Given any permutation $\sigma \in S_N$ and the associated Weyl group element $S_\sigma \in W$ one simply has
\[ S_\sigma(\epsilon_i) = \epsilon_{\sigma(i)} \quad (9) \]
Given this formula, we can deduce the Weyl group action on any weight $\mu = \sum_a c_i \epsilon_i$. Note that the labels $c_i$ are, a priori, only defined up to a simultaneous shift. We can nevertheless arrive at a unique description by imposing the “gauge” $\sum_i c_i = 0$, and the latter will be assumed from now on. With these conventions the new labels are related to the standard Dynkin labels $\mu_a$ as
\[ c_i = -\sum_{a=1}^{N-1} \frac{a}{N} \mu_a + \sum_{a=i}^{N-1} \frac{N-a}{N} - \mu_a \quad (10) \]
This relation can be derived using the explicit form of the roots in terms of Dynkin labels, compare the expression for the Cartan matrix above.

A second reason for using the epsilon basis is that $\epsilon_i(H^\rho)$ and $\epsilon_i(H^\rho)$ can be easily calculated. The former evaluates to $\epsilon_i(H^\rho) = \delta_{i,a} - \delta_{i,a+1}$, while the latter is $\epsilon_i(H^\rho) = N+1-i$. Note that a shift in the index $i$ translates directly to a shift in $\epsilon_i(H^\rho)$. More precisely, let $\sigma_m \in S_N$ be the cyclic permutation defined by $\sigma_m(i) = i + m$ (modulo $N$). Then
\[ \epsilon_{\sigma_m(i)}(H^\rho) = \epsilon_i(H^\rho) - m + N \theta(i + m - N) \quad (11) \]
Here, $\theta$ is the Heaviside step function with $\theta(0) = 0$. 
D. Classes of representations

As was discussed in detail in our previous article, the representations \( \lambda \) of \( su(N) \) (and hence of \( SU(N) \)) fall into \( N \) different classes which can be interpreted as elements of the group \( P/Q \), the quotient of the weight lattice \( P \) by the root lattice \( Q \). In terms of its Dynkin labels the class of the representation \( \lambda = (\lambda_1, \ldots, \lambda_{N-1}) \) is defined by

\[
[\lambda] \equiv \sum_{a=1}^{N-1} a\lambda_a \mod N . \tag{12}
\]

When representations are specified using Young tableaux, the class of a representation can be expressed as the number of boxes modulo \( N \). Even though Eq. (12) was introduced for highest weights, it can be extended to any weight since the expression on the right hand side is invariant under the action of the root lattice \( Q \). In other words, \([\mu] = [\lambda]\) for any weight \( \mu \) in a representation with highest weight \( \lambda \). As is illustrated in Figure 1, equation (12) divides the weight lattice of \( su(N) \) into \( N \) different sublattices.

The congruence class \([\lambda]\) of a representation \( \lambda \) determines whether the representation descends to quotients of the group \( SU(N) \). More precisely, the value of \([\lambda]\) fixes the action of the center \( Z_N \) of \( SU(N) \) on the representation \( \lambda \). Elements of \( Z_N \subset SU(N) \) are multiples of \( \Omega^kI_N \) of the identity matrix with \( \Omega = \exp(\frac{2\pi i}{N}) \) denoting the fundamental \( N \)th root of unity. In the representation \( \lambda \), this element is mapped to the complex phase \( \rho(\Omega^kI_N) = \Omega^k[\lambda] \). We conclude that representations \( \lambda \) with \([\lambda] \equiv 0 \) are linear representations of \( PSU(N) = SU(N)/Z_N \). Likewise we may ask whether a representation \( \lambda \) lifts to any of the groups \( SU(N)/Z_q \) where \( Z_q \subset Z_N \) is a subgroup of the center. This is the case if and only if \([\lambda] \equiv 0 \mod q \) (instead of using \( \mod N \)).

The connection to the classification of topological phases comes in since representations \( \lambda \) of \( SU(N) \) with \([\lambda] \neq 0 \) only define projective representations of \( PSU(N) \). If the physical Hilbert spaces \( \mathcal{H}_k \) transform in a linear representation of \( PSU(N) \), the (virtual) boundary spins might still transform in a projective representation of \( PSU(N) \) as was discussed in Section II B. The division of \( SU(N) \) representations into \( N \) distinct classes which is described by Eq. (12) in this way reflects the division of spin chains into \( N \) distinct topological classes.

Let us finally establish the connection to the physical spin chains which have been discussed in Section II B. Since we shall be dealing with \( PSU(N) \) spin chains in this paper, the physical Hilbert spaces \( \mathcal{H}_k \) (which are described by a highest weight \( \lambda \)) should all reside in the trivial class, i.e. \([\mathcal{H}_k] = [\lambda] \equiv 0 \). On the other hand, the auxiliary spaces \( \mathcal{H}_{(k,L/R)} \) can reside in non-trivial classes as long as their total class sums up to zero, \([\mathcal{H}_{(k,R)}] = -[\mathcal{H}_{(k,L)}] \). Together with the condition \([\mathcal{H}_{(k,R)}] = -[\mathcal{H}_{(k+1,L)}] \) which arises from the duality constraint \( \mathcal{H}_{(k,R)}^{(1)} = \mathcal{H}_{(k+1,L)}^{(1)} \) this means that the projective class of the left and right auxiliary spaces, respectively, is constant all along the chain.

III. A STRING ORDER PARAMETER FOR SU(N) SPIN CHAINS

In this Section we introduce a non-local string order parameter for \( SU(N) \) spin chains which reduces to the diluted anti-ferromagnetic order of Rommelse and den Nijs for \( N = 2 \). Using transfer matrix methods we evaluate the string order parameter on matrix product ground states and show that it may be used to extract a quantized topological order parameter. The latter is capable of distinguishing between the \( N \) different phases of \( PSU(N) \) invariant spin chains.

