Symmetry Protected Topological Phases of Spin Chains

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This thesis is dedicated to my brother Dolf, who sadly passed away in his beloved Alps.

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Abstract

Symmetry protected topological (SPT) phases are characterized by robust boundary features, which do not disappear unless passing through a phase transition. These boundary features can be quantified by a topological invariant which, in some cases, is related to a physical quantity, such as the spin conductivity for the quantum spin Hall insulators. In other cases, the boundary features give rise to new physics, such as the Majorana fermion. In all cases the boundary features can be analyzed with the help of an entanglement spectrum and their robustness make them promising candidates for storing quantum information. The topological invariant characterizing SPT phases is strictly only invariant under deformations which respect a certain symmetry. For example, the boundary currents of the quantum spin Hall insulator are only robust against non-magnetic, i.e. time-reversal invariant, impurities. In this thesis we study the SPT phases of spin chains.

As a result of our work we find a topological invariant for SPT phases of spin chains which are protected by continuous symmetries. By means of a non-local order parameter we find a way to extract this invariant from the ground state wave function of the system. Using density-matrix-renormalization-group techniques we verify that this invariant is a tool to detect transitions between different topological phases. We find a non-local transformation that maps SPT phases to conventional phases characterized by a local order parameter. This transformation suggests an analogy between topological phases and conventional phases and thus give a deeper understanding of the role of topology in spin systems.

Zusammenfassung

Symmetriegeschützte topologische Phasen (SPT-Phasen, von engl. symmetry protected topological) sind durch stabile Randeigenschaften bestimmt, die sich nur bei Quanten-Phasenübergängen ändern. Diese Eigenschaften können durch topologische Invarianten ausgedrückt werden, die in einigen Fällen in direkter Verbindung zu physikalischen Eigenschaften des betrachteten Systems stehen; ein Beispiel hierfür ist die Spin-Leitfähigkeit von Quanten-Spin-Hall-Isolatoren. In anderen Fällen äußern sie sich in Gestalt neuer Physik, beispielsweise Majorana-Fermionen. Die Randeigenschaften können mit Hilfe des Verschränkungsspektrums analysiert werden. Durch ihre Stabilität sind sie vielversprechende Kandidaten für die Speicherung von Quanteninformation. Die topologischen Invarianten sind strenggenommen nur für eine Klasse von symmetrieerhaltenden Deformationen invariant. Beispielsweise sind die Randströme in einem Quantum-Spin-Hall-Isolator nur stabil gegen nicht-magnetische Störstellen, d.h. solche, die die Zeitumkehrsymmetrie nicht brechen.

In der vorliegenden Arbeit untersuchen wir SPT-Phasen von Spinketten. Liegt der Stabilität eine kontinuierliche Symmetrie zugrunde, so geben wir eine topologische Invariante an, die mit Hilfe eines nichtlokalen Ordnungsparameters aus der Grundzustandswellenfunktion des System berechnet werden kann. Zur Überprüfung unserer theoretischen Vorhersage verwenden wir Dichtematrix-Renormierung und zeigen, dass sich diese Invariante zur Untersuchung von Übergängen zwischen verschiedenen topologischen Phasen eignet. Desweiteren geben wir eine nichtlokale Transformation an, mit deren Hilfe man SPT-Phasen auf solche abbilden kann, die durch einen lokalen Ordnungsparameter charakterisiert werden. Wir erhalten so eine Korrespondenz zwischen topologischen und konventionellen Phasen und gelangen auf diese Weise zu einem grundlegenderen Verständnis letzterer.

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Chapter 1

Introduction

Topological phases of matter have become of growing interest in the last couple of decades. They are often explained as phases that cannot be characterized by symmetry breaking, thus phases beyond the Landau paradigm [1]. This statement can be unsatisfying: it does not explain why these phases are coined *topological* and it does not enlighten us on any of the interesting properties of topological phases on which I will touch in this introduction.

In my thesis I will focus on a sub-topic of this growing field of topological phases: spin chains. Spin chains arise as models of 1-dimensional crystals in the limit of large on-site coulomb repulsion. Consider for example the Hubbard model, which describes the hopping of electrons and the Coulomb potential between two electrons if they occupy the same site. At half filling and small hopping amplitude compared to the Coulomb potential, this model describes a Mott insulator. Here electrons are essentially bound to a single site and each site is occupied by a single electron. They are effectively modeled by a spin 1/2 degree of freedom for each site. Exchange interactions, which can be thought of as virtual hoppings of electrons, lead to different types of couplings between neighboring electrons. A prime example is the Heisenberg model. The Hamiltonian describing this model is

$$H = J \sum_{i=1}^{L-1} \vec{S}_i \cdot \vec{S}_{i+1} \quad , \tag{1.1}$$

where J is the interaction strength, L is the number of electron sites and $\vec{S}_i$ denotes the operator that measures the spin direction of the i-th site. This model can be thought of as a quantum version of a chain of magnets. With a positive J these magnets prefer to anti-align to minimize the energy. It is important to understand the symmetry of this Hamiltonian. Since the Hamiltonian is a function of the relative orientation of neighboring spins, rotating all spins in the same manner will have no physical effect. Since spin rotations are given by the group $SU(2)$, this is also the symmetry group of this system. I have introduced the Heisenberg model by giving

the Hamiltonian of a spin 1/2 chain. This Hamiltonian can also be used to model crystals with more than one valence electron per ion. If S is the size of the effective electron spin on each site, we are dealing with a spin S chain.

Effects of topology already appear in the Heisenberg model. Haldane conjectured that the physics of the anti-ferromagnetic Heisenberg model is profoundly different for the cases when S is integer compared to the cases when S is half integer [2, 3]. If S is integer there is a finite energy difference (gap) between the ground state and the first excited state. This is evident if the size of the spin chain L is finite, however the gap persists even in the limit of infinite L. If S is half integer the anti-ferromagnetic Heisenberg model is gapless, meaning that the energy difference between the ground state and the first excited state vanishes as L goes to infinity. In the semiclassical limit, when the spin S is large, the conjecture is well established. The different behavior between integer and half integer spin systems can be explained by the presence or absence of a topological Θ-term in a non-linear sigma model of the spin chain. Later I will explain that the difference in behavior can also be understood by symmetry fractionalization.

In introducing the Heisenberg model, each ion of the crystal had an effective electronic spin of size S. Mathematically, spin S is a $(2S+1)$-dimensional representation of $SU(2)$. This $(2S+1)$-dimensional space, denoted by V_S, is called the on-site Hilbert space of the spin chain. The total Hilbert space is the tensor product of L copies of such spaces:

$$V_S^{[1]} \otimes V_S^{[2]} \otimes V_S^{[3]} \otimes V_S^{[4]} \otimes \cdots \otimes V_S^{[L]} = \bigotimes_{i=1}^{L} V_S^{[i]} \quad . \tag{1.2}$$

Here $V_S^{[i]}$ is the Hilbert space modeling the effective electronic degrees of freedom of the i-th site. By construction, this Hilbert space allows for an action of $SU(2)$. In the same manner, spin chains allowing for an action of any group, G, can be constructed. For example, the Hilbert space of an $SU(N)$ spin chain can be defined by tensoring L copies of a representation space of $SU(N)$. Whether such a chain is also $SU(N)$ invariant depends on the Hamiltonian of that system. Physically $SU(N)$ spin chains can arise in cold atom systems [4], created by atoms which are trapped in an optical lattice formed by lasers. (Note the similarities with electrons being trapped in a periodic Coulomb potential formed by a crystal of ions.) In earth-alkaline atoms the nuclear spin I is almost completely decoupled from the electronic angular momentum. Due to this decoupling, the $SU(2)$ symmetry is lifted to an $SU(N)$ symmetry where $N = 2I + 1$ and can be as large as 10.

The integer quantum Hall (IQH) effect is one of the first observed example of a topological phase [5]. It is an effect that arises when applying a large magnetic field to a 2-dimensional electron gas. This field gives rise to Landau levels with energy $\epsilon_m = \hbar\omega_c(m + 1/2)$, where ω_c is the cyclotron

frequency. The gap between the different Landau levels ensures that an IQH system is insulating if N levels are completely filled and the rest are empty. However, a current can be measured to flow along the boundaries of the sample with a Hall conductivity (σ_H) given by

$$\sigma_H = N\frac{e^2}{h} \quad . \tag{1.3}$$

Strikingly this conductivity is completely universal. It only depends on the number of filled Landau levels N and fundamental physical constants. It is independent of material details. The quantization of σ_H can be understood if one relates it to a topological invariant [6]. Via the Kubo formula, the Hall conductivity is shown to be proportional to the so called first Chern number. This number is an invariant of the topological space which models the electronic bands and only changes during a phase transition. In conclusion, the IQH effect gives rise to topological phases which differ in their boundary properties. This difference is quantified by a topological invariant N.

Related to the IQH effect is the fractional quantum Hall (FQH) effect. It is different in that N in Eq. (1.3) can now be some fraction ν. The first measurements were done with $\nu = 1/3$ [7], but FQH states with other fractional fillings have also been observed. The integer case can be understood by considering free electrons, in the fractional case however, interactions play a major role.

FQH states were one of the first to be analyzed by studying their entanglement spectrum [8], which is obtained by decomposing the Hilbert space $\mathcal{H}$ into two parts $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Spatial decompositions are most easily visualized. In Ref. [8] the FQH state was realized on a spherical geometry. A cut was created along the equator such that $\mathcal{H}_A$ is the northern and $\mathcal{H}_B$ the southern hemisphere. The ground state is described as

$$|\Psi\rangle = \sum_i e^{-\lambda_i/2}|\Psi_A^i\rangle \otimes |\Psi_B^i\rangle \quad . \tag{1.4}$$

The entanglement spectrum is given by the set $\{\lambda_i\}$. Remarkably, it contains information usable for characterizing the topological phase in which the state $|\Psi\rangle$ resides. As mentioned above, an IQH system is characterized by boundary currents, a sphere however, does not have boundaries. The decomposition into a northern and a southern hemisphere introduces an artificial boundary. The entanglement spectrum gives information on possible gapless boundary modes of a FQH state considered only on the northern or southern hemisphere. Indeed it was shown that the low lying energy levels of the entanglement spectrum $\{\lambda_i\}$ of a $\nu = 5/2$ FQH state coincide with the spectrum of a conformal field theory [8], which is always gapless.

Although I have not given a direct definition of what a topological phase is, the two previous examples indicate that in some cases it can be characterized by robust boundary properties, which persist throughout the phase.

These properties can be observed in a suitably chosen entanglement spectrum. I will continue this paradigm by considering yet another example of a topological phase that gives rise to exotic boundary physics.

In Ref. [9] a model of a quantum wire is discussed. It consists of spinless electrons obtained by applying a magnetic field to select one spin direction. The quantum wire is put onto a superconductor leading to electron pair creation and annihilation via the proximity effect. The Hamiltonian can be written in a compact form of coupled Majorana fermions. Let $c_n^\dagger$ create an electron on the n-th site. For each electron one can define two Majorana operators $\gamma_{n,1} = c_n + c_n^\dagger$ and $\gamma_{n,2} = i(c_n - c_n^\dagger)$, which are self adjoint ($\gamma_{n,i} = \gamma_{n,i}^\dagger$). For a certain choice of parameters the Hamiltonian is

$$H = -i \sum_{n=1}^{L-1} \gamma_{n,2}\gamma_{n+1,1} \quad . \tag{1.5}$$

The ground state of this Hamiltonian has the remarkable feature of having Majorana degrees of freedom localized at its boundary, see Fig. 1.1. This can be easily understood since the operators $\gamma_{1,1}$ and $\gamma_{L,2}$ do not enter in the Hamiltonian. Signals which could be remnants of these Majorana fermions have been recently measured in the lab [10]. Other than the emergence of these exotic boundary modes, I have not mentioned why this phase is topological. It is however separated by a quantum phase transition from the system described by the Hamiltonian [9]

$$H = -i \sum_{n=1}^{L-1} \gamma_{n,1}\gamma_{n,2} \quad . \tag{1.6}$$

Its ground state clearly does not have any Majorana fermions as boundary modes. Otherwise, both Hamiltonians are very similar in the sense that their ground states do not spontaneously break some symmetry of the Hamiltonian in different manners. However, both Hamiltonians describe systems residing in different phases since they can not be connected by a path of Hamiltonians without going through a phase transition [11, 12]. The above Hamiltonian describes a system in a topologically trivial phase whereas the Hamiltonian described by Eq. (1.5) describes a system in a topologically non-trivial phase.

The Majorana wire gives an example of a topological phase with boundary modes (Majorana fermions) which do not appear in the bulk of the wire. The Majorana fermions are not fundamental but rather emergent particles. In the bulk Majoranas pair up to form an electron. Those realized on the left and right boundary do not pair into an electron due to their spatial separation. This causes the Hamiltonian, given by Eq. (1.5), to have a completely delocalized electronic degree of freedom.

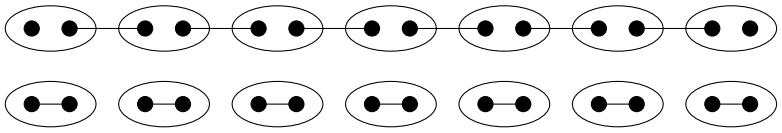

Figure 1.1: A graphical representation of the two phases of the quantum wire. Ellipses represent sites with a spinless electron. Each electron can be represented by two Majorana fermions (black dots). In the topological phase, Majorana fermions of different sites are coupled to each other (top) which results in boundary Majorana modes. In the trivial phase (bottom) these Majorana modes are not present.

Keeping the above discussion in mind I now to return to the topological phases in which spin chains can reside. Let G be the symmetry group of the spin chain. Recall that the Hilbert space of such a spin chain is modeled by a tensor product of L copies of a representation space of G, see Eq. (1.2). Naively, one would expect boundary modes to also transform according to this same representation. Let V_L and V_R be the representation spaces of the left and right boundary modes. Recently, it has been understood that for topologically phases, V_L and V_R need not be representations of G. Only the pair $V_L \otimes V_R$ is necessarily a representation of G [13, 14]. This is in complete analogy with the Majorana wire. Majoranas appear as emergent particles localized at the boundary although they are not the fundamental particles of the bulk. There is however one main difference. Topological phases of spin chains are only different phases (separated by a quantum phase transition) if one restricts to G invariant systems. This is why topological phases in spin chains are called symmetry protected.

Consider a $S = 1$ spin chain with a Hamiltonian given by

$$H = \sum_{i=1}^{L-1} \left[\vec{S}_i \vec{S}_{i+1} + \frac{1}{3} \left(\vec{S}_i \vec{S}_{i+1} \right)^2 \right] \quad . \tag{1.7}$$

Although it is not the same as the Heisenberg Hamiltonian given by Eq. (1.1), they both reside in the same symmetry protected topological (SPT) phase [15] that is called the Haldane phase. It is important to note that spin 1 is not only a representation of $SU(2)$ but also a faithful representation of $SO(3)$. It has the same structure as $SO(3)$ and not of $SU(2)$. (Note that $SU(2)$ is larger than $SO(3)$ since $SO(3) = SU(2)/\mathbb{Z}_2$.). It is thus more correct to call a spin 1 chain an $SO(3)$ chain.

Although the Hamiltonian described by Eq. (1.7) is an $SO(3)$ spin chain, it has boundary modes transforming according to the spin $1/2$ representation of $SU(2)$, which is clearly not a representation of $SO(3)$. However, both

boundary modes together pair into

$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1 \quad , \tag{1.8}$$

which is an $SO(3)$ representation. Here 0 and 1 denote the spin singlet and triplet representation. The spin 1 fractionalizes into two spin 1/2, just as an electron fractionalizes into two Majoranas. As explained with the FQH example, the entanglement spectrum can be used to observe this symmetry fractionalization. Indeed, the entanglement spectrum of systems in the Haldane phase consists of energy levels which are all even-fold degenerate [16]. This reflects the even dimensionality of half-integer spin representations, according to which artificial boundary modes of systems residing in the Haldane phase transform.

Similarly, on any $SO(3)$ invariant spin chain, Hamiltonians can be defined which have ground states with half-integer spin and fractionalized boundary modes. In contrast, half-integer boundary modes are not fractionalized on $SU(2)$ invariant spin chains since then the boundary modes transform under representations of the symmetry group. The fractionalized boundary modes occurring on integer spin chains can be related to the Haldane conjecture stating that the anti-ferromagnetic Heisenberg Hamiltonian is only gapped (topological phase) if defined on an such chains.

SPT phases do not only occur in spin chains. The quantum spin Hall (QSH) effect [17, 18] is another example of an SPT phase. It is a closely related to the IQH effect. In an IQH system time reversal symmetry is broken by the magnetic field, in a QSH system time reversal symmetry is not broken. Strong spin-orbit interactions can lead to chiral boundary modes. Here chiral means that the momentum is coupled to spin: spin up and down electrons travel in opposite directions. Two phases exist in QSH systems, depending on whether the number of boundary modes is odd or even. As long as time reversal is respected, these two phases cannot be connected without passing through a quantum phase transition. Similar effects were predicted in 3D topological insulating materials [19, 20, 21] and were first measured in bismuth antimony alloys [22].

The next Chapter of this thesis contains my three publications [DQ1, DQ2, DQ3]. In the first paper, *Topological phases of spin chains*, we discuss spin chains which are invariant under continuous symmetries described by a compact connected simple Lie group. We explicitly discuss the different phases that can arise in such systems and their characterizing features in terms of boundary modes. We generalize the statement that chains with an $SU(2)/\mathbb{Z}_2$ symmetry (being equal to $SO(3)$), allow for two phases, to; chains with an $SU(N)/\mathbb{Z}_N$ symmetry (being equal to $PSU(N)$), allow for N phases. This number N can in principle be any integer, which is remarkable when put into contrast to the periodic table of topological insulators [11, 12] where the non-trivial entries are $\mathbb{Z}_2$ and $\mathbb{Z}$, which implies only two or an

infinite number of phases.

In the second paper, *A discriminating string order parameter for topological phases of gapped $SU(N)$ spin chains*, we discuss a way to measure the features of the boundary modes that characterize the phase, by defining a topological invariant for the phases of $SU(N)$ spin chains. This invariant, which only changes during quantum phase transitions, can be extracted from a set of string order parameters in a novel way. Where other string order parameters are only able to distinguish between two phases by a zero/non-zero effect [23] or a positive/negative effect [24], our string order parameters can directly distinguish N phases.

In a third manuscript, *From symmetry-protected topological order to Landau order* we discuss a transformation which maps systems residing in SPT phases to systems residing in spontaneous symmetry breaking (SSB) phases and vice versa. Such a transformation was known for quite some time for the $SO(3)$ invariant spin 1 chain [25]. For the first time we generalize it such that it is applicable to spin chains invariant under a symmetry group of the form $\mathbb{Z}_N \times \mathbb{Z}_N$. This transformation gives a deeper understanding of SPT phases in terms of hidden symmetry breaking. Different SPT phases can be understood as phases in which the protected symmetry is broken in a different *hidden* manner. This symmetry breaking becomes apparent after applying our generalized transformation a different number of times. In the same manuscript we also argue that the SPT phases arising in spin chains protected by a symmetry G are also protected by a discrete subgroup of G, if G is a simple compact connected Lie group. In almost all cases (including $PSU(N)$) this subgroup is of the form $\mathbb{Z}_N \times \mathbb{Z}_N$ allowing to understand the corresponding SPT phases as to occur due to hidden symmetry breaking.

Chapters 3 to 5 contain relevant background information as well as some extending ideas. The first of these three chapters describes matrix product states (MPS). This name refers to a technique to cope with the exponentially increasing dimension of the Hilbert space of 1-dimensional quantum systems. It is the foundation of numerical tools such as DMRG [26] which can be used to calculate ground states with computation resources scaling only polynomially with system size. The framework of MPS is also useful as an analytical tool since it gives rise to gapped Hamiltonians with exactly known ground states and it allows for a direct access to the entanglement spectrum. In chapter 4 the classification of spin chains is discussed [13, 14]. Chapter 5 discusses some additional topics which go beyond my papers. Our $SU(N)$ string order parameter giving rise to a topological invariant can also be derived from a recently found selection rule for general string order parameters [27]. Also, some extra insights are discussed regarding the transformation defined in the third paper (which relates SPT phases to symmetry breaking phases).

Chapter 2

Publications

In this chapter the following three publications can be found:

1. K. Duivenvoorden and T. Quella, "Topological phases of spin chains," *Phys. Rev. B* 87 (2013) 125145.
2. K. Duivenvoorden and T. Quella, "A discriminating string order parameter for topological phases of gapped $SU(N)$ spin chains," *Phys. Rev. B* 86 (2012) 235142.
3. K. Duivenvoorden and T. Quella, "From symmetry-protected topological order to Landau order," *Phys. Rev. B* 88 (2013) 125115.

They are cited throughout the thesis as [DQ1, DQ2] and [DQ3].

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Discriminating string order parameter for topological phases of gapped $SU(N)$ spin chains

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One-dimensional gapped spin chains with symmetry $PSU(N) = SU(N)/\mathbb{Z}_N$ are known to possess N different topological phases. In this paper, we introduce a nonlocal string order parameter which characterizes each of these N phases unambiguously. Numerics confirm that our order parameter allows one to extract a quantized topological invariant from a given nondegenerate gapped ground state wave function. Discontinuous jumps in the discrete topological order that arise when varying physical couplings in the Hamiltonian may be used to detect quantum phase transitions between different topological phases.

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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.[1] 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 nontrivial 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.[2,3] While the exact ground state for the Heisenberg Hamiltonian is not known, the AKLT chain provides a convenient laboratory which allows one 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 nontrivial 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 nontrivial topological phases. It was later understood that the topological nature is due to symmetry fractionalization which allows the edge modes to carry a discrete $\mathbb{Z}_2$-valued topological quantum number.[4,5] Secondly, all these features can also be observed in a characteristic entanglement spectrum[6] 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 nonlocal string order parameter,[7] sensitive to a kind of diluted antiferromagnetic order, which allows one to distinguish the topologically trivial from the topologically nontrivial phase.

Various extensions of the AKLT setup to higher rank groups and supersymmetric systems have been considered (see, e.g., Refs. 3,8–11). Other generalizations include q deformations of the symmetry group which can be used to describe anisotropic spin chains.[12,13] In all these examples the matrix product (or valence bond) state formalism plays a crucial role.[14–17] The latter has also proven extremely useful in connection with the classification of symmetry protected topological phases in general one-dimensional (1D) spin systems.[4,5,18] 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. In addition, 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 for 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.[19–21] 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 nonlocal order parameters. Important progress in this direction has recently been achieved in Refs. 20 and 22 (see also Refs. 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 antiferromagnetic 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 $\mathbb{Z}_N$ of the group $SU(N)$ can be realized on possible boundary spins. Just as in the $SO(3) = SU(2)/\mathbb{Z}_2$ AKLT chain before, the situation can be understood as a fractionalization of the physical symmetry $PSU(N) = SU(N)/\mathbb{Z}_N$ 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 $\mathbb{Z}_N$. The string order parameter thus allows one to extract a discrete topological invariant which permits one 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 nontrivial phases of a $PSU(3)$ 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 $\vec{S}_1 \cdot \vec{S}_2$ 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 Fig. 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.[25,26] In addition, 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.[27] It should be noted that string order parameters have also been suggested for other systems (e.g., 1D Haldane Bose insulators).[28] Since the latter has been observed in experimental measurements[29] 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 Sec. 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, Sec. IV is devoted to the numerical study of a family of $PSU(3)$ symmetric spin chains which interpolates between two topologically nontrivial 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 appendixes.

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 outline 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 more 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 $su(N)$ 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 Sec. IV B.

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 nondegenerate finitely correlated state[14–16] (nondegenerate 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 antiferromagnetic 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,

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

with nearest neighbor interactions. The coupling constant J is assumed to be positive, thereby favoring antiparallel 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. In addition, 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 $\mathcal{V}$.[30] For other representations, the existence of a gap can be proven in the limit of "large spin" using a mapping to a σ-model with a topological Θ-term.[31–33] More recently, the question of the Haldane gap has been revisited in Refs. 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.[2,3] These Hamiltonians arise as "parent Hamiltonians" of specific matrix product states (MPS).[14–17] 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 Sec. 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[17]

$$|\phi\rangle = \sum_{i_1,\ldots,i_L} \mathrm{tr}(A^{[1]i_1} \cdots A^{[L]i_L}) \, |i_1 \cdots i_L\rangle, \tag{2}$$

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.[14–16] 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 (2) 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 $|I_k\rangle = \sum_q |q\rangle\langle q| \in \mathcal{H}_{(k,R)} \otimes \mathcal{H}_{(k+1,L)}$ where $|q\rangle$ refers to an orthonormal basis of $\mathcal{H}_{(k,R)}$. The matrices $A^{[k]}$ can be regarded as linear maps from $\mathcal{H}_{(k,L)} \otimes \mathcal{H}_{(k,R)}$ to $\mathcal{H}_k$. The state $|\phi\rangle$ is the image of the tensor product $|I\rangle = |I_1\rangle \otimes \cdots \otimes |I_{L-1}\rangle$ of completely entangled pairs under the map $\mathfrak{A} = A^{[1]} \otimes \cdots \otimes A^{[L]}$. The application of the map $\mathfrak{A}$ to the product of completely entangled pairs $|I\rangle$ 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 $|\phi\rangle$ should be invariant under the action of $SU(N)$.[35] These two properties imply the existence of additional structures which are realized on the data of an MPS. Let $R^{[k]}(g)$ denote the representation of $SU(N)$ on the space $\mathcal{H}_k$. According to Ref. 36, this on-site symmetry lifts to the auxiliary level as

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

thereby promoting $\mathcal{H}_{(k,L)}$ and $\mathcal{H}_{(k,R)}$ to representations of $SU(N)$.[37] 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 (3) 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 statement, let us for a moment assume that $D^{[k]} = D^{[k+1]}$ 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 $\mathbb{Z}_N$ of the symmetry group $SU(N)$. In other words, $R^{[k]}$ descents to a linear representation of the quotient group $PSU(N) = SU(N)/\mathbb{Z}_N$ while no such requirement exists for the matrix $D^{[k]}$. The latter only needs to implement a *projective representation* of $PSU(N)$,

$$\begin{aligned} &D(g_1)D(g_2) = \omega(g_1,g_2)\, D(g_1 g_2), \\ &\text{with} \quad g_1, g_2 \in PSU(N) \quad \text{and} \quad \omega(g_1,g_2) \in U(1), \end{aligned} \tag{4}$$

that is, 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 $SU(N)/\Gamma$ on the physical Hilbert spaces $\mathcal{H}_k$, where $\Gamma \subset \mathbb{Z}_N$ is an arbitrary subgroup of the center of $SU(N)$. It can be shown that the group $SU(N)/\Gamma$ has $|\Gamma|$ distinct classes of projective representations.[21]

In a series of papers,[4,5,18] 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 $|\phi\rangle$ of the form (2) there exists a local Hamiltonian with the following two properties:[17] The state $|\phi\rangle$ 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 $\mathcal{B}_L = \mathcal{H}_{(1,L)}$ and $\mathcal{B}_R = \mathcal{H}_{(L,R)}$. 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. 38 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 $(E^{ab})_{cd} = \delta_{ac}\delta_{bd}$ with a single nonzero 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 $\rho_V(H^a)$. 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 μ provided that

$$H^a v = \mu(H^a)v =: \mu_a v. \tag{5}$$

The different eigenvalues μ_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 ω_a which are dual to the Cartan generators in the sense that $\omega_a(H^b) = \delta_a^b$. 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,

$$V = \bigoplus_{\mu \in \mathfrak{h}^*} V_\mu. \tag{6}$$

In a finite dimensional representation all weights μ 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 λ whose Dynkin labels λ_a are all nonnegative 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 λ, the different weights are all related by the application of roots α. 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 μ in the representation λ one has $\lambda - \mu \in Q$ where Q is the root lattice which is generated by the (finite) set of roots α.

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 $X \mapsto \mathrm{ad}_X = [X, \cdot\,]$. The nonzero weights of the adjoint representation are precisely the roots α. The $N - 1$ simple roots have weights α_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 $\rho = \frac{1}{2}\sum_{\alpha>0}\alpha = (1, \ldots, 1)$, the so-called Weyl vector, which has a scalar product $(\rho, \alpha_a) = 1$ with each of the simple roots α_a. The dual generator $H^\rho \in \mathfrak{h}$ is characterized by the property,

$$\alpha_a(H^\rho) = 1, \tag{7}$$

for all $a = 1, \ldots, N - 1$. This generator will play an important role in the definition of the string order parameter in Sec. III. With the previous choice of simple roots one can find the following explicit expression for the diagonal entries of the matrix $H^\rho = \mathrm{diag}(H_1^\rho, \ldots, H_{N-1}^\rho) \in \mathfrak{h}$,

$$H_a^\rho = \frac{N+1}{2} - a. \tag{8}$$

Indeed, one can easily check that this defines the unique traceless diagonal matrix with $H_a^\rho - H_{a+1}^\rho = 1$, 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 $S \in \mathcal{W}$ 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 ϵ_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 $\epsilon_i(H) = H_{ii}$. 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 ϵ_i. However, this disadvantage is compensated by the simple transformation behavior under the action of the Weyl group $\mathcal{W}$ 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 $S_\sigma \in \mathcal{W}$ one simply has

$$S_\sigma(\epsilon_i) \;=\; \epsilon_{\sigma(i)}. \tag{9}$$

Given this formula, we can deduce the Weyl group action on any weight $\mu = \sum_i c_i \epsilon_i$. 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 μ_a as

$$c_i \;=\; -\sum_{a=1}^{i-1} \frac{a}{N}\mu_a + \sum_{a=i}^{N-1} \frac{N-a}{N}\mu_a. \tag{10}$$

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 $\epsilon_i(H^a)$ and $\epsilon_i(H^\rho)$ can be easily calculated. The former evaluates to $\epsilon_i(H^a) = \delta_{i,a} - \delta_{i,a+1}$, while the latter is $\epsilon_i(H^\rho) = \frac{N+1}{2} - i$. 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,

$$\epsilon_{\sigma_m(i)}(H^\rho) \;=\; \epsilon_i(H^\rho) - m + N\,\theta(i + m - N). \tag{11}$$

Here, θ is the Heaviside step function with $\theta(0) = 0$.

D. Classes of representations

As was discussed in detail in our previous article,[21] the representations λ 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

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

When representations are specified using Young tableaux, the class of a representation can be expressed as the number of boxes modulo N.[21] 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 μ in a representation with highest weight λ. As is illustrated in Fig. 1, Eq. (12) divides the weight lattice of $su(N)$ into N different sublattices.

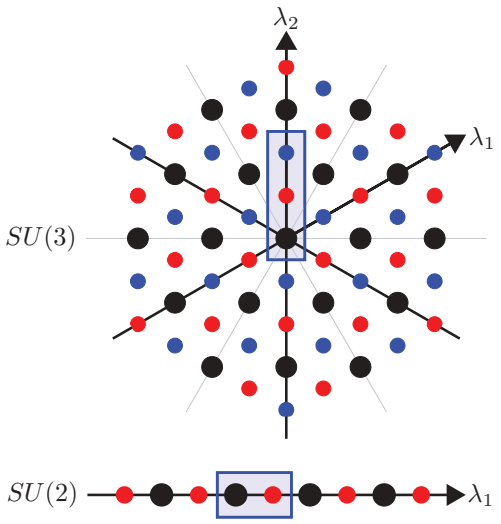


FIG. 1. (Color online) Visualization of different congruence classes for $SU(2)$ and $SU(3)$ in terms of colors. The shaded blue boxes are possible representatives of topological classes.

The congruence class $[\lambda]$ of a representation λ determines whether the representation descends to quotients of the group $SU(N)$. More precisely, the value of $[\lambda]$ fixes the action of the center $\mathbb{Z}_N$ of $SU(N)$ on the representation λ. Elements of $\mathbb{Z}_N \subset SU(N)$ are multiples $\Omega^k I_N$ of the identity matrix with $\Omega = \exp(\frac{2\pi i}{N})$ denoting the fundamental N^{th} root of unity. In the representation λ, this element is mapped to the complex phase $\rho(\Omega^k I_N) = \Omega^{k[\lambda]}$. We conclude that representations λ with $[\lambda] \equiv 0$ are linear representations of $PSU(N) = SU(N)/\mathbb{Z}_N$. Likewise we may ask whether a representation λ lifts to any of the groups $SU(N)/\mathbb{Z}_q$ where $\mathbb{Z}_q \subset \mathbb{Z}_N$ is a subgroup of the center. This is the case if and only if $[\lambda] \equiv 0 \bmod q$ (instead of using mod N).[21]

The connection to the classification of topological phases comes in since representations λ of $SU(N)$ with $[\lambda] \not\equiv 0$ 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 Sec. 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 Sec. 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 λ) 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 nontrivial 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 $\mathcal{H}^*_{(k,R)} =$

$\mathcal{H}_{(k+1,L)}$ 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 nonlocal string order parameter for $SU(N)$ spin chains which reduces to the diluted antiferromagnetic order of Rommelse and den Nijs[7] 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 Sec. 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 nonlocal string order operator,

$$\sigma_{ij}^{ab} \;=\; H_i^a \exp\!\left[\frac{2\pi i}{N}\sum_{k=i+1}^{j-1} H_k^\rho\right] H_j^b \quad (\text{for} \quad i<j), \tag{13}$$

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^ρ refers to the Cartan operator associated with the Weyl vector ρ (see Sec. II C). For $SU(2)$, expression (13) reduces to the string order $S_i^z \exp(i\pi\sum S^z) S_j^z$ introduced by Rommelse and den Nijs.[7]

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

$$T^{ab} = \lim_{|i-j|\to\infty}\langle\sigma_{ij}^{ab}\rangle \;=\; C_{ij}\,\Omega^{t(a-b)}, \qquad \text{with} \quad \Omega = \exp\frac{2\pi i}{N}. \tag{14}$$

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 nontrivial phase the prefactor is expected to be nonzero.[40] 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 $\Omega^{t(a-b)}$. 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 $T^{21}/T^{11} = \Omega^t$. 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.

B. 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 $J_{j,R}$ can be dealt with analogously.

1. 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 Sec. 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,

$$H_k^a\,\mathfrak{A} \;=\; \mathfrak{A}\big(H_{k,L}^a + H_{k,R}^a\big), \tag{15}$$

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

$$H_{k,R}^a|I\rangle \;=\; -H_{k+1,L}^a|I\rangle, \tag{16}$$

one easily sees that the phase factors in the string order operator σ_{ij}^{ab} cancel out pairwise except for the two boundaries. We then immediately find

$$\big\langle\sigma_{ij}^{ab}\big\rangle \;=\; \frac{\langle\phi|\sigma_{ij}^{ab}\mathfrak{A}|I\rangle}{\langle\phi|\phi\rangle} \;=\; \frac{\langle\phi|\mathfrak{A}J_{i,L}^a J_{j,R}^b|I\rangle}{\langle\phi|\phi\rangle}, \tag{17}$$

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

$$J_{i,L}^a \;=\; \big(H_{i,L}^a + H_{i,R}^a\big)\,\Omega^{-H_{i,R}^\rho}, \qquad \text{and} \tag{18}$$

$$J_{j,R}^b \;=\; \Omega^{-H_{j,L}^\rho}\big(H_{j,L}^b + H_{j,R}^b\big). \tag{19}$$

Note that each of these operators acts locally on two *auxiliary* sites. However, neither of them can be lifted to an operator acting locally on *physical* sites, that is, there is no way to commute them back through $\mathfrak{A}$ without rebuilding the original nonlocal string.

Now that we could eliminate the nonlocal string connecting the two sites i and j we can evaluate the string order parameter using standard transfer matrix techniques.[14] For that purpose, we write

$$\begin{aligned}&\langle\phi|\mathfrak{A}J^a_{i,L}J^b_{j,R}|I\rangle\\&\quad=\mathrm{tr}\big(\cdots E^{[i-1]}E^{[i]}_{J^a_L}E^{[i+1]}\cdots E^{[j-1]}E^{[j]}_{J^b_R}E^{[j+1]}\cdots\big),\end{aligned}\tag{20}$$

$$\langle\phi|\phi\rangle=\mathrm{tr}(E^{[1]}\cdots E^{[L]}),\tag{21}$$

where

$$\big(E^{[k]}_X\big)_{\alpha\beta,\mu\nu}=\sum_{s,\gamma,\rho}(\bar{A}^{[k]})^s_{\alpha\mu}(A^{[k]})^s_{\gamma\rho}\,\langle\gamma\rho|X|\beta\nu\rangle,\tag{22}$$

and $E^{[k]}=E^{[k]}_{\mathbb{1}}$. A pictorial interpretation of the expectation value is provided in Fig. 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 $\mathcal{H}_{(k,R)}$ to matrices acting on the auxiliary space $\mathcal{H}_{(k,L)}$.[41] 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 $\dim\mathcal{H}_k/\dim\mathcal{H}_{(k,L)}$ and $\dim\mathcal{H}_k/\dim\mathcal{H}_{(k,R)}$,

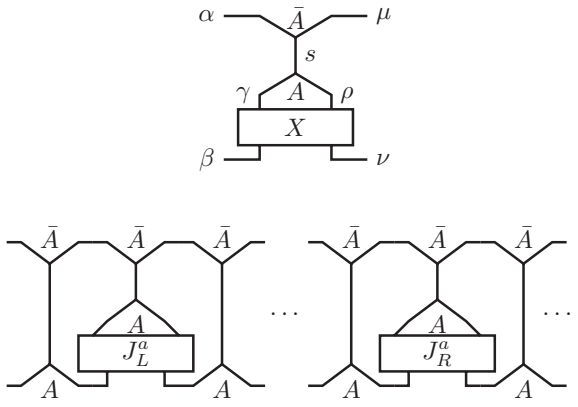


FIG. 2. Sketch of the one-site transfer matrix $E^{[k]}_X$ (upper diagram) and of the expectation value (20) (lower diagram). For the latter, periodic boundary conditions are assumed.

respectively. Indeed, due to Schur's Lemma we have

$$E^{[k]}_{\alpha\beta,\mu\nu}\,\mathbb{1}_{\mu\nu}=C_R\,\mathbb{1}_{\alpha\beta},\qquad\text{and}\tag{23}$$

$$\mathbb{1}_{\alpha\beta}\,E^{[k]}_{\alpha\beta,\mu\nu}=C_L\,\mathbb{1}_{\mu\nu}.\tag{24}$$

Moreover, it is obvious that

$$\begin{aligned}\dim(\mathcal{H}_k)&=\mathbb{1}_{\alpha\beta}\,E^{[k]}_{\alpha\beta,\mu\nu}\,\mathbb{1}_{\mu\nu}=C_R\,\mathrm{tr}_{\mathcal{H}_{(k,R)}}(\mathbb{1})\\&=C_R\,\dim(\mathcal{H}_{(k,R)}),\end{aligned}\tag{25}$$

and similarly for C_L. Since $E^{[k]}$ is a completely positive map it is guaranteed that there is no greater eigenvalue (Ref. 42, Prop 3.6). On the other hand, due to our mass gap assumption this eigenvalue is nondegenerate, even in absolute value.[17]

In the limit of large separation, $|i-j|\gg 1$, we can rewrite the desired expectation value in a factorized form as

$$\begin{aligned}\big\langle\sigma^{ab}_{ij}\big\rangle&=\frac{\langle\mathbb{1}_{\mathcal{H}_{(i,L)}}|E^{[i]}_{J^a_L}|\mathbb{1}_{\mathcal{H}_{(i,R)}}\rangle}{\dim\mathcal{H}_i}\,\frac{\langle\mathbb{1}_{\mathcal{H}_{(j,L)}}|E^{[j]}_{J^b_R}|\mathbb{1}_{\mathcal{H}_{(j,R)}}\rangle}{\dim\mathcal{H}_j}\\&=\big\langle J^a_{i,L}\big\rangle\big\langle J^b_{j,R}\big\rangle.\end{aligned}\tag{26}$$

We note that the result still depends on the representation spaces describing the start and the end point of the original string.