A. Definition and interpretation

Let \( |\phi\rangle \) be the unique ground state of our spin system. We will assume that the system has a symmetry group \( PSU(N) \) and that \( |\phi\rangle \) is in a definite topological phase described by a constant \( t \in \mathbb{Z}_N \) (regarded as an additive group). Following the reasoning of Section II B the constant \( t \) will be identified with the projective class \([\mathcal{H}_{(k,R)}] \) of the right auxiliary representations arising in the matrix product state representation of \( |\phi\rangle \).

In what follows we shall prove that the ground state expectation value \( \langle \sigma_{ij}^{ab} \rangle \) of the non-local string order operator

\[
\sigma_{ij}^{ab} = H_i^a \exp \left[ \frac{2\pi i}{N} \sum_{k=i+1}^{j-1} H_k^\rho \right] H_j^b \quad (\text{for } i < j) \tag{13}
\]
contains all information required to reconstruct the value of \( t \). It serves as a convenient tool for the measurement of the topological phase of the system, even in cases where the matrix product state representation of \( |\phi\rangle \) is not known or where the nature of the auxiliary spaces – regarded as a representation of \( SU(N) \) – is unclear. In the previous formula, \( H^p \) refers to the Cartan operator associated with the Weyl vector \( p \) (see Section H.C). For \( SU(2) \), expression (13) reduces to the string order \( S_i^z \) exp \((i\pi \sum S^z_i S^z_j)\) introduced by Rommelse and den Nijs.24

In the following Section it will be proven that, in the limit \( |i-j| \to \infty \), the dependence of the string order parameter \( \langle \sigma_{ij}^{ab} \rangle \) on \( a \) and \( b \) converges exponentially to

\[
T^{ab} = \lim_{|i-j| \to \infty} \langle \sigma_{ij}^{ab} \rangle = C_{ij} \Omega^{t(a-b)}
\]

with \( \Omega = \exp \frac{2\pi i}{N} \). (14)

The prefactor \( C_{ij} \) can be used as a first rough indication of whether the system resides in a topologically trivial phase or not. In a trivial phase we will always obtain \( C_{ij} = 0 \) while in a non-trivial phase the prefactor is expected to be non-zero20. Up to this point, the discussion completely parallels the analysis of the conventional \( SU(2) \) string order. For \( SU(N) \), however, the most important information resides in the off-diagonal entries, the complex phases \( \Omega_{i,a-b} \). Obviously, the constant \( t \) entering this expression is only defined modulo \( N \). In fact, as we shall see below, it takes values in \( \mathbb{Z}/N \) just as desired. It characterizes the projective class according to which (virtual) edge modes transform and it thereby determines the topological phase of the state \( |\phi\rangle \). Whenever \( C_{ij} \neq 0 \), the value of \( t \) can be extracted unambiguously by calculating (or measuring) two different matrix elements and taking their quotient. For instance one immediately finds \( T^{21}/T^{11} = \Omega \). Let us emphasize that a transition from one topological phase to another enforces the prefactor \( C_{ij} \) to vanish since otherwise the parameter \( t \) cannot change its value.

In the way it was introduced, the constant \( t \in \mathbb{Z}/N \) determines the projective class of (virtual) edge modes with respect to the minimal quotient \( PSU(N) = SU(N)/\mathbb{Z}/N \) of \( SU(N) \). In a concrete physical realization it might happen that the actual symmetry group is not \( PSU(N) \) but rather a different quotient \( SU(N)/\mathbb{Z}/q \) where \( \mathbb{Z}/q \subset \mathbb{Z}/N \). In this case, the projective classes are described by \( \mathbb{Z}/q \), not by \( \mathbb{Z}/N \), and \( t \) has to be considered modulo \( q \), see Ref. 21.

The attentive reader may wonder why the expectation value (14) still depends on \( i \) and \( j \) even after taking the limit \( |i-j| \to \infty \). The answer is simple: The result of the calculation depends on the representation spaces used at sites \( i \) and \( j \) and hence on how the limit is performed. The dependence will disappear if the system is translation invariant.

\section{Evaluation}

The proof of Eq. (14) will proceed in two steps. We first prove the factorization of the matrix \( \langle \sigma_{ij}^{ab} \rangle = \langle J_{i,L}^a \rangle \langle J_{j,R}^b \rangle \) in the thermodynamic limit, up to exponentially small corrections. This step uses transfer matrix techniques and it is intimately related to the matrix product state structure of \( |\phi\rangle \). In a second step we use the Weyl symmetry of the weight lattice to reduce \( J_{i,L}^a \) to a simpler expression. The latter is further analyzed in a third step from which we conclude that \( \langle J_{i,L}^a \rangle \) depends on \( a \) as \( \langle J_{i,L}^a \rangle \propto \Omega^{at} \). The case \( J_{j,R}^b \) can be dealt with analogously.

\subsection{Step 1: Factorization}

To prove the factorization of the matrix \( T^{ab} \) we express the ground state \( |\phi \rangle = \mathfrak{A}|I\rangle \) in terms of the maximally entangled state \( |I\rangle \), see Section II.B. The possibility to write \( |\phi \rangle \) in this form is a direct consequence of the fact that \( |\phi \rangle \) can be written as a matrix product state. In the next step we use the intertwining property

\[
H_i^a \mathfrak{A} = \mathfrak{A}(H_{i,L}^a + H_{i,R}^a)
\]

which expresses the physical spin operator \( H_i^a \) as a sum of spin operators \( H_{i,L}^a \) and \( H_{i,R}^a \) on the two corresponding auxiliary sites. Using the singlet property of \( |I\rangle \),

\[
H_{i,R}^a |I\rangle = -H_{i+1,L}^a |I\rangle,
\]

one easily sees that the phase factors in the string order parameter \( \sigma_{ij}^{ab} \) cancel out pairwise except for the two boundaries. We then immediately find

\[
\langle \sigma_{ij}^{ab} \rangle = \frac{\langle \phi | \sigma_{ij}^{ab} \mathfrak{A} |I\rangle \langle I| \phi \rangle}{\langle \phi | \phi \rangle} = \frac{\langle \phi | \mathfrak{A} J_{i,L}^a J_{j,R}^b |I\rangle \langle I| \phi \rangle}{\langle \phi | \phi \rangle}.
\]

where the two operators \( J_{i,L}^a \) and \( J_{j,R}^b \) are defined by

\[
J_{i,L}^a = (H_{i,L}^a + H_{i+1,L}^a) \Omega^{-H_{i,L}^a} \quad \text{and} \quad J_{j,R}^b = \Omega^{-H_{j,R}^b} (H_{j,L}^b + H_{j+1,L}^b) \, . \]

Note that each of these operators acts locally on two auxiliary sites. However, neither of them can be lifted to \( \mathfrak{A} \) without rebuilding the original non-local string.

Now that we could eliminate the non-local string connecting the two sites \( i \) and \( j \) we can evaluate the string order parameter using standard transfer matrix techniques22. For that purpose, we write

\[
\langle \phi | \mathfrak{A} J_{i,L}^a J_{j,R}^b |I\rangle = \text{tr} \left( \cdots E^{[i-1]} E^{[i]} E^{[i+1]} \cdots E^{[j-1]} E^{[j]} E^{[j+1]} \cdots \right),
\]

\[
\langle \phi | \phi \rangle = \text{tr} (E^{[1]} \cdots E^{[L]}),
\]

for all sites \( i \) and \( j \). This is a consequence of the fact that the expectation value (14) still depends on \( i \) and \( j \) even after taking the limit \( |i-j| \to \infty \). The answer is simple: The result of the calculation depends on the representation spaces used at sites \( i \) and \( j \) and hence on how the limit is performed. The dependence will disappear if the system is translation invariant.
where
\[
(E_X^{[k]})_{\alpha\beta,\mu\nu} = \sum_{s,\gamma,\rho} \langle A^{[k]} \rangle_{\alpha\mu}^{s} \langle A^{[k]} \rangle_{\gamma\rho}^{s} |X|\beta\nu \tag{22}
\]
and \(E^{[k]} = E^{[k]}_X\). A pictorial interpretation of the expectation value is provided in Figure 2. The two traces can be evaluated by diagonalization of the transfer matrices \(E^{[k]}\), considered as an operator mapping matrices on the auxiliary space \(H_{(k,R)}\) to matrices acting on the auxiliary space \(H_{(k,L)}\). In the thermodynamic limit and with \(|i - j| \to \infty\), the only contribution will come from the highest eigenvalue. All other contributions are suppressed exponentially due to our mass gap assumption. It can easily be seen that the identity matrices on the auxiliary spaces are left and right “eigenvectors” with eigenvalues \(\dim H_k / \dim H_{(k,L)}\) and \(\dim H_k / \dim H_{(k,R)}\), respectively. Indeed, due to Schur’s Lemma we have
\[
E^{[k]}_{\alpha\beta,\gamma\rho} I_{\mu\nu} = C_R I_{\alpha\beta} \quad \text{and} \quad I_{\alpha\beta} E^{[k]}_{\gamma\rho,\mu\nu} = C_L I_{\mu\nu} . \tag{23}
\]
Moreover it is obvious that
\[
\dim(H_k) = I_{\alpha\beta} E^{[k]}_{\alpha\beta,\mu\nu} = C_R \text{tr}_{H_{(k,R)}}(I) = C_R \dim(H_{(k,R)}) , \tag{24}
\]
and similarly for \(C_L\). Since \(E^{[k]}\) is a completely positive map it is guaranteed that there is no greater eigenvalue (Ref. [22] Prop. 3.6). On the other hand, due to our mass gap assumption this eigenvalue is non-degenerate, even in absolute value.\(\blacksquare\)

In the limit of large separation, \(|i - j| \gg 1\), we can rewrite the desired expectation value in a factorized form as
\[
\langle \sigma_{ij}^{ab} \rangle = \frac{\langle I_{H_{(i,L)}} E^{[k]}_{j,R} I_{H_{(i,R)}} \rangle \langle I_{H_{(j,L)}} E^{[j]}_{i,L} I_{H_{(j,R)}} \rangle}{\dim H_i \dim H_j} = \langle J_{i,L}^a \rangle \langle J_{j,R}^* \rangle . \tag{25}
\]
We note that the result still depends on the representation spaces describing the start and the end point of the original string.

**Step 2: Employing Weyl symmetry**

In the second part of the derivation we focus on the \(a\) dependence of the expectation value \(J^a \coloneqq \langle J_{i,L}^a \rangle\) which we claim to be proportional to \(\Omega^{bt}\) with \(t = [H_{(i,R)}]\). The same reasoning can be used to derive that \(\langle J_{i,R}^b \rangle \propto \Omega^b[H_{(i,L)}] = \Omega^{-bt}\) from which the main result, Eq. [14], follows. Here we used the chain of equalities \([H_{(j,L)}] = [H_{(j,R)}] = -[H_{(i,R)}] = -t\).

Since the operators \(J_{i,L}^a\) contain Cartan elements only, their expectation value can be calculated most easily in an orthonormal basis \(|\alpha\beta\rangle\) of the auxiliary space \(H_{(i,L)} \otimes H_{(i,R)}\) which respects the weight space decomposition. In such a basis the operator \(J_{i,L}^a\) is represented by a diagonal matrix with components \(J_{a\alpha\beta}\). In order to keep the notation simple we shall use the abbreviation \(\alpha \in \mu\) if \(|\alpha\rangle\) is contained in the weight space with weight \(\mu\) (of \(H_{(i,L)}\) in this case). Moreover, we wish to recall that the matrices \((\langle A^{[k]} \rangle)_{\alpha\beta}^s\) are SU(\(N\)) invariant projections from auxiliary space to physical space which can be represented as the matrix element \(\langle s|\alpha\beta\rangle\).