2. *Step 2: Employing Weyl symmetry*

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

Since the operators $J^a_{i,L}$ contain Cartan elements only, their expectation value can be calculated most easily in an orthonormal basis $|\alpha\beta\rangle$ of the auxiliary space $\mathcal{H}_{(i,L)}\otimes\mathcal{H}_{(i,R)}$ which respects the weight space decomposition. In such a basis the operator $J^a_{i,L}$ 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 μ (of $\mathcal{H}_{(i,L)}$ in this case). Moreover, we wish to recall that the matrices $(A^{[k]})^s_{\alpha\beta}$ 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 definition of the expectation values J^a in Eq. (26) we immediately conclude

$$\begin{aligned}J^a&=\frac{1}{\dim\mathcal{H}_i}\sum_{s,\alpha,\beta}|\langle s|\alpha\beta\rangle|^2J^a_{\alpha\beta}\\&=\frac{1}{\dim\mathcal{H}_i}\sum_{\mu,\nu}\sum_{\substack{\alpha\in\mu,\beta\in\nu\\ s\in\mu+\nu}}|\langle s|\alpha\beta\rangle|^2J^a_{\alpha\beta}.\end{aligned}\tag{27}$$

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 α and β, but only on the weight space they

belong to. We may thus define

$$J^a_{\mu\nu} := J^a_{\alpha\beta} \qquad \text{with} \qquad \alpha \in \mu, \beta \in \nu. \tag{28}$$

Furthermore, it is convenient to introduce the abbreviation,

$$P(\mu,\nu) := \sum_{\substack{\alpha \in \mu, \beta \in \nu \\ s \in \mu+\nu}} |\langle s|\alpha\beta\rangle|^2, \tag{29}$$

such that above expression can be written as

$$J^a = \frac{1}{\dim \mathcal{H}_i} \sum_{\mu,\nu} P(\mu,\nu) J^a_{\mu\nu}. \tag{30}$$

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 μ and ν 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 $\mathcal{W}_{\mu+\nu} \subset \mathcal{W}$. This procedure yields

$$\begin{aligned} J^a &= \frac{1}{\dim \mathcal{H}_i} \sum_{\substack{\mu,\nu \\ \mu+\nu \in P^+}} \frac{1}{|\mathcal{W}_{\mu+\nu}|} \sum_{S \in \mathcal{W}} P(S\mu, S\nu) J^a_{S(\mu),S(\nu)} \\ &= \frac{1}{\dim \mathcal{H}_i} \sum_{\substack{\mu,\nu \\ \mu+\nu \in P^+}} \frac{P(\mu,\nu)}{|\mathcal{W}_{\mu+\nu}|} \sum_{S \in \mathcal{W}} J^a_{S(\mu),S(\nu)} \\ &= \frac{1}{\dim \mathcal{H}_i} \sum_{\substack{\mu,\nu \\ \mu+\nu \in P^+}} \frac{P(\mu,\nu)}{|\mathcal{W}_{\mu+\nu}|} K^a_{\mu,\nu}. \end{aligned} \tag{31}$$

In the second equation the Weyl invariance of $P(\mu,\nu)$ is used: $P(\mu,\nu) = P(S\mu,S\nu)$ for all $S \in \mathcal{W}$. 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 $K^a_{\mu,\nu}(a) \propto \Omega^{a[\nu]} = \Omega^{at}$. The identification of $[\nu]$ with t follows since the label $[\nu]$ is the same for all weights ν appearing in the decomposition of the $su(N)$ representation $\mathcal{H}_{(i,R)}$. This is a direct consequence of the fact that the ground state $|\phi\rangle$ was assumed to be in a well-defined topological phase.

3. *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):

$$K^a_{\mu,\nu} = \sum_{S \in \mathcal{W}} S(\mu+\nu)(H^a)\, \Omega^{-S(\nu)(H^\rho)}. \tag{32}$$

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

$$\begin{aligned} K^a_{\mu,\nu} &= \sum_k d_k \sum_{\sigma(k)=a} \Omega^{\wedge}\Big(-\sum_l c_l \epsilon_{\sigma(l)}(H^\rho)\Big) \\ &\quad - \sum_k d_k \sum_{\sigma(k)=a+1} \Omega^{\wedge}\Big(-\sum_l c_l \epsilon_{\sigma(l)}(H^\rho)\Big) \\ &= \sum_k d_k \big(Q^{(a)}_k - Q^{(a+1)}_k\big). \end{aligned} \tag{33}$$

Let us now focus on the sum over the different permutations σ which has been abbreviated by $Q^{(a)}_k$ 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 σ_a and of Eq. (11),

$$\begin{aligned} Q^{(a)}_k &= \sum_{\sigma(k)=a} \Omega^{\wedge}\Big(-\sum_l c_l \epsilon_{\sigma(l)}(H^\rho)\Big) \\ &= \sum_{\sigma(k)=N} \Omega^{\wedge}\Big(-\sum_l c_{\sigma^{-1}(l)} \epsilon_{\sigma_a(l)}(H^\rho)\Big) \\ &= \sum_{\sigma(k)=N} \Omega^{\wedge}\Bigg(-\sum_l c_l \epsilon_{\sigma(l)}(H^\rho) + a\sum_l c_l \\ &\quad - \sum_{l=N-a+1}^{N} N c_{\sigma^{-1}(l)}\Bigg) \\ &= \Omega^{a[\nu]}\, Q^{(N)}_k. \end{aligned} \tag{34}$$

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" $\sum_l c_l = 0$. The third sum contains the information we are after. Formula (10) implies the relation $-Nc_k = \sum_a a\nu_a = [\nu]$ (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,

$$J^a = \frac{\Omega^{at}(1-\Omega^t)}{\dim \mathcal{H}_i} \sum_{\substack{\mu,\nu \\ \mu+\nu \in P^+}} \frac{P(\mu,\nu)}{|\mathcal{W}_{\mu+\nu}|} \sum_k d_k Q^{(N)}_k, \tag{35}$$

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 analog 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.[4]

It should be emphasized that the integer number t associated with our string order parameter (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., Refs. 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^a. 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 Sec. 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 nontrivial 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. (12) 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,

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

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 $\bar{3}$ and 3 of $SU(3)$, with highest weight (0,1) and (1,0), respectively. The matrices A correspond to the $SU(3)$ invariant projections $A : \bar{3} \otimes 3 \to 8$ as described in Sec. II. By construction, the state $|\phi_1\rangle$ resides in the nontrivial 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 $\bar{3}$ 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 $\bar{3}$ in the auxiliary space need to be treated on a different footing. Since the ground state is required to be nondegenerate, 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 nontrivial 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.[2,3] Our goal is to find concrete expressions for the Hamiltonians H_1 and H_2 as well as for the interpolating 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:

$$\begin{aligned}(1,1) \otimes (1,1) = (0,0) \oplus (1,1)_s \oplus (1,1)_a \\ \oplus (3,0) \oplus (0,3) \oplus (2,2).\end{aligned} \tag{37}$$

The subscripts in $(1,1)_s$ and $(1,1)_a$ refer to the symmetric and to the antisymmetric 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 2×2 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 $\vec{S}_1$ and $\vec{S}_2$ on the two sites.

The basic objects we have at our disposal are the expression $Q_{12} = \vec{S}_1 \cdot \vec{S}_2$ which is related to the quadratic Casimir $(\vec{S}_1 + \vec{S}_2)^2$ as well as the cubic terms $C_{112} = d_{rst} S_1^r S_1^s S_2^t$ and $C_{122} = d_{rst} S_1^r S_2^s S_2^t$ 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

$$C^{(2)} := d_{rst} d_{uvw} S_1^r S_1^u S_1^v S_2^w S_2^s S_2^t. \tag{38}$$

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

$$\begin{aligned} &\big\langle 1\,,\, Q_{12}\,,\, Q_{12}^2,\, Q_{12}^3,\, C_s = C_{112} + C_{122},\\ &C_a = C_{112} - C_{122},\, C^{(2)},\, [C_a, C^{(2)}]\big\rangle. \end{aligned} \tag{39}$$

The action of some of these operators on the constituents of the tensor product (37) is summarized in Fig. 3. Note that C_a is an operator which exchanges the symmetric and the antisymmetric 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[43]

$$\begin{aligned} H(c) = 1 &+ \frac{9}{56}\vec{S}_1 \cdot \vec{S}_2 - \frac{5}{112}(\vec{S}_1 \cdot \vec{S}_2)^2 \\ &- \frac{1}{112}(\vec{S}_1 \cdot \vec{S}_2)^3 + (1-2c)\frac{2}{7}C_a - \frac{4}{63}C^{(2)}. \end{aligned} \tag{40}$$

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 Fig. 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,

$$H_{\text{trunc}}(c) = 1 + \frac{9}{56}\vec{S}_1 \cdot \vec{S}_2 + (1-2c)\frac{2}{7}C_a. \tag{41}$$

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.

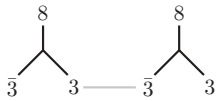
C. Evaluation of the topological order parameter and discussion

For different values of c in Eq. (41), we have calculated the ground state using DMRG techniques.[44] 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 $\langle \sigma_{ij}^{ab} \rangle$ numerically, for the specific sites $i = 5$ and $j = 15$. We compared the resulting matrix to the expression

$$\overline{\langle \sigma_{ij} \rangle} = -R \begin{pmatrix} 1 & \Omega^{2t} \\ \Omega^t & 1 \end{pmatrix} \quad \text{with} \quad \Omega = \exp\frac{2\pi i}{3}, \tag{42}$$

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 $d\sigma = \langle \sigma_{ij}^{ab} \rangle - \overline{\langle \sigma_{ij}^{ab} \rangle}$. The results are plotted in Fig. 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



Tensor product	$8 \otimes 8 = (1,1) \otimes (1,1)$					
Irrep λ	$(0,0)$	$(1,1)_s$	$(1,1)_a$	$(3,0)$	$(0,3)$	$(2,2)$
Q_λ	0	$6\,(\begin{smallmatrix}1&0\\0&1\end{smallmatrix})$		12	12	16
$\vec{S}_1 \cdot \vec{S}_2$	-6	$-3\,(\begin{smallmatrix}1&0\\0&1\end{smallmatrix})$		0	0	2
C_λ	0	$(\begin{smallmatrix}0&0\\0&0\end{smallmatrix})$		9	-9	0
$C^{(2)}$	$\frac{45}{8}$	$-\frac{9}{2}\,(\begin{smallmatrix}1&0\\0&0\end{smallmatrix})$		0	0	$\frac{9}{8}$
C_a	0	$\frac{3}{4}\sqrt{5}\,(\begin{smallmatrix}0&1\\1&0\end{smallmatrix})$		0	0	0

FIG. 3. Construction of the two-site Hamiltonian.

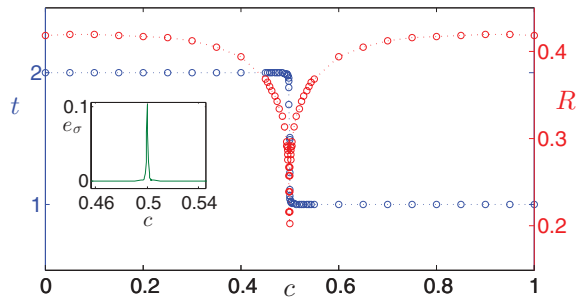


FIG. 4. (Color online) A phase transition between two topological phases. The diagram shows the c dependence of the parameters t (blue, squares) and R (red, circles). The inlet shows the deviation of the measured form of the string order matrix from its analytical form. We used adapted increments in the vicinity of the phase transition.

length increases. Let us summarize two observations which provide evidence for this assertion. First of all, the error bars in Fig. 4 which quantify the discrepancy of the numerical result from the analytical expression (42) 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 one 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 nontrivial topological classes 1 and 2, respectively.

V. CONCLUSIONS

In our paper, we have searched for a physical observable which allows one to distinguish the N different topological phases of $PSU(N)$ spin chains. To achieve this goal we have proposed a nonlocal string order operator in Eq. (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 nontrivial 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, Fig. 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 nontrivial 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 nontrivial 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 (41) 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.[45,46] 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.[47]

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 $\mathbb{Z}_N$ 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[21] that two and three distinct *nontrivial* 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.[20,22] 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 nontrivial Rommelse-Den Nijs string order[7] is equivalent to the breaking of a discrete hidden symmetry $\mathbb{Z}_2 \times \mathbb{Z}_2$.[48–51] This intimate relationship can be made manifest by means of a *nonlocal* 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.[21] The relationship between string order and discrete hidden symmetries for higher rank groups was also discussed in Ref. 52.

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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 μ and ν. Note that the expression can be rewritten as a trace over three orthogonal projections:

$$P(\mu,\nu) \;=\; \sum_{\substack{i\,\in\,\mu,\,j\,\in\,\nu\\ s\,\in\,\mu+\nu}} |\langle s|ij\rangle|^2 \;=\; \mathrm{tr}(\Pi_{\mu\nu}\Pi_{\mathcal{H}}\Pi_{\mu\nu}). \qquad \text{(A1)}$$

Recall that $\mathcal{H}_k \subset \mathcal{H}_{(k,L)} \otimes \mathcal{H}_{(k,R)}$: $\Pi_{\mathcal{H}}$ 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: $\mathcal{W} = N(T)/Z(T)$. 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 $\mathfrak{h}^*$, elements of the maximal torus have a simple action on states v_λ with a well-defined weight λ. For $h = \exp H$ ($H \in \mathfrak{h}$) one simply obtains

$$\rho(h)v_\lambda \;=\; \exp\lambda(H)v_\lambda. \qquad \text{(A2)}$$

Let $\sigma : SU(N) \supset N(T) \to \mathcal{W} \to \mathrm{Aut}(\Gamma_V)$, where Γ_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

$$P(\sigma_w\mu,\sigma_w\nu) \;=\; P(\mu,\nu). \qquad \text{(A3)}$$

The advantage of this approach is that since $w \in SU(N)$, the action of the Weyl group is trivial to implement on $V_1 \otimes V_2$. Denote $\rho_i : SU(N) \to V_i$ for $i \in \{1,2\}$. Using this action we aim to show that

$$\rho_i(w)\Pi_\mu\rho_i(w)^{-1} \;=\; \Pi_{\sigma_w\mu}. \qquad \text{(A4)}$$

Since if this holds, the Weyl transformed function P can be rewritten as

$$\begin{aligned} &P(\sigma_w\mu,\sigma_w\nu)\\ &\quad= \mathrm{tr}(\Pi_{\sigma_w\mu\sigma_w\nu}\Pi_{\mathcal{H}}\Pi_{\sigma_w\mu\sigma_w\nu})\\ &\quad= \mathrm{tr}(\rho_{12}(w)\Pi_{\mu\nu}\rho_{12}(w)^{-1}\Pi_{\mathcal{H}}\rho_{12}(w)\Pi_{\mu\nu}\rho_{12}(w)^{-1})\\ &\quad= \mathrm{tr}(\Pi_{\mu\nu}\rho_{12}(w)^{-1}\Pi_{\mathcal{H}}\rho_{12}(w)\Pi_{\mu\nu})\\ &\quad= \mathrm{tr}(\Pi_{\mu\nu}\Pi_{\mathcal{H}}\Pi_{\mu\nu}) \;=\; P(\mu,\nu), \end{aligned} \qquad \text{(A5)}$$

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 $\rho_{12}(w)^{-1}$. In the fourth equality we make use of the fact that $\rho_{12}(w)$ and $\Pi_{\mathcal{H}}$ 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,

$$\begin{aligned} \rho(h)\rho(w)v_\mu &= \rho(w)\rho(w^{-1}hw)v_\mu\\ &= \mu(w^{-1}hw)\rho(w)v_\mu\\ &= \sigma_w\mu(h)\rho(w)v_\mu, \end{aligned} \qquad \text{(A6)}$$

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 nondegenerate invariant form and can be expressed as $\vec{S}^2 = \kappa_{rs}S^rS^s$ where κ_{rs} is an invariant symmetric rank two tensor. The second Casimir is a cubic invariant $(\vec{S},\vec{S},\vec{S}) = d_{rst}S^rS^sS^t$ which can be constructed from a nonvanishing 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,

$$t^{a_1\cdots a_n} \;=\; \mathrm{tr}(S^{a_1}\cdots S^{a_n}). \qquad \text{(B1)}$$

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 λ^r (see, e.g., Ref. 8). One then defines

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

$$d^{rst} = \tfrac{1}{4}\mathrm{tr}(\{\lambda^r,\lambda^s\}\lambda^t). \qquad \text{(B3)}$$

By construction, κ^{rs} and d^{rst} are manifestly symmetric. The matrices κ^{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 κ_{rs} and $d_{rst} = \kappa_{ru}\kappa_{sv}\kappa_{tw}d^{uvw}$.

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,

$$Q = 4\,\kappa_{rs}S^rS^s \quad \text{and} \quad C = 8\,d_{rst}S^rS^sS^t, \tag{B4}$$

on the irreducible representation with highest weight λ are given by

$$\begin{aligned} Q_\lambda &= (\lambda,\lambda+2\rho) \\ &= \frac{2}{3}\left(\lambda_1^2+\lambda_2^2+\lambda_1\lambda_2+3\lambda_1+3\lambda_2\right) \quad \text{and} \end{aligned} \tag{B5}$$

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

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

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Topological phases of spin chains

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Symmetry-protected topological phases of one-dimensional spin systems have been classified using group cohomology. In this paper, we revisit this problem for general spin chains which are invariant under a continuous onsite symmetry group G. We evaluate the relevant cohomology groups and find that the topological phases are in one-to-one correspondence with the elements of the fundamental group of G if G is compact, simple, and connected and if no additional symmetries are imposed. For spin chains with symmetry $PSU(N) = SU(N)/\mathbb{Z}_N$, our analysis implies the existence of N distinct topological phases. For symmetry groups of orthogonal, symplectic, or exceptional type, we find up to four different phases. Our work suggests a natural generalization of Haldane's conjecture beyond $SU(2)$.

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I. INTRODUCTION

The integer quantum Hall effect is the best-known example of a condensed matter system where a physical observable, the electric conductance, can be expressed in terms of a discrete, $\mathbb{Z}$-valued topological invariant. The interest in such topological phases of matter was renewed with the prediction of a spin quantum Hall effect and an associated $\mathbb{Z}_2$ topological invariant in graphene with time-reversal-invariant spin-orbit interactions.[1] Soon after, a generalization of the spin quantum Hall effect to three dimensions was found.[2] By now, a comprehensive classification of noninteracting fermionic systems is available which describes various types of topological insulators and superconductors.[3–6] These results have been motivated by the symmetry classification of quadratic random Hamiltonians à la Altland and Zirnbauer.[7,8]

More recently, the focus shifted towards interacting systems. Due to strong correlations between the electrons, the notion of a band structure ceases to be valid and alternative methods to detect and to classify topological phases have to be sought. The bulk-boundary correspondence, i.e., the prediction of massless surface modes at the interface between two topologically distinct bulk systems, serves as a useful guiding principle. Evidence may also be gained from characteristic entanglement spectra[9,10] which contain information about potential surface modes by introducing virtual interfaces into the system or from single-particle Green's functions.[11] The first systematic studies of topological phases of interacting fermions have been concerned with Majorana chains.[12–14] For these chains, it was shown that the $\mathbb{Z}$ classification of the corresponding noninteracting symmetry class is reduced to a $\mathbb{Z}_8$ classification. Similar results for other systems have been obtained in Refs. 15,16.

Topologically nontrivial phases are not confined to fermionic systems but they also arise naturally in bosonic models, e.g., in interacting spin systems. A specific deformation of the $SU(2)$-invariant antiferromagnetic Heisenberg spin chain with spin $S = 1$, the so-called Affleck-Kennedy-Lieb-Tasaki (AKLT) spin chain,[17,18] was probably the first example of this type. This system exhibits the following hallmarks of a topological phase: with periodic boundary conditions there is a gap above a unique ground state,[18] one has a bulk-boundary correspondence: open boundary conditions imply massless edge modes carrying a topological quantum number,[19] the ground state leads to a characteristic entanglement spectrum,[20,21] and last but not least there exists a nonlocal string order parameter.[22]

Various extensions of the AKLT setup to higher-rank groups and supersymmetric systems have been considered (see, e.g., Refs. 18,23–26). Other generalizations include q deformations of the symmetry group which can be used to describe anisotropic spin chains.[27–29] In all these examples, the matrix product (or valence bond) state formalism plays a crucial role.[30–33] Indeed, the latter is extremely useful when classifying symmetry-protected topological phases of one-dimensional spin systems since boundary and entanglement properties are almost trivial to access.[34–36] In the meantime, also proposals have been presented on how to address fermionic systems in this framework and how to lift the classification to higher-dimensional systems using projective entangled pairs and, more generally, tensor network states[35,37,38] (see also Ref. 39 for a C^*-algebraic point of view).

In this paper, we are considering gapped antiferromagnetic spin chains which are invariant under the action of an arbitrary compact connected simply connected simple Lie group G. In contrast, we do not impose any additional symmetries such as time-reversal or inversion symmetry. Under these conditions, the general classification predicts that the distinct topological phases are labeled by the elements of a certain cohomology group.[34,35] Depending on the concrete system under study, the relevant cohomology groups are $H^2(G/\Gamma, U(1))$ where $\Gamma \subset \mathcal{Z}(G)$ denotes a central subgroup of G. Elements of this cohomology label the distinct classes of projective representations of G/Γ. The group Γ is determined by the representations of G which are used to describe the physical spins.

To our knowledge, so far explicit results on the cohomology groups $H^2(G/\Gamma, U(1))$ have only appeared in the condensed matter literature for the orthogonal groups $SO(N) = \mathrm{Spin}(N)/\mathbb{Z}_2$ where two topological phases have been found.[40] In addition, the cohomologies for the classical groups $SU(N)$ and $SP(N)$ (corresponding to $\Gamma = \{1\}$) have been written in Ref. 37. However, the corresponding phases all turn out to be topologically trivial, at least in one dimension. In our paper, we will fill this gap and show that the cohomology group $H^2(G/\Gamma, U(1))$ is isomorphic to Γ, which can also be

interpreted as the fundamental group of G/Γ [see Eq. (11)]. Hence, there are $|\Gamma|$ distinct topological phases. This number becomes maximal for $\Gamma = \mathcal{Z}(G)$ in which case the resulting group $PG = G/\mathcal{Z}(G)$ is called the projective group associated with G. For $PSU(N)$, for instance, our result implies the existence of N distinct topological phases.

Aside from stating an abstract classification result, we also discuss how each nontrivial topological phase can be engineered using matrix product states. For this purpose, we state an explicit formula which determines the projective class of a representation of G if it is interpreted as a projective representation of PG [see Eq. (14)]. The topological phases fall into different hierarchies with regard to different choices of central subgroups $\Gamma \subset \mathcal{Z}(G)$. This information is sufficient to determine the projective class with respect to any of the quotients G/Γ. While, from a mathematical perspective, we are merely summarizing well-known facts, we hope that the explicitness of our presentation will be useful to the practitioner.

Our paper ends with a discussion of physical implications. We first reveal a physical interpretation for the hierarchy of topological phases. More importantly, the mere existence of such a hierarchy suggests a natural generalization of Haldane's conjecture[41,42] to arbitrary symmetry groups. In particular, we conjecture the existence of confined spinon phases in spin chains with $SO(2N)$ symmetry and long-range interactions. Even though spin chains with higher-rank symmetry groups such as $SU(N)$ or $SO(2N)$ 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.[43–46] Also, special points in the moduli space of spin chains and spin ladders might exhibit an enhanced symmetry. This for instance happens for $SU(2)$ spin chains which are known to possess an $SU(3)$-symmetric point for a certain value of the couplings.[47]

The paper is organized as follows. In Sec. II, we present a number of physical and mathematical prerequisites. From a physical perspective, this includes a precise definition of the setup, a brief review of the classification of topological phases in terms of the second cohomology of the symmetry group, and the general definition of matrix product states. The mathematical part is concerned with the relation between a Lie algebra $\mathfrak{g}$ and its various associated compact connected Lie groups, which can all be represented as a quotient G/Γ of a simply connected universal covering group G. We introduce the congruence class $[\lambda]$ of an irreducible representation λ of $\mathfrak{g}$. The value of $[\lambda]$ measures whether the representation can be lifted to a linear representation of PG or not. We also recall the intimate connection between central extensions and covering groups.

Section III contains the main result of the paper: We identify the second cohomology of the groups G/Γ with their fundamental group Γ, thereby giving a direct classification of topological phases. In a case-by-case study, we afterwards determine the number of topological phases and their characteristics for each compact connected simple Lie group. Our presentation includes explicit formulas for the congruence class of representations which may be used to characterize gapless edge modes. In Sec. IV, we return to the physical realization of topologically nontrivial phases in spin chains. We give a physical interpretation for the mathematical hierarchy of topological phases in terms of a blocking procedure. Otherwise, the main focus centers around a generalization of Haldane's conjecture to spin chains with arbitrary continuous symmetry. Section V features an application of our formalism to $SU(N)$ spin chains that arise in the context of cold-atom systems. Our results support the observation of Ref. 46 that nontrivial topological phases should be realizable in such systems. Finally, Sec. VI provides a summary and concluding remarks. In particular, we briefly sketch the modification of our classification when space-time symmetries are enforced.

II. PHYSICAL AND MATHEMATICAL PREREQUISITES

The first half of this section is used to define one-dimensional (1D) spin systems with continuous symmetries and to briefly review the classification of topological phases in such systems by means of cohomology groups. For later convenience, we also recall the characterization of nontrivial topological phases in terms of massless edge modes. In the second half, we present some important facts on Lie algebras and Lie groups which are well known in mathematics but required for a self-contained presentation of our results. Our main focus is the relation between Lie algebras and Lie groups. We discuss which groups can be obtained by exponentiating a given Lie algebra $\mathfrak{g}$ and which representations of $\mathfrak{g}$ lift to which of these groups, possibly projectively. For this purpose, we introduce congruence classes of $\mathfrak{g}$ representations. Finally, we discuss the relation between finite coverings of Lie groups and their central extensions.

A. Physical setup

We base the definition of 1D spin chains on the following data: A simple Lie algebra $\mathfrak{g}$ of symmetries, a representation $\mathcal{H}_k$ of $\mathfrak{g}$ attached to each of the sites k, and a Hamiltonian $H \in \mathrm{End}_{\mathfrak{g}}(\mathcal{H})$ which acts on the total Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_L$ of the system and which commutes with the action of $\mathfrak{g}$. In addition, one might wish to impose specific boundary conditions (open, periodic, ...) which are compatible with the action of $\mathfrak{g}$. For physical reasons, the Hamiltonian should be local, i.e., one should be able to write it as a sum $H = \sum_k H_k$ where each summand H_k only affects a finite number of sites. Since the quadratic Casimir is the only second-order invariant of a simple Lie algebra, every Hamiltonian with two-body interactions will be a function of the product $\vec{S}_k \cdot \vec{S}_l$ of the two "spin operators" on the sites k and l.

Given this setup, it is important to note that $\mathfrak{g}$ alone does not (necessarily) determine the full symmetry of the system. In particular, there might be discrete symmetries (e.g., translations but also onsite symmetries) which necessarily need to be described by a group. They can not be captured by the symmetry algebra $\mathfrak{g}$ but may well be relevant for a characterization and/or classification of topological phases. Aside from the choice of $\mathfrak{g}$, also the choice of representations $\mathcal{H}_k$ will play a crucial role in the discussion of discrete symmetries. To give just one trivial example, translations by one site only have a chance to be a symmetry of the system

if all spaces $\mathcal{H}_k$ are chosen to be isomorphic and periodic boundary conditions are imposed.

More important for the purpose of this paper, when lifting the symmetry described in terms of the Lie algebra $\mathfrak{g}$ to a group symmetry G, one might have several choices and not all of them will lead to a faithful representation of G on the spaces $\mathcal{H}_k$. A simple example is the $S = 1$ representation of $SU(2)$ which can not distinguish the two central elements $\pm 1 \in SU(2)$ and hence only corresponds to a faithful representation of $SU(2)/\mathbb{Z}_2 = SO(3)$. In Secs. II E and II F and then in Sec. III, we will discuss additional (and less familiar) examples of this type. Being aware of subtle differences such as those just mentioned is the key to the classification of topological phases in the presence of continuous symmetries.

B. Classification of topological phases

A complete classification of one-dimensional gapped spin systems has been obtained in Refs. 34–36. We use this and the following section to review these results. In case one is only interested in topological phases sharing the same onsite symmetry group G, the classification is particularly simple: Different topological classes are in one-to-one correspondence with the cohomology group $H^2(G,U(1))$ [with trivial action of G on $U(1)$]. If, in addition, space-time symmetries are taken into account, the classification becomes more complicated.[36] In this paper, we wish to keep the presentation simple, thus neglecting potential space-time symmetries throughout the main part of the text. Necessary modifications arising from the presence of space-time symmetries will be briefly discussed in the Conclusions.

Before we proceed, let us briefly recall the definition of the cohomology group $H^2(G,U(1))$. For this purpose, let us consider maps $\omega : G \times G \to U(1)$ which are solutions to the cocycle equation

$$\omega(g_1,g_2)\,\omega(g_1g_2,g_3) \;=\; \omega(g_2,g_3)\,\omega(g_1,g_2g_3). \qquad (1)$$

The set of cocycles forms an Abelian group $\mathcal{G}$ under pointwise multiplication. Furthermore, there are trivial solutions of the cocycle condition which, for $f : G \to U(1)$, have the form

$$\omega(g_1,g_2) \;=\; f(g_1g_2)/f(g_1)f(g_2). \qquad (2)$$

Solutions of this form are called coboundaries and they form a subgroup $\mathcal{K}$ of $\mathcal{G}$. The cohomology group above is defined as the quotient $H^2(G,U(1)) = \mathcal{G}/\mathcal{K}$. In the cases of interest, this is a finite Abelian group (Proposition 2.2 of Ref. 48).

Cocycles arise naturally from projective representations of G, i.e., from maps $D : G \to U(N)$ satisfying

$$D(g_1)D(g_2) \;=\; \omega(g_1,g_2)\,D(g_1g_2). \qquad (3)$$

From this point of view, the cocycle condition (1) is just the associativity condition for the multiplication law (3), while the identification of coboundaries with the trivial cocycle arises from the desire to trivialize the transformation $D(g) \to f(g)D(g)$.

From a physical perspective, the relevance of the second cohomology group $H^2(G,U(1))$ can be understood as follows: Each element $\Omega \in H^2(G,U(1))$ labels a different central extension $\tilde{G}(\Omega)$ of G. If $\omega \in \Omega$ is a representative of the class Ω, this central extension $\tilde{G}(\Omega)$ is defined as the set $G \times U(1)$ with group multiplication

$$(g,\alpha)\cdot(h,\beta) \;:=\; [gh,\alpha\beta\,\omega(g,h)/\omega(1,1)]. \qquad (4)$$

One can check that cocycles ω belonging to the same class Ω give rise to isomorphic central extensions. The choice $\omega(g_1,g_2) = 1$ corresponds to the trivial central extension $\Omega = [0]$. Now the important point is the following: While the total system is invariant under the symmetry group G, the system will exhibit gapless edge modes when considered with open boundary conditions.[34,35] The latter transform under one of the enhanced symmetries $\tilde{G}(\Omega)$ if the system is in a topologically nontrivial phase. If the system has periodic boundary conditions, the same reasoning applies. However, now the edge modes are not real but they rather appear virtually in the bipartite entanglement spectrum after part of the system has been traced out.[20,21] The two possibilities are sketched in Fig. 1.

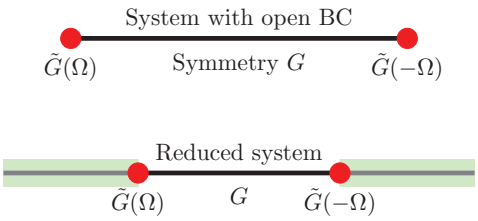

FIG. 1. (Color online) Physical and virtual edge modes (red dots) in topologically nontrivial spin chains. For simplicity of illustration, the spin chain is depicted as a continuous system.

So far, we have not discussed the class of functions that we wish to allow for the cocycles $\omega : G \times G \to U(1)$ and the functions $f : G \to U(1)$ entering Eqs. (1) and (2). For the finite groups mostly used in Refs. 34–36 there is actually no restriction. However, since our paper is concerned with continuous groups, one should impose additional regularity conditions. Demanding continuity turns out to be too restrictive. Indeed, all we need is that linear and projective representations are implemented in terms of continuous homomorphisms $R : G \to U(N)$ and $D : G \to PU(N)$, respectively, where $PU(N) = U(N)/U(1)$. In this formulation, any reference to cocycles is missing altogether. In fact, in order to be admissible, the cocycles only have to respect a Borel structure on the relevant groups G and $U(1)$, i.e., they have to be measurable functions. Since a Borel structure is less restrictive than a topology, this opens the possibility for discontinuous jumps on sets of measure zero. Fortunately, these rather technical aspects are not relevant for the further presentation of the subject. For this reason, we refer interested readers to the more detailed expositions available in the original literature.[48–50]

C. Matrix product states

The previous statements can be motivated most easily in the language of matrix product states (MPS).[34,35] Since all its characteristics should be visible at zero temperature, we expect the topological phase of a system to be fully encoded in its ground state $|\psi\rangle$. In this paper, we will throughout assume the absence of spontaneous symmetry breaking such that the ground state is unique (the more general case can be considered

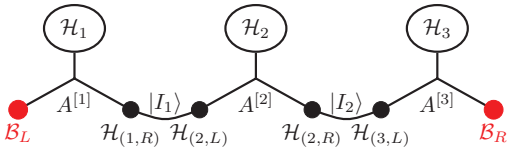

FIG. 2. (Color online) Sketch of a matrix product state for a system with open boundary conditions. The states in the boundary spaces $\mathcal{B}_L$ and $\mathcal{B}_R$ (red) correspond to massless edge modes.

along the lines of Refs. 35 and 36). It is also crucial to require an energy gap between the ground state and the first excited state, even in the thermodynamic limit, since otherwise long-range correlations would exist which might spoil the existence of a topological invariant altogether. We regard the requirement of having a gap as being equivalent to demanding a finite correlation length.

As is well known, any state, including the ground state $|\psi\rangle$, on a periodic chain of length L can be represented as a matrix product state of the form[33]

$$|\psi\rangle = \sum_{i_1,\ldots,i_L} \mathrm{tr}(A^{[1]i_1}\ldots A^{[L]i_L})\,|i_1\ldots i_L\rangle, \qquad (5)$$

where the vectors $|i_k\rangle$ constitute an orthonormal basis of the Hilbert space $\mathcal{H}_k$. If the dimension of the matrices $A^{[k]}$ remains bounded uniformly when L is sent to infinity, it makes sense to speak about the thermodynamic limit of the state $|\psi\rangle$. One can then specify very precise conditions under which the state defines correlation functions with a finite correlation length.[32,33] At the same time, they ensure the existence of a mass gap even in the thermodynamic limit. Throughout the paper, we are only interested in situations where $|\psi\rangle$ is finitely correlated and invariant under the action of G.

From a mathematical perspective, matrix product states arise by associating two auxiliary sites (k,L) and (k,R) to each physical site k which carry a Hilbert space $\mathcal{H}_{(k,L)}$ and $\mathcal{H}_{(k,R)}$. Moreover, we demand that $\mathcal{H}_{(k,R)} = \mathcal{H}^*_{(k+1,L)}$. This guarantees the existence of intertwiners $I_k : \mathbb{C} \to \mathcal{H}_{(k,R)} \otimes \mathcal{H}_{(k+1,L)}$. Alternatively, one has a state $I_k(1) = |I_k\rangle \in \mathcal{H}_{(k,R)} \otimes \mathcal{H}_{(k+1,L)}$, a completely entangled pair, which is invariant under the action of G. Under these prerequisites, the matrices $A^{[k]}$ can be regarded as intertwiners from $\mathcal{H}_{(k,L)} \otimes \mathcal{H}_{(k,R)}$ to $\mathcal{H}_k$. The state $|\psi\rangle$ can then be viewed as the image of a product $|I\rangle = |I_1\rangle \otimes \ldots \otimes |I_{L-1}\rangle$ of completely entangled pairs under the map $A^{[1]} \otimes \ldots \otimes A^{[L]}$. By construction, the state $|\psi\rangle$ is invariant under the action of G. The construction of a matrix product state is sketched in Fig. 2.

Let $R^{[k]} : G \to U(\mathcal{H}_k)$ be a unitary representation of G on $\mathcal{H}_k$ and let, similarly, $D^{[k]} : G \to U(\mathcal{H}_{(k,L)})$ be a unitary (potentially projective) representation on $\mathcal{H}_{(k,L)}$. The intertwining property for the homomorphisms $A^{[k]}$ translates into the equation (see also Ref. 51)

$$R^{[k]}(g) \cdot A^{[k]} = D^{[k]}(g) A^{[k]} D^{[k+1]}(g)^{-1}. \qquad (6)$$

In this equation, the maps $A^{[k]}$ are interpreted as homomorphisms from $\mathcal{H}_{(k,R)} = \mathcal{H}^*_{(k+1,L)}$ to $\mathcal{H}_{(k,L)}$ with values in $\mathcal{H}_k$. It should be emphasized that the auxiliary space $\mathcal{H}_{(k,L)} \otimes \mathcal{H}_{(k,R)}$ can always be regarded as a representation of G even when the two auxiliary spaces $\mathcal{H}_{(k,L)}$ and $\mathcal{H}_{(k,R)}$ themselves are only projective representations of G (as long as their projective class sums up to the trivial one). This is due to the fact that potential phase factors arising in the multiplication law (3) are canceling out on the right-hand side of Eq. (6).

In a chain with open boundary conditions, the auxiliary spaces $\mathcal{B}_L = \mathcal{H}_{(1,L)}$ and $\mathcal{B}_R = \mathcal{H}_{(L,R)}$ at the two boundaries are associated with the massless edge modes and, as advertised before, these are capable of carrying a projective representation of G. This is equivalent to the statement that they carry a linear representation of two centrally extended groups $\tilde{G}(\Omega)$ and $\tilde{G}(-\Omega)$, respectively (if the system is not in a superposition of topological phases). The situation is pictured in Fig. 1.

It was the remarkable insight of Refs. 34 and 35 that the (discrete) projective class Ω is invariant under continuous deformations of the physical system. For this reason, it can be viewed as a quantitative measure for the topological phase the system resides in. The continuity of the deformation is equivalent to the preservation of a gap. Moreover, it is important to emphasize that the previous classification only holds as long as we restrict ourselves to deformations which retain the full original symmetry group G.

If we view the same system from the angle of a different symmetry G' and if we allow for deformations which preserve G' instead of G, the classification of topological phases will change. In particular, one and the same system can belong to different topological classes, depending on the symmetry group under consideration. It is thus incorrect to think about Ω as being an inherent property of the physical system, without specifying the precise symmetry group the classification refers to. This basic but important observation will play a key role in Sec. IV.[52]

It should finally be noted that the dimension of the spaces $\mathcal{B}_L$ and $\mathcal{B}_R$ alone is not sufficient to discriminate between topological phases.[53–55] It really requires knowledge of the full representation type $\Omega \in H^2(G,U(1))$. In principle, the latter should be measurable by a suitable nonlocal order parameter.[40,54,55] In contrast, it is not clear to us whether this knowledge can be inferred unambiguously from (a nonspecialized version of) the entanglement spectrum.