From the discussion of the expectation values \(J^a\) in Eq. [26] we immediately conclude
\[
J^a = \frac{1}{\dim H_i} \sum_{s,\alpha,\beta} |\langle s|\alpha\beta\rangle|^2 J_{a\alpha\beta} \tag{26}
\]
In the second equality, instead of summing directly over all basis vectors, we first sum over weight spaces followed by a sum over vectors spanning a certain weight space. We also used an obvious selection rule for the weights entering the Clebsch-Gordan coefficients \(\langle s|\alpha\beta\rangle\). The values \(J_{a\alpha\beta}\) do not directly depend on \(\alpha\) and \(\beta\), but only on the weight space they belong to. We may thus define
\[
J_{\mu\nu}^a \coloneqq J_{a\alpha\beta} \quad \text{with} \quad \alpha \in \mu, \quad \beta \in \nu . \tag{27}
\]
Furthermore, it is convenient to introduce the abbreviation
\[
P(\mu, \nu) \coloneqq \sum_{\alpha \in \mu, \beta \in \nu} |\langle s|\alpha\beta\rangle|^2 \tag{28}
\]
such that above expression can be written as
\[
J^a = \frac{1}{\dim H_i} \sum_{\mu, \nu} P(\mu, \nu) J_{\mu\nu}^a . \tag{29}
\]
At this point we split the sum into orbits with respect to the Weyl group. To be more precise, we simplify Eq. (30) by restricting the summation to those weights $\mu$ and $\nu$ such that their sum is in the fundamental Weyl chamber, $\mu + \nu \in P^+$. All the other terms are obtained using the action of the Weyl group. Since the weights at the boundary of $P^+$ are invariant under a subgroup of the Weyl group this leads to an overcounting which is compensated by dividing through the order of the stabilizer subgroup $W_{\mu + \nu} \subset W$. This procedure yields

$$J^a = \frac{1}{\dim H_i} \sum_{\mu, \nu} \frac{1}{|W_{\mu + \nu}|} \sum_{S \in W} P(S\mu, S\nu) J^a_{S(\mu), S(\nu)}$$

$$= \frac{1}{\dim H_i} \sum_{\mu, \nu} \frac{P(\mu, \nu)}{|W_{\mu + \nu}|} \sum_{S \in W} J^a_{S(\mu), S(\nu)}$$

$$= \frac{1}{\dim H_i} \sum_{\mu, \nu} \frac{P(\mu, \nu)}{|W_{\mu + \nu}|} K^a_{\mu, \nu} ,$$

(31)

In the second equation the Weyl invariance of $P(\mu, \nu)$ is used: $P(\mu, \nu) = P(S\mu, S\nu)$ for all $S \in W$. This is proven in Appendix A. The third equation defines $K^a_{\mu, \nu}$. Since $P(\mu, \nu)$ is independent of $a$, we are left to show that $K^a_{\mu, \nu}(a) \propto \Omega^a[\nu]$. The identification of $[\nu]$ with $t$ follows since the label $[\nu]$ is the same for all weights $\nu$ appearing in the decomposition of the $su(N)$ representation $H_{(t,R)}$. This is a direct consequence of the fact that the ground state $|\phi\rangle$ was assumed to be in a well-defined topological phase.

**Step 3: Weyl group gymnastics**

At this point, all ingredients are set to show that $K^a_{\mu, \nu} \propto \Omega^a[\nu]$, where $K^a_{\mu, \nu}$ is defined by Eq. (31):

$$K^a_{\mu, \nu} = \sum_{S \in W} S(\mu + \nu)(H^a\nu) \Omega^{-S(\nu)(H^a)} .$$

(32)

Writing the weights as $\nu = \sum \epsilon_i$ and $\mu + \nu = \sum d_k \epsilon_k$ (with the “gauge fixing” $\sum \epsilon_i = 0$), respectively, and using the Weyl group action specified in Eq. 9 allows us to rewrite this expression in the form

$$K^a_{\mu, \nu} = \sum_k d_k \sum_{\sigma(k) = a} \Omega^\epsilon_\sigma(\nu)(H^a)$$

$$- \sum_k d_k \sum_{\sigma(k) = a + 1} \Omega^\epsilon_\sigma(\nu)(H^a)$$

$$= \sum_k d_k (Q_k^a - Q_k^{a+1}) .$$

(33)

Let us now focus on the sum over the different permutations $\sigma$ which has been abbreviated by $Q_k^a$ in the previous formula. Our goal is to remove the constraint involving the index $a$ in the summation over the permutations and to convert it into an explicit dependence of the whole expression. This can be achieved by the following simple resummation which makes use of the cyclic permutations $\sigma_a$ and of Eq. (11):

$$Q_k^a = \sum_{\sigma(k) = a} \Omega^\epsilon\left( - \sum_l \epsilon_l \sigma(\epsilon_l)(H^a) \right)$$

$$= \sum_{\sigma(k) = a} \Omega^\epsilon\left( - \sum_l \epsilon_l \sigma(\epsilon_l)(H^a) \right) + a \sum_l \epsilon_l H^a$$

$$= \sum_{l=N-a+1}^{N} N \epsilon_l \sigma(\epsilon_l)(H^a)$$

$$= \Omega^a[\nu] Q_k^{N(a)} .$$

(34)

The last expression arises from the following simplifications on the third row. The first sum in the exponent of the last equation is independent of $a$. The second sum vanishes due to our choice of “gauge fixing” $\sum \epsilon_l = 0$. The third sum contains the information we are after. Formula (10) implies the relation $-N c_k = \sum \epsilon_l \epsilon_a = [\nu]$ (modulo $N$) for any index $k$. Hence each term in this sum is equal to $[\nu] = t$. Moreover, there are exactly $a$ of these terms in this sum. This gives the desired dependence of $K^a_{\mu, \nu} \propto \Omega^a[\nu]$ on the index $a$. The equation

$$J^a = \frac{\Omega^a(1 - \Omega^t)}{\dim H_i} \sum_{\mu, \nu} \frac{P(\mu, \nu)}{|W_{\mu + \nu}|} \sum_k d_k Q_k^{N(a)}$$

(35)

follows immediately. We have thus confirmed that the string order parameter is given by Eq. (14) and that it is a suitable tool for measuring the topological phase of a state on a spin chain. Moreover, the previous equation also implies that the string order operator always has a vanishing expectation value as long as the edge modes transform according to a linear representation of $PSU(N)$, i.e. when the system is in a topologically trivial phase with $t = 0$.