As we have just reviewed, the general principles leading to the classification of symmetry protected topological phases are well known. What is currently still missing is an explicit evaluation of the cohomology groups $H^2(G,U(1))$ for general continuous groups G. Moreover, for the purpose of constructing nontrivial topological phases it will be important to have an explicit map between the boundary representations $\mathcal{B}_L$ and $\mathcal{B}_R$ and their associated projective classes Ω and $-\Omega$. Section III will provide a complete solution to both problems. However, before we can state our results, we first need to recall some facts about the structure of continuous groups.

D. Review of *SU*(2) spin chains: The difference between *SU*(2) and *SO*(3)

In an $SU(2)$ spin chain, the spin operators $\vec{S}_k$ on each site take values in the spin algebra $su(2)$. The relevant irreducible representations are labeled by the spin $S \in \{0,1/2,1,3/2,\ldots\}$. By definition, the spin chain possesses an $SU(2)$ symmetry if the total spin generator $\vec{S} = \sum_k \vec{S}_k$ commutes with the Hamiltonian H.

For the classification of topological phases, we need to carefully consider which symmetry group G is entering the cohomology group $H^2(G,U(1))$. If the physical spins transform in half-integer spin representations, the group $SU(2)$ is acting faithfully and there is only one topological phase. Indeed, it is well known that $SU(2)$ only admits the trivial central extension $SU(2) \times U(1)$.

The situation is different if the physical spins transform in integer spin representations. In that case, $SU(2)$ does *not* act faithfully and the actual symmetry is only $SO(3) = SU(2)/\mathbb{Z}_2$. However, the edge modes can transform in projective representations of $SO(3)$ and all of them can be thought of as ordinary representations of $SU(2)$. We now thus find two different topological classes, corresponding to edge modes transforming either in integer or in half-integer representations of $SU(2)$.[34] The two central extensions [by $U(1)$] corresponding to these two classes are $SO(3) \times U(1)$ and $U(2)$.[56] It should be noted that the difference can already be seen in the two central extensions of $SO(3)$ by $\mathbb{Z}_2$, namely, $SO(3) \times \mathbb{Z}_2$ and $SU(2)$.

In view of the envisaged generalization to spin chains based on $SU(N)$ and other Lie groups, it is useful to understand the difference between $SU(2)$ and $SO(3)$ more precisely in topological terms. When viewed as geometric manifolds, $SU(2)$ and $SO(3)$ look identical locally, i.e., they have the same underlying Lie algebra $su(2)$. However, they differ in their global topology. While $SU(2)$ is simply connected, the group $SO(3)$ is not simply connected, i.e., it admits nontrivial loops which can not be contracted to a point. Phrased more mathematically, $SO(3)$ has fundamental group $\pi_1[SO(3)] = \mathbb{Z}_2$ while $\pi_1[SU(2)] = \{1\}$. In other words, $SU(2)$ can be viewed as a twofold covering of the group $SO(3)$. As we will review in the following section, the close tie between fundamental groups and covering groups extends to other symmetry groups, e.g., to $SU(N)$.

E. From Lie algebras to Lie groups

Let us now consider a general spin chain whose spin operators take values in a Lie algebra $\mathfrak{g}$.[57] For convenience, we will assume $\mathfrak{g}$ to be simple. The rank of $\mathfrak{g}$ will be denoted by r. The finite-dimensional irreducible representations of $\mathfrak{g}$ are labeled by integrable weights λ, i.e., by r-tuples of non-negative integers. Denote this set by P^+. By relaxing the positivity condition, one obtains the weight lattice P. The root lattice will be denoted by Q. It is a sublattice of P and both can be regarded as Abelian groups. In Sec. III, we shall show that, under certain natural assumptions, the topological classes of $\mathfrak{g}$-symmetric spin chains are in one-to-one correspondence with the elements in the quotient P/Q.[58]

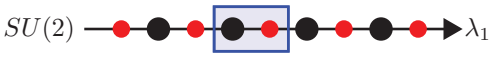

FIG. 3. (Color online) Visualization of different congruence classes for $SU(2)$. The picture shows the weight lattice P (all spins) in terms of colored dots. The root lattice Q (integer spins) corresponds to the large black dots. Different colors indicate different congruence classes. The shaded blue box is a possible representative of P/Q.

In the case $\mathfrak{g} = su(2)$, the weight lattice[59] is given by $P = \mathbb{Z}$, while the root lattice is given by $Q = 2\mathbb{Z}$ such that $P/Q = \mathbb{Z}_2$ (see Fig. 3). This reproduces the classification we obtained for the symmetry group $SO(3)$ but not that for $SU(2)$ even though both are associated with the same Lie algebra $su(2)$. If at all, our assertion can thus only be true for a subset of symmetry groups with Lie algebra $\mathfrak{g}$. In what follows, we review the classification and construction of such Lie groups. We also single out a Lie group PG which arises naturally from a physical perspective and whose second cohomology group coincides with the quotient P/Q.

Any simple Lie algebra $\mathfrak{g}$ can be exponentiated to a compact connected Lie group. However, as we have just seen in Sec. II D, several distinct Lie groups might have the same underlying Lie algebra $\mathfrak{g}$. The Lie groups associated with $\mathfrak{g}$ all look the same locally but they differ in their global topological properties, more precisely in their fundamental group.[60] To obtain a description of all Lie groups belonging to $\mathfrak{g}$, we start with the unique simply connected Lie group G. The Lie group G serves as a universal cover, i.e., all other Lie groups belonging to $\mathfrak{g}$ can be obtained by taking quotients $G_\Gamma = G/\Gamma$ where $\Gamma \subset \mathcal{Z}(G)$ is an arbitrary nontrivial subgroup of the center of G. The groups G_Γ have center $\mathcal{Z}(G_\Gamma) = \mathcal{Z}(G)/\Gamma$ and fundamental group $\pi_1(G_\Gamma) = \Gamma$. It is custom to denote the centerless Lie group with Lie algebra $\mathfrak{g}$ by the symbol $PG = G/\mathcal{Z}(G)$ and to call it the projective group belonging to G.[61] Among the Lie groups associated with $\mathfrak{g}$ it has the maximal fundamental group $\mathcal{Z}(G)$, i.e., its topology is the most complicated. A list of all classical simple Lie algebras $\mathfrak{g}$ and the associated simply connected group G can be found in Table I, together with the relevant data for P/Q and $\mathcal{Z}(G)$. For readers not dealing with Lie theory every day, we should stress that the simply connected double cover of $SO(N)$ is known as Spin(N).

F. Lifting representations

In the following paragraphs, we will compare the representation theory of the groups G and G_Γ (especially PG) and relate it to the representation theory of $\mathfrak{g}$. By considering infinitesimal group actions, it is clear that any finite-dimensional

TABLE I. Simple Lie algebras $\mathfrak{g}$ and their associated compact connected simply connected Lie group G. The table also contains the congruence group P/Q of $\mathfrak{g}$ and the center $\mathcal{Z}(G)$ of G.

Lie algebra $\mathfrak{g}$	A_n	B_n	C_n	D_n	E_6	E_7	E_8	F_4	G_2
Other name	$su(n+1)$	$so(2n+1)$	$sp(2n)$	$so(2n)$					
G	$SU(n+1)$	Spin$(2n+1)$	$Sp(2n)$	Spin$(2n)$	E_6	E_7	E_8	F_4	G_2
$P/Q \cong \mathcal{Z}(G)$	$\mathbb{Z}_{n+1}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_4$ (n odd) $\mathbb{Z}_2 \times \mathbb{Z}_2$ (n even)	$\mathbb{Z}_3$	$\mathbb{Z}_2$	$\{1\}$	$\{1\}$	$\{1\}$

representation of G, G_Γ, or PG must also be a representation of $\mathfrak{g}$. In contrast, the opposite conclusion only holds for the simply connected Lie group G, the universal cover of all the groups G_Γ. This restriction arises from the fact that the center $\mathcal{Z}(G) \subset G$ might act nontrivially on a representation, thus preventing it from descending to the quotient $G_\Gamma = G/\Gamma$. Nevertheless, the latter can still be regarded as a projective representation of G_Γ.

In order to study this issue more systematically, let us consider an irreducible representation V_λ of $\mathfrak{g}$ (and hence G) with highest weight $\lambda \in P^+$. As a consequence of Schur's lemma, the elements of the center $\mathcal{Z}(G)$ are represented by multiples of the identity operator. Put differently, V_λ can be viewed as $\dim(V_\lambda)$ copies of one and the same one-dimensional representation $[\lambda]$ of the Abelian group $\mathcal{Z}(G)$.[62] We call $[\lambda]$ the *congruence class* of λ. $[\lambda]$ can be interpreted as an element $[\lambda] \in \mathrm{Hom}(\mathcal{Z}(G), U(1))$ of the character group of $\mathcal{Z}(G)$. In our situation, with $\mathcal{Z}(G)$ being finite, the character group $\mathrm{Hom}\big(\mathcal{Z}(G), U(1)\big)$ is isomorphic to the center $\mathcal{Z}(G)$ itself, albeit the identification is not canonical.

We note that the algebraic structures on P^+ and on $\mathrm{Hom}(\mathcal{Z}(G), U(1))$ (considered as an additive group) are compatible with the embedding specified above in the sense that $[\lambda + \mu] \equiv [\lambda] + [\mu]$. Indeed, the left-hand side of this equation is determined by the action of $\mathcal{Z}(G)$ on the irreducible representation $V_{\mu+\lambda}$. However, the latter can be realized as an invariant subspace of the tensor product $V_\lambda \otimes V_\mu$ on which the two actions of $\mathcal{Z}(G)$ on the individual factors just multiply trivially, leading to the class $[\lambda] + [\mu]$. Since the trivial representation of G is associated with the trivial representation $[0]$ of $\mathcal{Z}(G)$, the previous relation can be used to extend the definition of $[\,\cdot\,]$ from P^+ to the full weight lattice P. This is also consistent with the observation that if λ^+ denotes the representation conjugate to λ, one easily finds $[\lambda^+] \equiv [\lambda]^+ \equiv -[\lambda]$, as is implied by the existence of the trivial representation inside of $V_\lambda \otimes V_\lambda^*$. Moreover, all groups G_Γ admit an action on $\mathfrak{g}$ by conjugation which is insensitive to the action of the center. Since the generators of $\mathfrak{g}$ can be interpreted as elements of Q, this means that the root lattice Q is mapped to $[0]$ and, in fact, one obtains a homomorphism $P/Q \to \mathrm{Hom}(\mathcal{Z}(G), U(1))$. A closer inspection shows that the homomorphism just constructed is actually an isomorphism (Ref. 63, Theorem 8.30).[64] Summarizing our previous discussion, we obtain an isomorphism

$$P/Q \;\cong\; \mathrm{Hom}(\mathcal{Z}(G), U(1)) \;\cong\; \mathcal{Z}(G). \tag{7}$$

Any representation λ of G with $[\lambda] \equiv [0]$ is a linear representation of PG, while all the other ones are only projective representations.

Similar considerations apply to any subgroup $\Gamma \subset \mathcal{Z}(G)$ of the center. By the same arguments as above, we can define a surjective homomorphism $[\,\cdot\,]_\Gamma : P \to \mathrm{Hom}(\Gamma, U(1))$. Since all the groups involved are Abelian, one can regard the character group $\mathrm{Hom}(\Gamma, U(1))$ of Γ as a quotient of the character group $\mathrm{Hom}(\mathcal{Z}(G), U(1))$ [see also Eq. (35)] and hence as a sublattice of P/Q. If Q_Γ denotes the kernel of the map $[\,\cdot\,]_\Gamma$, we obviously obtain the isomorphisms

$$P/Q_\Gamma \;\cong\; \mathrm{Hom}(\Gamma, U(1)) \;\cong\; \Gamma. \tag{8}$$

All linear representations λ of G_Γ satisfy $[\lambda]_\Gamma \equiv [0]$. If this equation is not satisfied, λ is a projective representation of G_Γ. Note that any representation with $[\lambda] \equiv [0]$ automatically satisfies $[\lambda]_\Gamma \equiv [0]$ for all $\Gamma \subset \mathcal{Z}(G)$. More generally, the relation $[\lambda]_\Gamma \equiv [0]$ implies $[\lambda]_{\Gamma'} \equiv [0]$ for all $\Gamma' \subset \Gamma \subset \mathcal{Z}(G)$. Additional details on the relationship between the maps $[\,\cdot\,]_\Gamma$ and $[\,\cdot\,]_{\Gamma'}$ for different choices of Γ and Γ' can be found in Sec. IV. In the next section, we will argue that all the groups appearing in Eq. (8) can also be identified with the cohomology group $H^2(G_\Gamma, U(1))$, thus relating our findings to the classification of topological phases.

G. Central extensions of compact Lie groups

As discussed in Sec. II B, central extensions of an arbitrary group K are classified by the cohomology group $H^2(K, U(1))$. For a finite group K, the determination of the second cohomology group essentially reduces to a purely combinatorial problem. The situation is very different for continuous groups since now cocycles and coboundaries have to be measurable functions of continuous variables, resulting in an infinite number of constraints.

For concreteness, we assume all Lie groups to be finite dimensional, compact, and connected in what follows. In this case, the cohomology $H^2(K, U(1))$ receives contributions from two sources: there might be local obstructions to the trivialization of cocycles. These are classified by central extensions of the Lie algebra belonging to K and they are absent if K is semisimple. Moreover, there might be global obstructions arising from the existence of noncontractible loops in K, i.e., from a nontrivial fundamental group $\pi_1(K)$.[65]

Our previous statements can brought into a mathematically precise form and they result in the following proposition (for a proof, see e.g. Ref. 48, Proposition 2.1):

Proposition 1. Let K be a finite-dimensional compact connected simple Lie group; then, there is a canonical isomorphism

$$H^2(K, U(1)) \;\cong\; \mathrm{Hom}(\pi_1(K), U(1)). \tag{9}$$

Since $\pi_1(K)$ is finite and Abelian in the cases of interest, the right-hand side actually consists of *all* representations of $\pi_1(K)$ and can be identified with the group $\pi_1(K)$ itself (even though not in a canonical way).

Let us now discuss the implications of the previous proposition for simply connected simple Lie groups G. Since the fundamental group is trivial, one immediately finds that $H^2(G, U(1))$ is trivial as well. In other words, G neither admits nontrivial central extensions nor nontrivial projective representations. All finite-dimensional representations of the underlying Lie algebra $\mathfrak{g}$ lift to linear representations of G.

In the next step, we drop the simply connectedness, i.e., we allow for noncontractible loops. As was recalled in Sec. II E, every simple Lie group can be written as $G_\Gamma = G/\Gamma$ where G is its simply connected universal cover and $\Gamma \subset \mathcal{Z}(G)$ is a subgroup of the center of the latter. The fundamental group of G_Γ can be written as $\pi_1(G_\Gamma) = \Gamma$. In order to illustrate the content of Proposition 1, we are now constructing the central extensions of G_Γ explicitly. Fix an element $\Omega \in H^2(G_\Gamma, U(1))$ and interpret it as a representation

$\Omega : \Gamma \to U(1)$. The associated central extension is given by

$$\tilde{G}_\Gamma(\Omega) = [G \times U(1)]/\Gamma \ , \tag{10}$$

where the central subgroup $\Gamma \subset \mathcal{Z}(G)$ of G is embedded diagonally into $G \times U(1)$ according to the prescription $\gamma \mapsto [\gamma, \Omega(\gamma)]$. Our previous arguments also imply that the projective representations of G_Γ are just the representations of G (or $\mathfrak{g}$) themselves. Different projective classes correspond to different actions of the subgroup Γ. Indeed, due to Schur's lemma, the center Γ can always be interpreted as being embedded in $U(1)$ (possibly not injectively) when acting on an irreducible representation.

III. TOPOLOGICAL PHASES OF GAPPED SPIN CHAINS

In this section, we will give a classification of topological phases in gapped spin chains whose spin operators belong to an arbitrary simple Lie algebra $\mathfrak{g}$. This is achieved by evaluating the cohomology groups $H^2(G_\Gamma, U(1))$ explicitly by relating them to the central subgroup $\Gamma \subset \mathcal{Z}(G)$ defining G_Γ. We also provide a dictionary that characterizes massless boundary modes according to the congruence class of their representation. We conclude with a detailed application of our general result to each individual simple Lie group. Among these, the symmetry group $PSU(N)$ is the most interesting since the number of distinct topological phases turns out to increase with N. Also, the symmetry groups $PSO(2n)$ stand out since their four topological phases are characterized by either $\mathbb{Z}_2 \times \mathbb{Z}_2$ or $\mathbb{Z}_4$, depending on whether n is even or odd.

A. Topological classes for spin chains with general Lie group symmetry

In all that follows, we use the notation introduced in Secs. II E and II F. We shall assume that the physical onsite Hilbert spaces $\mathcal{H}_k$ can be regarded as linear representations of the group G_Γ. In particular, the central subgroup $\Gamma \subset \mathcal{Z}(G)$ acts trivially on each $\mathcal{H}_k$ such that these spaces are associated with the class $[0] \in P/Q_\Gamma$.

We are now prepared to present the main result of the paper. Combining the statements of Secs. II F and II G, the classification of topological phases can be obtained from the following chain of isomorphisms:

$$H^2(G_\Gamma, U(1)) \ \cong \ \mathrm{Hom}(\Gamma, U(1)) \cong \Gamma \ \cong \ P/Q_\Gamma. \tag{11}$$

In other words, the different topological phases of a spin chain with symmetry group G_Γ are in one-to-one correspondence with the elements of its fundamental group Γ. In particular, the topological phases of a system with PG symmetry can be identified with the center of G. In this case, the previous equation reduces to

$$H^2(PG, U(1)) \ \cong \ \mathrm{Hom}(\mathcal{Z}(G), U(1)) \cong \mathcal{Z}(G) \ \cong \ P/Q. \tag{12}$$

The interpretation of the center as the quotient of the weight lattice P of $\mathfrak{g}$ modulo its root lattice Q is sometimes useful for the concrete evaluation of $\mathcal{Z}(G)$, e.g., for exceptional groups such as E_6. More importantly, it provides the avenue for a characterization of topological phases in terms of edge modes as will be explained in Sec. III B. The relevant data for P/Q [and hence $\mathcal{Z}(G)$] for different choices of $\mathfrak{g}$ can be found in Table I. The important question as to how to determine the relevant symmetry group G_Γ entering Eq. (11) will be addressed in Sec. IV. Let us just emphasize here that one can be certain not to miss a possible phase if one employs Eq. (12) instead. In this sense, the symmetry group PG can be regarded as a kind of master symmetry.

B. Edge-mode representations as an indicator for the topological phase

We will argue in Sec. IV that the topological phases of systems with G_Γ symmetry admit, in many cases, a natural embedding into the topological phases of systems with PG symmetry. Hence, we will restrict the following analysis to the symmetry group PG.

Let us thus consider a PG-symmetric gapped spin chain with a unique PG-invariant ground state which resides in a well-defined topological class. According to our previous discussions, this statement has three implications. First, all irreducible representations λ appearing in the decomposition

$$\mathcal{H}_k \ = \ \bigoplus_\lambda V_\lambda \tag{13}$$

of the physical onsite Hilbert spaces $\mathcal{H}_k$ should belong to the trivial class $[0] \in P/Q$. Second, there should exist a unique class $\Omega \in \mathrm{Hom}(\mathcal{Z}(G), U(1))$ labeling the topological phase.[66] Third, the edge modes (possibly virtual) on the left-hand side and on the right-hand side of the (reduced) system should transform in representations which correspond to the projective classes $\Omega \in P/Q$ and $-\Omega \in P/Q$, respectively.[67] If we decompose the auxiliary Hilbert space $\mathcal{B}_L = \mathcal{H}_{(1,L)}$ (or $\mathcal{B}_R = \mathcal{H}_{(L,R)}$) at the boundary into irreducible representations of $\mathfrak{g}$ similar to Eq. (13), then all the λ should belong to the same class $\Omega \in P/Q$ (or $-\Omega \in P/Q$). The previous few lines clearly exhibit the need for an efficient way of determining the projective class of a given representation λ of $\mathfrak{g}$.

Fortunately, there exists an explicit formula which determines the congruence classes $[\lambda] \in P/Q$ of any irreducible representation λ of $\mathfrak{g}$.[68] If $\lambda = (\lambda_1, \ldots, \lambda_r) \in P^+$ denotes the associated integrable weight, one simply finds

$$[\lambda] \ \equiv \ \sum_{i=1}^{r} \lambda_i \nu_i \mod M, \tag{14}$$

where the congruence vectors ν are summarized in Table II. In all cases but $so(4n)$ $(= D_{2n})$, the class $[\lambda]$ is specified by a

TABLE II. Congruence vectors for simple Lie algebras (Ref. 68).

Lie algebra	Congruence vector(s) ν	Modulus M
A_n	$(1,2,\ldots,n)$	$n+1$
B_n	$(0,\ldots,0,1)$	2
C_n	$(1,0,1,0,\ldots)$	2
D_{2n+1}	$(0,\ldots,0,1,1)$	2
	$(2,0,2,\ldots,2,2n-1,2n+1)$	4
D_{2n}	$(0,\ldots,0,1,1)$	2
	$(2,0,2,\ldots,2,0,2n-2,2n)$	4
E_6	$(1,-1,0,1,-1,0)$	3
E_7	$(0,0,0,1,0,1,1)$	2

single number. Only for $so(4n)$ are there two choices of (ν, M) one has to consider at the same time. In this case, the class is given by a tuple $[a,b]$ of two numbers. Since formula (14) is pretty abstract, we will use the subsequent sections to evaluate it in great detail for all relevant groups. We shall begin with $SU(N)$ and continue with all the remaining simple simply connected Lie groups, including Spin(N) [the twofold cover of $SO(N)$] and $SP(2N)$ as well as the exceptional groups E_6 and E_7. The remaining exceptional Lie groups E_8, F_4, and G_2 have a trivial center and hence do not allow for nontrivial topological phases.

C. Topological classes for *SU(N)* spin chains

We assume that $N \geqslant 2$ since $SU(1)$ is just the trivial group. The group $SU(N)$ is simply connected and it has a center $\mathbb{Z}_N$. When defined in matrix form, the center consists of the matrices $\omega^l \mathbb{1}$ with $\omega = \exp(2\pi i/N)$ and $l = 0, \ldots, N-1$. The restriction of the prefactor to the N distinct Nth roots of unity is implied by the requirement that $SU(N)$ matrices should have unit determinant.

The group $SU(N)$ serves as the universal cover of the projective special unitary group $PSU(N) = SU(N)/\mathbb{Z}_N$. According to our general result (12), topological phases of $SU(N)$ spin chains are classified by the cohomology group

$$H^2(PSU(N), U(1)) \cong \mathbb{Z}_N. \tag{15}$$

In other words, there are N distinct topological phases. For $N = 2$, this reproduces the familiar result for $PSU(2) = SO(3)$ (see also Sects. II D and III D).

Let us now describe which type of edge mode indicates the presence of which topological phase. As explained in Sec. III B, this requires knowledge about the congruence class of all irreducible representations of $SU(N)$. Representations of $SU(N)$ can be described in terms of integrable weights $\lambda = (\lambda_1, \ldots, \lambda_{N-1})$ as above or, alternatively, in terms of Young tableaux $\lambda = \{l_1; \ldots; l_{N-1}\}$. In terms of the weight, the partition of the associated Young tableau is specified by the numbers

$$l_i = \sum_{k=i}^{N-1} \lambda_k. \tag{16}$$

By definition, the number l_i determines the number of boxes in the ith row of the tableau.

According to our general result (14) and Table II, the projective class of a representation λ is given by

$$[\lambda] \equiv \sum_{k=1}^{N-1} k\lambda_k \mod N. \tag{17}$$

This formula divides the weight lattice P into N sublattices, each of them labeled by an element of P/Q. An illustration of this fact is shown in Fig. 3 and in Fig. 4 for the particular cases of $SU(2)$ and $SU(3)$, respectively.

We will now briefly recall in which way the N different classes of $SU(N)$ representations correspond to the N different representations of the center $\mathbb{Z}_N \subset SU(N)$. If $\rho : SU(N) \to U(V_\lambda)$ denotes the irreducible representation with highest weight λ, the center will act as follows:

$$\rho(\omega^l \mathbb{1}) = \omega^{l[\lambda]} \mathbb{1}. \tag{18}$$

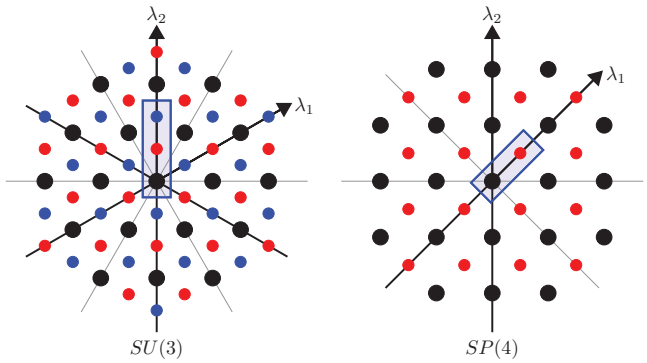

FIG. 4. (Color online) Visualization of different congruence classes for $SU(3)$ and $SP(4)$. The pictures show the respective weight lattice P in terms of colored dots. The root lattice Q corresponds to the large black dots. Different colors indicate different congruence classes. The shaded blue boxes are possible representatives of P/Q. We clearly see that, for $SP(4)$, the topological class is independent of λ_2.

This equation is evident for the trivial representation and for the fundamental representation $\lambda = (1,0,\ldots,0)$ (which has $[\lambda] \equiv 1$ and can thus be regarded as the generator of $\mathbb{Z}_N$). The general validity follows from linear extrapolation (i.e., from taking multiple tensor products of the fundamental representation).

We wish to emphasize that formula (17) admits a nice interpretation in terms of Young tableau: The projective class of a representation λ just corresponds to the number of boxes $|\lambda|$ modulo N. Indeed, a simple rewriting of Eq. (17) using the identity (16) yields

$$[\lambda] \equiv \sum_{i=1}^{N-1} l_i \mod N \equiv |\lambda| \mod N. \tag{19}$$

This result can also be understood as follows. The basic representation of $SU(N)$ is the N-dimensional fundamental representation. It is represented by a Young tableau with a single box. Hence, it has $[\lambda] \equiv 1$ and can be regarded as the generator of the group $\mathbb{Z}_N$. All the other representations of $SU(N)$ can be found in iterated tensor product of the fundamental representation with itself. By the Littlewood-Richardson rule for calculating tensor products, the number of boxes (and hence the projective class) increases by one unit in each iteration until we eventually reach the Nth power of the tensor product. Here, the phase is reset to zero and the counting starts anew. In the process of calculating tensor products, one might need to delete columns with N boxes. However, deleting N boxes does not have an effect if the number of boxes is only counted modulo N anyway.

D. Topological classes for Spin(*N*) spin chains

Let us now look at the orthogonal symmetry groups $SO(N)$. In what follows, we restrict our attention to $N \geqslant 3$ since $SO(1) = \mathbb{Z}_2$ is discrete and $SO(2) = U(1)$ fails to be simple. Since $SO(N)$ is not simply connected, it is more appropriate for the purpose of our paper to speak about the universal covering group Spin(N) which is a twofold cover of $SO(N)$. As usual, the covering implies the identity

$SO(N) = \mathrm{Spin}(N)/\mathbb{Z}_2$. For $N = 3$, we recover the familiar case $\mathrm{Spin}(3) = SU(2)$ with $SO(3) = \mathrm{Spin}(3)/\mathbb{Z}_2$.

Surprisingly, the groups $\mathrm{Spin}(N)$ fall into two (actually three) separate families with rather different properties as can be inferred from Table I. For odd $N = 2n+1$ ($n \geqslant 1$), the center is $\mathbb{Z}_2$, while for even $N = 2n$ the center is $\mathbb{Z}_4$ for odd values of n and $\mathbb{Z}_2 \times \mathbb{Z}_2$ for even n. The cohomology groups classifying the topological phases of $\mathrm{Spin}(N)$ symmetric spin chains are thus given by

$$\begin{aligned} H^2(SO(2n+1),U(1)) &\cong \mathbb{Z}_2, \\ H^2(SO(2n)/\mathbb{Z}_2,U(1)) &\cong \begin{cases} \mathbb{Z}_4, & n \text{ odd} \\ \mathbb{Z}_2 \oplus \mathbb{Z}_2, & n \text{ even.} \end{cases} \end{aligned} \tag{20}$$

In particular, there are four phases if N is even and two phases if N is odd. We will treat these two cases separately in what follows. A partial classification, focusing on $SO(N)$, has previously appeared in Ref. 40.

1. Case Spin($n+1$)

For odd $N = 2n+1$ ($n \geqslant 1$), the center is $\mathbb{Z}_2$ and there are two different classes of representations. They can be distinguished by the last entry of the Dynkin label $\lambda = (\lambda_1, \ldots, \lambda_n)$,

$$[\lambda] \equiv \lambda_n \mod 2. \tag{21}$$

If γ is the generator of $\mathbb{Z}_2 \subset \mathrm{Spin}(N)$ and $\rho : \mathrm{Spin}(N) \to U(V_\lambda)$ denotes the irreducible representation with highest weight λ, the center is represented by

$$\rho(\gamma) = (-1)^{[\lambda]} \mathbb{1}. \tag{22}$$

Accordingly, the situation is very similar to that of $SU(2)$. Representations with $[\lambda] \equiv 0$ are linear representations of $\mathrm{Spin}(N)$ and of $SO(N)$. On the other hand, representations with $[\lambda] \equiv 1$ are spinorial, i.e., they are linear representations of $\mathrm{Spin}(N)$ but only projective ones of $SO(N)$. Since the center of $SO(N)$ is trivial for $N = 2n+1$, this covers all possible cases.

2. Case Spin($2n$)

The treatment of $SO(N)$ with even $N = 2n$ ($n \geqslant 2$) becomes slightly more involved but also more interesting. In this case, the center of $\mathrm{Spin}(N)$ is $\mathbb{Z}_2 \times \mathbb{Z}_2$ for even n and $\mathbb{Z}_4$ for odd n.[69] This observation in particular implies that the groups $SO(N) = \mathrm{Spin}(N)/\mathbb{Z}_2$ have a center $\mathbb{Z}_2$ themselves such that one also needs to consider the group $PSO(2n) = SO(2n)/\mathbb{Z}_2$.[70] In order to determine the class of a representation $\lambda = (\lambda_1, \ldots, \lambda_n)$, we have to calculate the $\mathbb{Z}_2 \oplus \mathbb{Z}_4$-valued quantity

$$\begin{aligned} [\lambda] &= \begin{bmatrix} [\lambda]_1 \\ [\lambda]_2 \end{bmatrix} \\ &\equiv \begin{bmatrix} \lambda_{n-1} + \lambda_n & \mod 2 \\ 2\lambda_1 + 2\lambda_3 + \ldots + (n-2)\lambda_{n-1} + n\lambda_n & \mod 4 \end{bmatrix}. \end{aligned} \tag{23}$$

The first entry $[\lambda]_1$ determines whether the representation is a linear representation of $SO(2n)$ ($[\lambda]_1 \equiv 0$) or rather a projective one ($[\lambda]_1 \equiv 1$). The second entry $[\lambda]_2$ is required to produce the correct group structure of $\mathcal{Z}(\mathrm{Spin}(2n))$ and it is relevant when it comes to determining whether λ is a representation of $PSO(2n)$. For simplicity of presentation, we shall treat the cases n even and n odd separately.

We start with n even. Note that the second entry $[\lambda]_2$ is always even in this case. Moreover, both components of $[\lambda]$ are completely independent. Hence, precisely four of the eight possibilities,

$$[0,0],\ [0,2],\ [1,0],\ [1,2], \tag{24}$$

are realized and one can easily check that they satisfy an addition law corresponding to $\mathbb{Z}_2 \oplus \mathbb{Z}_2$ (considered as a subgroup of $\mathbb{Z}_2 \oplus \mathbb{Z}_4$). If $\gamma = [1,0]$ and $\epsilon = [0,2]$ denote the generators of these two central subgroups $\mathbb{Z}_2 \subset \mathrm{Spin}(2n)$, their action on an irreducible representation $\rho : \mathrm{Spin}(2n) \to U(V_\lambda)$ of highest weight λ is given by

$$\rho(\gamma) = (-1)^{[\lambda]_1} \mathbb{1} \quad \text{and} \quad \rho(\epsilon) = e^{\frac{i\pi}{2}[\lambda]_2} \mathbb{1}. \tag{25}$$

Representations λ of $\mathrm{Spin}(2n)$ with $[\lambda] = [0,0]$ are linear representations of $PSO(2n)$. All the remaining ones correspond to projective representations of $PSO(2n)$.

If we turn to n odd, the analysis becomes even simpler. Now, the two entries $[\lambda]_1$ and $[\lambda]_2$ of $[\lambda]$ are either both even or both odd. Put differently, the first component $[\lambda]_1$ is completely determined by the second $[\lambda]_2$ by taking its value modulo two. This again realizes four of the eight possibilities,

$$[0,0],\ [1,1],\ [0,2],\ [1,3], \tag{26}$$

but now with an addition law corresponding to $\mathbb{Z}_4$ (again considered as a subgroup of $\mathbb{Z}_2 \oplus \mathbb{Z}_4$), the generator being $\eta = [1,1]$. On an irreducible representation $\rho : \mathrm{Spin}(2n) \to U(V_\lambda)$ of highest weight λ, the center acts as

$$\rho(\eta) = e^{\frac{i\pi}{2}[\lambda]_2} \mathbb{1}. \tag{27}$$

The generator η^2 of the subgroup $\mathbb{Z}_2 \subset \mathbb{Z}_4 \subset \mathrm{Spin}(2n)$ which needs to be used to descend from $\mathrm{Spin}(2n)$ to $SO(2n)$ is mapped to $\pm\mathbb{1}$ under ρ, depending on whether $[\lambda]_2$ is even or odd. We thus obtain the following three-level hierarchy: representations of $\mathrm{Spin}(2n)$ with $[\lambda]_2 \equiv 0$ are linear representations of $SO(2n)$ and $PSO(2n)$. If $[\lambda]_2 \equiv 2$, one deals with a linear representation of $SO(2n)$ which is only a projective representation of $PSO(2n)$. And in the two remaining cases, one has a projective representation of $SO(2n)$ and $PSO(2n)$.

We note that in both of the superordinate cases treated, even and odd n, there exist modifications of formula (23) which give the classification of topological phases in a more direct and canonical way: in the first case one could divide the second component by two and in the second case one could restrict the attention to the second component from the very beginning. We decided to present both cases on the same footing in order to stay close to the original reference.[68] It seems plausible that our results also have a natural explanation in terms of Young tableaux. However, in this paper we refrain from adopting this perspective.

E. Topological classes for *SP(2N)* spin chains

The group $SP(2N)$ is simply connected and its center is isomorphic to $\mathbb{Z}_2$. We should carefully note that there we are talking about the *compact* symplectic group $SP(2N)$ of rank N

(see below for a brief comment on the noncompact version). As usual, the topological phases are classified by the cohomology group

$$H^2(SP(2N)/\mathbb{Z}_2, U(1)) \cong \mathbb{Z}_2. \tag{28}$$

We thus have two distinct topological phases. Given any weight $\lambda = (\lambda_1, \ldots, \lambda_N)$, the associated congruence class is determined by the number[71]

$$[\lambda] \equiv \lambda_1 + \lambda_3 \mod 2. \tag{29}$$

The two different values of $[\lambda]$ divide the weight lattice P into two sublattices. For $SP(4)$, this is depicted in Fig. 4. In an irreducible representation V_λ of highest weight λ, the center $\mathbb{Z}_2 \subset SP(2N)$ is implemented in the same fashion as in Eq. (22). Representations with $[\lambda] \equiv 0$ are representations of $SP(2N)$ and $SP(2N)/\mathbb{Z}_2$ while $[\lambda] \equiv 1$ leads to linear representations of $SP(2N)$ which are projective representations of $SP(2N)/\mathbb{Z}_2$.

In order to prevent potential confusion, let us finally comment on the (probably more familiar) *noncompact* group $SP(2N,\mathbb{R})$. This group arises as the symmetry group of a symplectic form defined on a $2N$-dimensional real vector space. The fundamental group of $SP(2N,\mathbb{R})$ is given by $\pi_1(SP(2N,\mathbb{R})) = \mathbb{Z}$. In order to arrive at a simply connected group, one thus needs to pass on to an infinite cover of $SP(2N,\mathbb{R})$. The group also has a well-known double cover, the so-called metaplectic group. From a representation theoretic point of view, the transition from the compact instance of a group to a noncompact version requires one to replace finite-dimensional representations with infinite-dimensional ones, just alone for reasons of unitarity. The topological classification of systems involving infinite-dimensional representations is beyond the scope of this paper. However, our example shows that one needs to be very precise about the real form and the global structure of the symmetry group under consideration.

F. Topological classes for E_6 and E_7 spin chains

Just for completeness, we also treat the two exceptional cases in the E series. By abuse of notation, we also use the symbols E_6 and E_7 for the simply connected groups associated with the corresponding Lie algebras. From Table I we infer that the respective centers of these groups are given by $\mathbb{Z}_3$ and $\mathbb{Z}_2$. We immediately conclude that the cohomology groups classifying the topological phases are given by

$$\begin{aligned} H^2(E_6/\mathbb{Z}_3, U(1)) &\cong \mathbb{Z}_3, \\ H^2(E_7/\mathbb{Z}_2, U(1)) &\cong \mathbb{Z}_2. \end{aligned} \tag{30}$$

Hence, there are three topological phases of E_6-invariant and two phases of E_7-invariant spin chains.

Let us discuss the E_6 case first. The representations $(\lambda_1, \ldots, \lambda_6)$ of E_6 fall into three different classes according to the value of

$$[\lambda] \equiv \lambda_1 - \lambda_2 + \lambda_4 - \lambda_5 \mod 3. \tag{31}$$

If $\gamma \in \mathbb{Z}_3 \subset E_6$ is the generator of the center, the action in an irreducible representation $\rho : E_6 \to U(V_\lambda)$ of highest weight λ is determined by

$$\rho(\gamma) = e^{\frac{2\pi i}{3}[\lambda]} \mathbb{1}. \tag{32}$$

Representations with $[\lambda] \equiv 0$ are linear representations of the projective group $E_6/\mathbb{Z}_3$. The remaining two classes are only linear representations of E_6 but projective representations of $E_6/\mathbb{Z}_3$.

Let us now turn our attention to E_7. The representations $(\lambda_1, \ldots, \lambda_7)$ of E_7 fall into two different classes according to the value of

$$[\lambda] \equiv \lambda_4 + \lambda_6 + \lambda_7 \mod 2. \tag{33}$$

The action of the generator $\gamma \in \mathbb{Z}_2 \subset E_7$ on an irreducible representation of highest weight λ is specified by formula (22). Representations with $[\lambda] \equiv 0$ are linear representations of E_7 and $E_7/\mathbb{Z}_2$. In contrast, representations with $[\lambda] \equiv 1$ are linear representations of E_7 but only projective representations of $E_7/\mathbb{Z}_2$.

IV. PHYSICAL PERSPECTIVES

In Sec. III, we classified topological phases for all spin chains whose spins belong to a simple Lie algebra $\mathfrak{g}$. The classification was intimately related to a division of representations of $\mathfrak{g}$, thought of as becoming manifest in gapless edge modes, into different classes of projective representations of a Lie group G_Γ associated with $\mathfrak{g}$. In this section, we will analyze which of the possible Lie groups G_Γ is actually the relevant symmetry. We will also investigate the hierarchy of topological phases that arises by considering one and the same system from different perspectives, based on symmetries G_Γ and $G_{\Gamma'}$ where Γ and Γ' are related by the inclusion $\Gamma' \subset \Gamma \subset \mathcal{Z}(G)$. Moreover, we point out an interesting connection of our results with a natural generalization of Haldane's conjecture to arbitrary spin chains. In the final part of this section, we illustrate our general considerations with two examples.

A. Identification of the symmetry group

In the following, we will consider a fixed gapped spin system with spin operators in a simple Lie algebra $\mathfrak{g}$ and a Hamiltonian that commutes with all elements of $\mathfrak{g}$. Furthermore, we assume the action of $\mathfrak{g}$ on the total Hilbert space to be faithful and the existence of a unique and $\mathfrak{g}$-invariant ground state. The precise symmetry group which is relevant for the classification of potential topological phases [see Eq. (11)] depends on the nature of the onsite Hilbert spaces $\mathcal{H}_k$.[72] The simply connected Lie group G can always be regarded as a symmetry of the system. However, its action on the Hilbert spaces $\mathcal{H}_k$ might not be faithful, leading to the existence of nontrivial kernels Γ_k. Whenever $\mathfrak{g}$ acts faithfully on the total Hilbert space, this kernel will be a subgroup $\Gamma_k \subset \mathcal{Z}(G)$ of the center of G. Under these circumstances, the *actual* symmetry group (neglecting symmetries not related to $\mathfrak{g}$) is $G_A = G/\Gamma_A$, with $\Gamma_A = \cap_k \Gamma_k$ being the intersection of all kernels Γ_k, and it is *this* group which enters the calculation of the cohomology group (11) that characterizes potential topological phases. Note that the actual symmetry group as defined above might (and will generally) differ from that obtained by identifying Γ with the kernel of G that arises when acting on the total

Hilbert space $\mathcal{H} = \bigotimes_k \mathcal{H}_k$.[73] It is thus important to distinguish between the overall symmetry and symmetries that are realized locally, even in the absence of translation invariance.

Our previous statements can easily be connected to our discussion of congruence classes of representations of G in Sec. III. The system has symmetry $G_\Gamma = G/\Gamma$ if *all* physical onsite Hilbert spaces $\mathcal{H}_k$ are linear representations of G_Γ, i.e., if $[\mathcal{H}_k]_\Gamma \equiv [0]$. In contrast, it is *not* required that *all* these representations are faithful. Instead, we are searching for the "smallest" among the groups G_Γ which is still linearly represented on *all* spaces $\mathcal{H}_k$. Inverting the logic, the *actual* symmetry group $G_A = G/\Gamma_A$ of the system is associated with the maximal subgroup $\Gamma_A \subset \mathcal{Z}(G)$ such that $[\mathcal{H}_k]_{\Gamma_A} \equiv [0]$.

B. Hierarchies of topological phases

As a physical system can be invariant under more than one of the groups G_Γ, it seems appropriate to discuss the relation between the potential topological phases predicted for different choices of $\Gamma \subset \mathcal{Z}(G)$ (keeping the system fixed). Let us thus consider a central subgroup Γ which is contained in Γ_A such that $\Gamma \subset \Gamma_A \subset \mathcal{Z}(G)$. In what follows, we wish to argue that this inclusion of subgroups gives rise to a natural inclusion of topological phases. For the two symmetries G_A and G_Γ, the topological phases are described by

$$\begin{aligned} H^2(G_A, U(1)) &\cong \mathrm{Hom}(\Gamma_A, U(1)), \\ H^2(G_\Gamma, U(1)) &\cong \mathrm{Hom}(\Gamma, U(1)). \end{aligned} \tag{34}$$

We expect that G_A provides a finer resolution of topological phases than G_Γ. In other words, from the perspective of G_Γ, some of the original topological phases can not be distinguished and need to be identified. It turns out that this identification is done via the Abelian group Γ_A/Γ which measures to which extent Γ_A is larger than Γ. This suggests a relation of the form $H^2(G_\Gamma, U(1)) \cong H^2(G_A, U(1))/(\Gamma_A/\Gamma)$ and indeed a simple calculation yields

$$\begin{aligned} \mathrm{Hom}(\Gamma, U(1)) &\cong \mathrm{Hom}(\Gamma_A/(\Gamma_A/\Gamma), U(1)) \\ &\cong \mathrm{Hom}(\Gamma_A, U(1))/(\Gamma_A/\Gamma). \end{aligned} \tag{35}$$

By considering embedding chains of central subgroups, the previous procedure yields a whole hierarchy of topological phases.

In the previous example, it was straightforward to change the perspective from G_A to G_Γ with $\Gamma \subset \Gamma_A$ and then back from G_Γ to G_A. In many situations, however, it is even possible to change the perspective from G_A to a smaller group G_Γ right away. In this case, the latter is obtained from a central subgroup Γ satisfying $\Gamma_A \subset \Gamma \subset \mathcal{Z}(G)$. For instance, a fixed system with symmetry G can (under certain circumstances) be interpreted as a system with symmetry PG (or any of the other groups G_Γ). This requires no modification of the physical system, but rather a reinterpretation of its underlying Hilbert space by means of a blocking procedure in which several sites are combined into one. Under blocking, certain tensor products of G_A representations indeed lift to a representation of G_Γ since the individual projective classes (with respect to Γ) add up and might eventually give $[0] \in H^2(G_\Gamma, U(1))$.

For the sake of concreteness, we explain the idea in a simple example. Most antiferromagnetic spin chains are modeled using a chain of onsite Hilbert spaces $\mathcal{H}_k$ which are alternating between a representation space $\mathcal{H}$ and its dual $\mathcal{H}^*$, both having a well-defined congruence class with respect to the action of $\mathcal{Z}(G)$. Let us assume that the actual symmetry group is G_A, with a specific central subgroup $\Gamma_A \subset \mathcal{Z}(G)$. In this situation, we can combine two neighboring sites $\mathcal{H}$ and $\mathcal{H}^*$ into a single site $\mathcal{H}_{\mathrm{block}} = \mathcal{H} \otimes \mathcal{H}^*$ which resides in the trivial class $[\mathcal{H}_{\mathrm{block}}] \equiv [\mathcal{H}] + [\mathcal{H}^*] \equiv [0]$ with respect to PG. Blocking thus allows us to move within the hierarchy of topological phases. It might happen, e.g., in spin ladders, that the Hilbert space $\mathcal{H}$ decomposes into several irreducible representations of G which belong to distinct congruence classes. In this situation, blocking does not give rise to a symmetry PG. Examples for hierarchies of topological phases are presented in Sec. IV D.

Parts of our discussion might look very academic at first sight. However, there are also direct physical implications. Imagine two spin chains with actual symmetry groups G_A and G_B. If we couple the two chains, thus building a spin ladder, the actual symmetry group of the complete system will be determined by the intersection $\Gamma_{A\cup B} = \Gamma_A \cap \Gamma_B \subset \mathcal{Z}(G)$. In the case of $SU(2)$ spin ladders involving a mixture of integer and half-integer spin representations, the intersection is trivial, thus confirming the observation of Ref. 74 that edge modes are not topologically protected.

C. A generalization of Haldane's conjecture to arbitrary groups

As we will now explain, our analysis hints towards a natural generalization of Haldane's conjecture. In its original formulation for the thermodynamic limit of the antiferromagnetic $SU(2)$ Heisenberg Hamiltonian for spin S representations, it consists of the following two statements:[41,42] First of all, there is a unique ground state which is translation invariant. Second, there is a gap above the ground state if S is integer and the chain is gapless if S is half-integer (i.e., if $2S$ is odd). Manifold evidence has been found to support the conjecture. In particular, it is well motivated in the semiclassical limit where the spin S is large and where one can derive an effective description in terms of nonlinear σ models with or without Θ term.[41,42] Also, the absence of a gap could be proved using the nontrivial action of the center of $SU(2)$ on representations with half-integer spin.[75,76] On the other hand, a rigorous mathematical proof of the existence of a mass gap for integer spins still seems to be open. The invention of the AKLT chain (in which a mass gap can be proven[18]) was an attempt to cure this unsatisfactory situation. In any case, the relevance of the center of $SU(2)$ and of its action on specific representations already indicates a close relation to our present work.

Rather recently, the existence of Haldane gaps was revisited for different types of $SU(N)$-invariant spin chains[23,77] (see Ref. 47 for some older work). In particular, the authors of Refs. 23 and 77 claimed that $SU(N)$ chains with two-site interactions possess a Haldane-type gap due to spinon confinement if the physical sites are described by an irreducible representation λ whose Young tableau possesses a number $|\lambda|$ of boxes which can be divided by N. In view of our discussion in Sec. III C, this just corresponds to the statement that $[\lambda] \equiv [0]$, i.e., the representation of $SU(N)$ needs to descend to a representation of $PSU(N)$. With $PSU(N)$ playing the

same role as $SO(3)$, this suggests an obvious generalization of Haldane's original conjecture to an arbitrary simply connected symmetry group G: The center $\mathcal{Z}(G)$ should act trivially, $[\lambda] \equiv 0$, in order to find a Haldane phase.

However, the authors of Refs. 23 and 77 noted something even more interesting: A confinement similar to the one above can also be observed whenever $|\lambda|$ and N have a nontrivial common divisor different than N. With an important difference to the previous case, the ground state is degenerate now and the interaction needs to encompass $N/q + 1$ sites where $q = \gcd(|\lambda|, N)$. Our discussion of the hierarchy of topological phases immediately exhibits: Under the conditions specified, the representation λ is a linear representation of the group $SU(N)/\mathbb{Z}_q$. Since the second cohomology of this group is isomorphic to $\mathbb{Z}_q$, this still gives potential edge modes the chance to transform in a nontrivial projective representation, thus providing a topological argument for the presence of a Haldane gap. Proving the absence of a mass gap in systems where $|\lambda|$ and N do not have common divisors appears to be a more challenging endeavor (see, however, Ref. 76 for two-site interactions).

An extrapolation of our previous arguments suggests that spinon confinement (for a suitable interaction range) exists if and only if the physical system allows for a nontrivial way of enhancing its symmetry at (virtual) edges. Equivalently, the physical Hilbert spaces $\mathcal{H}_k$ have to belong to the trivial congruence class $[\mathcal{H}_K]_\Gamma \equiv [0]$ with respect to at least one nontrivial central subgroup $\Gamma \subset \mathcal{Z}(G)$ such that the relevant symmetry of the system is G_Γ, a proper quotient of G. For matrix product states, the existence or absence of a mass gap (with respect to a specific model Hamiltonian) is intimately related to the possibility of realizing it in an "injective" way.[33,51] Most likely, a suitable adaption of these arguments provides the route for a proof of our statement.

A nontrivial test of our conjecture should be possible along the lines of Refs. 23 and 77 for the groups Spin($4n$) (see Sec. III D). In this case, the center is given by $\mathbb{Z}_2 \times \mathbb{Z}_2$ and it admits three inequivalent embeddings $\mathbb{Z}_2 \subset \mathbb{Z}_2 \times \mathbb{Z}_2$, either into the left or right factor or diagonally. It turns out that among the three quotients Spin($4n$)$/\mathbb{Z}_2$, two are isomorphic, leading to the so-called semispinor group $SS(4n)$, while the remaining one is isomorphic to $SO(4n)$ [but not isomorphic to $SS(4n)$ as long as $n \neq 2$].[60] The resulting hierarchy of quotients is displayed in Fig. 5. One can thus imagine to build spin chains based on linear representations of $SO(4n)$ or $SS(4n)$ which are only projective representations of $PSO(4n)$. It is likely that some of these chains would enjoy topological protection, resulting in nontrivial edge modes transforming in a projective representation of $SO(4n)$ or $SS(4n)$, respectively. *A priori*, it is not clear whether gapped spin chains of this type can be realized with two-site interactions. Block renormalization and the experience with $SU(N)$, however, suggest that such spin chains should exist if interactions across several sites are permitted. Similar remarks apply to Spin($4n + 2$) which has a nontrivial central subgroup $\mathbb{Z}_2 \subset \mathbb{Z}_4$.

D. Two illustrative examples: *SU*(6) and *SU*(12) spin chains

In this section, we wish to focus on spin chains with $SU(6)$ symmetry. This example nicely illustrates the technical aspects and the physical implications of our work. The group $SU(6)$ has center $\mathbb{Z}_6$. We have three different choices for nontrivial subgroups Γ. Either we choose $\mathbb{Z}_2$, $\mathbb{Z}_3$, or the full group $\mathbb{Z}_6$ itself. Depending on the choice of physical Hilbert spaces $\mathcal{H}_k$, one then ends up with one of four symmetry groups: $SU(6)$, $PSU(6)$, $SU(6)/\mathbb{Z}_2$, or $SU(6)/\mathbb{Z}_3$.

The topologically richest systems are those with $PSU(6)$ symmetry. In this case, we expect six different topological phases which manifest themselves in the congruence class $[\mathcal{B}] \in \mathbb{Z}_6$ of (virtual) edge modes. They are labeled by $[\mathcal{B}] \in \{[0],[1],[2],[3],[4],[5]\}$. In systems with $SU(6)/\mathbb{Z}_3$ symmetry, we still have three distinct topological phases, which are labeled by $[\mathcal{B}]_{\mathbb{Z}_3} \in \{[0],[1],[2]\}$. Since the center of $SU(6)/\mathbb{Z}_3$ is isomorphic to $\mathbb{Z}_2$ and the double quotient gives rise to $\left[SU(6)/\mathbb{Z}_3\right]/\mathbb{Z}_2 = PSU(6)$, the phases of $PSU(6)$ can be identified with the phases of $SU(6)/\mathbb{Z}_3$ up to the identifications $[0] \sim [3]$, $[1] \sim [4]$, and $[2] \sim [5]$, thus $[\mathcal{B}]_{\mathbb{Z}_3} \equiv [\mathcal{B}] \mod 3$. Conversely, if we have a topological phase $[\mathcal{B}]_{\mathbb{Z}_3}$, there is a chance (but no need) that it admits an interpretation as a phase of type $[\mathcal{B}]$ or $[\mathcal{B}] + [3]$ in a $PSU(6)$ chain.

Similarly, a system with $SU(6)/\mathbb{Z}_2$ has two distinct topological phases labeled by $[\mathcal{B}]_{\mathbb{Z}_2} \in \{[0],[1]\}$. Now, we have $PSU(6) = [SU(6)/\mathbb{Z}_2]/\mathbb{Z}_3$ and $[\mathcal{B}]_{\mathbb{Z}_2} \equiv [\mathcal{B}] \mod 2$. The whole hierarchy of topological phases for $SU(6)$ is depicted in Fig. 6. We can easily confirm that Haldane phases should exist for representations with $[\mathcal{B}] \in \{[0],[2],[3],[4]\}$ albeit they are protected by different symmetries. These numbers are precisely those having nontrivial common divisors with 6 [the 6 of $SU(6)$], in accord with the results of Refs. 23 and 77. They are represented in black color in the lower line of Fig. 6. For higher-rank groups, the hierarchies becomes more involved, but they can be derived following the same principles. In Fig. 7, the hierarchy for the group $SU(12)$ is depicted. The extra structure arises from the fact that $\mathbb{Z}_{12}$ has subgroups, for example $\mathbb{Z}_3$ and $\mathbb{Z}_4$, that are not subgroups of each other.

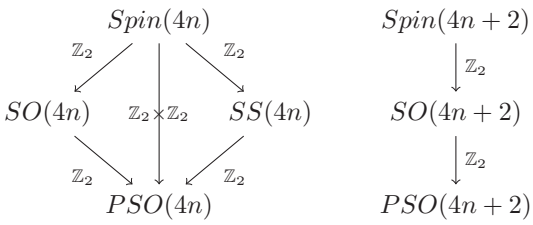

FIG. 5. The hierarchy of topological phases in Spin($2n$) spin chains.

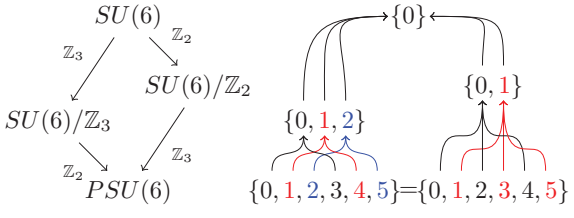

FIG. 6. (Color online) The hierarchy of topological phases in $SU(6)$ spin chains.

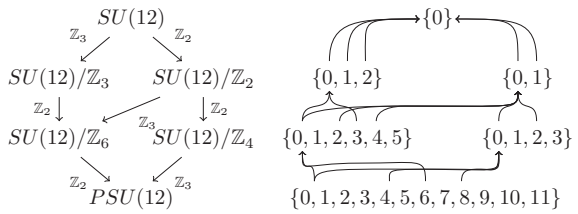

FIG. 7. The hierarchy of topological phases in $SU(12)$ spin chains.

V. APPLICATION TO COLD-ATOM SYSTEMS

The final section of our paper is devoted to the application of our general formalism to the study of quantum magnetism in cold-atom systems. The continuous symmetries relevant in this context are $SP(4)$ [or, equivalently, Spin(5)] and $SU(N)$, with even values of N up to $N = 10$.[44–46] In what follows, we shall focus on the series $SU(N)$. We first outline how the Heisenberg Hamiltonian arises as a particular limit of a Fermi-Hubbard model. Afterwards, we discuss how particular examples fit into our general framework.

A. *SU(N)* Heisenberg model from cold atoms

The realization of an $SU(N)$ symmetry requires a large number of degenerate energy levels. As was emphasized in Ref. 44, the latter arise naturally in earth-alkaline atoms. Since the nuclear spin I reaches values up to $I = \frac{9}{2}$ (for ^{87}Sr), one can easily achieve degeneracies up to $2I + 1 = 10$. The resulting states can be identified with the N-dimensional fundamental representation of $SU(N)$, with $N = 2I + 1$. Earth-alkaline systems exhibit an almost perfect decoupling of nuclear and electronic spin degrees of freedom. In practice, this means that the degeneracy is not lifted by interactions. For this reason, the $SU(N)$ symmetry is still reflected in the Hamiltonian describing the dynamics of the atoms in an optical lattice. Effectively, one thus arrives at an $SU(N)$-symmetric Fermi-Hubbard model. Similar to the familiar case of the Mott insulator phase, there exists a certain parameter range where the model can be approximated in terms of an $SU(N)$ antiferromagnetic Heisenberg spin chain.[44,46]

B. Realization of topologically nontrivial phases

For the physics of the system, it is essential to know the $SU(N)$ representation on which the spin operators act. This representation is determined by the occupation number per site.[44,46] The situation that will be of interest for us is the two-orbital case at half-filling, i.e., with N atoms per site. As was argued in Ref. 46, the relevant $SU(N)$ representation λ is then specified by a Young tableau with two columns and $N/2$ rows. Using the general formula (19), we find that $[\lambda] \equiv [0]$. Accordingly, λ can not only be interpreted as a representation of $SU(N)$ but it also descends to the quotient group $PSU(N) = SU(N)/\mathbb{Z}_N$. It is thus natural to ask which of the N possible topological phases is actually realized by the cold-atom system.

The authors of Ref. 46 argued that the system realizes a topologically nontrivial phase. This claim was supported by the existence of AKLT-type Hamiltonians which act on the same physical Hilbert space and which are utilizing an auxiliary representation $\mathcal{B}$ which is described by a Young tableau with $N/2$ rows in a single column. With our formula (19), we easily verify that $[\mathcal{B}] \equiv [N/2]$, i.e., the AKLT-type system indeed corresponds to a nontrivial topological phase. Since the AKLT-type Hamiltonian for $N = 4$ provides a close approximation to the Heisenberg Hamiltonian, the same nontrivial topology was conjectured for the cold-atom system in the relevant range of parameters.[46]

At this moment of time, it is still an open question as to whether the Heisenberg Hamiltonian and the AKLT-type Hamiltonian really belong to the same topological phase. On the other hand, it is known that the topological phase can be extracted unambiguously from a suitable string order parameter.[55] Our current work thus provides an important step towards settling this crucial issue. Moreover, it suggests the existence of other topological phases of $PSU(N)$ spin chains which might be realizable in cold-atom systems. A more detailed discussion of these aspects will be reported elsewhere.

VI. CONCLUSIONS

In our paper, we revisited the classification of topological phases in gapped spin chains with continuous symmetry group. We identified and evaluated the relevant cohomology groups $H^2(G_\Gamma, U(1))$ and showed that they are isomorphic to the central subgroup $\Gamma \subset \mathcal{Z}(G)$ defining $G_\Gamma = G/\Gamma$ as a quotient of its simply connected cover G. For a number of symmetries, among them $PSU(N)$ and $PSO(2N)$, we found more than one topologically nontrivial phase. In particular, we wish to emphasize the remarkable fact that for $PSU(N)$, the number of topological phases is N and hence increases with the rank of the symmetry group. For the projective groups $PG = G/\mathcal{Z}(G)$, a complete summary of our classification result can be read off from Table I. The cohomology groups $H^2\big(G_\Gamma, U(1)\big)$ exhibit mathematical relations when considered for different choices of the subgroup $\Gamma \subset \mathcal{Z}(G)$. These dependencies lead to a natural hierarchy of topological phases. In Sec. IV, we managed to explain this hierarchy from a physical perspective by considering blocking procedures and the combination of spin chains into spin ladders.

Our classification of topological phases, and the distinguished role played by the central subgroups $\Gamma \subset \mathcal{Z}(G)$, led us to propose a natural generalization of Haldane's conjecture[41,42] to arbitrary symmetry groups (see Sec. IV C). In our more general setup, the original distinction between half-integer and integer spin S of $SU(2)$ is replaced by whether a representation λ is a linear representation of *any* of the groups G_Γ (i.e., $[\lambda]_\Gamma \equiv [0]$) where $\Gamma \subset \mathcal{Z}(G)$ is a nontrivial central subgroup of G. Our proposal is in complete accord with a recent analysis of Haldane phases in $SU(N)$ spin chains by Greiter and Rachel.[23] We believe that their analysis can be carried over to groups of type Spin($2N$), thus providing a nontrivial check of our conjecture.

Let us briefly discuss the implications of our results for the study of concrete physical systems, possibly from a numerical point of view. In our opinion, it can not be overemphasized that in many spin chains there are *more than two distinct* topological phases. While it is a relatively simple task to distinguish between a topologically trivial and a nontrivial phase, e.g., using a suitable string order parameter[22] (for a general discussion, see Ref. 78), the definition of a quantity

which can be calculated efficiently and which can discriminate between all different topologically nontrivial phases is still an open problem. Significant progress with regard to such order parameters has recently been made in Refs. 40 and 54. However, both papers focused on discrete symmetries and an application of similar ideas to the cases at hand remains to be worked out. In a companion paper,[55] we will fill this gap and provide an explicit expression for a string order parameter for $SU(N)$ spin chains which can easily be evaluated once the ground state is known. It will be proven that our order parameter is sensitive to the projective class describing the topological phase and that it allows us to discriminate all N distinct phases of $PSU(N)$ spin chains. The string order parameter may therefore be used to verify the claim of Ref. 46 that nontrivial topological phases of $PSU(N)$ spin chains can be simulated in cold-atom systems (see also Sec. V).

Our analysis calls for extensions in several directions. First of all, our classification was concerned with continuous onsite symmetries only. Taking into account additional discrete symmetries such as translation symmetry, time-reversal symmetry, or inversion symmetry will modify the classification.[34,36] In order to gain some intuition for the underlying reasons, let us briefly discuss the effects of imposing either time-reversal or inversion symmetry (or both), in addition to the onsite symmetry G. According to Ref. 36, apart from the cohomology groups $H^2(G,U(1))$, another important ingredient is the space of one-dimensional representations of G. For simple Lie groups G, the only one-dimensional representation is the trivial representation. Hence, these data do not give rise to additional topological phases in our situation.

On the other hand, it was observed that the projective class $[\lambda]$ describing the boundary modes has to satisfy $2[\lambda] \equiv 0$ in the presence of either inversion or time-reversal symmetry. This leads to a possible reduction in the number of topological phases. Actually, the constraint $2[\lambda] \equiv 0$ can be understood quite easily from the matrix product state construction reviewed in Sec. II C. It is obvious for instance that inversion symmetry requires the auxiliary spaces to be self-conjugate, $\lambda = \lambda^+$, since they are exchanged under inversion. In view of the general relation $[\lambda^+] = -[\lambda]$, this condition immediately implies $2[\lambda] \equiv 0$. Similar remarks apply to time reversal.

As we have just seen, enforcing the presence of additional symmetries may drastically reduce the number of topological phases which can exist in spin chains with continuous symmetry. In particular, for $PSU(N)$, there are no nontrivial inversion-symmetric topological phases if N is odd. Indeed, the construction of the two nontrivial topological phases in a $PSU(3)$ spin chain that was presented in Ref. 55 explicitly required to break inversion symmetry. On the other hand, there is precisely one topologically nontrivial inversion-symmetric phase if N is even. An explicit realization of this phase has been constructed in Ref. 46. Using the results of Ref. 34 and our own classification, it is a straightforward exercise to work out all topological phases which are protected by a combination of continuous onsite symmetries G and/or time-reversal or inversion symmetry.

Another interesting open point concerns the interplay of continuous symmetries with discrete internal symmetries, arising e.g. in spin ladders. The presence of these additional symmetries will lead to adjustments (see, e.g., Ref. 79) which require a separate analysis, depending on the precise type of model under consideration. We believe that the results presented here will be helpful in accomplishing this task.

It seems feasible to generalize our results to supersymmetric and q-deformed spin chains. We hope to report on this in the near future. On the other hand, an extension to noncompact groups appears to be more challenging from a technical point of view. While the mathematical part of the story, the topology of noncompact groups and the division of representations into congruence classes, seems to be well understood, the complications arise on the physical side. In particular, it is evident that noncompact groups come hand in hand with infinite-dimensional representations, together with all their functional analytic intricacies. For example, it is not clear to us at the moment whether in the infinite-dimensional setup symmetry-preserving matrix product states can be constructed which admit a parent Hamiltonian describing a gapped phase.

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[57]The background on Lie theory needed for this section can for instance be found in Refs. 60,63, and 80.
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[71]For $N = 2$, the second contribution involving λ_3 is omitted.
[72]We note in passing the following important facts: When the symmetries are restricted to groups of type G_Γ, i.e., as long as potential space-time symmetries and internal symmetries are disregarded, what matters are really only the Hilbert spaces under

consideration. As an operator, the Hamiltonian H itself will transform as $H \mapsto gHg^{-1}$ and will be insensitive to the action of the center $\mathcal{Z}(G) \subset G$. Put differently, if H commutes with all elements of the Lie algebra $\mathfrak{g}$, then it will be invariant under the action of all elements $g \in G_\Gamma$ for any choice of $\Gamma \subset \mathcal{Z}(G)$. This simple observation has its origin in Schur's lemma and in the fact that irreducible representations of G_Γ are a subset of irreducible representations of $\mathfrak{g}$. Similarly, if the ground state is $\mathfrak{g}$ invariant, it will also automatically be G_Γ invariant.

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From symmetry-protected topological order to Landau order

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Focusing on the particular case of the discrete symmetry group $\mathbb{Z}_N \times \mathbb{Z}_N$, we establish a mapping between symmetry-protected topological phases and symmetry-broken phases for one-dimensional spin systems. It is realized in terms of a nonlocal unitary transformation which preserves the locality of the Hamiltonian. We derive the image of the mapping for various phases involved, including those with a mixture of symmetry breaking and topological protection. Our analysis also applies to topological phases in spin systems with arbitrary continuous symmetries of unitary, orthogonal, and symplectic type. This is achieved by identifying suitable subgroups $\mathbb{Z}_N \times \mathbb{Z}_N$ in all these groups, together with a bijection between the individual classes of projective representations.

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I. INTRODUCTION

Symmetry-protected topological phases have received a lot of interest recently due to their characteristic properties such as the existence of massless boundary modes. Prominent examples are various types of topological insulators[1,2] and spin systems such as the AKLT model.[3,4] In contrast to purely topological phases such as the fractional or integer quantum Hall effect, in these systems the robustness of boundary modes is directly tied to the presence of symmetries.

For one-dimensional spin systems a complete classification of gapped symmetry-protected topological and symmetry-broken phases has been established in Refs. 5–8. Restricting one's attention to on-site symmetries G only, the phases are fully characterized by the spontaneous symmetry breaking of G to a subgroup K, together with an element from the cohomology group $H^2(K,U(1))$. The latter labels the distinct classes of projective representations of K and can be thought of as being a discrete topological invariant attached to edge modes of the system.[9]

In the present paper we shall focus on the particular symmetry group $\mathbb{Z}_N \times \mathbb{Z}_N$. It is the smallest Abelian group which exhibits up to N distinct topological phases. At the same time, it allows us to study topological phases in combination with the phenomenon of spontaneous symmetry breaking if N has nontrivial divisors. While information about the latter can be inferred from suitable local Landau order parameters, the detection of topological phases in 1D systems requires the use of nonlocal string order parameters (see, e.g., Refs. 10–15). As we shall see later, discrete groups of type $\mathbb{Z}_N \times \mathbb{Z}_N$ also play a distinguished role when extending our considerations to continuous symmetry groups.

Before we proceed, let us briefly review the specific case of the dihedral group $D_2 = \mathbb{Z}_2 \times \mathbb{Z}_2$ which historically arose in connection with the $SO(3)$ AKLT model.[3,4] It is well known that the AKLT model realizes the Haldane phase of $S = 1$ spin models. It exhibits topological order which can be detected using the nonlocal string order parameter suggested by Rommelse and Den Nijs.[10] Soon after, it was discovered that the presence of topological order could be interpreted as the spontaneous breaking of a "hidden" $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry which is related to the occurrence of two spin-1/2 degrees of freedom at the edges of the chain.[16] This symmetry breaking becomes manifest after a nonlocal unitary transformation which maps the original string order parameter to a local Landau order parameter. This mapping can also be understood as disentangler,[17] transforming the entangled AKLT state into a product state. It is known that this observation extends to AKLT chains based on higher integer spins S.[18] However, it only became clear later that the topological protection does in fact not rely on the full $SO(3)$ symmetry but that it can already be achieved by restricting one's attention to a discrete subgroup $\mathbb{Z}_2 \times \mathbb{Z}_2$.[19,20] The nontrivial elements of this group can be thought of as rotations by π around three mutually orthogonal axes. This group also appears in connection to the cluster state, where in a similar way it protects the topological order.[21]

In this paper, we generalize the previous ideas to arbitrary groups $\mathbb{Z}_N \times \mathbb{Z}_N$. In the process we face two difficulties: First of all, these groups allow for more complicated patterns of spontaneous symmetry breaking, giving rise to a whole hierarchy of phases. And second, a more refined version of string order parameter has to be used. Indeed, while for $\mathbb{Z}_2 \times \mathbb{Z}_2$ one only has to distinguish between two topological phases (trivial and nontrivial), we now have to discriminate N distinct phases which are labeled by a parameter $t \in \mathbb{Z}_N$. It should be obvious that such a number cannot be extracted from a single expectation value since there is no reason why the latter should be quantized.

As it turns out, the method of choice is to employ the selection rule procedure of Ref. 14.[22] Our analysis starts with a specific (string) order parameter $S(a,b)$ which depends on two parameters $a,b \in \mathbb{Z}_N$ and which vanishes except if the selection rule $a + tb = 0$ modulo N is satisfied. While $S(a,b)$ is nonlocal for $b \neq 0$ it becomes local for $b = 0$. Determining $S(a,b)$ for various choices of a and b, one can thus extract information about the topological phase t and about the potential existence of spontaneous symmetry breaking. We then construct a nonlocal unitary transformation U_N which maps $S(a,b)$ to $S(a,a+b)$. We analyze the implications of this mapping and find that purely topologically phases are mapped to symmetry-breaking ones. The transformation U_N thus allows us to reinterpret topological order in terms of standard local Landau order. More generally, we work out the effect of acting with U_N on almost all phases of $\mathbb{Z}_N \times \mathbb{Z}_N$ spin chains, including those with a mixture of topological protection and spontaneous symmetry breaking to a subgroup $\mathbb{Z}_r \times \mathbb{Z}_r$.[23]

As the original example of the $SO(3)$ AKLT model suggests, the results we derive may equally well be applied to the detection of topological order in systems with continuous symmetry groups. This is due to the fact that each continuous symmetry group which permits nontrivial topological phases (see Ref. 8) contains a nontrivial subgroup of the form $\mathbb{Z}_N \times \mathbb{Z}_N$ for a suitable choice of $N \geqslant 2$. Moreover, the projective representations characterizing the topological phases with regard to either the continuous group or its discrete subgroup are in bijection.[24] For all groups of unitary, orthogonal, and symplectic type the relevant subgroups are constructed explicitly in Sec. V.

The paper is structured as follows. In Sec. II we introduce the group $\mathbb{Z}_N \times \mathbb{Z}_N$ and we discuss its projective representations. Furthermore, we introduce the (string) order parameter $S(a,b)$ and explain how it can be used to characterize the distinct topological and symmetry-broken phases of $\mathbb{Z}_N \times \mathbb{Z}_N$-invariant spin systems. The construction of the nonlocal unitary transformation U_N which maps purely topological phases to symmetry-broken ones is the content of Sec. III. In Sec. IV we analyze the fate of each individual phase under the action of U_N. Finally, Sec. V discusses the implications of our results for continuous groups. We conclude with a brief summary and an outlook to future directions.

II. PRELIMINARIES

Different phases of one-dimensional quantum systems can either arise due to symmetry breaking, due to topology, or a combination thereof. We will consider systems with an on-site symmetry G, but we will not impose space-time symmetries such as translation invariance, time reversal, or inversion symmetry. If the ground state of the system breaks the symmetry to a subgroup $K \subset G$, then the possible topological phases are given by different classes of projective representations of K.[6,7]

The group $\mathbb{Z}_N \times \mathbb{Z}_N$ has N different projective classes. Let R and $\tilde{R}$ be the generators of this group and let R' and $\tilde{R}'$ be projective representations of these generators. The phases $R'^N = e^{i\theta}$ and $\tilde{R}'^N = e^{i\tilde{\theta}}$ can be removed by a redefinition (gauge transformation) of R' and $\tilde{R}'$. However, the phase $R'\tilde{R}'R'^{-1}\tilde{R}'^{-1} = e^{i\phi}$ is gauge invariant and determines the projective class of the corresponding representation. Moreover, ϕ is an integer multiple of $\frac{2\pi}{N}$ due to the cyclic property of the group $\mathbb{Z}_N$. Thus the projective class $t \in \mathbb{Z}_N$ of a representation of $\mathbb{Z}_N \times \mathbb{Z}_N$ can be obtained from the relation

$$R'\tilde{R}' = \omega^t \tilde{R}'R'. \tag{1}$$

Here, we used the abbreviation $\omega = \exp(2\pi i/N)$.

The special case of $N = 2$ arises in $S = 1$ spin chains in which $\mathbb{Z}_2 \times \mathbb{Z}_2$ is a subgroup of $SU(2)$ generated by $R^x = \exp(i\pi S^x)$ and $R^z = \exp(i\pi S^z)$. In these systems two phases can occur: a topological trivial and a nontrivial (Haldane) phase. The latter is characterized by a hidden symmetry breaking which becomes manifest after applying a nonlocal unitary transformation (NL-UT).[16] The NL-UT can be written as[18]

$$U_2 = \prod_{i<j} \exp\left(\pi i S_i^x S_j^z\right). \tag{2}$$

This transformation preserves the symmetry and maps local invariant Hamiltonians (such as that of the XYZ or the bilinear biquadratic model) to local Hamiltonians. Most importantly, it maps the string order parameter $S_i^a \prod_{i\leqslant k<j} R_k^a S_j^a$ to a Landau order parameter $S_i^a S_j^a$ for $a = x$ or z, which explains that string order and hidden symmetry breaking are one-to-one related to each other.[25]

Our attempt to generalize the previous considerations to $\mathbb{Z}_N \times \mathbb{Z}_N$ heavily used the string order selection rules introduced in Ref. 14. In order to explain the underlying ideas, let us consider a spin chain which is invariant under two commuting transformations $\mathcal{X}$ and $\mathcal{Y}$. It is known that the action of these operators on the boundary modes can be factorized according to

$$\mathcal{X} = \mathcal{X}''\mathcal{X}' \quad \text{and} \quad \mathcal{Y} = \mathcal{Y}''\mathcal{Y}', \tag{3}$$

where the operators $\mathcal{X}''$ and $\mathcal{Y}''$ act on the left boundary modes and $\mathcal{X}'$ and $\mathcal{Y}'$ on the right boundary modes. The factorization leads to a phase ambiguity which implies that the boundary modes only need to transform projectively. In other words, we have that $\mathcal{X}'\mathcal{Y}' = e^{i\phi}\mathcal{Y}'\mathcal{X}'$ where the phase ϕ determines the projective class of the representation of the right boundary mode. The phase ϕ thus also determines the topological phase of the system. Let us now consider a string order parameter

$$O_i^L \prod_{i\leqslant k<j} \mathcal{X}_k \, O_j^R. \tag{4}$$

A nonvanishing expectation value of such a string order parameter in the limit $|i-j| \to \infty$ implies invariance under the transformation $\mathcal{X}$, but stated as such it contains no information on the topological phase.[11] However, the latter can be gained from a group theoretical selection rule.[14] If the operators O^L and $(O^R)^\dagger$ have the same quantum number with respect to $\mathcal{Y}$,

$$\mathcal{Y}^{-1} O^L \mathcal{Y} = e^{i\sigma} O^L \quad \text{and} \quad \mathcal{Y}^{-1} O^R \mathcal{Y} = e^{-i\sigma} O^R, \tag{5}$$

then the selection rule states that the string order parameter can only be nonzero if $\sigma = \phi$.

For the case of systems with symmetry $\mathbb{Z}_N \times \mathbb{Z}_N$ the role of $\mathcal{X}$ and $\mathcal{Y}$ are played by R and $\tilde{R}$, respectively. We define operators X^a which are invariant under R but which have a specific quantum number with respect to $\tilde{R}$:

$$\tilde{R}^{-1} X^a \tilde{R} = \omega^{-a} X^a, \quad [R, X^a] = 0. \tag{6}$$

Using these operators, we introduce the string order parameter

$$S(a,b) = X_i^a \prod_{i\leqslant k<j} R_k^b \left(X_j^a\right)^{-1}. \tag{7}$$

We note that this operator becomes local for $b = 0$. The selection rule for string order states that the expectation value

$$\Sigma(a,b) = \lim_{|i-j|\to\infty} \langle S(a,b) \rangle \tag{8}$$

can only be nonzero if $a + tb = 0$ modulo N, where t is the projective class of the right boundary mode;[14] see Eq. (1).

For the validity of our arguments below it is essential that all ground states of the system give rise to the *same* expectation value $\Sigma(a,b)$. This is due to the invariance of the string order parameter $S(a,b)$ under conjugation by R and $\tilde{R}$. This invariance implies that all ground states related by broken

symmetries lead to the same result. On the other hand, ground states in a well-defined gapped topological phase which are not related by such transformations only differ locally at the edges (see, e.g., Ref. 26), and the expectation value $\Sigma(a,b)$ is insensitive to such differences.