**C. Properties**

The string order parameter that is derived from Eq. (13) has a number of desired features that one expects for a quantity capable of measuring a topological property. First of all, the factorization (26) implies the invariance under arbitrary block renormalization between the end points in questions. From a mathematical perspective this is the analogue of invariance under continuous deformations or choice of metric. Even though the
factorized expression resembles a local correlation function one should bear in mind that the invariance of the ground state under $PSU(N)$ leads to a subtle entanglement which propagates from site to site and cannot be removed by block renormalization.\cite{12}

It should be emphasized that the integer number $t$, associated with our string order parameter \cite{14} gives a reliable answer about the precise type of the topological phase. In contrast, entanglement entropies and spectra only encode information about the number of massless edge modes but not (at least not directly) about their representation type (see e.g. Ref. [19] and [20]). Indeed, even when only considering irreducible representations of $SU(N)$, the dimension is not sufficient to distinguish between a representation and its dual for instance. A systematic search for even more convincing examples already succeeds for $SU(3)$: This group has four different 15-dimensional irreducible representations labeled by $(2, 1)$ and $(4, 0)$ as well as their conjugates. While $(2, 1)$ and $(4, 0)$ belong to the class $[1] \in \mathbb{Z}_3$, the representations $(1, 2)$ and $(0, 4)$ belong to the class $[2] \in \mathbb{Z}_3$. So, even when forgetting about the possibility to form direct sums of irreducible representations we recognize that the dimension of a representation alone might not be sufficient to specify the topological phase it is associated with.

The formula we derived for the string order and its interpretation in a sense assumes an ideal measurement. The form of the outcome and the particular dependence of the complex phase factor on the label $a$ rely on a very specific and fixed choice of basis for the Cartan generators. In a real physical measurement in a laboratory one will generally measure the expectation value for a linear combination of operators which slightly deviates from $H^0$. A more detailed analysis of this effect, just as of finite size corrections, is beyond the scope of the present article.

IV. NUMERICAL VERIFICATION

In this Section, it will be verified in a concrete physical setup that the string order parameter defined in Section III is capable of measuring the topological order of a spin chain. For this purpose we define a family of $PSU(3)$ invariant Hamiltonians which smoothly interpolates between two distinct topologically non-trivial phases. We determine the ground states numerically using DMRG and study the behavior of the string order parameter and its associated topological order parameter $t$. The numerical results clearly confirm our theoretical predictions. The complex phase of the string order parameter is quantized and jumps at the phase transition.

A. Setup and idea

In what follows, we shall consider a family of $PSU(3)$ invariant spin chains with periodic boundary conditions. The on-site Hilbert spaces are all chosen to be equal to the eight-dimensional adjoint representation of $SU(3)$, which is described by the highest weight $(1, 1)$. Since Eq. (1) implies $[(1, 1)] \equiv 0$, this is clearly a representation of $PSU(3)$. We start with a discussion of two particular states $|\phi_1\rangle$ and $|\phi_2\rangle$ and their associated parent Hamiltonians $H_1$ and $H_2$. For these two systems we have full analytical control over all relevant properties such as the energy gap and the topological phase. We then consider the family of Hamiltonians

$$H(c) = cH_1 + (1-c)H_2 \quad \text{with} \quad c \in [0, 1] . \quad (36)$$

Our basic idea is to determine the ground state and the string order parameter numerically as a function of $c$. Since, however, the structure of the Hamiltonian $H(c)$ is quite complicated we will instead implement the numerics using a truncated version $H_{\text{trunc}}(c)$ which exhibits the same qualitative behavior.

The state $|\phi_1\rangle$ is a matrix product state defined as follows: As the left and right auxiliary spaces we choose the two distinct three-dimensional representations $3$ and $3'$ of $SU(3)$, with highest weight $(0, 1)$ and $(1, 0)$, respectively. The matrices $A$ correspond to the $SU(3)$ invariant projections $A : 3 \otimes 3 \to 8$ as described in Section II. By construction, the state $|\phi_1\rangle$ resides in the non-trivial topological phase $t = [(1, 0)] = 1$. As is well known, the parent Hamiltonian for an open chain of this form will lead to massless boundary spins transforming in the representations $3$ and $3'$, respectively. With periodic boundary conditions however, we end up with a unique ground state. A state which belongs to the topological class $t = 1$ necessarily breaks inversion symmetry since the representations $3$ and $3'$ in the auxiliary space need to be treated on a different footing. Since the ground state is required to be non-degenerate, this actually provides an interesting challenge for the construction of a suitable two-site Hamiltonian as will be discussed below.

The state $|\phi_2\rangle$ is obtained from $|\phi_1\rangle$ by inversion. In particular, the left auxiliary space of each site is interchanged with the right auxiliary space. As should be clear from the exchange of auxiliary spaces, the new state $|\phi_2\rangle$ resides in the non-trivial topological phase $t = [(0, 1)] = 2$. Of course we can also apply the inversion to the Hamiltonian $H_1$, resulting in a new Hamiltonian $H_2$ of which $|\phi_2\rangle$ is the unique ground state.

B. A family of Hamiltonians

We are now making the preceding statements more explicit, following the standard strategy of the AKLT construction.\cite{12} Our goal is to find concrete expressions for the Hamiltonians $H_1$ and $H_2$ as well as for the in-
terpolating Hamiltonian $H(c)$ defined in (36). This requires introducing the concept of Casimir operators (see also Appendix B) and the calculation of a few tensor products. It turns out that we can restrict our attention to Hamiltonians involving nearest neighbor interactions only.