III. A NONLOCAL UNITARY TRANSFORMATION FOR $\mathbb{Z}_N \times \mathbb{Z}_N$

In this section we aim to generalize the NL-UT given in Eq. (2), such that it is applicable to systems with $\mathbb{Z}_N \times \mathbb{Z}_N$ symmetry. Recall that this group is generated by the symmetries R and $\tilde{R}$. Furthermore we consider two operators O and $\tilde{O}$ which have the properties $R = \omega^O$ and $\tilde{R} = \omega^{\tilde{O}}$, with $\omega = \exp(2\pi i/N)$ as in the previous section. These operators will generalize S^x and S^z. We then define a NL-UT as

$$U_N = \prod_{i<j} \omega^{O_i \tilde{O}_j}. \tag{9}$$

All terms in the above product commute with each other. Commutators which are possibly nonzero are of the form $[\omega^{O_i \tilde{O}_j}, \omega^{O_j \tilde{O}_k}]$. They can be rewritten as $[\tilde{R}_j^{O_i}, R_j^{\tilde{O}_k}]$, from which it is clear that also these commutators are zero since R and $\tilde{R}$ commute. Using similar arguments it is easily shown that both R and $\tilde{R}$ commute with U_N. Thus U_N preserves the $\mathbb{Z}_N \times \mathbb{Z}_N$ symmetry generated by these two transformations.

Consider a $\mathbb{Z}_N \times \mathbb{Z}_N$-invariant local Hamiltonian H_0. We will now show that the transformed Hamiltonian $H_1 = U_N^{-1} H_0 U_N$ is also local. More precisely, n-body terms (which act on n consecutive sites) will be mapped to n-body terms. We will show this for $n = 2$. Let $h_{i,i+1}$ be a term acting on sites i and $i+1$. This term is transformed as follows:

$$\begin{aligned} U_N^{-1} h_{i,i+1} U_N &= P^\dagger \omega^{-O_i \tilde{O}_{i+1}} h_{i,i+1} \omega^{O_i \tilde{O}_{i+1}} P \\ &= \omega^{-O_i \tilde{O}_{i+1}} h_{i,i+1} \omega^{O_i \tilde{O}_{i+1}}, \end{aligned} \tag{10}$$

with

$$P = \prod_{j>i+1} (R_i R_{i+1})^{\tilde{O}_j} \prod_{j<i} (\tilde{R}_i \tilde{R}_{i+1})^{O_j}. \tag{11}$$

The simplification in Eq. (10) is due to the $\mathbb{Z}_N \times \mathbb{Z}_N$ invariance of the Hamiltonian. The result is clearly a local 2-body term. The generalization to n-body Hamiltonians is straightforward.

In the previous section it was explained that the string order parameter $S(a,b)$ is able to detect topological order via the selection rule. We will now discuss the transformation rule of $S(a,b)$. The operators X^a appearing in $S(a,b)$ transform as

$$U_N^{-1} X_i^a U_N = \prod_{j<i} \tilde{R}_i^{-O_j} X_i^a \prod_{j<i} \tilde{R}_i^{O_j} = \prod_{j<i} \omega^{-aO_j} X_i^a. \tag{12}$$

In these equalities we have used Eq. (6), in particular that X^a and R commute. With this transformation rule it follows that

$$\begin{aligned} U_N^{-1} S(a,b) U_N &= U_N^{-1} X_i^a \prod_{i\leqslant k<j} \omega^{bO_k} X_j^{-a} U_N \\ &= X_i^a \prod_{i\leqslant k<j} \omega^{(a+b)O_k} X_j^{-a} = S(a,a+b). \end{aligned} \tag{13}$$

Applying U_N sufficiently many times (n times, such that $b + na = 0$ modulo N), the result will eventually be $U_N^{-n} S(a,b) U_N^n = S(a,0) = X_i^a X_j^{-a}$. The operator U_N^n thus relates the string order parameter which is capable of detecting topological phases to a Landau order parameter measuring symmetry breaking. Indeed, a nonzero $S(a,b)$ gives information on the topological phase through the selection rule, whereas a nonzero $S(a,0)$ gives information on the breaking of the symmetry generated by $\tilde{R}$.

Just as before, we can define the string order parameter $\tilde{S}^{(a,b)} = \tilde{X}_i^a \prod_{i\leqslant k<j} \tilde{R}_k^b \tilde{X}^{-a}$ with operators $\tilde{X}^a$ satisfying $R^{-1} \tilde{X}^a R = \omega^a \tilde{X}^a$ and $[\tilde{X}^a, \tilde{R}] = 0$. Similar to Eq. (13) we have the transformation rule $U_N^{-1} \tilde{S}^{(a,b)} U_N = \tilde{S}^{(a,a+b)}$. In the topological phase labeled by t both $S^{(a,b)}$ and $\tilde{S}^{(a,b)}$ can be nonzero (when their arguments satisfy $a + tb = 0 \bmod N$). If both string order parameters are zero, the unbroken symmetry transformations of the U_N-transformed system form a group of the form $\mathbb{Z}_r \times \mathbb{Z}_r \subset \mathbb{Z}_N \times \mathbb{Z}_N$.

IV. A MAPPING OF PHASES

In this section we will discuss in detail what will happen to the symmetries after performing the NL-UT. That is, we start with a system with symmetry $\mathbb{Z}_N \times \mathbb{Z}_N$ whose ground states spontaneously break the symmetry to $\mathbb{Z}_{r_0} \times \mathbb{Z}_{r_0}$, with $q_0 r_0 = N$. We furthermore assume that the system is in the topological phase t_0, defined by the projective class of the right boundary modes. In the previous section it was argued that the transformed system, obtained by applying the NL-UT defined in Eq. (9), could show a different pattern of symmetry breaking and could reside in a different topological phase. It was also argued that the group of unbroken symmetries of the transformed system is of the form $\mathbb{Z}_{r_1} \times \mathbb{Z}_{r_1}$, with $q_1 r_1 = N$. Let t_1 label the topological phase of the transformed system. We aim to find the explicit form of the relation

$$f_N : (r_0, t_0) \xrightarrow{U_N} (r_1, t_1). \tag{14}$$

As a warmup we will first assume that N is prime. In this case, there is either no symmetry breaking or symmetry is fully broken. From the selection rule we conclude that only the string order parameter of the form $S(at_0, -a)$ can be nonzero. This string order parameter is mapped to $U_N^{-1} S(at_0, -a) U_N = S(at_0, a(t_0 - 1))$. As long as $t_0 \neq 1$ no symmetry is broken ($r_1 = N$). The topological phase can be deduced from the selection rule: $t_0 + t_1(t_0 - 1) = 0 \bmod N$. In the exceptional case of $t_0 = 1$, the operator $S(at_0, -a)$ is mapped to a Landau order parameter measuring symmetry breaking ($r_1 = 1$ and trivially $t_1 = 0$). Conversely, if we start with a symmetry-breaking phase, $S(a,0) \neq 0$, the transformed system will have nonzero string order parameter $S(a,a)$ from which it follows that $t_1 = N - 1$. Note that the trivial phase is always mapped to the trivial phase. In Table I the action of the map f_N is illustrated for $N = 5$.

The discussion is slightly more involved when N is not prime because topological order can then be mixed with symmetry-breaking order. The first step in the analysis is to use the selection rule to determine when $S(a,b)$ is possibly nonzero. Note that b is always a multiple of q_0 ($b = n_1 q_0$). The transformations R^b and $\tilde{R}^q$ restricted to the right boundaries

TABLE I. Mapping of symmetry-breaking and topological phases of a $\mathbb{Z}_5 \times \mathbb{Z}_5$ (left) and a $\mathbb{Z}_6 \times \mathbb{Z}_6$ (right) invariant system. With SSB we refer to the phase characterized by full spontaneous symmetry breaking.

$\mathbb{Z}_5 \times \mathbb{Z}_5$		
t_0		t_1
0	→	0
1	→	SSB
2	→	3
3	→	1
4	→	2
SSB	→	4
$\mathbb{Z}_6 \times \mathbb{Z}_6$		
(r_0,t_0)		(r_1,t_1)
(6,0)	→	(6,0)
(6,1)	→	(1,0) SSB
(6,2)	→	(6,4)
(6,3)	→	(3,0)
(6,4)	→	(2,0)
(6,5)	→	(3,2)
(3,0)	→	(6,3)
(3,1)	→	(6,1)
(3,2)	→	(2,1)
(2,0)	→	(6,2)
(2,1)	→	(3,1)
(1,0) SSB	→	(6,5)

do not commute but give rise to a phase factor. This complex phase depends on the topological phase t_0 via Eq. (1):

$$\exp(2\pi i/r_0)^{t_0 n_1} = \omega^{t_0 b}. \tag{15}$$

Moreover, from Eq. (6) it follows that transforming X^a by $\tilde{R}^{q_0}$ gives rise to the phase ω^{-aq_0}. The selection rule states that the string order parameter $S(a,b)$ is nonzero only if these two phases coincide, thus if $t_0 b + q_0 a = 0 \mod N$. We conclude that nonzero string order parameters are of the form $S(n_1 t_0 + n_2 r_0, -n_1 q_0)$. An extra term $n_2 r_0$ in the first argument is allowed since X^{r_0} commutes with $\tilde{R}^{q_0}$. Setting $n_1 = 0$ results in a nonzero Landau order parameter $S(n_2 r_0, 0)$, which is consistent with symmetry breaking at hand. This string order parameter is mapped to

$$\begin{aligned} &S(n_1 t_0 + n_2 r_0, -n_1 q_0) \\ &\xrightarrow{U_N} S(n_1 t_0 + n_2 r_0, n_1(t_0 - q_0) + n_2 r_0). \end{aligned} \tag{16}$$

The transformed string order parameter is a Landau order parameter if its second argument vanishes (modulo N). This can only happen if $n_1(t_0 - q_0) = 0 \mod r_0$. The smallest n_1 which fulfills this equation is given by $n_1 = r_0/\gcd(t_0 - q_0, r_0)$. The corresponding symmetry-breaking operator X^a is determined by $a = n_1 t_0 + n_2 r_0 = n_1 q_0 = N/\gcd(t_0 - q_0, r_0)$. We conclude that the symmetry of the transformed system is determined by

$$r_1 = \frac{N}{\gcd(t_0 - q_0, r_0)}. \tag{17}$$

Note that the second argument of the transformed string operator is a multiple of $q_1 = \gcd(t_0 - q_0, r_0)$. Thus the selection rule can be used to determine the topological phase t_1 of the transformed system. From this rule we have that

$$(n_1 t_0 + n_2 r_0) q_1 = -t_1 [n_1(t_0 - q_0) + n_2 r_0]. \tag{18}$$

The solution for t_1 should be independent of n_1 and n_2. Thus factoring these constants out we obtain two equations

$$0 = t_1(t_0 - q_0) + t_0 q_1 \mod N, \tag{19}$$

$$0 = r_0(q_1 + t_1) \mod N. \tag{20}$$

From the second equation we deduce that t_1 is equal to $-q_1$ modulo q_0 thus $t_1 = n q_0 - q_1$. Substituting in the first and simplifying results in $n(t_0 - q_0) = -q_1 \mod r_0$. This equation has a solution for n due to the definition of $q_1 = \gcd(t_0 - q_0, r_0)$. In Table I the map f_N is worked out for $N = 6$.

Let us finally comment on a subtle technical issue. Our derivation of the map f_N hinges on the presence of (string) order via the selection rule. However, the selection rule only gives a necessary but not a sufficient condition on the nonvanishing of the (string) order. It can be accidentally absent at specific points in the phase diagram where one would have expected it to occur from the selection rule. To resolve this problem, we recall that the map f_N is not a statement about specific points in a phase but rather about phases as a whole. Assuming the existence of some point in the phase diagram where the ground state leads to a nonvanishing string order is enough to show that the map f_N is valid for the whole phase.

Note that from Table I it can be seen that f_N is bijective for $N = 5$ and $N = 6$. This is as expected since the spectrum and thus phase transitions should be invariant under the NL-UT. Also it has been checked numerically for values of N up to 100 that indeed f_N is bijective.

In Ref. 27 a different NL-UT transformation, mapping topological phases to symmetry breaking phases, is discussed. The main difference is that we discuss one single NL-UT whereas in Ref. 27 the NL-UT $\mathcal{D}_t$ depends on the topological phase t at hand. The map $\mathcal{D}_t$ always maps a pure topological phase to the phase where the full symmetry is spontaneously broken (SSB phase), whereas U_N maps phases characterized by a mixture of symmetry breaking and topology to each other. Under certain conditions one can map such phases to the SSB phase applying the transformation U_N sufficiently many times. Indeed, from Eq. (16) we have that

$$\begin{aligned} &S(n_1 t_0 + n_2 r_0, -n_1 q_0) \\ &\xrightarrow{U_N^u} S(n_1 t_0 + n_2 r_0, n_1(u t_0 - q_0) + n_2 u r_0), \end{aligned} \tag{21}$$

where u is the number of times U_N is applied. An arbitrary phase is mapped to the SSB phase if its string order parameters are mapped to Landau order parameters, that is, if $n_1(u t_0 - q_0) + n_2 u r_0 = 0 \mod N$ for all values of n_1 and n_2. From this we have the conditions that $u t_0 = q_0 \mod N$ and $u = 0 \mod q_0$. The first condition can only be satisfied if $\gcd(t_0, r_0) = 1$. This is equivalent to stating that the projective representations of $\mathbb{Z}_{r_0} \times \mathbb{Z}_{r_0}$ in class t_0 are *maximally noncommutative*,[27] a requirement for defining the map $\mathcal{D}_{t_0}$. The second condition can be verified by considering orbits of f_N containing the SSB phase. For example, taking $N = 6$ this orbit is

$$\text{SSB} \to (6,5) \to (3,2) \to (2,1) \to (3,1) \to (6,1) \to \text{SSB}.$$

V. RELEVANCE TO SYSTEMS WITH CONTINUOUS SYMMETRY GROUPS

Although the previous section gives a better understanding of the connection between symmetry-breaking order and topological order, as it stands it is only applicable to systems with the specific symmetry $\mathbb{Z}_N \times \mathbb{Z}_N$. In this section, however, we will argue that almost all connected and compact simple Lie groups G_Γ (with only one exception) contain a subgroup of the form $\mathbb{Z}_N \times \mathbb{Z}_N$ which is sensitive to the projective classes of G_Γ. More precisely, we will be discussing subgroups $F_\Gamma \subset G_\Gamma$ such that the homomorphism

$$\tau : H^2(G_\Gamma, U(1)) \to H^2(F_\Gamma, U(1)) \tag{22}$$

is bijective and use a case-by-case argument to show that F_Γ can be chosen to be of the form $\mathbb{Z}_N \times \mathbb{Z}_N$. Topological order can thus also be understood as "hidden" symmetry breaking if it is protected by a continuous symmetry. Note that this is not in contradiction with the Mermin-Wagner theorem[28] (stating that spontaneous symmetry breaking does not occur in one-dimensional quantum systems with continuous symmetry) since the NL-UT only preserves the discrete subgroup $\mathbb{Z}_N \times \mathbb{Z}_N$ but not the full continuous symmetry.

As was explained in great detail in Ref. 8, a connected compact simple Lie group can be written as a a quotient $G_\Gamma = G/\Gamma$ (which motivates the notation) where G is the universal cover of G_Γ and Γ is a subgroup of the center $\mathcal{Z}(G)$ of G. All projective representations ρ of G_Γ originate from linear representations of G. The projective class of a representation of G_Γ can be deduced from the action of Γ on the corresponding linear representation of G [denoted by $\rho : \Gamma \to U(1)$]. With only one exception [occurring for $G = Spin(4n)$], Γ is of the form $\mathbb{Z}_N$. In these cases we choose a generator $\gamma \in \Gamma$ and define the projective class of a representation by $\rho(\gamma) = \omega^t$ with $\omega = \exp(2\pi i/N)$. The main strategy in defining F_Γ is to start by choosing $R, \tilde{R} \in G$ such that $R^N \in \Gamma$ and $\tilde{R}^N \in \Gamma$ (moreover, N should be the smallest nonzero integer for which this holds). Furthermore, $R\tilde{R}R^{-1}\tilde{R}^{-1}$ should generate Γ. Thus $R\tilde{R}R^{-1}\tilde{R}^{-1} = \gamma^m$ with $\gcd(N,m) = 1$. Let F be generated by R and $\tilde{R}$. Clearly $\Gamma \subset F$. Furthermore $F/\Gamma = F_\Gamma = \mathbb{Z}_N \times \mathbb{Z}_N$ is a finite Abelian group.

It is now not to hard to see that with this choice of F_Γ the map τ is bijective. Let ρ be a representation of G in the projective class t [$\rho(\gamma) = \omega^t$ for $\gamma \in \mathcal{Z}(G)$]. Restrict this representation to F. The projective class of this restricted representation is determined by the phase obtained upon commuting R and $\tilde{R}$ or, in other words, by $\rho(\gamma^m) = \omega^{tm}$. As a consequence we find $\tau : t \to tm$ which is bijective under the assumption that $\gcd(N,m) = 1$.

It remains to show that symmetry generators R and $\tilde{R}$ with the desired properties indeed exist. In what follows, we will provide an explicit realization for G being equal to either of the groups $SU(N)$, $Sp(N)$, or $Spin(N)$. A summary of the possible quotient groups to be considered can be found in Ref. 8.

(1) *Case* $G_\Gamma = SU(N)/\mathbb{Z}_N$. The subgroup $\mathbb{Z}_N$ is generated by $\omega\mathbb{I}$, where $\omega = \exp(2\pi i/N)$. We will give matrix representations of R and $\tilde{R}$ acting on $\mathbb{C}^N$. Let v_i denote the standard orthonormal basis of this space. Choose R to be proportional to the linear map $v_i \to \omega^i v_i$. The proportionality constant c should be chosen such that R has determinant 1, thus $c^N = (-1)^{N+1}$. Similarly, let $\tilde{R}$ be proportional to the linear map $v_i \to v_{i+1}$ (and $v_N \to v_1$) with the same proportionality constant c. These matrices obey $R^N = \tilde{R}^N = (-1)^{N+1}\mathbb{I}$ and $R\tilde{R} = \omega\tilde{R}R$.

(2) *Case* $G_\Gamma = SU(N)/\mathbb{Z}_q$. The subgroup $\mathbb{Z}_q$ is generated by $\omega\mathbb{I}$, where $\omega = \exp(2\pi i/q)$. Choose the generators of F to be the block diagonal matrices $R = \mathrm{diag}(R_q, \ldots, R_q)$ and $\tilde{R} = \mathrm{diag}(\tilde{R}_q, \ldots, \tilde{R}_q)$ where R_q and $\tilde{R}_q$ are defined just as for the case $SU(q)/\mathbb{Z}_q$ discussed before. From the previous paragraph we then directly conclude that $R^q = \tilde{R}^q = (-1)^{q+1}\mathbb{I}$ and $R\tilde{R} = \omega\tilde{R}R$.

(3) *Case* $G_\Gamma = Sp(2N)/\mathbb{Z}_2$. The group $Sp(2N)$ consists of complex unitary $2N \times 2N$ matrices M which preserve a symplectic form Q (i.e., $M^T Q M = Q$, where Q is a nonsingular skew symmetric matrix). Choose a basis such that $Q = \left(\begin{smallmatrix} 0 & -\mathbb{I} \\ \mathbb{I} & 0 \end{smallmatrix}\right)$. The group $\mathbb{Z}_2$ is $\{\mathbb{I}, -\mathbb{I}\}$. Let the generators of F be $R = \left(\begin{smallmatrix} i\mathbb{I} & 0 \\ 0 & -i\mathbb{I} \end{smallmatrix}\right)$, and $\tilde{R} = Q$. Clearly $R^2 = \tilde{R}^2 = -\mathbb{I}$ and $R\tilde{R} = -\tilde{R}R$.

(4) *Case* $G_\Gamma = Spin(N)/\mathbb{Z}_2 = SO(N)$, $N \geqslant 3$. The group $Spin(N)$ is most easily understood by first considering its Lie algebra $so(N)$. Let e_i be an orthonormal basis of $\mathbb{R}^N$. The Clifford algebra $\mathrm{Cl}(N)$ is generated by this basis together with the relations $\{e_i, e_j\} = 2\delta_{ij}$. The Lie algebra $so(N) \subset \mathrm{Cl}(N)$ is generated by the operators $S_{ij} = \frac{i}{2}e_i e_j$ (with $i \neq j$). These operators generate rotations in the (i,j) plane: $T_{ij}(\theta) = e^{i\theta S_{ij}} = \cos(\frac{\theta}{2})\mathbb{I} - \sin(\frac{\theta}{2})e_i e_j$. The group $\mathbb{Z}_2$ is $\{\mathbb{I}, -\mathbb{I}\}$. The generators of F can be chosen to be $R = e_1 e_2$ and $\tilde{R} = e_2 e_3$. These elements square to $-\mathbb{I}$ and anticommute. From the perspective of $SO(N)$, they correspond to π rotations in two orthogonal planes with a one-dimensional intersection.

(5) *Case* $G_\Gamma = Spin(N)/\mathbb{Z}_4 = PSO(N)$, $N = 4n+2$. In this case the center of $Spin(N)$ is isomorphic to $\mathbb{Z}_4$ and is generated by the element $\gamma = \prod_i e_i$ (indeed $\gamma^2 = -\mathbb{I}$). The generators of F can be chosen to be $R = 2^{-1/2}(1 + e_{N-1}e_N)\prod_{i=1}^n e_{4i-2}e_{4i}$ and $\tilde{R} = 2^{-n}e_{N-2}e_N\prod_{i=1}^{2n}(1 + e_{2i-1}e_{2i})$. One can check that $R^4 = \tilde{R}^4 = -\mathbb{I}$ and that $R\tilde{R} = \gamma\tilde{R}R$.

(6) *Case* $G_\Gamma = Spin(N)/(\mathbb{Z}_2 \times \mathbb{Z}_2) = PSO(N)$, $N = 4n$. This is the only exception to the above recipe since the center of $Spin(N)$ is no longer of the form $\mathbb{Z}_q$ if N is a multiple of four. However we can still give a flavor of how this exception should be treated. Again, let $\gamma = \prod_i e_i$. The center is generated by γ and $-\mathbb{I}$ (indeed $\gamma^2 = \mathbb{I}$). The projective class of a representation ρ is determined by both $\rho(\gamma) = \pm\mathbb{I}$ and by $\rho(-\mathbb{I}) = \pm\mathbb{I}$. In this case we shall thus need two string order parameters to determine both prefactors via the selection rule. One could define two different NL-UTs mapping these string order parameters to Landau order parameters. In order to define both the string order parameters as well as the NL-UTs, one would need to go through the above procedure twice. That is, define $R_i, \tilde{R}_i \in Spin(N)$ for $i = 1,2$ such that $R_1\tilde{R}_1 = -\tilde{R}_1 R_1$ and $R_2\tilde{R}_2 = \gamma\tilde{R}_2 R_2$. Let $R_1 = R_2 = \prod_{i=1}^n e_{4i-2}e_{4i}$, $\tilde{R}_1 = e_1 e_2$, and $\tilde{R}_2 = 2^{-n}\prod_{i=1}^{2n}(1 + e_{2i-1}e_{2i})$, which satisfy the desired conditions [together with $R_1^2 = (-1)^n\mathbb{I}$, $\tilde{R}_1^2 = -\mathbb{I}$ and $\tilde{R}_2^2 = \gamma$].

(7) *Case* $G_\Gamma = Spin(N)/\mathbb{Z}_2 = SS(N)$, $N = 4n$. As discussed before, the group $Spin(N)$ has center $\{\mathbb{I}, -\mathbb{I}, \gamma,$

$-\gamma\} = \mathbb{Z}_2 \times \mathbb{Z}_2$. After dividing out $\{\mathbb{I},\gamma\}$ or $\{\mathbb{I}, -\gamma\}$ (which are both isomorphic to $\mathbb{Z}_2$) one obtains the group $SS(N)$ also known as the semi-spinor group (see, e.g., Ref. 8). In the former case one could define $R = R_2$ and $\tilde{R} = \tilde{R}_2$, where R_2 and $\tilde{R}_2$ have been defined in the previous paragraph. Using the same reasoning as before, we directly obtain $R\tilde{R} = \gamma\tilde{R}R$ and $\tilde{R}^2 = \gamma\mathbb{I}$. However, $R^2 = -\mathbb{I} \notin \Gamma$. Thus although $F_\Gamma = \mathbb{Z}_4 \times \mathbb{Z}_2$ constructed in this way does lead to an bijective τ, it is not of the form $\mathbb{Z}_r \times \mathbb{Z}_r$. In principle the results discussed in Secs. III and IV cannot be directly applied. However, Eq. (9) can still be used to define a NL-UT and an analysis similar to Sec. IV can be performed to find out what type of symmetry-breaking phase the topological nontrivial phase is mapped to by such a NL-UT. In the case where $\Gamma = \mathbb{Z}_2 = \{\mathbb{I}, -\gamma\}$ similar problems occur. One could still define $R = R_2$ and $\tilde{R} = e_1e_2\tilde{R}_2$ such that $R\tilde{R} = -\gamma\tilde{R}R$ and $\tilde{R}^2 = -\gamma\mathbb{I}$. But also in this case $R^2 = -\mathbb{I} \notin \Gamma$ such that $F_\Gamma = \mathbb{Z}_4 \times \mathbb{Z}_2$.

VI. CONCLUSIONS AND OUTLOOK

We presented a nonlocal unitary transformation which maps topological phases of $\mathbb{Z}_N \times \mathbb{Z}_N$ spin chains to symmetry-breaking ones. Since the map transfers nonlocal string order to the more familiar local Landau order it provides a useful alternative characterization of topological phases. Our result may be regarded as a twofold generalization of the "hidden" symmetry breaking that is familiar from the AKLT model.[16] First of all, our method is able to deal with the existence of several distinct nontrivial topological phases, not just a single one. Moreover, in view of the existence of nontrivial subgroups $\mathbb{Z}_r \times \mathbb{Z}_r \subset \mathbb{Z}_N \times \mathbb{Z}_N$, we are also capable of characterizing phases which exhibit a mixture of topological protection and spontaneous symmetry breaking.

As pointed out in Sec. V, our previous considerations lead to a full characterization of topological phases in spin systems with continuous symmetry groups. This observation relies on the existence of discrete subgroups of type $\mathbb{Z}_N \times \mathbb{Z}_N$ in all classical groups of unitary, orthogonal, or symplectic type. Besides constructing these subgroups explicitly, we also showed that the projective representations of the continuous groups and their subgroups are (with one exception) in one-to-one correspondence if N is chosen properly. For the stability of edge modes it is thus not important to preserve the full continuous symmetry group. Rather it is sufficient to preserve the corresponding discrete subgroup. This phenomenon has been known for some time in the case of $SO(3)$[19,20] but the picture that emerges from our paper is somewhat more complete.

As a by-product, our analysis provides a complementary perspective on the hierarchy of topological phases that was pointed out in Ref. 8. As was shown in Ref. 8, there is an injection of topological phases when viewing the same system from the perspective of either G_Γ or $G_{\Gamma'}$, with $\Gamma' \subset \Gamma \subset \mathcal{Z}(G)$ being two central subgroups of G. In Sec. V we have shown that G_Γ has a subgroup F_Γ that can be used to characterize the topological phases, and a similar statement holds for Γ'. From the construction of F_Γ it is clear that $F_{\Gamma'} \subset F_\Gamma$. The original hierarchy of topological phases is thus also reflected on the level of "hidden" symmetry breaking.

We would like to stress that our results from Sec. V also provide a precise route to embed spin systems with discrete spin degrees of freedom into spin systems with continuous symmetry. While *a priori* the latter appear to be more constrained, this reformulation may nevertheless be useful with regard to constructing effective low-energy topological field theories in terms of nonlinear σ models. In this sense, it may be used to make some of the ideas discussed in Ref. 29 more precise. It remains to be clarified, however, whether the embeddings just mentioned only capture the features of topological protection with regard to continuous symmetry groups in one-dimensional systems or whether the correspondence also lifts to higher dimensions.

Note added. Recently Ref. 27 appeared which has considerable overlap with our own results. Let us briefly summarize the main differences. Our setup is, in a sense, more limited. Instead of considering arbitrary Abelian groups, we restrict our attention to groups of type $\mathbb{Z}_N \times \mathbb{Z}_N$. Besides, the authors of Ref. 27 construct a different nonlocal unitary transformation for each individual purely topological phase which can be used to map it to a phase with *full* spontaneous symmetry breaking. In contrast, we keep the nonlocal unitary transformation fixed and investigate the fate of various phases under this map. This allows us to investigate phases which involve a mixture of topological protection and symmetry breaking. At the end of Sec. IV we determine precise conditions under which a given phase can possibly be mapped to a fully symmetry broken one. Finally, our treatment of continuous groups exhausts *all* classical cases and does not just cover $PSU(N)$ and $SO(2N + 1)$ as in Ref. 27.

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Chapter 3

One-Dimensional Gapped Systems

The origin of the complexity of quantum spin systems is the exponential growth of the dimension of the Hilbert space with respect to the physical system size. However, for all physical models interactions are local. This locality should somehow be reflected in some property of the corresponding ground states: it is reflected in the behavior of the von Neumann entropy of the ground states. Let R denote a spatial region of a quantum spin system and let ρ_R be the reduced density matrix of the corresponding ground state with respect to this region. It is obtained from the density matrix ρ of the ground state by tracing over all degrees of freedom in the complement of R (denoted by $\backslash R$): $\rho_R = \mathrm{Tr}_{\backslash R}\,\rho$. The von Neumann entropy $S(\rho_R) = -\mathrm{Tr}(\rho_R \log \rho_R)$ is a measure of entanglement between R and its complement. For generic quantum states, this entropy can be as large as $|R| \log d$, where d is the dimension of an on-site Hilbert space and $|R|$ the number of sites contained in region R. However, for one dimensional gapped systems, it has been shown that the von Neumann entropy is bounded by a constant which depends only on the energy gap and the correlation length [28]. Generalizing to higher dimensions, ground states seem to obey an area law [29] which states that the entropy scales as the boundary $|\partial R|$ of the region R, with possibly logarithmic corrections for gapless systems. Note that $|\partial R|$ is constant in the one dimensional case.

Matrix product states (MPS) offer an efficient way to parametrize the set of states which obey an area law. Indeed, they were introduced to describe ground states of finitely-ranged gapped Hamiltonians [30, 31]. Moreover the inverse has also been shown: each MPS gives rise to a gapped Hamiltonian which has this state as a ground state [32, 31, 33, 34]. They also lie at the heart of the density-matrix-renormalization-group algorithm (DMRG) [26], which has been proven to be very successful in computing the ground state and low lying excited states in various models. These three

topics - matrix product states, parent Hamiltonians and the density-matrix-renormalization-group algorithm - will be discussed in detail in this chapter.

3.1 Matrix Product States

The Hilbert space of a physical spin chain is described by a tensor product of on-site Hilbert spaces $\mathcal{H}_n$,

$$\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_L \quad , \tag{3.1}$$

where L is the length of the spin chain. Let $|i_n\rangle$ be an orthonormal basis for $\mathcal{H}_n$. The tensor product $|i_1 \dots i_L\rangle = |i_1\rangle \otimes \cdots \otimes |i_L\rangle$ forms an orthonormal basis for the total Hilbert space. Quantum states which are most resemblant to classical states are those without entanglement, i.e. separable states. They can be most easily written as a product:

$$|\Psi\rangle = \sum_{i_1 \dots i_L} A^{[1]}_{i_1} \dots A^{[L]}_{i_L} |i_1 \dots i_L\rangle \quad . \tag{3.2}$$

Note that the coefficients $A^{[n]}_{i_n}$ appearing in the above equation depend on a single site only. The total number of coefficients to be determined is $d \cdot L$, where d is the dimension of an on-site Hilbert space. This is a great contrast to a generic quantum state:

$$|\Psi\rangle = \sum_{i_1 \dots i_L} C_{i_1 \dots i_L} |i_1 \dots i_L\rangle \quad . \tag{3.3}$$

Any form of entanglement can be encoded in such a state. The total number of coefficients to be determined equals the dimension of the total Hilbert space which is d^L. To overcome this exponential growth, one could study a generalization of separable states, such that each coefficient $A^{[n]}_{i_n}$ depends on an extra parameter shared with its neighbor:

$$|\Psi\rangle = \sum_{\alpha,\beta,\dots,\delta} \sum_{i_1 \dots i_L} A^{[1]}_{i_1,(\alpha\beta)} A^{[2]}_{i_2,(\beta\gamma)} \dots A^{[L]}_{i_L,(\delta\alpha)} |i_1 \dots i_L\rangle \quad . \tag{3.4}$$

These extra parameters encode entanglement between neighboring sites. Restricting these parameters to the integers smaller or equal to a constant D, one can interpret the coefficients $A^{[n]}_{i_n,(\alpha\beta)}$ as a set of d matrices of size $D \times D$. These matrices are multiplied to obtain the resulting coefficients of the state $|\Psi\rangle$. Hence the name matrix product state (MPS) [35]. The state $|\Psi\rangle$ is determined by a total of $D^2 \cdot d \cdot L$ coefficients, a number which scales linearly with system size. The constant D can be site dependent. That is for each site we define a "left" integer $D_{(n,l)}$ and a "right" integer $D_{(n,r)}$ such that the parameters appearing in $A^{[n]}_{i_n,(\alpha\beta)}$ are restricted to $\alpha \leq D_{(n,l)}$ and $\beta \leq D_{(n,r)}$.

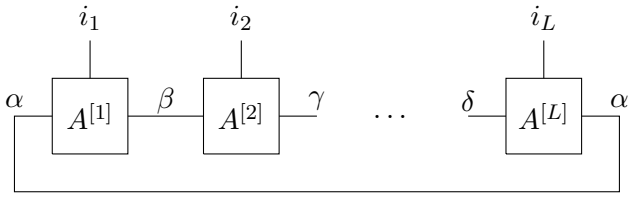


Figure 3.1: A diagrammatic representation of a matrix product state.

Of course these constants are related by $D_{(n,r)} = D_{(n+1,l)}$. For systems with open boundary conditions there is no reason for the boundary sites to be entangled. In this case the constants $D_{(1,l)}$ and $D_{(L,r)}$ are set to 1.

Another popular way to explain MPSs is to introduce two auxiliary spaces $\mathcal{H}_{(n,l)}$ and $\mathcal{H}_{(n,r)}$ for each site n. These spaces have dimensions $D_{(n,l)}$ and $D_{(n,r)}$, respectively. These spaces model the entanglement of the n-th site with its two neighbors. All the spaces $\mathcal{H}_{(n,l/r)}$ together form an auxiliary spin chain twice as long as the original spin chain. Neighboring auxiliary spaces should be dual to each other $\mathcal{H}_{(n+1,l)} = \mathcal{H}^*_{(n,r)}$. This allows to construct maximally entangled states on auxiliary spaces of sites n and $(n+1)$: $|I_n\rangle = \sum_\alpha |\alpha\rangle\langle\alpha| \in \mathcal{H}_{(n,r)} \otimes \mathcal{H}_{(n+1,l)}$. A maximally entangled state can also be defined on the left and right most auxiliary spaces: $|I_n\rangle \in \mathcal{H}_{(1,l)} \otimes \mathcal{H}_{(L,r)}$. Together these states define a state on the auxiliary spin chain: $|\Psi_A\rangle = \bigotimes_n |I_n\rangle$. A state on the physical spin chain $|\Psi\rangle$ is defined by a set of maps

$$A^{[n]} : \mathcal{H}_{(n,l)} \otimes \mathcal{H}_{(n,r)} \to \mathcal{H}_n \quad , \tag{3.5}$$

where $\mathcal{H}_n$ denotes the Hilbert space of the n-th site. The state $|\Psi\rangle$ is obtained by $|\Psi\rangle = \left(\bigotimes_n A^{[n]}\right)|\Psi_A\rangle$. The maps $A^{[n]}$ can be related to the matrices introduced in Eq. (3.4) through

$$A^{[n]}_{i_n,(\alpha\beta)} = \langle i_n | A^{[n]} | \alpha\beta \rangle \quad . \tag{3.6}$$

where $|\alpha\beta\rangle = |\alpha\rangle \otimes |\beta\rangle \in \mathcal{H}_{(n,l)} \otimes \mathcal{H}_{(n,r)}$.

For a first encounter with MPSs, it is insightful to have a diagrammatic picture in mind. The object $A^{[n]}_{i_n,(\alpha\beta)}$ has three indices and is thus represented by a box with three outgoing lines. Each time indices are contracted, their corresponding lines are connected. In Fig. 3.1 these rules are used to depict the product of matrices appearing in Eq. (3.4).

3.1.1 Success of matrix product states

MPSs were introduced to describe states obeying an area law. If R is a region consisting of the sites between (and including) sites n and m, the von Neumann entropy of an MPS with respect to R is bounded by $\log D_{(n,l)} +$

$\log D_{(m,r)}$. This can be explained by first observing that the reduced density matrix ρ_R with respect to region R has a dimension smaller or equal to $D_{(n,l)} \cdot D_{(m,r)}$. The von Neumann entropy is maximal if all the eigenvalues of ρ_R are equal, that is equal to $(D_{(n,l)} \cdot D_{(m,r)})^{-1}$. This calculation shows that MPSs indeed obey an area law. But does the contrary also hold? Can each state obeying an area law efficiently be modeled by an MPS? Certainly any state on a finite chain can be written as an MPS, given that the dimension of the auxiliary spaces is big enough ($D = d^{L/2}$). The key point is that, using a much smaller auxiliary dimensions ($D \ll d^{L/2}$), one can already approximate any finitely correlated state with high precision.

Let $|\Psi_0\rangle$ be some state on a chain that we want to approximate with an MPS $|\Psi\rangle$. To simplify notation, assume open boundary conditions, that is $D_{(1,l)} = 1$. Again consider a region consisting of the first n sites. The entanglement of $|\Psi_0\rangle$ between this region and its complement depends on the Schmidt coefficients λ_i obtained by computing a singular value decomposition

$$|\Psi_0\rangle = \sum_{i=1}^{k} \lambda_i |\phi_i^R\rangle |\phi_i^{\backslash R}\rangle \quad , \tag{3.7}$$

where $\{|\phi_i^R\rangle\}_i$ is a set orthonormal states in region R and similarly for $\{|\phi_i^{\backslash R}\rangle\}_i$. The Schmidt coefficients are assumed to be sorted in decreasing order of magnitude. The number of Schmidt coefficients k is bounded by the dimensions of the Hilbert spaces of both region R and its compliment. Consider $|\Psi\rangle$ obtained by taking only the first $D_{(n,l)} < k$ Schmidt coefficients. Thus, the entanglement between R and its compliment is now modeled by a space of dimension $D_{(n,l)}$ instead of k, exactly what an MPS does. The error made in this approximation is bounded by [36]:

$$\| |\Psi_0\rangle - |\Psi\rangle \| \leq \sum_{i=D_{(n,l)}+1}^{k} \lambda_i^2 \quad . \tag{3.8}$$

The success of MPS lies in the fact that, for states obeying the area law the Schmidt coefficients decay exponentially. More precisely, it was shown in Ref. [28] that the sum of all but the first D Schmidt coefficients between region R and its complement depends on D, the correlation length ξ and the von Neumann entropy $S = S(\rho_R)$ as:

$$\sum_{i>D} \lambda_i^2 \leq C \left(\frac{e^{2S}}{2D} \right)^{1/(\xi \log d)} \quad , \tag{3.9}$$

where d is the dimension of the on-site Hilbert space and C is some constant that depends only on the correlation length. Note that even if the entropy S

scales logarithmically (which is the case for ground states of critical systems [37]) in the size of R ($\sim L/2$), the numerator of the fraction appearing in Eq. (3.9) still scales linearly in L. In Ref. [36] a bound on the sum of all but the largest D Schmidt coefficient was found in terms of the Renyi entropy $S(\alpha) = \frac{1}{1-\alpha} \log \mathrm{tr}(\rho_R^\alpha)$:

$$\sum_{i>D} \lambda_i^2 \leq \left(\frac{1-\alpha}{D}\right)^{\frac{1-\alpha}{\alpha}} \exp\left(\frac{1-\alpha}{\alpha} S(\alpha)\right) \quad , \tag{3.10}$$

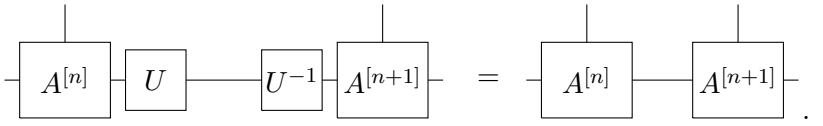
where $0 < \alpha < 1$. Note that this bound is independent of the correlation length ξ. Strictly speaking, it is only a bound of the Renyi entropy from which approximability of an MPS follows. That is, in order to approximate a (critical) ground state with precision ϵ, the corresponding bond dimension D must scale polynomially in L and $1/\epsilon$. Thus, the total number of parameters ($= D^2 \cdot d \cdot L$) must scale polynomially in L and $1/\epsilon$, which is in contrast to the exponentially increasing size of the total Hilbert space. In Ref. [38], examples of states with an area law in term of von Neumann entropy are discussed that can not be approximated efficiently with an MPS.

3.1.2 A standard form of MPSs

Although an MPS is a unique state, any state can be represented by various different MPSs. The origin of this degree of freedom is the invariance of the maximally entangled state under the gauge transformation $U \otimes U^{-1} |\alpha\rangle\langle\alpha|$. This degree of freedom translates to an invariance of an MPS under the transformation of its matrices

$$A^{[n]} \to A^{[n]} \circ \left(U_{(n,l)} \otimes U_{(n,r)}\right) \quad , \tag{3.11}$$

such that $U_{(n+1,l)} = U_{(n,r)}^{-1}$. One can also understand this diagrammatically:



The boxes U and U^{-1} cancel, explaining the invariance of the MPS. The notation U is short for $U_{(n,r)}$. Different MPSs can describe the same quantum state. However, it is convenient for calculations to use MPSs with certain additional properties. In this section I will show that any MPS can be brought into standard form [35] obeying

$$\sum_{i_n} A_{i_n}^{[n]} A_{i_n}^{[n]\dagger} = \mathbb{I} \quad , \tag{3.12}$$

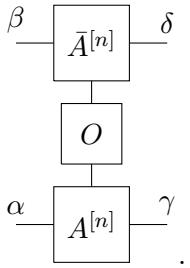
$$\sum_{i_n} A_{i_n}^{[n]\dagger} (\Gamma^{[n]})^2 A_{i_n}^{[n]} = (\Gamma^{[n+1]})^2 \quad , \tag{3.13}$$

for some diagonal real non-negative matrices $\Gamma^{[n]}$.

I will start by defining the transfer matrix:

$$E_{O\ \alpha\beta,\gamma\delta}^{[n]} = \sum_{i_n,j_n} A_{i_n,(\alpha\gamma)}^{[n]} O_{i_n j_n} \bar{A}_{j_n,(\beta\delta)}^{[n]} \quad , \tag{3.14}$$

where $O_{i_m j_n} = \langle j_n|O|i_m\rangle$ are the matrix elements of some operator O. This expression can be depicted diagrammatically as



The transfer matrix with unit operator $E^{[n]} := E_{\mathbb{I}}^{[n]}$ acts as

$$E^{[n]} : \mathrm{End}(\mathcal{H}_{(n,r)}) \to \mathrm{End}(\mathcal{H}_{(n-1,r)}) \quad . \tag{3.15}$$

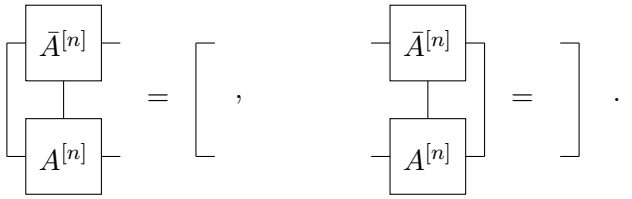
Using the gauge degree of freedom of MPSs one can right-normalize the transfer matrices such that $\tilde{E}^{[n]}(\mathbb{I}) = \mathbb{I}$ which is equivalent to Eq. (3.12). Let $C_r^{[n]} : \mathcal{H}_{(n,r)} \otimes \mathcal{H}_n \to \mathcal{H}_{(n-1,r)}$ be the mapping obtained from $A^{[n]}$ through

$$\langle\alpha|C_r^{[n]}|i_n\beta\rangle = A_{i_n,(\alpha\beta)}^{[n]} \quad . \tag{3.16}$$

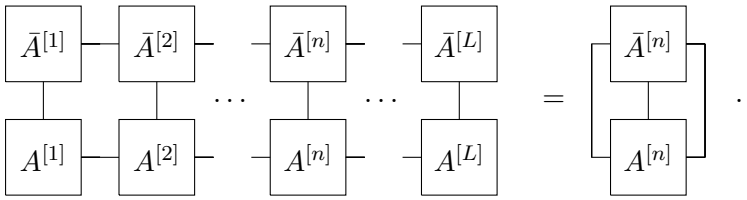
Its singular value decomposition is $C_r^{[n]} = U\Lambda^{[n]}\tilde{A}^{[n]}$, where U and $\tilde{A}^{[n]}$ are isometries and $\Lambda^{[n]}$ is a diagonal matrix with the singular values of $C_r^{[n]}$ as its diagonal entries. More explicitly

$$A_{i_n,(\alpha\beta)}^{[n]} = U_{\alpha\gamma}\lambda_\gamma^{[n]}\tilde{A}_{i_n,(\gamma\beta)}^{[n]} \quad , \tag{3.17}$$

with $\lambda_\gamma^{[n]} = \Lambda_{\gamma\gamma}^{[n]}$. Saying that the matrices $\tilde{A}^{[n]}$ are isometric means that the matrix M with entries $(M)_{\gamma,i_n\beta} = \tilde{A}_{i_n,(\gamma\beta)}^{[n]}$ obeys $MM^\dagger = \mathbb{I}$. Here i_n and β combine to form the second index. Similarly $U^\dagger U = \mathbb{I}$. Using these property, it can easily be shown that it gives rise to a right-normalized transfer matrix. The matrix $\tilde{A}^{[n-1]}$ should be transformed accordingly to keep the total MPS invariant. Similarly, one could left-normalize a transfer matrix such that it obeys $\sum_\alpha E_{\alpha\alpha,\gamma\delta}^{[n]} = \delta_{\gamma\delta}$. Diagrammatically, the left- and right-normalized transfer matrices obey:



Normalizing transfer matrices simplifies calculations. For example, calculating the norm of an MPS $|\Psi\rangle$ with transfer matrices $E^{[i]}$ which are left-normalized for $i < n$ and right-normalized for $i > n$ results in $\langle\Psi|\Psi\rangle = \mathrm{Tr}E^{[n]}(\mathbb{I}) = \sum_{i_n,\alpha,\beta} |A^{[n]}_{i_n,(\alpha\beta)}|^2$. Diagrammatically:



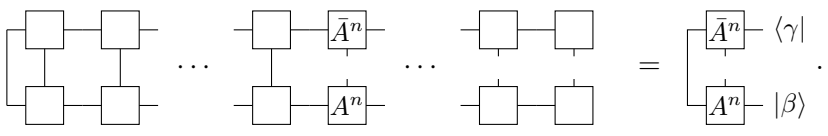
The calculation of reduced density matrices is also simplified if transfer matrices are normalized. Consider an MPS with open boundary conditions ($D_{(1,l)} = D_{L,r)} = 1$). Let R_n be the region of the last $L - n + 1$ sites. Its complement consists of the first $n - 1$ sites. If the transfer matrices $E^{[i]}$ are left-normalized for $i < n$ and right-normalized for $i > n$, the expression for the reduced density matrix ρ_{R_n} will simplify as follows:

$$\begin{aligned}
\rho_{R_n} &= \mathrm{Tr}_{\setminus R_n} \sum_{i_1\ldots i_L, j_1\ldots j_L} \bar{A}^{[1]}_{j_1}\ldots\bar{A}^{[L]}_{j_L} A^{[1]}_{i_1}\ldots A^{[L]}_{i_L} |i_1\ldots i_L\rangle\langle j_1\ldots j_L| \\
&= \sum_{i_1\ldots i_L, j_n\ldots j_L} \bar{A}^{[1]}_{i_1}\ldots\bar{A}^{[n-1]}_{i_{n-1}}\bar{A}^{[n]}_{j_n}\ldots\bar{A}^{[L]}_{j_L} A^{[1]}_{i_1}\ldots A^{[L]}_{i_L} |i_n\ldots i_L\rangle\langle j_n\ldots j_L| \\
&= \sum_{i_n j_n \alpha\beta} \bar{A}^{[n]}_{j_n,(\alpha\gamma)} A^{[n]}_{i_n,(\alpha\beta)} |i_n\beta\rangle\langle j_n\gamma| \quad . \qquad (3.18)
\end{aligned}$$

The vectors $|\beta\rangle$ are obtained through:

$$|\beta\rangle = A^{[n+1]}_{i_{n+1},(\beta\delta)}\ldots A^{[L]}_{i_L,(\epsilon)} |i_{n+1}\ldots i_L\rangle \quad . \qquad (3.19)$$

All the matrices $A^{[a]}_{i_a}$ in the above equation can be viewed as unitary mappings since their corresponding transfer matrices are right-normalized. Thus, the vectors $|\beta\rangle$ form an orthonormal basis. The same argument holds for $\langle\gamma|$. This equation can be written diagrammatically as



The reduced density matrix ρ_{R_n} can also be written in terms of the mappings $C^{[n]}_r$ defined in Eq. (3.16): $\rho_{R_n} = C^{[n]\dagger}_r C^{[n]}_r$. The eigenvalues of ρ_{R_n} are exactly the square of the singular values of $C^{[n]}_r$. From Eq. (3.18) it follows that $\rho_{R_{n+1}} = \sum_{i_n}\langle i_n|\rho_{R_n}|i_n\rangle = \sum_{i_n} A^{[n]\dagger}_{i_n} A^{[n]}_{i_n}$ results in the reduced

density matrix of R_{n+1} having eigenvalues values $(\lambda_i^{[n+1]})^2$. Furthermore, the matrices $A^{[n]}$ can also be right-normalized by means of Eq. (3.17). Thus the matrices $A^{[n]}$ can be transformed to obey Eq. (3.13).

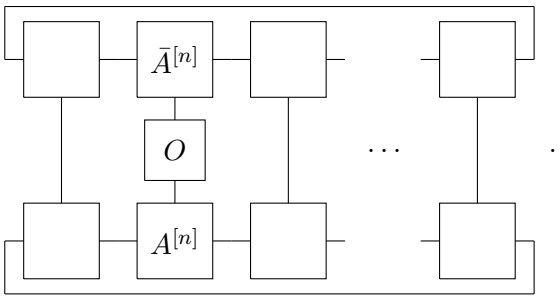
All right-normalized matrices can be transformed to obey Eq. (3.13) where $(\Lambda^{[n]})^2$ is a diagonal matrix containing the eigenvalues of the reduced density matrix ρ_{R_n}. The right-normalized matrix $\tilde{A}^{[n]}$ can also be obtained by computing the right-eigenvectors of ρ_{R_n}.

I stated before that bringing an MPS in the standard form of Eqs. (3.12) and (3.13) can simplify further calculations. Indeed the reduced density matrix can easily be computed by means of Eq. (3.18). In the following I will show that expectation values and correlation functions can also be more easily computed if an MPS is brought into the standard form.

The expectation value of an operator O_n acting on the n-th site is calculated as follows:

$$\langle\Psi|O_n|\Psi\rangle = \mathrm{Tr}\left(\prod_{i=1}^{n-1} E^{[i]} E_O^{[n]} \prod_{i=n+1}^{L} E^{[i]}\right) \quad , \tag{3.20}$$

where $E^{[i]} = E_{\mathbb{I}}^{[i]}$. This expression can be depicted diagrammatically as



Correlations between two operators L and R acting on two sites n and m can also be easily calculated using transfer matrices:

$$\langle L_n R_m\rangle = \frac{\mathrm{Tr}\left(E_L E^j E_R E^{L-j-2}\right)}{\mathrm{Tr}E^L} \quad . \tag{3.21}$$

Here we assume that all transfer matrices are site independent: $E_O^{[i]} = E_O$. Thus we are dealing with a translational invariant MPS. Furthermore $j = m - n - 1$ is the number of sites between sites n and m. Now for simplicity assume that E has a non degenerate largest eigenvalue λ_1 with right and left eigenvectors $|r\rangle$ and $\langle l|$ and rescale the MPS such that $\lambda_1 = 1$. Eq. (3.21) then simplifies to

$$\langle L_n R_m\rangle = \langle l|E_L|r\rangle\langle l|E_R|r\rangle + \sum_{k>1} \lambda_k^j \langle l|E_L|r_k\rangle\langle l_k|E_R|r\rangle \quad , \tag{3.22}$$

where λ_k are the other eigenvalues of E with corresponding right and left eigenvectors $|r_k\rangle$ and $\langle l_k|$. This implies an exponentially decaying correlation. The exponent is in this case determined by λ_2: in general it is determined by the ratio between the first and second largest eigenvalue. This statement also holds for MPS with a transfer matrix with degenerate largest eigenvalue. In this case one obtains more than one constant non-decaying term. The other terms still decay exponentially.

3.1.3 The AKLT-state

The AKLT-state is defined on a spin-1 spin chain and is the unique ground state of the $SO(3)$ invariant AKLT-Hamiltonian:

$$H_{AKLT} = \sum_{\langle i,j\rangle} \left(\frac{1}{3} + \frac{1}{2}\vec{S}_i\vec{S}_j + \frac{1}{6}(\vec{S}_i\vec{S}_j)^2 \right) \quad , \tag{3.23}$$

with periodic boundary conditions. It was studied by Affleck, Kennedy, Lieb and Tasaki [15] because the correlation length and a lower bound on its gap can be exactly calculated. Moreover this state lies in the Haldane phase, thus it allows to verify the statement that the Heisenberg model on integer spin chains is gapped and short range correlated [3]. Alternatively, the AKLT-Hamiltonian with open boundary conditions has a four-fold degenerate ground state.

The AKLT-Hamiltonian is a sum of terms, each acting on a space $V_2 \otimes V_2 = V_0 \oplus V_2 \oplus V_4$ where V_λ is the $(\lambda+1)$-dimensional spin-$\lambda/2$ representation of $SU(2)$. The action of $\vec{S}_i\vec{S}_j$ on each of these three spaces can be calculated by

$$\begin{aligned} \vec{S}_i\vec{S}_j v &= \frac{1}{2}\left((\vec{S}_i + \vec{S}_j)^2 - \vec{S}_i^2 - \vec{S}_j^2 \right) v \\ &= (\lambda(\lambda+2)/8 - 2)\, v \quad , \end{aligned} \tag{3.24}$$

for all $v \in V_\lambda$. Using this equation for $\lambda = 0, 2$ or 4, it follows that the AKLT-Hamiltonian is a projection on V_4. Thus a state which does not contribute to the spin 2 sector ($\mathrm{Tr}_{V_4}\rho_R = 0$ where R is a region of two neighboring sites) has zero energy and is thus a ground state.

Consider an MPS whose auxiliary spaces are spin 1/2 representations and whose matrices $A^{[n]} = A$ are site independent $SU(2)$ invariant projectors $A : V_1 \otimes V_1 \to V_2$, see Fig. 3.2. Let R' be a region of the auxiliary spin chain consisting of four sites corresponding to two neighboring physical sites. The reduced density matrix $\rho'_{R'}$ of the ground state on the auxiliary spin chain with respect to region R' only contributes to the spaces $V_1 \otimes V_0 \otimes V_1 = V_0 \oplus V_2$ due to the singlet between neighboring auxiliary sites of different physical sites. Thus $\mathrm{Tr}_{V_4}\rho'_{R'} = 0$. But since the mappings A are $SU(2)$ invariant, it follows that $\mathrm{Tr}_{V_4}\rho_R = 0$, where R is the region corresponding to two

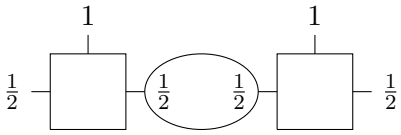


Figure 3.2: A graphical representation of two sites of the AKLT state (denoted by a "1") and their corresponding auxiliary spaces (denoted by a "$\frac{1}{2}$"). The boxes represent the SU(2) invariant projection. The ellipse represents the spin singlet.

neighboring physical sites. Thus this MPS is indeed a ground state of the AKLT-Hamiltonian. It was shown in Ref. [15] that it is the unique ground state.

3.2 Parent Hamiltonians

Up to now we have considered MPSs as approximate or exact solutions of gapped Hamiltonians. One can turn the question around: given an MPS, what is a corresponding gapped Hamiltonian with exactly this MPS as unique ground state. This Hamiltonian is called the parent Hamiltonian. Such a study is motivated by the fact that it gives rise to toy models with exactly known ground states. For example, in Ref. [DQ2] we used parent Hamiltonians to study models in a specific topological phase.

Again, let $|\Psi\rangle$ be an MPS and let R be a region of sites m to n. The rank of the reduced density matrix ρ_R is at most $D_{(m,l)}D_{(n,r)}$ which is smaller than the dimension of the Hilbert space belonging to region R ($\dim\mathcal{H}_R = d^l$) for a certain size $l = m-n+1$ of R. Consider the positive-semidefinite operator h_R acting in R with the property $\ker(h_R) = \mathrm{im}(\rho_R)$. The MPS $|\Psi\rangle$ is, by construction, a ground state of $h_R \otimes \mathbb{I}_{\setminus R}$ (where $\setminus R$ denotes the complement of R) and thus also of

$$\sum_i h_{R_i} \otimes \mathbb{I}_{\setminus R_i} \quad , \tag{3.25}$$

where R_i is some covering of the chain. This Hamiltonian is frustration free in the sense that its ground state minimizes each term in the above sum. Note that this is exactly how one can obtain the AKLT-Hamiltonian as the parent Hamiltonian of the AKLT-state (if one sums over regions of neighboring sites).

Nothing guarantees that the Hamiltonian constructed in this manner has a unique ground state. Consider for example the GHZ state (after Greenberger, Horne and Zeilinger). It is a periodic state defined on a spin-1/2 chain given by $|\uparrow\uparrow\cdots\uparrow\rangle + |\downarrow\downarrow\cdots\downarrow\rangle$. Its corresponding MPS representation is given by the site independent matrices $A_\pm = \mathbb{I} \pm \sigma_z$, where the subscript

"±" refers to spin-up and spin-down. The reduced density matrix of any region R is given by $\rho_R = |\Uparrow\rangle\langle\Uparrow| + |\Downarrow\rangle\langle\Downarrow|$ where $|\Uparrow\rangle$ ($|\Downarrow\rangle$) refers to the state in region R of all spins up (down). Its image space is clearly 2-dimensional and is spanned by $|\Uparrow\rangle$ and $|\Downarrow\rangle$. The Hamiltonian given by expression (3.25) will be of Ising type, having a two fold degenerate ground state.

The Hamiltonian of the GHZ state, constructed using Eq. (3.25), does not have a unique ground state because any reduced density matrix ρ_R has rank 2. However, the entanglement between region R and its complement is modeled by two auxiliary spaces, both of dimension 2. Thus it is modeled by a 4-dimensional space. I will discuss a sufficient condition for an MPS to have a parent Hamiltonian, a Hamiltonian that has this MPS as its *unique* ground state. Let $|\Psi\rangle$ be an MPS with matrices $A^{[n]}_{i_n,(\alpha\beta)}$ and let R be a region from site m to site n, with corresponding Hilbert space $\mathcal{H}_R$. Consider the map $\Gamma_R : \mathcal{H}_{(m,l)} \otimes \mathcal{H}_{(n,r)} \to \mathcal{H}_R$ from the boundaries of R into R given by

$$\Gamma_R|\alpha\epsilon\rangle = A^{[m]}_{i_m,(\alpha\beta)} A^{[m+1]}_{i_{m+1},(\beta\gamma)} \dots A^{[n]}_{i_n,(\delta\epsilon)} |i_m i_{m+1} \dots i_n\rangle \quad . \tag{3.26}$$

Region R is said to be injective if the above mapping is injective. An MPS is said to be injective if it has a disjoint covering of injective regions [34]. Each injective MPS has a parent Hamiltonian given by

$$\sum_{\langle i,j\rangle} h_{R_i \bigcup R_j} \otimes \mathbb{I}_{\setminus(R_i \bigcup R_j)} \quad , \tag{3.27}$$

such that its ground state is unique [32]. Here h_R is a projection with the property $\ker(h_R) = \mathrm{im}(\Gamma_R)$.

We can check that the MPS of the GHZ state (defined by the matrices $A_\pm = \mathbb{I} \pm \sigma_z$) is not injective. Indeed, for any region R we have $\Gamma_R(\begin{pmatrix}1&0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}) = 0$, proving that Γ_R is not injective. For the AKLT state, each region R consisting of two neighboring sites is injective. Indeed the corresponding map $\Gamma_R = V_1 \otimes V_1 \to V_2 \otimes V_2$ is injective. Regions R consisting of only 1 site are not injective. Note that Eq. (3.27) implies a parent Hamiltonian with 4-site interactions.

3.2.1 Translationally invariant systems

Translationally invariant states can be written in terms of site independent maps A acting on site independent auxiliary spaces $\mathcal{H}_l \otimes \mathcal{H}_r$, with $\mathcal{H}_r = \mathcal{H}_l^*$. In the previous section it was already shown that each MPS can be brought into standard form (obeying Eqs. (3.12) and (3.13)). In Ref. [35] it is shown that each MPS can be brought into a block form. Let the left and right auxiliary space split into $\mathcal{H}_l = \oplus_k \mathcal{H}_l^k$ and $\mathcal{H}_r = \oplus_k \mathcal{H}_r^k$. The matrices A_i can

be written as

$$A_i = \begin{pmatrix} A_i^1 & 0 & 0 \\ 0 & A_i^2 & 0 \\ 0 & 0 & \ddots \end{pmatrix} \quad , \tag{3.28}$$

such that each set of matrices $\{A_i^k\}_i$ obeys Eqs. (3.12) and (3.13). Moreover, the unit matrix is the *unique* eigenvector of the transfer matrix E^k : $\mathrm{End}(\mathcal{H}_r^k) \to \mathrm{End}(\mathcal{H}_r^k)$ given by

$$E^k(X) = \sum_i A_i^k X A_i^{k\dagger} \quad , \tag{3.29}$$

with eigenvalue 1, for each k. This standard form directly gives insight into the degeneracy of the ground state of its parent Hamiltonian. The idea is that each of the matrices A^k defines an injective MPS with injective regions of some size L_k, which depends on the block k. The Hamiltonian defined in Eq. (3.27), where the regions R_i have size $\max_k L_k$, has each of these MPSs as ground states [31, 33, 35]. This directly explains why the parent Hamiltonian of the GHZ state described above has a two fold degenerate grounds state.

This statement does not hold if a transfer matrix E^k has more than one eigenvalue of magnitude 1 for some k. Consider for example the Majumdar-Ghosh model [39]. It is defined on a spin 1/2 spin chain and consists of nearest and next-nearest neighbor interactions:

$$H_{\mathrm{MG}} = \sum_{\langle i,j \rangle} \vec{S}_i \vec{S}_j + \frac{1}{2} \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \vec{S}_j \quad . \tag{3.30}$$

It has a two-fold degenerate ground state consisting of singlets between neighboring sites. The ground states are only invariant under a translation of an even number of sites. The equal weight superposition of these two ground states has an MPS representation with matrices

$$A_\downarrow = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{and} \qquad A_\uparrow = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad . \tag{3.31}$$

One obtains only a single block upon bringing these matrices into the form given by Eq (3.28). The corresponding transfer matrix has eigenvalues 1 and -1 (after renormalization). By blocking two sites into one, one considers the square E^2 of the transfer matrix E, which of course has a twofold degenerate eigenvalue 1. Indeed, this transfer matrix can be written in block form with $k = 2$ such that the number of blocks is consistent with the number of ground states.

In Ref. [33] the statement on a parent Hamiltonian is generalized to non-injective systems, being indeed that the number of ground states equals

the number of blocks k in the decomposition of the transfer matrix (when translational symmetry is not broken). And more recently, in Ref. [34] the condition for a parent Hamiltonian has been generalized to incorporate higher dimensional systems in the framework of projected entangled pair states (PEPS) [40].

3.2.2 Gap in translationally invariant systems

Throughout this whole Chapter we are dealing with gapped system. The gap of a one dimensional translationally invariant system is defined in the limit of large system size:

$$\Delta = \lim_{L\to\infty} (e_2 - e_1) \quad . \tag{3.32}$$

Here e_1 and $e_2 \neq e_1$ are the two lowest eigenvalues up to degeneracies. Thus a degenerate ground state does not imply a zero gap.

In Ref. [31] a lower bound for the gap of a parent Hamiltonian of an injective MPS is found. It is given by:

$$\Delta \geq \frac{\Delta_{2p}}{2}\left(1 - 2c\lambda^p \frac{1+c\lambda^p}{1-c\lambda^p}\right) \quad . \tag{3.33}$$

Here λ is the second largest eigenvalue of the transfer matrix, $c = \mathrm{Tr}\rho^{-1}$ where ρ is the left non-zero fixed point of the transfer matrix ($\rho = \sum_i A_i^\dagger \rho A_i$) and $p \geq l$ where l is the size of the smallest region R which is injective. The gap Δ_{2p} is the gap of the same system restricted to $2p$ sites. In determining λ and c, it assumed that the transfer matrix is right-normalized.

Note that λ also determines the correlation length via Eq. (3.22). Thus these two important physical quantities - gap and correlation length - are directly related to each other.

3.3 DMRG

In the following I will describe an algorithm to find an MPS with minimal energy with respect to some Hamiltonian [41, 42]. This algorithm is closely related to the Density-Matrix-Renormalization-Group (DMRG) algorithm [26]. It consists of three steps: (1) Start with a random MPS $|\Psi\rangle$. (2) Keeping all other matrices fixed, find the set of matrices belonging to a site n (given by $A^{[n]}$) such that $|\Psi(A^{[n]})\rangle$ has minimal energy. (3) Repeat step 2 for all sites sufficiently often, until some stopping criteria are met.

An MPS $|\Psi\rangle$ depends linearly on the matrix coefficients $A^{[n]}_{i_n,(\alpha\beta)}$. These coefficients can be understood to form a vector a ($a_{i_n\alpha\beta} = A^{[n]}_{i_n,(\alpha\beta)}$). Finding $|\Psi(a)\rangle$ with minimal energy amounts to minimizing $\langle\Psi|H|\Psi\rangle$ which is quadratic in a and can be written as $a^\dagger X a$. Normalization of $|\Psi(a)\rangle$ gives

rise to a constraint also of quadratic form: $1 = \langle\Psi|\Psi\rangle =: a^\dagger Y a$. This problem can be solved using a Lagrange multiplier λ:

$$L(a, \lambda) = a^\dagger X a + \lambda(1 - a^\dagger Y a) \quad . \tag{3.34}$$

The minimum of this Lagrangian is determined by the generalized eigenvalue equation $Xa = \lambda Y a$.

There are a few issues that should be taken care of before being able to implement the above algorithm in an efficient way. I will discuss two important issues. The first issue arises when optimizing an MPS with periodic boundary conditions ($D_{(1,l)} = D_{(L,r)} \neq 1$). I will discuss that the matrix Y has a chance of being badly conditioned leading to numerical errors. In the second section I will discuss how symmetries can be used to reduce the computational costs. However, this give rise to a new problem, the algorithm might get stuck in a certain "symmetry sector". I will also discuss how this problem can be helped.

3.3.1 Periodic versus open boundary conditions

When solving this generalized eigenvalue problem numerically one should take care that the matrix Y is well conditioned [43]. The condition number is the ratio between the largest and the smallest eigenvalue. Given the equation $b = Ya$, the condition number of Y gives a bound on the dependence of the solution a on deviations of b. For systems with open boundary conditions this is however not a issue. One could transform the matrices as explained in Sect 3.1.2 such that $\langle\Psi|\Psi\rangle := a^\dagger a$ or in other words Y is unity.

For systems with periodic boundary conditions more care should be taken. Note that Y is a Hermitian matrix acting on the space $\mathcal{H}_{(n,l)} \otimes \mathcal{H}_{(n,r)} \otimes \mathcal{H}_n$. It can be decomposed into the sum of tensor products

$$Y = \sum_i \lambda_i L_i \otimes R_i \otimes \mathbb{I} \quad , \tag{3.35}$$

such that L_i and R_i are also Hermitian and normalized with respect to the Frobenius norm. (The Frobenius norm of X is given by $\sqrt{\mathrm{tr}(XX^\dagger)}$.) For systems without periodic boundary conditions, the left and right part are completely separated, the previous sum will consist of only one term with $L_1 = 1/\sqrt{D_{(n,l)}} \prod_{i<n} E^{[n]}$ and $R_1 = 1/\sqrt{D_{(n,r)}} \prod_{i>n} E^{[n]}$. However, with periodic boundary conditions there exists some "entanglement" between the left and right part leading to more than one non-zero singular value λ_i. The singular values are expected to decay exponentially in system size due to the finite correlation length [43]. Gauge invariance of the MPS allows to transform the matrix Y as:

$$Y \to (U_L^\dagger \otimes U_R^\dagger \otimes \mathbb{I}) Y (U_L \otimes U_R \otimes \mathbb{I}) \quad . \tag{3.36}$$

Choosing U_L such that $U_L U_L^\dagger = L_1$ and U_R such that $U_R U_R^\dagger = R_1$ will result in a Y close to unity and thus well conditioned.

3.3.2 Symmetries

After optimizing the n-th site one continues to optimize the $(n+1)$-th site and so on until the L-th site is reached. After this "right-sweep" all sites are optimized again in decreasing order. In this way, the effort in calculating the matrices X and Y is minimized, since only the matrices $A^{[n]}$ has to be left- (or right-) normalized after optimization during a "right- (or left-) sweep" [41]. After solving the generalized eigenvalue equation given by Eq. (3.34), the matrices on site n should be right-normalized to prepare the minimization of the $(n-1)$-st site (or left-normalized, depending on the direction of optimization). As described in Sect. 3.1.2, the reduced density matrix ρ_{R_n} described in Eq. (3.18) should be diagonalized to obtain right normalized matrices $\tilde{A}^{[n]}$.

As with all diagonalization algorithms, great improvement with regard to computational cost is achieved by making use of symmetries. Assume for the following that a $U(1)$ symmetry generated by S^z is conserved: $[H, S^z] = 0$. Not only is it useful to choose a basis of the on-site Hilbert spaces $\mathcal{H}_n$ in which S^z is diagonal (such that each basis vector is labeled by an S^z quantum number), but also the auxiliary spaces can be chosen to have a basis for which S^z is diagonal.[1] Using the quantum numbers of S^z, both ρ_{R_n} and the matrix X appearing in Eq. (3.34) can be block diagonalized. Moreover, if it is known that the ground state is in a certain symmetry sector it is sufficient to diagonalize only the corresponding block of the matrix X.

Optimizing the matrices $A^{[n]}$ does not change the distribution of quantum labels of the auxiliary spaces. If one starts with a certain state with certain corresponding distributions of quantum labels for the auxiliary spaces, which is different for the optimal state, this optimal state will not be reached. The algorithm is thus prone to getting trapped in a wrong "symmetry sector". Note that quantum numbers of the auxiliary space $\mathcal{H}_{(n,l)}$ are the sum of the quantum numbers of the region R_n consisting of the last $L-n+1$ sites. Quantum numbers of this auxiliary space are changed due to those part of the Hamiltonian which acts on both R_n and its complement. In Ref. [44] a method to prevent trapping is proposed which makes use of this fact. Decompose the Hamiltonian H into a part $H_{(n,l)}$ acting on the first $n-1$ sites and $H_{(n,r)}$ acting on all other sites. Thus:

$$H = \sum_i H^i_{(n,l)} \otimes H^i_{(n,r)} \quad . \tag{3.37}$$

[1] Consider the case where $D_{(n,l)} = D_{(L,r)} = 1$. The first and last auxiliary space are trivial and thus have quantum number 0. The right-normalized matrices induce an isometry C_r given by Eq. (3.16) which can be obtained from a reduced density matrix commuting with the symmetry. Thus C_r commutes with the symmetry. This implies an S^z action on $\mathcal{H}_{(n,r)}$ given an S^z action on $\mathcal{H}_{(n+1,r)}$. The same argument can be used in case of left-normalized matrices. They imply a S^z action on $\mathcal{H}_{(n,l)}$ given an S^z action on $\mathcal{H}_{(n-1,l)}$.

The second part of the Hamiltonian, given by $H^i_{(n,r)}$, is used to perturb the reduced density matrix ρ_{R_n} obtained after optimization

$$\hat{\rho}_{R_n} = \rho_{R_n} + \alpha \sum_i H^{i\,\dagger}_{(n,r)} \rho_{R_n} H^i_{(n,r)} \quad , \tag{3.38}$$

where the weight α is small ($10^{-4} - 10^{-8}$ [44]). This new reduced density matrix should be diagonalized to obtain right normalized matrices $\tilde{A}^{[n]}$. It may in general have more than $D_{(n,l)}$ eigenvalues. Only the largest $D_{(n,l)}$ should be kept, which may correspond to a different set of quantum numbers compared to before optimization.

Chapter 4

Symmetry Protected Topological Order in One Dimensional Systems

Topological order [1] is a concept to describe distinct quantum phases with equal symmetry breaking, which cannot be described by Landau theory. Quantum phases can be defined in different ways. One definition is that two gapped Hamiltonians H_0 and H_1 describe the same quantum phase if there exist a continuous path of Hamiltonians $H(q)$ with $H(0) = H_0$ and $H(1) = H_1$ such that $H(q)$ is gapped for each value of q. Another definition, shown to be equivalent [45], is to say that two systems are in the same quantum phase if their ground states are related by a unitary transformation U_t generated by the time evolution of a local Hamiltonian. This locality restriction only makes sense if one studies systems in some thermodynamic limit.

From the second definition it directly follows that all states obtained by transforming a separable (classical) state with some U_t reside in the same phase: the trivial phase. Since a separable state is not entangled, states in this trivial phase are called short ranged entangled. Long range entanglement in two-dimensional systems results in a universal constant term in the von Neumann entropy: $S(R) = c|\partial R| + \gamma$, [46, 47]. In one-dimensional spin systems long range order does not exist [13]. Or in other words, topological order does not exist in spin chains. This is because every ground state can be written as a matrix product state (MPS) as explained in the previous chapter. And as explained in Ref. [13] each MPS can be mapped to a separable state by essentially mapping the singlets between auxiliary spaces of different physical sites to singlets between auxiliary spaces of a single physical site, see Fig.4.1.

In some cases one cannot use an arbitrary unitary transformation U_t to connect different systems in the same phase. Symmetry might restrict

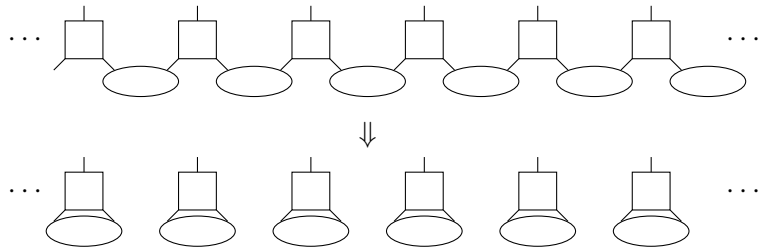


Figure 4.1: A graphical explanation why every MPS can be mapped to a separable state. Squares represent maps from auxiliary spaces to physical spaces, ellipses represent singlets.

the choice of U_t. Having less options for U_t could result in more quantum phases. These are called symmetry protected topological (SPT) phases [48]. An example of an SPT phase is the Haldane phase appearing in spin 1 spin chains. In this case the $SO(3)$ symmetry restricts the possible transformations U_t. The Haldane phase is separated by a quantum phase transition from for example a dimerized phase (being the topological trivial phase). Recently, a classification of all SPT phases has been found [13, 14]: given a group G of unitary symmetries acting globally, the different phases are classified by the elements of the group $H^2(G, U(1))$, being the second group cohomology of G with values in $U(1)$. The group $H^2(G, U(1))$ also classifies the different projective representations of G, being representations up to a phase. The idea behind the classification of SPT phases is that in the context of an MPS a symmetry can be thought to act on not only the physical sites but also on the auxiliary spaces. Since each physical site has two corresponding auxiliary sites the symmetry $u(g)$ acting on a single site fractionalizes $u(g) \to V_l(g) \otimes V_r(g)$ into actions $V_l(g)$ and $V_r(g)$ acting on the corresponding left and right auxiliary space. This fractionalization gives the auxiliary spaces $\mathcal{H}_{(n,l)}$ and $\mathcal{H}_{(n,r)}$ the possibility to be projective representations. The type of projective representation that the auxiliary spaces are, is directly related to the type of SPT in which the system resides.

Before discussing the classification of SPT phases I will introduce the concept of central extensions which can be used to explain projective representations. To get a good understanding of projective representations I will discuss them for the case of finite Abelian groups and of simple Lie groups. In the second part of this Chapter I will first discuss quite rigorously why symmetry fractionalizes. In a more hand waving manner I will prove the statement that SPT phases are classified by $H^2(G, U(1))$. Finally I will discuss in more detail the consequences of having time reversal or inversion symmetry.

4.1 Projective representations

As mentioned in the introduction, projective representations are classified by the second group cohomology $H^2(G, U(1))$, which in turn determines the different extensions of G by $U(1)$. Before introducing projective representations I will first introduce group extensions.

4.1.1 Central extensions

An extension of a group G over A is a group E together with homomorphisms ι and σ determining the following short exact sequence:

$$1 \to A \xrightarrow{\iota} E \xrightarrow{\sigma} G \to 1 \quad . \tag{4.1}$$

That is, the map ι is injective, the map σ is surjective and thus $E/A = G$. As a set, E is just the direct product $A \times G$ and its elements can be written as (a, g). In this notation the map σ is just $(a, g) \to g$. Let $\tau : G \to E$ select a representative (a_g, g) for each coset in G. It follows that $\sigma \circ \tau = \mathbb{I}_G$. The map τ is in general not a homomorphism. If there exist a homomorphism τ the extension E is said to be split, being isomorphic to a semi-direct product $A \rtimes G$. Multiplication is given by $(a_1, g_1)(a_2, g_2) = (a_1 \phi_{g_1}(a_2), g_1 g_2)$ where the map $\phi : G \to \mathrm{Aut}(A)$ is defined as $\phi_g(a) = \tau(g) a \tau(g)^{-1}$. From this point on I will assume A is in the center of G, which defines central extensions. In this case ϕ would always map to the trivial automorphism and thus it follows that every split central extension is isomorphic to the direct product $A \times G$.