The two-site Hilbert space decomposes as follows,

$$(1,1) \otimes (1,1) = (0,0) \oplus (1,1)_s \oplus (1,1)_a \oplus (3,0) \oplus (0,3) \oplus (2,2).$$

(37)

The subscripts in $(1,1)_s$ and $(1,1)_a$ refer to the symmetric and to the anti-symmetric part of the tensor product. Schur’s Lemma implies that $su(3)$ invariant Hamiltonians cannot change the type of representation. This leaves one parameter for each of the representations which occur with multiplicity one but four parameters for the representation $(1,1)$ which appears with multiplicity two. The latter can be thought of as the entries of a $2 \times 2$ matrix which acts on the multiplicity space of the representation $(1,1)$. In total, there is thus an eight-dimensional space of two-body Hamiltonians which commute with the action of $su(3)$. In what follows, we will express these explicitly in terms of invariant combinations of the spin operators $\hat{S}_1$ and $\hat{S}_2$ on the two sites.

The basic objects we have at our disposal are the expression $Q_{12} = \hat{S}_1 \cdot \hat{S}_2$, which is related to the quadratic Casimir $(\hat{S}_1^2 + \hat{S}_2^2)$ as well as the cubic terms $C_{112} = d_{rst}S_1^rS_2^sS_2^t$ and $C_{122} = d_{rst}S_1^rS_2^sS_2^t$ which are defined using a symmetric invariant rank three tensor $d_{rst}$, see Appendix B. In addition, we need to consider polynomials in these objects, potentially with permutations in the order of the operators. One example for such an operator would be

$$C^{(2)} := d_{rst}d_{uvw}S_1^rS_1^uS_2^sS_2^vS_2^wS_2^t.$$  

(38)

A careful analysis shows that the eight-dimensional space of invariant operators acting on the tensor product $(1,1) \otimes (1,1)$ is spanned by

$$\langle 1, Q_{12}, Q_{12}^2, Q_{12}^3, C_s = C_{112} + C_{122},$$

$$\langle C_a = C_{112} - C_{122}, C^{(2)}, [C_a, C^{(2)}] \rangle.$$  

(39)

The action of some of these operators on the constituents of the tensor product (37) is summarized in Figure 3. Note that $C_a$ is an operator which exchanges the symmetric and the anti-symmetric part of the tensor product. After some linear algebra, it turns out that a good choice for the interpolating two-site Hamiltonian entering (36) is given by

$$H(c) = 1 + \frac{9}{56}\hat{S}_1 \cdot \hat{S}_2 - \frac{5}{112}(\hat{S}_1 \cdot \hat{S}_2)^2$$

$$- \frac{1}{112}(\hat{S}_1 \cdot \hat{S}_2)^3 + (1 - 2c)^2 \frac{2}{7} C_a - \frac{4}{63} C^{(2)}.$$  

(40)

We note that the deformation parameter $c$ only multiplies the term $C_a$ which explicitly breaks inversion symmetry. It is not obvious at all, but an explicit calculation shows that the Hamiltonian above reduces to a projector for $c = 0$ and for $c = 1$ (see the table in Figure 3). In both cases it projects onto the subspace generated by $(3,0) \oplus (0,3) \oplus (2,2)$ as well as two (different) one-dimensional subspaces in the two-dimensional multiplicity space of $(1,1)_s \oplus (1,1)_a$. The latter single out a specific copy of $(1,1)$ inside of $(1,1)_s \oplus (1,1)_a$. In other words, the space of zero-energy states (for two sites) is given by $(0,0)$ and states in a complementary copy of $(1,1)$ within $(1,1)_s \oplus (1,1)_a$ for $c = 0$ and $c = 1$. This is precisely the content of $(1,0) \otimes (0,1)$, i.e. the contribution of the four auxiliary sites with the singlet constraint imposed, thus showing that the Hamiltonians $H(0)$ and $H(1)$ are of AKLT-type.

Since the numerical evaluation of the Hamiltonian (40) is quite time-consuming we shall henceforth work with the following family of truncated Hamiltonians,

$$H_{\text{trunc}}(c) = 1 + \frac{9}{56}\hat{S}_1 \cdot \hat{S}_2 + (1 - 2c)^2 \frac{2}{7} C_a .$$  

(41)

In view of the structural similarity with the Hamiltonian (40), we believe that both share the same qualitative features. Evidence for this assertion comes from the exact diagonalization on a chain of $L = 6$ sites.

C. Evaluation of the topological order parameter and discussion

For different values of $c$ in Eq. (41), we have calculated the ground state using DMRG techniques. We have considered a chain of length $L = 20$ and worked with an auxiliary space of dimension $D = 400$. We calculated the expectation value of the string order parameter $\langle \sigma_{i,j}^{ab} \rangle$ numerically, for the specific sites $i = 5$ and $j = 15$. We compared the resulting matrix to the expression

$$\langle \sigma_{ij} \rangle = -R \left( \begin{array}{c} 1 \\ \Omega^t \\ 1 \end{array} \right)$$

with $\Omega = \exp \frac{2\pi i}{3}$,  

(42)
which is the theoretical prediction for the string order parameter in the limit of an infinite chain (see Eq. (14)). The numerical values of the parameters $R$ and $t$ have been estimated by minimizing $e_{\sigma} = \text{tr}(d\sigma \cdot d\sigma^\dagger)$, with $d\sigma = (\sigma_{ij}^{ab}) - (\sigma_{ij}^{\text{eq}})$. The results are plotted in Figure 4 and they are in perfect agreement with the theory. The parameter $t$ is quantized and restricted to the numbers 1 and 2, thus providing the desired label for the topological class of the system. Moreover, this parameter changes discontinuously at the value $c = 1/2$.

The failure of finding $R = 0$ at the phase transition is probably due to finite bond dimension and finite system size. Indeed, apart from potential numerical deficiencies there are finite size corrections which have been neglected in the derivation of Eq. (14). These finite size effects become more important as the mass gap goes to zero and the correlation length increases. Let us summarize two observations which provide evidence for this assertion. First of all, the error bars in Figure 4 which quantify the discrepancy of the numerical result from the analytical expression grow significantly close to the transition point. In addition, we compared the numerical results for $R$ at $c = 1/2$ using two different bond dimensions $D = 200$ and $D = 400$. The drop from $R = 0.31$ to $R = 0.20$ is another signal of finite size effects.