Since τ is in general not a homomorphism, the element

$$\omega(g, h) = \tau_g \tau_h \tau_{gh}^{-1} \quad , \tag{4.2}$$

is not necessarily equal to the unit element in E. Following [49], I use the notation $\tau_g = \tau(g)$ and $\tau_{gh}^{-1} = (\tau(gh))^{-1}$ as the inverse element of τ_{gh} in G. However, $\omega(g, h)$ is an element of $\ker \sigma$ and thus of A. Note that the map ω depends on the map τ. A different choice of representatives given by $\tau'_g = \theta(g)\tau_g$ (where $\theta : G \to A$) will lead to a different map ω' related to ω by:

$$\omega'(g, h) = \theta(g)\theta(h)\theta(gh)^{-1}\omega(g, h) \quad . \tag{4.3}$$

From the associativity in E and G it follows that ω obeys a cocycle condition:

$$\omega(f, gh)\omega(g, h) = \omega(f, g)\omega(fg, h) \quad . \tag{4.4}$$

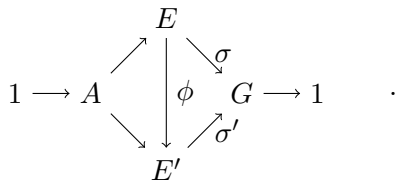
Maps $\omega : G \times G \to A$ satisfying the cocycle condition form a group under point wise multiplication which is denoted by $Z^2(G, A)$. Each map $\theta : G \to A$ defines a map $d\theta : G \times G \to A$ by $d\theta(g, h) = \theta(g)\theta(h)\theta(g, h)^{-1}$. The image

of this map is a subgroup of $Z^2(G,A)$ and is denoted by $B^2(G,A)$. Their quotient gives the group cohomology $H^2(G,A) = Z^2(G,A)/B^2(G,A)$. This can be put in a more general setting of a cochain complex. Let C^n be the Abelian groups of maps $\theta : G^n \to A$ and let $d_n : C^n \to C^{n+1}$ be given by:

$$\begin{aligned} d_n\theta(g_1,\ldots,g_n,g_{n+1}) =& \theta(g_1,\ldots,g_n)\theta(g_2,\ldots,g_{n+1})^{(-1)^{n+1}} \times \\ & \prod_{i=1}^{n} \theta(g_1,\ldots,g_ig_{i+1},\ldots,g_{n+1})^{(-1)^i} \quad . \end{aligned} \tag{4.5}$$

Define $B^n = \operatorname{im} d_{n-1}$ and $Z^n = \ker d_n$. Since $d_{n+1} \circ d_n = 1$ it follows that $B^n \subset Z^n$ which allows us to define $H^n(G,A) = Z^n/B^n$ as the n-th group cohomology of G over A.

Not only does a central extension of G give rise to an element $\omega \in H^2(G,A)$, also every $\omega \in Z^2(G,A)$ gives rise to a central extension E with multiplication rule $(a_1,g_1)(a_2,g_2) = (a_1a_2\omega(g_1,g_2),g_1g_2)$. Moreover, two maps ω and ω' satisfying $\omega(\omega')^{-1} \in B^2(G,A)$ give rise to isomorphic central extensions. Note that two groups related by the isomorphism $\phi : E \to E'$ are isomorphic central extensions if the following diagram commutes:



Thus the group $H^2(G,A)$ exactly gives the central extensions of G over A up to isomorphisms.

4.1.2 Representation of central extensions

Projective representations ρ_p of a group G are group homomorphism to the projective linear group $PGL(V) = GL(V)/\mathbb{C}^*$. The group $GL(V)$ itself is a central extension of $PGL(V)$, giving rise to a (non-homomorphic) map t which fixes a phase for each representation matrix $\rho_p(g)$. Let $U(g)$ denote $t(\rho_p(g))$ (these maps are also depicted in the diagram below). Due to the non-homomorphicity of t we have that:

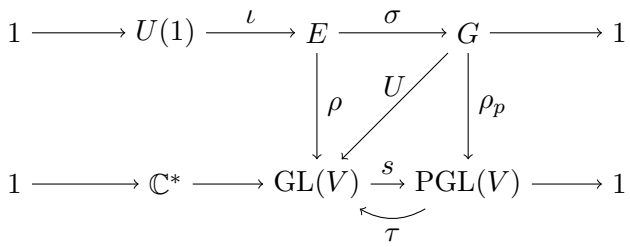
$$U(g)U(h) = \omega(g,h)U(gh) \quad , \tag{4.6}$$

where $\omega(g,h) = \omega(\rho(g),\rho(h))$ is defined through Eq. (4.2). Thus projective representations are also said to be representations up to a phase.

A projective representation can be lifted to a linear representation of a central extension. Let s be the homomorphism from $GL(V)$ to $PGL(V)$. Following Ref. [49], let E be the group defined as:

$$E = \{(U,g) \in GL(V) \times G \,|\, \rho_p(g) = s(U)\} \quad . \tag{4.7}$$

Defined as such E is a group since both ρ_p and s are homomorphisms. Furthermore the maps $\sigma = pr_2$ and $\iota : \lambda \to (\lambda \mathbb{I}_V, \mathbb{I}_G)$ are surjective and injective, respectively, from which follows that E is indeed an extension of G. These maps can be depicted diagrammatically as:



Also on the level of this central extension a non-homomorphic map $\tau : G \to E$ can be constructed. If one chooses the map $t(g) = (U(g), g)$ it follows that the central extension of G has the same structure as the central extension of $PGL(V)$. That is:

$$(U(g), g) \cdot (U(h), h) = (U(g)U(h), gh) = (\omega(g, h)U(gh), gh) \quad . \tag{4.8}$$

Projective representations are said to be equivalent if they are linear representations of the same (isomorphic) central extension. Thus the set of equivalence classes of projective representations of G, which I denote with $\{[\omega]\}$, equals $H^2(G, U(1))$. The group structure of $H^2(G, U(1))$ is also present in $\{[\omega]\}$ and is defined by the tensor product:

$$U_{\omega_1} \in [\omega_1] \text{ and } U_{\omega_2} \in [\omega_2] \implies U_{\omega_1} \otimes U_{\omega_2} \in [\omega_1\omega_2] = [\omega_1] + [\omega_2] \quad , \tag{4.9}$$

where U_ω is the projective representation $U : G \to GL(V)$ satisfying Eq. (4.6).

4.1.3 Projective representations of finite Abelian groups

For finite groups, finding all inequivalent projective representations reduces to the problem of finding a finite site of suitable phases $\omega(g, h)$ satisfying some given relations. Let g_i be some ordered set of generators for the group G. Note that the projective class $[\omega]$ is fully determined by the functions of the form $\omega(g_i, h)$. Any other function $\omega(g, h)$ can be determined by applying the cocycle condition given by Eq. (4.4) sufficiently often. Consider a representative ω for each class $[\omega]$ satisfying

$$h = \prod_{k \geq i} g_k^{m_k} \implies \omega(g_i, h) = 1 \quad . \tag{4.10}$$

Each class $[\omega']$ has such a representative since a g_i and an h of the given form give rise to a unique element $g_i h$ and a $\theta \in B^2(G, U(1))$ can be defined such

that $\theta(g_i h) = \omega(g_i, h)\theta(g_i)\theta(h)$. Such a θ will relate ω' to an ω satisfying Eq. (4.10).

From the above statement it directly follows that cyclic groups don't allow for non trivial central extensions. Or in other words, $H^2(\mathbb{Z}_n, U(1)) = 1$. Each ω satisfying Eq. (4.10) is fully determined by the functions of the form $\omega_{ji} = \omega(g_j, g_i)$ with $j > i$. These functions determine how g_j and g_i "commute" with each other. Let n_i be the order of g_i. It then follows that

$$1 = \omega(g_j, g_i^{n_i}) = \omega(g_j, g_i)\omega(g_i g_j, g_i^{n_i - 1}) = \omega_{ji}\omega(g_j, g_i^{n_i - 1}) = \omega_{ji}^{n_i} \quad . \tag{4.11}$$

The third equality is due to the fact that $\omega(g_i, g_j g_i^{n_i - 1}) = 1$. And the fourth equality is obtained by induction. Thus ω_{ji} is an n_i-th root of unity. It is also a n_j-th root of unity where n_j is the order of g_j. Let q be the number of generators of a finite Abelian group. A projective representation is determined by $q(q-1)/2$ phases ω_{ji} satisfying

$$\omega_{ji}^{\gcd(n_i, n_j)} = 1 \quad . \tag{4.12}$$

It remains to show that these projective representations are all inequivalent. For that matter consider the ratio $f(g, h) = \omega(g, h)/\omega(h, g)$. This function is the same for all other $\omega' \in [\omega]$. And since $f(g_j, g_i) = \omega_{ji}$ for $j > i$ it follows that a different choice of phases ω_{ij} leads to a representative of a different class of projective representations.[2]

4.1.4 Projective representations of simple Lie groups

Every simple Lie group G_Γ can be written as the quotient of its universal cover G and some subgroup Γ of the center of G. That is $G_\Gamma = G/\Gamma$. Such Lie groups are also simply-connected if and only if $\Gamma = \{\mathbb{I}_G\}$. In this case G_Γ does not allow for non-trivial central extensions [50]. This statement allows for a straightforward classification of projective representations of simple Lie groups. The idea is that all (projective) representations of G_Γ give rise to (projective) representations of G. And since G only allows for trivial projective representations, it follows that the set of all projective representations of G_Γ is equal to the set the representations of G. It remains to study which representations of G are equivalent as projective representations of G_Γ.

The reason representations of G lift to projective representations of G_Γ is the non trivial action of Γ on such representations. Let $\gamma \in \Gamma$ and let P denote the weight lattice of G. Due to Schur's lemma, the action of $\rho(\gamma)$ on some irreducible representation V_μ with highest weight $\mu \in P^+$,

[2] Note that this argument is only complete if all orders n_i are different. I have neglected that different choices of some ordered set of generators and a different choice of ω can still lead to the same projective representations. For example if $G = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ than clearly the projective representation $\omega_{21} = -1$ and $\omega_{31} = \omega_{32} = 1$ is equivalent to the projective $\omega'_{31} = -1$ and $\omega'_{21} = \omega'_{32} = 1$ representation.

equals a multiple of the identity. This allows me to introduce the map $c : P \to \mathrm{Hom}(\Gamma, U(1))$, thus which maps $\mu \to c_\mu$ where $c_\mu(\gamma)$ is defined by the action of $\rho(\gamma)$ on vectors $v \in V_\mu$:

$$c_\mu(\gamma)v = \rho(\gamma)v \quad \text{for} \quad v \in V_\mu \quad . \tag{4.13}$$

The map c is a homomorphism. Since firstly if $v \in V_\mu$ and $w \in V_\nu$ we have that $\rho(\gamma)v \otimes w = c_\mu(\gamma)c_\nu(\gamma)v \otimes w$ and secondly $V_{\mu+\nu}$ is an invariant subspace of $V_\mu \otimes V_\nu$. Thus $c_{\mu+\nu}(\gamma) = c_\mu(\gamma)c_\nu(\gamma)$. Moreover, Γ always acts trivially on the one dimensional representation V_0 which allows to extend the map c to the negative weights by $c_{-\mu} = c_\mu^*$. Let Q_Γ be the kernel of this map. It consist of exactly those weights μ which are highest weights of some representation V_μ of G on which Γ acts trivially. Thus if $\mu \in Q_\Gamma$ (and μ positive or zero) then V_μ is a linear representation of G_Γ.

For those V_μ which are not a representation of G_Γ due to a non-trivial phase $c_\mu(\gamma)$ we can construct a central extension E of G_Γ of the form:

$$1 \to U(1) \xrightarrow{\iota} \frac{U(1) \times G}{\Gamma} \xrightarrow{\sigma} G_\Gamma \to 1 \quad , \tag{4.14}$$

such that V_μ is a representation of E. In the quotient defining E the subgroup $\Gamma \subset U(1) \times G$ is defined diagonally, consisting of the elements of the form $(c_\mu^*(\gamma), \gamma)$. Clearly the maps ι and σ are injective and surjective, respectively. Moreover, the representation ρ_μ of E defined as $\rho_\mu(\lambda, g) = \lambda\rho_\mu(g)$ is well defined in the sense that the subgroup Γ acts trivially on ρ_μ. Thus ρ_μ, being a projective representation of G_Γ, is a representation of the above constructed extension of G_Γ.

The different central extensions are thus given by the different maps in $\mathrm{Hom}(\Gamma, U(1))$ which in its turn is isomorphic to P/Q_Γ. Vice versa, different maps $\mathrm{Hom}(\Gamma, U(1))$ give rise to inequivalent central extensions since the central extension given in Eq. (4.14) is only trivial if $c \in \mathrm{Hom}(\Gamma, U(1))$ is the trivial map. Also, since Γ is finite, it is isomorphic to $\mathrm{Hom}(\Gamma, U(1))$. In conclusion we have that:

$$H^2(G_\Gamma, U(1)) \cong P/Q_\Gamma \cong \Gamma \quad . \tag{4.15}$$

As an example consider the Lie group $SU(3)$ with $\Gamma = \mathbb{Z}_3$ generated by $\omega\mathbb{I}_3$, where ω is a third root of unity. The group $SU(3)/\mathbb{Z}_3$ allows for three different central extensions. Its projective representations fall into three classes. In Fig. 4.2 these classes are depicted by giving the highest weight projective representation in different classes a different color.

4.2 Classification of topological order

In this section I will discuss in detail one of the main topics of the thesis: the classification of symmetry protected topological (SPT) phases in one-dimensional spin systems. I will focus on periodic systems having a ground

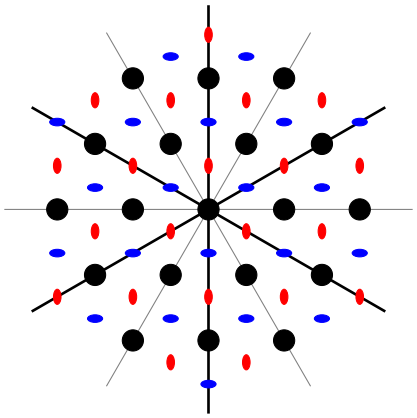


Figure 4.2: The weight lattice P of the group SU(3). The black dots represent weights which are highest weights of representations of $SU(3)/\mathbb{Z}_3$. The red/vertical and blue/horizontal ellipses represent weights which are highest weights of projective representations of $SU(3)/\mathbb{Z}_3$.

state $|\Psi\rangle$ which can be represented by an injective MPS. This implies that it is the unique ground state of some parent Hamiltonian but may allow for boundary modes if the terms in the parent Hamiltonian connecting the first and last site are omitted.

4.2.1 Action of the symmetry

As described in the introduction, no topological phases exist without restricting paths to connect different systems by symmetries. I assume that the system has a symmetry described by the group G. Thus $[H, U(g)] = 0$. Uniqueness of the ground state implies: $U(g)|\Psi\rangle = \alpha(g)|\Psi\rangle$ where $\alpha(g)$ is some one-dimensional representation of G. I consider symmetries which can be realized by a product of copies of the same unitary transformation, which all act on a different single site. Thus I consider symmetries which can be written in the form: $U(g) = \bigotimes_n u_n(g)$. Here the unitary $u_n(g)$ acts on the site $\mathcal{H}_n$, being a representation space of G and L is the length of the system.

From Eq. (3.11) it follows that if $u(g)$ commutes with the maps A defining the MPS representation of $|\Psi\rangle$ as:

$$u(g) \circ A = \alpha'(g) A \circ (V_l(g) \otimes V_r(g)) \quad , \tag{4.16}$$

with $V_l(g) = V_r(g)^{-1}$ then $|\Psi\rangle$ is invariant under $U(g)$ up to a phase $\alpha(g) = \alpha'^L(g)$. Following Ref. [51] I will now show that the reverse also holds. If two MPSs with maps A and $A' = u \circ A$ describe the same state $|\Psi\rangle$ and $|\Psi'\rangle = \alpha|\Psi\rangle$ up to a phase α an action V_l and V_r on the left and right auxiliary spaces can be defined such that Eq. (4.16) is satisfied. Moreover $V = V_l = V_r^\dagger$ is unitary and unique up to a phase.

First assume that the matrices A_i are right normalized obeying the following two equations:

$$\sum_i A_i A_i^\dagger = \mathbb{I} \quad , \quad \sum_i A_i^\dagger \Lambda A_i = \Lambda \quad . \tag{4.17}$$

where Λ is a diagonal matrix whose eigenvalues are strictly greater than zero. Uniqueness of the ground state implies that $\mathbb{I}$ is the only eigenvector of the transfer matrix $E(X) = \sum_i A_i X A_i^\dagger$ with eigenvalue 1 and that Λ is the unique solution to the second of the above two equations. Furthermore let $|i\rangle$ be eigenvectors of U with eigenvalues $e^{i\theta_i}$. The transfer matrix $E_U(X)$ as defined in Eq. (3.14) can be written as:

$$E_U(X) = \sum_j e^{i\theta_j} A_j X A_j^\dagger \quad . \tag{4.18}$$

We will first prove that the spectral radius $\rho(E_U)$ of E_U, is bounded by 1. Moreover $\rho(E_U) = 1$ if and only if there exists a unitary V such that the following equation holds:

$$e^{i\theta_j} A_j V = \alpha V A_j \quad . \tag{4.19}$$

with $|\alpha| = 1$. From this Eq. (4.16) follows with $V_l = V_r^\dagger = V$ if $\rho(E_U)$ equals to 1. This is indeed the case since the overlap $\langle \Psi | U | \Psi \rangle$, which has magnitude unity, can be written in terms of powers of $\rho(E_U)$. From this it follows that $\rho(E_U)$ has at least one non-zero fixed point.

I will now prove that the spectral radius of $\rho(E_U)$ is bounded by 1. Consider an eigenvector V of E_u with eigenvalue λ: $\lambda V = E_U V$. Multiplying with $\Lambda V^\dagger$ (Λ is determined by Eq. (4.17)), taking traces and absolute values one obtains:

$$|\lambda| \mathrm{tr}(V \Lambda V^\dagger) = |\sum_j \mathrm{tr}(e^{i\theta_j} A_j V A_j^\dagger \Lambda V^\dagger)| \quad . \tag{4.20}$$

Note that $\mathrm{tr}(V \Lambda V^\dagger)$ is a positive number since it is the Frobenius norm squared of the matrix $V \Lambda^{1/2}$. Define the vectors $X_{j,\alpha\beta} = (\Lambda^{1/2} A_j V^\dagger)_{\alpha\beta}$ and $Y_{j,\alpha\beta} = e^{i\theta_j} (\Lambda^{1/2} V^\dagger A_j)_{\alpha\beta}$. The r.h.s. of the above equation is just the norm squared of the inner product of these two vectors. From the Cauchy-Schwarz inequality it follows that

$$\begin{aligned} |\lambda| \mathrm{tr}(V \Lambda V^\dagger) \leq \|X\| \|Y\| =& \sqrt{\sum_j \mathrm{tr}(V A_j^\dagger \Lambda A_j V^\dagger)} \sqrt{\sum_j \mathrm{tr}(A_j A_j^\dagger V \Lambda V^\dagger)} \\ =& \mathrm{tr}(V \Lambda V^\dagger) \quad . \end{aligned} \tag{4.21}$$

In the second equality Eq. (4.17) has been used. This proves that the spectral radius of E_u is less or equal to one. Moreover, λ is only equal to one

if X and Y are parallel. Thus if an α exist such that $e^{i\theta_j}V^\dagger A_j = \alpha A_j V^\dagger$. Multiplying both sides with their adjoint, summing over j, taking traces and using Eq. (4.17) one can show that $|\alpha|$=1. Since Λ is invertible Eq. (4.19) follows. Using this equation to compute $E(V^\dagger V)$ one obtains that $E(V^\dagger V) = V^\dagger V$. We also assumed that $\mathbb{I}$ is the only eigenvector of the transfer matrix E with eigenvalue 1. It thus follows that V is unitary.

The phases $\alpha(g)$ defined in Eq. (4.16) form a one dimensional representation of G. Since the matrices $V_l(g)$ and $V_r(g)$ are only defined up to a phase they define projective representations of G. Their projective classes are related by $[V_r] = -[V_l]$ and I will denote $[V_r]$ by t.

In the more general case without translational invariance the actions on auxiliary spaces would be site dependent. Due to the relation $V_{(n+1,l)}(g) = V_{(n,r)}(g)^{-1}$ the projective classes of all auxiliary spaces are connected to each other. I can still define a t such that

$$t = [V_{(n,r)}] = -[V_{(n,l)}] \quad , \tag{4.22}$$

for all n.

It is this $t \in H^2(G, U(1))$ that determines the phase in which the state $|\Psi\rangle$ resides. To show this I will use the arguments described in Ref. [13] and Ref. [14].

4.2.2 Equivalence of phases

First of all I will show that two ground states $|\Psi\rangle$ and $|\Psi'\rangle$ with equal projective classes of auxiliary spaces ($t = t'$) reside in the same phase. This can be shown be finding a symmetry preserving local unitary transformation U relating the two states. As described in the introduction, with locality I mean that it is the time evolution of some local Hamiltonian. More concretely I will take a $U(\tau) = \prod_n U_n(\tau)$ such that each term $U_n(\tau)$ acts on only two sites. Most importantly $|\Psi(\tau)\rangle = U(\tau)|\Psi\rangle$ is symmetric during the transformation.

In what follows I will describe the unitary transformations $U_n(\tau)$. Let $A^{[n]}$ be the maps defining an MPS representation of $|\Psi\rangle$ and similarly, let $B^{[n]}$ define $|\Psi'\rangle$. Since it was assumed that $|\Psi\rangle$ and $|\Psi'\rangle$ are injective I can also assume that the maps $A^{[n]}$ and $B^{[n]}$ are injective. One can achieve this by possibly blocking injective regions to one site. The difference between $|\Psi\rangle$ and $|\Psi'\rangle$ is two fold. Not only are they defined by different maps, these maps are also defined to act on different auxiliary spaces, denoted by $\mathcal{H}_{(n,l/r)}$ for $|\Psi\rangle$ and by $\mathcal{H}'_{(n,l/r)}$ for $|\Psi'\rangle$. The idea is to use $U_1(\tau)$ to change the auxiliary spaces between the first and second site, use $U_2(\tau)$ to change the auxiliary space between the second and third site, and so on. Thus to use $U_n(\tau)$ to change the auxiliary spaces between the n-th and $n+1$-th site. This give rise to the following complication: after the first transformation $U_1(\tau)$ the

auxiliary spaces of the first site are $\mathcal{H}_{(1,l)}$ and $\mathcal{H}'_{(1,r)}$. To define an MPS at this stage we will need a map $T_{12}^{[1]}$ which act as:

$$T_{12}^{[1]} : \mathcal{H}_{(1,l)} \otimes \mathcal{H}'_{(1,r)} \to \mathcal{H}_1 \quad , \tag{4.23}$$

which should be injective and respect the symmetries (that is obey Eq. (4.16)). Similarly we shall need to define a $T_{21}^{[n]}$ acting as

$$T_{21}^{[n]} : \mathcal{H}'_{(n,l)} \otimes \mathcal{H}_{(n,r)} \to \mathcal{H}_n \quad , \tag{4.24}$$

which should also be injective and equivariant. These maps will be used to define $U_n(t)$ and appear in the MPS representation of intermediates states $|\Psi_n\rangle$:

$$|\Psi_n\rangle = \mathrm{Tr}(T_{12}^{[1]} B^{[2]} \dots B^{[n]} T_{21}^{[n+1]} A^{[n+2]} \dots A^{[L]}) |i_n \dots i_L\rangle \quad . \tag{4.25}$$

A few of these states have been depicted in Fig. 4.3. Note that $|\Psi_0\rangle = |\Psi\rangle$ and $|\Psi_L\rangle = |\Psi'\rangle$.

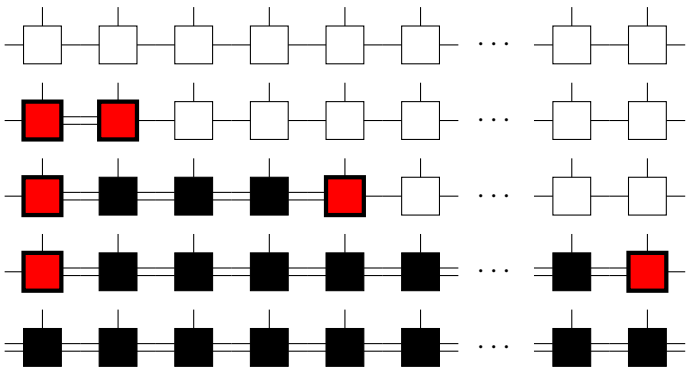


Figure 4.3: A schematic representation of the state $|\Psi_n\rangle$ for n equal to 0 , 1, 4, $L-1$ and L. The white boxes represent matrices $A^{[n]}$, the black boxes $B^{[n]}$ and the red boxes $T^{[n]}$. The single horizontal lines represent completely entangled pairs between $\mathcal{H}_{(n,r)}$ and $\mathcal{H}_{(n+1,l)}$ whereas the double horizontal lines represent completely entangled pairs between $\mathcal{H}'_{(n,r)}$ and $\mathcal{H}'_{(n+1,l)}$.

In more detail the maps $U_n(t)$ satisfy:

$$U_n(\tau) = \begin{cases} \mathbb{I} \quad \text{for} \quad \tau < n-1 \\ U_n(n) := U_n \quad \text{for} \quad \tau > n \end{cases} \quad , \tag{4.26}$$

such that they act in increasing order. Or in other words we have the equations $|\Psi_n\rangle = \prod_n U_n |\Psi\rangle = U_n |\Psi_{n-1}\rangle$. The unitary $U_n(t)$ will thus interpolate between $|\Psi_{n-1}\rangle$ and $|\Psi_n\rangle$. During this interpolation only the matrices of the sites $n+1$ and $n+2$ will change. The auxiliary space between these two

sites will be enlarged to $\mathcal{H}_{(n+1,r)} \oplus \mathcal{H}'_{(n+1,r)}$. Let the matrices on these sites depend on $\gamma = t - n - 1$ as:

$$(1-\gamma)T_{21}^{[n+1]} + \gamma B^{[n+1]} \quad , \tag{4.27}$$

$$(1-\gamma)A^{[n+2]} + \gamma T_{21}^{[n+2]} \quad . \tag{4.28}$$

Since both the maps T_{21}, A and B are assumed to be injective, the above linear combinations are also injective except for $\gamma = 0$ or 1. However this is only due to the too large auxiliary space which should be reduced again to $\mathcal{H}_{(n+1,r)}$ or $\mathcal{H}'_{(n+1,r)}$. Injectivity ensures that the gap does not close during the transformation.

For the above argument it is crucial that the maps $T_{12}^{[n]}$ and $T_{21}^{[n]}$ can be defined. This is not always the case. Consider for example an $SU(3)$ invariant spin chain with $\mathcal{H}_n = 1 \oplus 8 \oplus 27$ (irreps of $SU(3)$ are labeled by their dimensions). Let $|\Psi\rangle$ have auxiliary space $\mathcal{H}_{(n,l)} = 3$ and $\mathcal{H}_{(n,r)} = \bar{3}$ and be defined by the $SU(3)$ invariant projection $3 \otimes \bar{3} \to 1 \oplus 8$. Similarly let $|\Psi'\rangle$ have auxiliary space $\mathcal{H}'_{(n,l)} = \bar{6}$ and $\mathcal{H}'_{(n,r)} = 6$ and be defined by the $SU(3)$ invariant projection $\bar{6} \otimes 6 \to 1 \oplus 8 \oplus 27$. A $SU(3)$ invariant injective projection $T_{12} : \mathcal{H}_{(n,l)} \otimes \mathcal{H}'_{(n,r)} \to \mathcal{H}_n$ does not exist since $10 \subset 3 \otimes 6$ and $10 \not\subset \mathcal{H}_n$. This problem can however be cured by again blocking two sites into one since $10 \subset \mathcal{H}_n \otimes \mathcal{H}_n$.

I do not prove that $T_{12}^{[n]}$ and $T_{21}^{[n]}$ can be defined. However, if we are dealing with two states with different auxiliary spaces belonging to different projective classes ($t \neq t'$) then these maps can certainly not be defined. Since in that case $[\mathcal{H}_{(n,l)}] + [\mathcal{H}'_{(n,r)}] \neq 0$ whereas we have trivially that $[\mathcal{H}_n] = 0$. In the following we will argue that indeed two such states reside in different SPT phases.

4.2.3 Inequivalence of phases

In what follows I will give an idea of a proof that if two states are related by a local unitary transformation $|\Psi'\rangle = U|\Psi\rangle$ where $U = e^{iH}$ is a finite time evolution ($\Delta\tau = 1$) of some local Hamiltonian H, then the projective classes of the auxiliary spaces of $|\Psi\rangle$ and $|\Psi'\rangle$ are the same ($t = t'$). I will assume that H is a nearest neighbor Hamiltonian, a property that can be achieved after blocking sufficiently many sites. The idea is that the time evolution $U(\tau) = e^{i\tau H}$ can be approximated by a product of unitary operators acting on two sites only. This statement has been proven in the quantum information community in order to show that one-dimensional quantum systems can be simulated by a quantum circuit [52]. Thus we have that

$$U(\tau)|_{\tau=1} = e^{iH} = \prod_i U_i^{[n_i]} \quad , \tag{4.29}$$

where $U_i^{[n_i]}$ acts only on the sites n_i and n_i+1. Since the unitaries $U_i^{[n_i]}$ are all local, they can not change the projective class of all auxiliary spaces, see Fig. 4.4. Changing the projective class of all auxiliary spaces would require a unitary transformation acting on all sites.

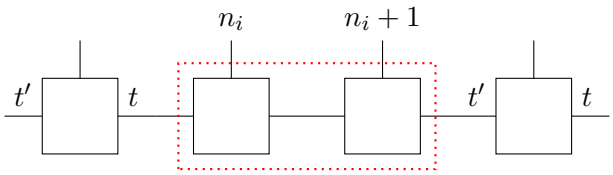


Figure 4.4: A schematic picture of a part of an MPS. The red dotted rectangle depicts the two sites on which $U_i^{[n_i]}$ acts. The projective class of the corresponding auxiliary spaces is fixed by the auxiliary spaces of the two neighboring sites and are thus unaltered.

To get a better understanding of Eq. (4.29), denote $H = H_1 + H_2$ where H_1 consists of terms acting on sites $2i$ and $2i+1$ and H_2 consist of terms acting on sites $2i-1$ and $2i$. One can approximate the time evolution $U(\tau)|_{\tau=1}$ with

$$e^{i(H_1+H_2)} \approx \left(e^{iH_1/m}e^{iH_2/m}\right)^m \quad , \tag{4.30}$$

in which the error scales inversely proportional to m (and quadratic in $\|H_1\|$ and $\|H_2\|$) [52]. Since the two-body terms in the Hamiltonian H_1 commute with each other it can be written as a product of unitaries acting on two sites only, and similarly for H_2. Thus Eq. (4.29) could have been written as:

$$e^{iH} = \prod_{i=1}^{2m} U_i^{\text{disj}} \quad , \tag{4.31}$$

where U_i^{disj} is a a product of unitaries acting on disjoint regions. The above argument stating that the transformation $U_i^{[n_i]}$ does not change the projective class of auxiliary spaces, can also be applied to U_i^{disj}. In this case the auxiliary spaces connecting the disjoint regions are still left unaltered. This argument should be applied $2m$ times. This should be put in comparison with the case in which H is non-local. Since in principle any Hamiltonian can be simulated by a quantum circuit. Thus for any Hamiltonian, Eq. (4.29) holds and it seems that locality is a superfluous assumption. However, the number of unitaries needed to simulate an arbitrary Hamiltonian generally scales exponentially with the system size whereas the number of unitaries needed to simulate a local Hamiltonian only depends on the desired accuracy, as explained by Eq. (4.30). Thus for non-local Hamiltonians the decomposition into local unitaries is ill defined in the thermodynamic limit, which is not the case for local Hamiltonians.

4.3 Time reversal and inversion symmetry

Both time reversal and inversion symmetry are exceptions to the symmetries I discuss in Sect. 4.2.1. Time reversal is anti-unitary and inversion symmetry is not of the form $U(g) = u(g)^{\otimes L}$ since it maps site i to $L - i$. I discuss in the following that this will give further restrictions on the maps V acting on auxiliary space.

Time reversal T can be modeled by a unitary transformation u_T combined with a complex conjugation K ($T = u_T K$). Eq. (4.16) will thus be modified to

$$u_T \circ \bar{A} = \alpha A \circ (V \otimes V^\dagger) \quad , \tag{4.32}$$

where V is again some unitary matrix acting on auxiliary space and α is some complex phase. Applying time reversal twice one obtains $T^2 A = A(V\bar{V}) \otimes (\bar{V}V)^\dagger$. Using Eq. (4.17) it follows that the matrix $\bar{V}V$ is a fixed point of the transfer matrix and thus by assumption a multiple of the identity. Together with the fact that V is unitary it follows that $\bar{V}V = e^{i\phi_T}\mathbb{I}$ with $\phi_T = 0$ or π. Just like the parameter t the phase ϕ_T can not jump unless the system goes through a phase transition [16]. Imposing invariance under time reversal thus gives rise to additional quantum phases. In more recent work time reversal is combined with on-site symmetries already on the group level ($T \in G$) [53]. In this case the definition of second group cohomology $H^2(G, U(1)_T)$ or that of projective representations is slightly altered to incorporate anti-unitary symmetries. Instead of considering the maps U and ρ_p to $GL(V)$ and $PGL(V)$ as discussed in Sect. 4.1.2 one should consider the map U to $U_{UA} = U(V) \cup U_A(V)$ and the map ρ_p to $PU_{UA} = U_{UA}/\mathbb{C}^*$ where $U_A(V)$ is the set of all anti-unitary operators acting on V [54]. The result is that all quantum phases, including those protected by time reversal, are classified by $H^2(G, U(1)_T)$.

Inversion symmetry has a very similar effect as time reversal. When translation symmetry is also imposed (and if one works with a translationally invariant MPS) inversion is just the transposition of the matrices A_i. Thus

$$A^T = \alpha A \circ (V \otimes V^\dagger) \quad . \tag{4.33}$$

Just as above, applying inversion twice one can show that $V\bar{V} = e^{i\phi_I}\mathbb{I}$. And thus it again follows that ϕ_I is either 0 or π. Just like ϕ_T it is argued in [16] that ϕ_I can only jump at a phase transition. Thus imposing inversion leads to a separation of a trivial phase from a non-trivial phase.

From the discussion above, it seems as if imposing either time reversal or inversion symmetry leads to a doubling of phases already present when these symmetries are not imposed due to the extra invariant ϕ_T or ϕ_I. However, not all SPT phases allow for time reversal or inversion symmetric states. Focus on inversion symmetry. A ground state residing in an SPT phase

characterized by the invariant t has right auxiliary spaces being projective representations in class t and left auxiliary spaces being in class $-t$. Inversion symmetry gives rise to the restriction that $t = -t$. Non-trivial solutions exist for example if $H^2(G, U(1)) = \mathbb{Z}_{2N}$, thus for example if $G = SU(2N)$. In that case states in the phase $t = N$ have a chance of being inversion symmetric.

For time reversal symmetry the same restriction for t holds. From Eq. (4.16) it follows that the the matrices $\bar{A}$ obey

$$\bar{u}(g) \circ \bar{A} = \bar{\alpha}'(g)\bar{A} \circ (\bar{V}_l(g) \otimes \bar{V}_r(g)) \quad , \tag{4.34}$$

Projectiveness of $\bar{V}_r$ gives rise to phases $\omega^{-1}(g, g')$ where ω is the factor system of the projective representation V_r. And from Eq. (4.9) it follows that $t = [\omega^{-1}] = -[\omega]$. To be time reversal symmetric t should obey $t = -t$.

Chapter 5

Measuring Order

In the previous chapter symmetry protected topological (SPT) order was discussed. A key point is that the ground state is invariant under the same symmetries as its Hamiltonian. This is in great contrast to spontaneous symmetry breaking (SSB) phases. Such phases have degenerate ground states which are not invariant under all symmetry transformation. Let $|\Phi\rangle$ be one of such ground states. Symmetry breaking of the ground state is made apparent by a non-zero expectation value of an order parameter X which changes under symmetry transformations. Thus if G were the group of symmetries and $U \in G$ is a symmetry transformation we have that:

$$\langle \Phi | X | \Phi \rangle = \langle X \rangle \neq \langle U^\dagger X U \rangle \quad . \tag{5.1}$$

From this property of X it follows directly that $[X, U] \neq 0$ and moreover that $|\Phi\rangle \neq U|\Phi\rangle$. One might wonder whether the state $\sum_{U \in G} U|\Psi\rangle$ is an invariant ground state (assuming G to be discrete). It is clearly invariant but not a macroscopic ground state since it is not stable under symmetry breaking fluctuations. It is crucial for this argument to hold that the system is infinite. A more formal treatment on spontaneous symmetry breaking can be found for example in [55]. Physically, ground states can be obtained by cooling the system in the presence of a small symmetry breaking exterior field, for example a magnetic field. In this manner a state $|\Phi\rangle$ is obtained which is not only the ground state of the Hamiltonian H but also of $H + \delta \sum_i X_i$, where X_i is the operator X acting on the i-th site and δ is the strength of the magnetic field.

Let G be the group of on-site symmetries of the Hamiltonian of a spin chain. These symmetries are all realized as unitary global transformations. Time reversal and inversion symmetry will not be considered in this Chapter. The SSB and SPT phases of the spin chain are classified by a subgroup $H \subset G$, describing the unbroken symmetries and a topological invariant $t \in H^2(H, U(1))$ describing the projective class of the boundary modes. By analyzing the behavior of suitable order parameters X the subgroup H can

be deciphered. Order parameters are used to detect symmetry breaking. In Ref. [27] a method is introduced to detect the invariant t by means of a suitable *string* order parameter in the case that G is a finite Abelian group.

It is understood that the Haldane phase occurring in $SO(3)$ invariant spin-1 chains can be explained by hidden symmetry breaking [25]. A non-local unitary (NL-UT) transformation is introduced which preserves the subgroup $\mathbb{Z}_2 \times \mathbb{Z}_2 \subset SO(3)$ of symmetries and the locality of $SO(3)$ invariant Hamiltonians. It is exactly this subgroup of symmetries which also protects the topological nature of the Haldane phase [56]. The NL-UT maps systems residing in the Haldane phase into systems which break the $\mathbb{Z}_2 \times \mathbb{Z}_2$. Essentially, the string order parameter measuring the Haldane phase [23] is mapped to a Landau order parameter measuring symmetry breaking. The four fold degeneracy of the AKLT Hamiltonian on an open chain is mapped to four states which all break the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. The Haldane phase is thus understood as a phase in which the $\mathbb{Z}_2 \times \mathbb{Z}_2$ is broken in a hidden manner. In Ref. [DQ3] we generalize these ideas to systems with $\mathbb{Z}_N \times \mathbb{Z}_N$.

In this Chapter, I will review the concept of string order parameters and discuss how the selection rule of Ref. [27] can be used to decipher t from the expectation values of suitably chosen string order parameters. In Ref. [DQ2] we have introduced a different string order parameter which is capable of determining the SPT phase of a system with $SU(N)$ symmetry. The behavior of this $SU(N)$ string order parameter can be derived from the selection rule which I present in Sect. 5.1.1. In Sect. 5.2 I will review the ideas of Ref. [DQ3] leading to our NL-UT and discuss that SPT phases can be explained by hidden symmetry breaking.