Of course, the transfer matrix method allows to compute the string order exactly, even for finite size of the system, once the eigenvalues and the eigenvectors of the transfer matrix have been determined. However, our numerical analysis here should merely be regarded as a proof of principle. A more accurate treatment will be left for future work. Despite our numerical limitations we still clearly see the crossover from one topological phase to another.

In addition to the previous investigations we applied the same method to the full parent Hamiltonians $H_1$ and $H_2$. Also in this case, the numerical analysis confirmed our analytical expectation that the corresponding ground states belong to the non-trivial topological classes 1 and 2, respectively.

V. CONCLUSIONS

In our paper, we have searched for a physical observable which allows to distinguish the $N$ different topological phases of $PSU(N)$ spin chains. To achieve this goal we have proposed a non-local string order operator in equation (13) and we have shown that its expectation value provides an unambiguous measure for the topological phase the chain resides in. In essence, our string order parameter extracts the projective class of the representations according to which potential (virtual) massless boundary modes transform in. It should be emphasized that, in contrast to earlier studies, our string order parameter is matrix valued. All matrix entries are equal in absolute value and identical to zero in the topologically trivial phase. The information about the quantized topological phase of the chain is contained in the relative complex phases between different matrix entries. More precisely, the quotient of two suitably chosen matrix elements is completely sufficient in order to extract the quantized topological order parameter determining the topological phase. Our analytical results are supported by the numerical study of a family of $PSU(3)$ Hamiltonians which interpolates between two distinct non-trivial topological phases. Since the realization of these two phases enforces the breaking of inversion symmetry, the Hamiltonian employs a new construction scheme making explicit use of higher order Casimir operators. We find full agreement between our analytical predictions and the numerical results. Indeed, Figure 4 clearly exhibits a robust quantization of the topological order parameter.

Even though tentative results have been included here, we believe that $SU(N)$ spin chains deserve further numerical study. First of all, our numerical investigation of the string order parameter only covered a special family of $SU(3)$ spin chains, the interpolation between two topologically non-trivial phases. While this provided the desired proof of principle that our method works in practice, one could similarly analyze the behavior of the string order parameter when interpolating between a non-trivial phase and the trivial phase. An important open problem in this context is the identification of the type of phase transitions that occur when crossing the boundary between two distinct topological phases. For our model Hamiltonian we analyzed the gap behavior in the vicinity of the transition point $c = 1/2$. However, at this point of time our DMRG results are not accurate enough to be able to draw a final conclusion. Another possible avenue to uncover the nature of the phase transition is the investigation of the scaling behavior of the entanglement entropy. The latter is directly accessible from the DMRG representation of the ground state. However, just as before accurate results would require increasing bond dimension and system size.
Another natural direction is the extension of our numerical study to larger values of $N$. Since $PSU(N)$ spin chains have $N$ distinct topological phases, we expect a complicated phase diagram with a large number of different phase transitions which might be implemented. It would be interesting to investigate whether each pair of mutually distinct phases is directly connected or whether they are only connected via a series of phase transitions each of which changes the $Z_N$ topological order by one unit for instance.

It is evident that systems which are invariant under continuous symmetries different than $SU(N)$ should also admit a string order parameter similar to the one described in the current paper. Even though the groups based on $SU(N)$ are the most interesting ones due to the large size of their center, it is known that two and three distinct non-trivial topological phases, respectively, also exist for the symmetry groups $E_6$ and $Spin(2N)$ (the universal cover of $SO(2N)$). Just as for $PSU(N)$ a single expectation value will not be sufficient to distinguish between different types of topological order for such symmetries. In addition, an extension to certain classes of supersymmetric or anisotropic systems looks feasible.

It should be noted, however, that the respective symmetries of these systems are described by supergroups or quantum groups and that a classification of topological phases is still missing in that context. Nevertheless, it seems likely that our formula (13) will be applicable in anisotropic spin chains with $SU_q(N)$ quantum group symmetry without modification.

It remains to be clarified how our string order parameter relates to other recent proposals for the determination of the projective class of (virtual) edge modes. While there is no fundamental obstruction in applying these techniques to the case of $PSU(N)$, the details still need to be worked out. In particular, we would like to remark that both Refs. 20 and 22 adopt a perspective which is somewhat different from ours: Their discussion is based on relations between discrete group elements (possibly interpreted as elements of subgroups of a continuous group), while our proposal only features the underlying Lie algebra and, in fact, only its abelian part.

As a result, our final formula (13) for the string order parameter is easy to evaluate on the standard basis of the spin states. This statement is independent of whether the ground state is represented as a matrix product state or not.

Let us finally address an interesting conceptual issue that arises in connection with our work. For the original $SU(2)$ AKLT chain it is well known that the existence of a non-trivial Rommelse-Den Nijs string order is equivalent to the breaking of a discrete hidden symmetry $\mathbb{Z}_2 \times \mathbb{Z}_2$. This intimate relationship can be made manifest by means of a non-local transformation of the spin chain. It would be very interesting to investigate whether a similar relationship exists for general $SU(N)$ spin chains and to analyze the symmetry breaking patterns of discrete groups that arise in this way when considering the full hierarchy of topological phases.\footnote{The relationship between string order and discrete hidden symmetries for higher rank groups was also discussed in Ref. 22.}

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Appendix A: Weyl group invariance of Clebsch-Gordan coefficients

In this Appendix it will be shown that the expression $P(\mu, \nu)$ defined in Eq. (29), is invariant under a Weyl transformation of the weights $\mu$ and $\nu$. Note that the expression can be rewritten as a trace over three orthogonal projections:

$$P(\mu, \nu) = \sum_{\lambda, \rho \in \mathcal{P}} |\langle \lambda | ij \rangle |^2 = \text{tr}(\Pi_{\lambda\mu} \Pi_H \Pi_{\mu\nu}) \ . \ (A1)$$

Recall that $\mathcal{H}_k \subset \mathcal{H}_{(k,L)} \otimes \mathcal{H}_{(k,R)}$: $\Pi_H$ denotes the orthogonal projection onto this subspace. $\Pi_{\mu\nu}$ denotes the orthogonal projections on the weight space $V_{\mu} \otimes V_{\nu} \subset \mathcal{H}_{(k,L)} \otimes \mathcal{H}_{(k,R)}$.

The Weyl group is not only the symmetry group of the root system, but it can also be defined as the quotient group of the normalizer of the maximal torus with the centralizer of the maximal torus: $W = N(T)/Z(T)$. The maximal torus of $SU(N)$ simply consists of all diagonal matrices with elements of $U(1)$ on the diagonal and determinant 1. Just like elements in the Cartan subalgebra $h^\ast$, elements of the maximal torus have a simple action on states $v_\lambda$ with a well defined weight $\lambda$. For $h = \exp H (H \in h)$ one simply obtains

$$\rho(h)v_\lambda = \exp \lambda(H)v_\lambda \ . \ (A2)$$

Let $\sigma : SU(N) \supset N(T) \to W \to \text{Aut}(\Gamma_V)$, where $\Gamma_V$ is the space of weights appearing in the representation $V$. Explicitly, $\sigma_w(\mu(h) = \mu(w^{-1}hw)$. Weyl invariance of $P(\mu, \nu)$ will follow from

$$P(\sigma_w\mu, \sigma_w\nu) = P(\mu, \nu) \ . \ (A3)$$

The advantage of this approach is that since $w \in SU(N)$, the action of the Weyl group is trivial to implement on
Since if this holds, the Weyl transformed function $P$ can be rewritten as

$$\rho_i(w) \Pi_{\mu, \nu} = \Pi_{\sigma_{w, \mu}}, \quad (A4)$$

which shows that $P(\mu, \nu)$ is Weyl invariant. In the second equality, $\rho_{12} = \rho_1 \otimes \rho_2$. In the third equality, we make use of the cyclic property of the trace to cancel the outer two maps $\rho_{12}(w)$ and $\Pi_{\mu, \nu}$ commute. We are left to check the validity of Eq. (A4). Let $v_{\mu} \in V_{\mu}$ and let $h$ be an element in the maximal torus. The chain of equalities

$$\rho(h) \rho(w) v_{\mu} = \rho(w) \rho(w^{-1} h w) v_{\mu} = \mu(w^{-1} h w) \rho(w) v_{\mu} = \sigma_{w, \mu} \rho(w) v_{\mu}, \quad (A6)$$

shows that $\rho(w) v_{\mu} \in V_{\sigma_{w, \mu}}$. From this, Eq. (A4) follows.

**Appendix B: Casimir operators of su(3)**

The Casimir elements of a Lie algebra are polynomials in its generators $S^r$ which are central, i.e., which commute with each of the generators. For $su(3)$ there are two algebraically independent Casimir operators. One is the usual square of the spin vector $\vec{S}^2$. It is associated with a non-degenerate invariant form, and can be expressed as $\vec{S}^2 = \kappa_{rs} S^r S^s$ where $\kappa_{rs}$ is an invariant symmetric rank two tensor. The second Casimir is a cubic invariant $\{ S^r, S^s, S^t \} = d_{rst} S^r S^s S^t$ which can be constructed from a non-vanishing invariant symmetric rank three tensor $d_{rst}$. Up to normalization, all invariant tensors of $su(3)$ are obtained by choosing suitable representations and by considering traces of the form

$$t^{a_1 \cdots a_n} = \text{tr}(S^{a_1} \cdots S^{a_n}) \quad (B1)$$

These tensors are not all independent. On the contrary, there exist algebraic relations between the tensors which may be used to reduce higher rank tensors to those of relatively low degree.

For $su(3)$ the most convenient way of finding explicit expressions for the tensors $[B1]$ is to employ the fundamental representation in which the spin operators $S^r = \lambda^r / 2$ are proportional to the Gell-Mann matrices $\lambda^r$ (see e.g. Ref. [5]). One then defines

$$\kappa^{rs} = \text{tr}(\lambda^r \lambda^s) = 2 \delta^{rs}, \quad (B2)$$

$$d^{rst} = \frac{1}{4} \text{tr}(\{ \lambda^r, \lambda^s \} \lambda^t) \quad (B3)$$

By construction, $\kappa^{rs}$ and $d^{rst}$ are manifestly symmetric. The matrices $\kappa^{rs}$ and its inverse, $\kappa_{rs} = \delta_{rs} / 2$, serve as a metric which can be used to raise and lower indices, just as in special and in general relativity. The tensors which are used for the construction of the Casimir operators are $\kappa_{rs}$ and $d_{rst} = \kappa_{ra} \kappa_{sb} \kappa_{tc} d^{aub}$.

Since Casimir operators commute with the action of $su(3)$, they are represented as scalars on irreducible representations. With our normalization conventions, the eigenvalues of the quadratic and the cubic Casimir operator,

$$Q = 4 \kappa_{rs} S^r S^s \quad \text{and} \quad C = 8 d_{rst} S^r S^s S^t \quad (B4)$$

on the irreducible representation with highest weight $\lambda$ are given by

$$Q_{\lambda} = \langle \lambda, \lambda + 2 \rho \rangle = \frac{2}{3} \left( \lambda_1^2 + \lambda_2^2 + \lambda_1 \lambda_2 + 3 \lambda_1 + 3 \lambda_2 \right) \quad (B5)$$

and

$$C_{\lambda} = \lambda \left( \lambda - \lambda_2 \right) \left[ \frac{2}{9} \left( \lambda_1 + \lambda_2 \right)^2 + \frac{1}{9} \lambda_1 \lambda_2 + \lambda_1 + \lambda_2 + 1 \right].$$

In contrast to $Q_{\lambda}$, the cubic Casimir $C_{\lambda}$ can distinguish between a representation $\lambda = (\lambda_1, \lambda_2)$ and its dual $\lambda^* = (\lambda_2, \lambda_1)$. We also see that $C_{\lambda}$ vanishes on all representations which are self-dual.

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