5.1 String order parameters

Consider the case where G is the finite Abelian group $\mathbb{Z}_N \times \mathbb{Z}_N$.[3] Let R and $\tilde{R}$ be generators of this group and let X and $\tilde{X}$ be order parameters which obey:

$$[X, R] = 0 \ , \qquad \tilde{R} X \tilde{R}^\dagger = \omega X \ , \tag{5.2}$$

$$[\tilde{X}, \tilde{R}] = 0 \ , \qquad R \tilde{X} R^\dagger = \omega^{-1} \tilde{X} \ , \tag{5.3}$$

where $\omega = \exp(\frac{2\pi i}{N})$. Since the order parameter X does not commute with $\tilde{R}$, it can be used to measure breaking of the symmetry generated by $\tilde{R}$. In the introduction it was mentioned that $\langle \Phi | X | \Phi \rangle \neq 0$ implies $|\Phi\rangle \neq \tilde{R}|\Psi\rangle$ if X and $\tilde{R}$ do not commute. Reversing the argument, in symmetric SPT phases the ground state is invariant under $\tilde{R}$ and thus the expectation value of the order

[3] In Ref. [DQ3] it is motivated that this is a very useful group to study since it can be defined to be a sub group of any (with one exception) compact connected group $G_\Gamma = G/\Gamma$ such that the SPT phases protected by G_Γ are also protected by the subgroup $\mathbb{Z}_N \times \mathbb{Z}_N$.

parameter X is necessarily zero: $\langle\Phi|X|\Phi\rangle = 0$. The idea of a string order parameter is that the string gives rise to an extra phase, compensating the ω appearing in Eq. (5.2), such that the string order parameter commutes with the symmetry. If the string order parameter commutes with the symmetry it can take on a non-zero expectation value and it can be used as a detection tool.

In general a string order parameter is of the form:

$$X_i \left(\prod_{k=i+1}^{j-1} U_k \right) Y_j \quad , \tag{5.4}$$

thus acting on sites i and j with some order parameter while transforming the spin chain between these two sites with the symmetry transformation U. The sites on which U act form a string between sites i and j, hence the name *string* order parameter. For the symmetry group at hand I will consider string order parameters of the following form

$$S_{ij}(a,b) = X_i^a \left(\prod_{k=i}^{j-1} R_k^b \right) (X_j^\dagger)^a \quad , \tag{5.5}$$

$$\tilde{S}_{ij}(a,b) = \tilde{X}_i^a \left(\prod_{k=i}^{j-1} \tilde{R}_k^b \right) (\tilde{X}_j^\dagger)^a \quad , \tag{5.6}$$

where X_i^a is the a-th power of the operator X acting on the i-th site. Similarly for $\tilde{X}$, R and $\tilde{R}$.

As was discussed in the previous Chapter, the group $\mathbb{Z}_N \times \mathbb{Z}_N$ has N classes of projective representations. Let P and $\tilde{P}$ be the action of the symmetry transformation on the right auxiliary spaces. The topological phase t is determined by the manner in which P and $\tilde{P}$ "commute" with each other. That is:

$$P\tilde{P} = \omega^t \tilde{P} P \quad . \tag{5.7}$$

It is exactly this phase that compensates the phase in Eq. (5.2). That is, following Ref. [27], I will now show that in the limit of large $|j-i|$ the string order $\langle S_{ij}(a,b)\rangle$ can only be non zero if $a + bt = 0$ modulo N. A non-zero string order parameter gives information about the type of topological phases in a very similar way that non-zero order parameters give information about symmetry breaking phases.

The first step in proving that a non-zero $S_{ij}(a,b)$ implies $a + bt = 0$ modulo N is similar to finding the t dependence of the string order parameter introduced in Ref. [DQ2]. It makes use of the MPS structure of the ground state. Instead of acting with R on all physical sites between sites i and j one could act with P on all auxiliary sites. However, almost all actions of P

cancel each other except for the one acting on left auxiliary space of the i-th site and the right auxiliary space of the $(j-1)$-th site. This step is clarified in Fig. 5.1. Thus we are left with:

$$\lim_{|j-i|\to\infty} \langle S_{ij}(a,b)\rangle = \mathrm{tr}\left(A^\dagger X_i^a A(P^{b\dagger}\otimes\mathbb{I})\right)\cdot \mathrm{tr}\left(A^\dagger (X_j^a)^\dagger A(P^b\otimes\mathbb{I})\right) \quad , \tag{5.8}$$

where A are maps defining the MPS. For notational simplicity I have assumed A to be site independent ($A^{[i]} = A^{[j]} = A$).

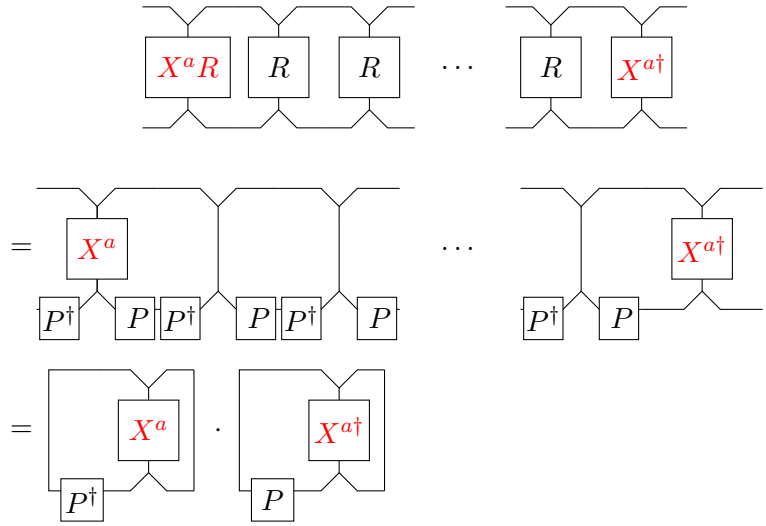


Figure 5.1: A diagrammatic derivation of Eq. (5.8). To simplify notations b has been set to 1.

A non-zero string order parameter implies a non-zero trace over the expression $A^\dagger X_i^a A(P^{b\dagger}\otimes\mathbb{I})$. Since the ground state is assumed to be symmetric under a global transformation $\tilde{R}$ it follows that the matrices A in Eq. (5.8) are equivariant, that is $A = \tilde{R}A(\tilde{P}^\dagger\otimes\tilde{P})$. Using Eqs. (5.2) and (5.7) it follows that:

$$\begin{aligned}\mathrm{tr}\left(A^\dagger X^a A(P^{b\dagger}\otimes\mathbb{I})\right) =& \omega^a \mathrm{tr}\left(A^\dagger \tilde{R}^\dagger X^a \tilde{R} A(P^{b\dagger}\otimes\mathbb{I})\right)\\ =& \omega^a \mathrm{tr}\left(A^\dagger X^a A(\tilde{P}P^{b\dagger}\tilde{P}^\dagger\otimes\tilde{P}^\dagger\tilde{P})\right)\\ =& \omega^{a+bt}\mathrm{tr}\left(A^\dagger X^a A(P^{b\dagger}\otimes\mathbb{I})\right) \quad .\end{aligned} \tag{5.9}$$

Thus indeed only if $a + bt = 0 \bmod N$ can the above trace and thus the string order parameter be non-zero. A non-zero string order parameter gives a selection rule of the possible SPT phases at hand [27]. Measuring different string order parameters for various values of a and b one could exactly determine the invariant t.

It should be emphasized that our notation treats string order parameters and Landau order parameters on the same footing. Indeed $S(a,b)$ is just a Landau order parameter when $b=0$. The string order parameter detects SPT phases analogous to Landau order parameters detecting SSB phases.

5.1.1 An *SU(N)* string order parameter

In Ref. [DQ2] we proposed a slightly different string order parameter suitable for detecting SPT phases of $SU(N)$ spin chains. I will first introduce this string order parameter after which I will show that its behavior (detecting SPT phases of $SU(N)$ spin chains) can be derived using the selection rule explained in the previous section.

Let $H^a = E^{aa} - E^{a+1,a+1}$ be $N-1$ generators of the Cartan subalgebra $\mathfrak{h}$ of $su(N)$. Here E^{ab} is a N by N matrix satisfying $(E^{ab})_{cd} = \delta_{ac}\delta_{bd}$. Since the operators H^a mutually commute, they can be diagonalized simultaneously. Every representation decomposes into eigenspaces of H^a or in other words, has a weight decomposition: $V = \oplus_\mu V_\mu$ such that:

$$Hv = \mu(H)v \ , \quad \forall\ v \in V_\mu \quad , \tag{5.10}$$

where $\mu \in \mathfrak{h}^*$ contains information about the eigenvalues of all $H \in \mathfrak{h}$. The weights of the adjoint representation $\mathrm{Ad}_X = [X,\cdot]$ are called roots and are denoted by α, that is $[H,X] = \alpha(H)X$ if $X \in V_\alpha$. Let α_a be the roots corresponding to the operators H^a: $H^a \in [V_{\alpha_a}, V_{-\alpha_a}]$. The operators H^a are chosen such that the roots α_a are a set of simple positive roots [57]. Let H^ρ be the element in the Cartan subalgebra defined uniquely by $\alpha_a(H^\rho) = 1$. It is dual to the Weyl vector ρ being half the sum of all positive roots (the positive roots are those roots which can be obtained by summing simple positive roots with non-negative coefficients). With the above definition for matrices H^a, H^ρ becomes a diagonal matrix with entries:

$$H^\rho_{ii} = \frac{N+1}{2} - i \quad . \tag{5.11}$$

The string order parameter discussed in Ref. [DQ2] is defined as[4]

$$S^{ab}_{ij} = H^a_i \prod_{k=i}^{j-1} \exp\left(\frac{2\pi i}{N} H^\rho_k\right) H^b_j \quad , \tag{5.12}$$

where H^ρ_k is the operator H^ρ acting on the k-th site. The operators H^a_j and H^b_j equal to H^a and H^b acting on the i-th and j-th site, respectively. In

[4] Actually, the $SU(N)$ string order parameter as defined in Ref. [DQ2] has a string running from $(i+1)$ instead of i. However, this does not alter its behavior. The string order parameter measures the projective class of the right auxiliary space of the i-th site: $t = [\mathcal{H}_{(i,r)}]$. It does so in Ref. [DQ2] by relating it to $-t = [\mathcal{H}_{(i+1,l)}]$. In the same way, one can relate it to $-t = [\mathcal{H}_{(i,l)}]$.

this article we proved that this string order parameter has a characteristic t dependence:

$$\lim_{|j-i|\to\infty} \langle S_{ij}^{ab} \rangle = C_{ij} \omega^{t(a-b)} \quad . \tag{5.13}$$

Again the number t defines the topological phase of the spin chain and can be obtained from the equation [DQ1]:

$$t = \sum_n n u_n \quad , \tag{5.14}$$

where u_n are the coefficients of the weight $\mu = \sum_n u_n \mu_n$ with respect to the basis $\{\mu_n\}$ of the weight lattice, which is dual to the basis $\{H^a\}$ of the Cartan subalgebra ($\mu_i(H^a) = \delta_{ia}$). The weight μ is the highest weight of the right most auxiliary space.

I will now show that the behavior of our string order parameter given by Eq. (5.13) can be derived from the selection rule discussed in Ref. [27]. Let $R = \exp\left(\frac{2\pi i}{N} H^\rho\right)$ and let $\tilde{R}$ be proportional to the matrix $E^{N,1} + \sum_a E^{a,a+1}$. Clearly these two matrices now obey $R\tilde{R} = \omega \tilde{R} R$. More generally, as discussed in Ref. [DQ3], how R and $\tilde{R}$ "commute" with each other depends on the projective class t of the representation ρ they act on:

$$\rho(R)\rho(\tilde{R}) = \omega^t \rho(\tilde{R})\rho(R) \quad \text{iff} \quad [\rho] = t \quad . \tag{5.15}$$

Note that the matrix representation of R and $\tilde{R}$ defined above is just the fundamental representation with $t = 1$. In order to use the selection rule we need to derive the transformation properties of the Cartan operators H^a under conjugation by $\tilde{R}$. Define the order parameter X which in the fundamental representation of $SU(N)$ are diagonal matrices with elements $X_{ii} = \omega^i$. This is a traceless matrix obeying Eq. (5.2). The matrices H^a can be written as a linear combination of powers of X:

$$H^a = \frac{1}{N} \sum_{b=1}^{N-1} \omega^{-ab} (1 - \omega^b) X^b \quad . \tag{5.16}$$

Now all the work is done. The last step consists of using this expression for H^a to rewrite our string order parameter given by Eq. (5.12) and using the selection rule to simplify the result:

$$\begin{aligned} \langle S_{ij}^{ab} \rangle &= \frac{1}{N^2} \sum_{cd} \omega^{-ac}(1-\omega^c)\omega^{-bd}(1-\omega^d) \langle X_i^c \prod R_k X_j^d \rangle \\ &\propto \omega^{at}\omega^{-bt}(1-\omega^{-t})(1-\omega^t) \quad , \end{aligned} \tag{5.17}$$

where I have used the selection rule Ref. [27] to conclude that $c = -t$ and $d = t$. This is exactly the t dependence which we derived in Ref. [DQ2] using different means. Note also that the $SU(N)$ string order parameter is zero if $t = 0$.

5.1.2 Accidental zero points

Not only is the $SU(N)$ string order parameter zero if the system is in the topological trivial phase, it can also be accidentally zero at specific isolated points in non-trivial phases. This idea was worked out after discussions with Norbert Schuch.

Let V_μ be the irreducible representation of $SU(2)$ with highest weight μ. I use the convention in which the dimension of V_μ equals $\mu + 1$, μ is twice the spin value of V_μ. Consider a spin chain with on-site Hilbert spaces $\mathcal{H}$ and left and right auxiliary spaces $\mathcal{H}_l$ and $\mathcal{H}_r$ as:

$$\mathcal{H}_l = \mathcal{H}_r = V_1 \oplus V_3 \quad , \tag{5.18}$$

$$\mathcal{H} = \mathcal{H}_l \otimes \mathcal{H}_r \quad . \tag{5.19}$$

Let the maps $A : \mathcal{H}_l \otimes \mathcal{H}_r \to \mathcal{H}$ defining the state be given by

$$A = \mathbb{I} \otimes (\lambda_1 P_1 + \lambda_3 P_3) \quad , \tag{5.20}$$

where P_i are projectors on the space $V_i \subset V_1 \oplus V_3$ for $i \in \{1, 3\}$. Again, for large $|j - i|$ the $SU(N)$ string order parameter $\langle S^{zz}_{ij} \rangle$ factorizes into $\langle J^z_{i,L} \rangle \langle J^z_{i,R} \rangle$. The left factors equals:

$$J^z_{i,L} = \mathrm{tr}(A^\dagger S^z_i A(\mathbb{I} \otimes U^z)) \quad , \tag{5.21}$$

with $U^z = \exp(-\pi i S^z)$. Using $S^z = S^z \otimes \mathbb{I} + \mathbb{I} \otimes S^z$ this simplifies to:

$$J^z_{i,L} = \mathrm{tr}(S^z)\mathrm{tr}(A^\dagger A U^z) + \mathrm{tr}(\mathbb{I})\mathrm{tr}(A^\dagger S^z A U^z) \quad . \tag{5.22}$$

The first term is zero since $\mathrm{tr}(S^z)$ is zero. The second term can be written as the sum of two traces over the different spaces V_1 and V_3. Also note that $\mathrm{tr}(\mathbb{I}) = 6$. Thus we obtain:

$$J^z_{i,L} = 6\left(|\lambda_1|^2 \mathrm{tr}_{V_1}(S^z U^z) + |\lambda_3|^2 \mathrm{tr}_{V_3}(S^z U^z)\right) \tag{5.23}$$

$$= 6\left(i|\lambda_1|^2 - 2i|\lambda_3|^2\right) \quad . \tag{5.24}$$

Thus choosing $\lambda_1 = \sqrt{2}\lambda_3$, the $SU(N)$ string order parameter will be zero (although the spin chain is in a topologically non-trivial phase).

Note that this feature only occurs at very specific point in phases space. Perturbing away from the point $\lambda_1 = \sqrt{2}\lambda_3$ automatically gives a non-zero string order parameter. It is for this reason that we still believe that string order parameters are suitable tools to detect SPT phases.

5.2 Non-local Unitary transformations

In Ref. [DQ3] a non-local unitary transformation (NL-UT) is discussed which maps between different models: the transformation does not commute with

the Hamiltonian. It is not only a map between models, it is also a map between phases: the SSB/SPT phase of the transformed system is uniquely determined by the SSB/SPT phase of the original system. In this section I will introduce this NL-UT transformation and outline how it is shown that phases are mapped to each other. Essentially what we show is that the NL-UT maps Landau order parameters into string order parameters and vice versa. Another way to understand the NL-UT is that it maps topologically protected edge modes to symmetry breaking bulk modes. This idea will be worked out in Sect. 5.2.1.

I will again restrict the discussion in this section to the finite Abelian group $\mathbb{Z}_N \times \mathbb{Z}_N$. Moreover I will discuss SSB phases, which are possibly also non-trivial as SPT phases, such that the symmetry is broken to the form $\mathbb{Z}_r \times \mathbb{Z}_r \subset \mathbb{Z}_N \times \mathbb{Z}_N$. These SSB phases split into r different topological phases which I specify by a number t running from 0 to $r-1$. Let O and $\tilde{O}$ be operators satisfying $R = \omega^O$ and $\tilde{R} = \omega^{\tilde{O}}$, where as in the previous section R and $\tilde{R}$ are the generators of $\mathbb{Z}_N \times \mathbb{Z}_N$. Note that R and $\tilde{R}$ are simultaneously diagonalizable and have eigenvalues being some integer power of ω. Thus O and $\tilde{O}$ have integer eigenvalues defined up to a multiple of N. The NL-UT discussed in Ref. [DQ3] is:

$$U_N = \prod_{i<j} \omega^{O_i \tilde{O}_j} \quad . \tag{5.25}$$

It is invariant under a change of an eigenvalue of either O or $\tilde{O}$ by a multiple of N. The NL-UT can be understood as: "Rotate on site i depending on a measurement on site j". This can be emphasized by the following notation

$$U_N = \prod_{i<j} (R_i)^n \tilde{\Pi}_j^n \quad , \tag{5.26}$$

where $\tilde{\Pi}_j^n$ is a projector projecting on the eigenspace of the operator $\tilde{R}_j$ acting on the j-the site corresponding to the eigenvalue ω^n.

It is discussed that this NL-UT is a mapping between SSB/SPT phases. The reasoning is as follows: a SSB/SPT phase is labeled by the two integers r and t. The integer r labels symmetry breaking of the form $\mathbb{Z}_r \times \mathbb{Z}_r \subset \mathbb{Z}_N \times \mathbb{Z}_N$ and the integer t labels the projective class of the representation of the right auxiliary spaces. In a certain phase, "topology" leads to possible non-zero string order parameters, denoted by $S(a,b)$ whereas symmetry breaking can lead to non-zero order parameters. Non zero order parameters are directly related to non-zero string order parameter of the form $S(a,0)$. The main step in Ref. [DQ3] is to show that

$$U_N^\dagger S(a,b) U_N = S(a, a+b) \quad . \tag{5.27}$$

Thus a non-zero string order parameter $S(a,b)$ in a certain system described by a Hamiltonian H is related to a non-zero string order parameter of the

form $S(a, a+b)$ in a transformed system $H' = U_N^\dagger H U_N$. From this slightly modified string order parameter conditions can be derived for the parameters r' and t' describing the phase of the transformed Hamiltonian. It should be noted that U_N preserves the $\mathbb{Z}_N \times \mathbb{Z}_N$ symmetry and locality of the Hamiltonian (if H is a nearest neighbor Hamiltonian then so is H'). In summary we have the two steps:

$$\text{Step 1 :} \qquad (r,t) \longrightarrow \langle S(a,b)\rangle \quad , \tag{5.28}$$

$$\text{Step 2 :} \qquad \langle S(a,a+b)\rangle' \longrightarrow (r',t') \quad . \tag{5.29}$$

There are some subtleties with the above derivation. Although non-zero string order parameters can give information on r' and t' (Step 2), information on r and t do not always imply non-zero string order parameters (Step 1). String order parameters can be accidentally zero at certain points in the phase diagram (as discussed in the previous section). However, since we are dealing with a mapping of phases, as long as there is a point in phase space such that all allowed string order parameters are indeed non-zero, the above reasoning can be used to derive which phases are mapped to each other.

In the second step [Eq. (5.29)], the prime in $\langle S(a,a+b)\rangle'$ indicates that the expectation value is taken with respect to a ground state of H'. And this brings me to the second subtlety. The ground states $|\Psi_i\rangle$ of H are mapped to $|\Phi_i\rangle = U_N^\dagger |\Psi_i\rangle$. The states $|\Psi_i\rangle$ and $|\Phi_i\rangle$ necessarily have the same symmetry breaking properties. However H and H' describe different symmetry broken phases if $r \neq r'$. In this case the states $|\Phi_i\rangle$ can not be macroscopic ground states of H'. Thus the intermediate step of $\langle S(a,b)\rangle \neq 0 \Rightarrow \langle S(a,a+b)\rangle' \neq 0$ is on loose grounds.

One could also discuss this problem as follows. As discussed in the introduction of this Chapter, I consider ground states of H as also being ground states of the perturbed Hamiltonian $H + \delta \sum_i X_i^a$, where X^a is a suitable order parameter coupled to a magnetic field with strength δ. Or, in other words, I use explicit symmetry breaking to ensure that I consider only ground states which break the symmetry. When sending δ to zero, these explicitly symmetry breaking ground states become SSB ground states. The order parameter X^a only needs to commute with $\tilde{R}^q$ where $q = N/r$ to ensure that the symmetries $\mathbb{Z}_r \subset \mathbb{Z}_N$ generated by $\tilde{R}^q$ are preserved. Thus a can be chosen to be a multiple of r. Similar arguments can be used to show that a perturbation $\delta \sum_i \tilde{X}_i^a$ should be added to the Hamiltonian to ensure that its ground state spontaneously breaks the symmetry generated by R and is only invariant under the subgroup $\mathbb{Z}_r \subset \mathbb{Z}_N$ generated by R^q with again $q = N/r$. Since U_N commutes with the symmetries $\mathbb{Z}_N \times \mathbb{Z}_N$, the transformed perturbation $U_N^\dagger \sum_i X_i^a U_N$ has the same symmetry properties as the original perturbation $\sum_i X_i^a$. Thus the ground states of H' can not be obtained by using the transformed perturbation and thus can not be

obtained by simply transforming the ground states of H by the NL-UT U_N.

The macroscopic ground states of H' are thus not given by $|\Phi_i\rangle = U_N^\dagger|\Psi_i\rangle$ but rather by a linear combination of these states: $|\Psi_i'\rangle = T_{ij}|\Phi_j\rangle$. In the following I will show that the expectation value of $S(a,b)$ is independent of the ground state, that is

$$\langle\Psi_i|S(a,b)|\Psi_i\rangle = \langle\Psi_j|S(a,b)|\Psi_j\rangle \quad . \tag{5.30}$$

From this statement it follows that the expectation value of the string order parameter can be written as $\langle S(a,b)\rangle = n_g^{-1}\sum_i\langle\Psi_i|S(a,b)|\Psi_i\rangle$ or in other words be related to the trace

$$\langle S(a,b)\rangle = \frac{1}{n_g}\mathrm{Tr}_{GS}S(a,b) \quad , \tag{5.31}$$

where the trace is take over the ground state sector and n_g is the ground state degeneracy. Since the trace is invariant under a basis transformation this cures the problem that macroscopic ground states $|\Psi_i'\rangle$ of the transformed system are linear combinations of the transformed ground states $|\Phi_j\rangle$ of the original system. Thus concluding that $\langle S(a,a+b)\rangle' = 0$ on the basis that $\langle S(a,b)\rangle = 0$ is valid.

The origin of ground state degeneracy is two-fold: symmetry and boundary modes. Let $|\Psi_{\alpha\beta nm}\rangle$ be a complete set of orthogonal ground states. The quantum numbers α and β specify the left and right boundary modes. The quantum numbers m,n specify the different symmetry breaking grounds states. That is:

$$R|\Psi_{\alpha,\beta,n,m}\rangle = |\Psi_{\alpha,\beta,n+1,m}\rangle \quad \text{and} \quad \tilde{R}|\Psi_{\alpha,\beta,n,m}\rangle = |\Psi_{\alpha,\beta,n,m+1}\rangle \quad . \tag{5.32}$$

The ground states are assumed to be invariant under the symmetry $\mathbb{Z}_r\times\mathbb{Z}_r$ generated by R^q and $\tilde{R}^q$ (with $q=N/r$), thus the quantum numbers n and m take value in $\mathbb{Z}_q$. First of all, the expectation value of the string order parameter can not depend on the quantum numbers specifying the boundary modes, since the ground states are finitely correlated. Secondly, since the string order parameter commutes with the symmetry, its expectation value cannot depend on the quantum numbers n and m. Combining these two arguments results in:

$$\langle\Psi_{\alpha,\beta,n,m}|S(a,b)|\Psi_{\alpha,\beta,n,m}\rangle = \langle\Psi_{\alpha',\beta',n',m'}|S(a,b)|\Psi_{\alpha',\beta',n',m'}\rangle \quad . \tag{5.33}$$

The NL-UT transformation is a transformation that maps different systems into each other such that their SSB and SPT phases are also mapped into each other. This gives a deeper understanding of SPT phases in terms of hidden symmetry breaking. For example when N is 5, spin chains with $\mathbb{Z}_5\times\mathbb{Z}_5$ symmetry allow for a trivial phase, four non-trivial SPT phases and a phase in which the full symmetry is spontaneously broken. I do not consider spontaneous symmetry breaking phases where the symmetry is broken

to a group not of the form $\mathbb{Z}_r \times \mathbb{Z}_r \subset \mathbb{Z}_N \times \mathbb{Z}_N$. In Ref. [DQ3] it was derived in which manner these phases are mapped into each other. In terms of the parameters (r, t) we have the following chain of phases:

$$(1,0) \longrightarrow (5,4) \longrightarrow (5,2) \longrightarrow (5,3) \longrightarrow (5,1) \longrightarrow (1,0) \quad . \tag{5.34}$$

Thus the SSB phase $(1,0)$ is mapped to the fourth non-trivial SPT phase and so on. The trivial phases in which no symmetry is broken $(5,0)$ is always mapped to itself. The different SPT phases can be understood as phases in which symmetry is broken in a different hidden manner. That is, for the different SPT phases one would need to perform the NL-UT transformation a different number of times to arrive at the SSB phase.

5.2.1 A disentangler

The NL-UT given by Eq. (5.25) has been discussed as a map between different SSB/SPT phases. In this paragraph I will explain the disentangling properties of the NL-UT following the ideas described in Ref. [58]. From this discussion it should become more evident that the NL-UT essentially maps protected edge modes to symmetry breaking bulk modes.

I will focus on the transformation of $(N,1) \to (1,0)$, thus from the first non trivial SPT phase to the phase in which the complete symmetry group is spontaneously broken. As in Ref. [58] I will discuss the consequence of the NL-UT on a single site by writing it as: $U_N = \prod_i U_i$ where U_i is

$$U_i = \prod_{j<i} R_j^{\tilde{O}_i} \prod_{j>i} \tilde{R}_j^{O_i} \quad . \tag{5.35}$$

The action of R and $\tilde{R}$ on the right auxiliary spaces are given by P and $\tilde{P}$ obeying Eq. (5.7), with $t = 1$. They generate a group which I will denote by G_P. The elements of this group can be written in the form $\omega^a P^b \tilde{P}^c$. It can be seen as a discrete subgoup of a central extension of $\mathbb{Z}_N \times \mathbb{Z}_N$ over $U(1)$. This group has N^2 1-dimensional irreps defined by $\rho_{mn}(P) = \omega^m$ and $\rho_{mn}(\tilde{P}) = \omega^n$ (and thus $\rho_{mn}(\omega) = 1$). Furthermore, the group G_P has $(N-1)$ N-dimensional irreps obeying $\rho_i(\omega) = \omega^i \mathbb{I}_N$. Only the representation ρ_1 can contribute to $\mathcal{H}_{(i,r)}$ in order for Eq. (5.7) to hold. Thus we can write the right auxiliary space as:

$$\mathcal{H}_{(i,r)} = V_\omega \otimes V_{(i,r)} \quad , \tag{5.36}$$

where V_ω is the representation space of ρ_1 and $V_{(i,r)}$ is some multiplicity space. The space V_ω is sometimes referred to as the protected or topological subsystem [59]. It is the origin of the multiplets seen in the entanglement spectrum of topological ordered systems [16]. The space $V_{(i,r)}$ is sometimes referred to as junk system.

Let V_{mn} be the representation space of ρ_{mn}. As explained above, it is spanned by the eigenvector $|mn\rangle$ of P and $\tilde{P}$ having eigenvalue ω^m and ω^n, respectively. Since the spaces $V_\omega^\dagger$ and V_ω combine to $V_\omega^\dagger \otimes V_\omega = \bigoplus_{mn} V_{mn}$ and since the matrices $A^{[i]}$ are $\mathbb{Z}_N \times \mathbb{Z}_N$ equivariant, the vectors $|mn\rangle$ all have an equal contribution to the ground state. Now consider the state after the transformation. Using Eq. (5.35) it can be understood that the matrix $A^{[i]}$ at site i are transformed by the NL-UT as follows:

$$A^{[i]} \to A'^{[i]} = \sum_{nm} A^{[i]}((P^m)^\dagger \otimes (\tilde{P}^n)^\dagger)\Pi_n\tilde{\Pi}_m \quad . \tag{5.37}$$

Here Π_n projects onto the eigenspace of R corresponding to the eigenvalue ω^n and similarly for $\tilde{\Pi}_n$. This can be understood as follows. If an eigenvalue of ω^m is measured by $\tilde{R}_i$, or if an eigenvalue of m is measured by $\tilde{O}_i$, all sites to the left of site i should be transformed by R^m. Using an argument similar to the one depicted in Fig. 5.1, it can be shown that transforming all sites to the left of i is equal to transforming the auxiliary spaces $\mathcal{H}_{(1,l)}$ and $\mathcal{H}_{(i,l)}$. Neglecting the effect of transforming boundary modes results in the above equation.

Eq. (5.37) is slightly misleading. On the one hand it tells to measure (using Π_n and $\tilde{\Pi}_m$) before transforming (using $(P^m)^\dagger$ and $(\tilde{P}^n)^\dagger$). On the other hand however, measuring takes place on physical space (after using the mapping $A^{[i]}$) and transforming happens on auxiliary space (before using the mapping $A^{[i]}$). This problem can be easily solved since the mapping $A^{[i]}$ is equivariant under the symmetry transformations $\mathbb{Z}_N \times \mathbb{Z}_N$. In other words, measuring can also take place on auxiliary space. Eq. (5.37) then becomes:

$$\sum_{nm} \left((P^m)^\dagger \otimes (\tilde{P}^n)^\dagger\right) \Pi_n\tilde{\Pi}_m \tag{5.38}$$

$$= \sum_{nm}\sum_{kl} \left((P^m)^\dagger\Pi_k\tilde{\Pi}_l \otimes (\tilde{P}^n)^\dagger\Pi_{n-k}\tilde{\Pi}_{m-l}\right) \tag{5.39}$$

$$= \sum_{nm}\sum_{kl} \left(\Pi_k\tilde{\Pi}_{l-m}(P^m)^\dagger \otimes \Pi_{-k}\tilde{\Pi}_{m-l}(\tilde{P}^n)^\dagger\right) \tag{5.40}$$

$$= \Pi_0\tilde{\Pi}_0 \sum_{nm} \left((P^m)^\dagger \otimes (\tilde{P}^n)^\dagger\right) \quad . \tag{5.41}$$

In the third line I have used the relations $\tilde{P}^\dagger\Pi_a = \Pi_{a-1}\tilde{P}^\dagger$ and $P^\dagger\tilde{\Pi}_a = \tilde{\Pi}_{a-1}P^\dagger$ which can derived from Eq. (5.7). The conditional projection given by Eq. (5.37) can thus be understood as a projection onto the eigenspace V_{00} of $\mathcal{H}_i$. This holds for all sites. Thus only those states in an on-site Hilbert space, which are vectors in the eigenspace V_{00} are entangled to each other. The entanglement between site i and its neighbors is modeled by the auxiliary spaces $\mathcal{H}_{(i,r)}$ and $\mathcal{H}_{(i,r)}$. In the topologically non-trivial phase $(N, 1)$ the protected subsystem is modeled by the N-dimensional space V_ω

whereas in a topologically trivial phase the protected subsystem is modeled by an irrep of $\mathbb{Z}_N \times \mathbb{Z}_N$ which is 1 dimensional. I conclude that the N fold degeneracy in the entanglement spectrum has been effectively removed since the space V_ω in the auxiliary spaces or the multiplicity in the entanglement spectrum has been effectively removed.

One might wonder what has happened to all other states in the eigenspaces V_{mn} with $m \neq 0$ and $n \neq 0$. For also these states should lie in the image of the NL-UT. I have neglected the transformation of the left and right most auxiliary spaces described by the term $P^m_{(1,l)} \otimes \tilde{\Pi}_m$ and $P^n_{(L,r)} \otimes \tilde{\Pi}_n$. These two extra conditional transformations alter the above result if the eigenvalues of the operators P and $\tilde{P}$ corresponding to the left and right boundary modes are different from 1. The NL-UT transformation maps boundary degrees of freedom (characterized by different eigenvectors of the boundary operators P and $\tilde{P}$) to bulk degrees of freedom (characterized by the different eigenspaces V_{mn}). We already stated that SPT phases are analogous to SSB phases in the sense that *string* order parameters exist that detect *hidden* symmetry breaking in the same manner that order parameters detect symmetry breaking. The above discussion suggest a further analogy in terms of their ground state degeneracy: in SSB phases ground state degeneracy occurs due to bulk degrees of freedom whereas in SPT phases it occurs due to boundary degrees of freedom. These different types of degrees of freedom are mapped into each other by the NL-UT.

Chapter 6

Conclusions

In this thesis I have discussed symmetry protected topological (SPT) phases of spin chains which are invariant under a symmetry group G. The phase of a spin chain is determined by properties of its boundary modes. In more detail, the boundary modes do not transform according to a representation of G but rather according to a *projective* representation of G. It is the projective class of this projective representation that determines the topological phase. Using the framework of matrix product states (MPS) it has been shown that the SPT phases of spin chains are classified by the second group cohomology of G with values in $U(1)$, denoted by $H^2(G, U(1))$ [13, 14]. Suitable chosen entanglement spectra can give evidence that boundary modes, reel or virtual (in case of periodic chains), transform according to a projective representation [16].

The main conclusions of this thesis are:

- We presented a way to characterize the SPT phases of spin chains with symmetries described by a simple connected compact Lie group [DQ1]. As an example, we showed that spin chains with $PSU(N)$ symmetry allow for N different SPT phases. Proposals to realize such spin chains in cold atom systems (for N up to 10) have already been made [4].

- We found a novel way to distinguish these N phases by measuring the expectation value of a suitable string order parameter [DQ2]. Comparable string order parameters are capable of only distinguishing two phases from each other [23, 24, 27].

- We found an analogy between SPT phases and spontaneous symmetry broken (SSB) phases [DQ3]. We defined a transformation mapping SPT phases to SSB phases and vice versa. The N different SPT phases can be understood to arise as N different ways a *hidden* symmetry is broken.

Results

We studied spin chains invariant under a continuous set of symmetries described by a compact connected simple Lie group G_Γ. This notation of the subscript Γ is motivated as follows: a compact connected simple Lie group G_Γ can always be written as the quotient of its universal cover G and a subgroup Γ of the center of G. Thus $G_\Gamma = G/\Gamma$. A well known example is $SO(3) = SU(2)/\mathbb{Z}_2$. We used that the second group cohomology $H^2(G_\Gamma, U(1))$ of G_Γ is isomorphic to Γ [DQ1]. This motivates the emphasis on Γ in the notation of the set symmetries of the spin chain, since Γ classifies the different SPT phases that can arise in spin chains invariant under G_Γ.

The group Γ is a subgroup of the center of a universal cover group G, which is by definition a compact *simply*-connected simple Lie group. In Ref. [DQ1] we remind the reader what the centers are of these different Lie groups. For example, the center of $SU(N)$ is the discrete group $\mathbb{Z}_N$. We concluded that spin chains which are topologically the richest are those based on $PSU(N) = SU(N)/\mathbb{Z}_N$ since these allow for N different phases. This is particularly interesting in light of recent proposals of constructing such spin chains in optical lattices [4]. Other groups that give rise to more than one non-trivial topological phase are $PSO(N)$ and the exceptional group E_6.

I emphasize again that the boundary mode of a spin chain can transform according to a *projective* representation of G_Γ. All projective representations of G_Γ are linear representation of G, which are well known due to Lie theory. They fall into different projective classes which are one-to-one related to the topological phases of the spin chain. The action of Γ on the respective representation gives rise to a topological invariant t which determines the projective class and hence the topological phase of the spin chain.

It can be enlightening to keep the example of $SO(3) = SU(2)/\mathbb{Z}_2$ in mind. Only the integer spins are representations of $SO(3)$, while the half-integer spins are projective representations of $SO(3)$. However, all spins are representations of $SU(2)$ and fall into two projective classes: the integer spins, and the half-integer spins. Thus a spin chain with a half-integer spin boundary mode resides in a topologically non-trivial phase.

After having discussed in detail which SPT phases can occur in spin chains invariant under G_Γ one would like to be able to determine the phase by measuring an associated invariant. We proposed a string order parameter that does exactly this: it is able to measure unambiguously in which SPT phase a $PSU(N)$ spin chains resides [DQ2]. This string order parameter is novel in the sense that it is able to distinguish N different phases from each other. It is a matrix valued order parameter and the absolute value of all matrix entries are equal. The complex phase between different matrix entries is uniquely related to the topological invariant t and thus determines the phase of the spin chain. An ordinary string order parameter [23] which is zero in a trivial SPT phase and non-zero in a non-trivial SPT phase will not

be able to distinguish $N-1$ non-trivial phases (when N is greater than 2). We verified the behavior of our string order parameter with numerical studies [DQ2]. Using the DMRG algorithm we studied a quantum phase transition between the two non-trivial phases of a $PSU(3)$ invariant spin chain. We verify that our string order parameter can be used to detect quantum phase transitions since we observe a discrete jump of the topological invariant t exactly at the expected transition point.

The Haldane phase occurring in $SO(3)$-invariant spin 1 chains is known to be protected by a subgroup $\mathbb{Z}_2 \times \mathbb{Z}_2 \subset SO(3)$ of the symmetry group [56]. We generalized this idea to all connected compact simple Lie groups G_Γ [DQ3]. That is, for each G_Γ we found a discrete finite Abelian subgroup F_Γ such that the SPT phases occurring in spin chains with symmetry group G_Γ are also protected by the symmetries determined by F_Γ. Moreover, we showed, with one exception being the groups $PSO(4N)$, that this subgroup can be chosen to be of the form $\mathbb{Z}_N \times \mathbb{Z}_N$ [DQ3]. This tremendously reduces the number of groups one has to consider to discuss all spin chains giving rise to SPT phases.

It was understood quite a while ago that the four-fold degeneracy of the AKLT state is due to hidden symmetry breaking [25]. By using a non-local unitary transformation (NL-UT) the AKLT state is mapped to a symmetry breaking state. Actually, every state in the Haldane phase is mapped to a state in the symmetry breaking phase. The topological feature of the Haldane phase can be understood by the concept of hidden symmetry breaking. We have generalized this non-local unitary transformation such that it is applicable to spin chains with $\mathbb{Z}_N \times \mathbb{Z}_N$ symmetry [DQ3]. Essentially, this transformation maps string order parameters (measuring SPT phases) to local order parameters (measuring spontaneous symmetry breaking). When N is prime, spin chains with $\mathbb{Z}_N \times \mathbb{Z}_N$ symmetry allow for a trivial phase, $(N-1)$ non-trivial SPT phases and a phase in which the full symmetry is spontaneously broken. These $(N+1)$ different phases are mapped to each other by our non-local unitary transformation. The different SPT phases can be understood as breaking the symmetry in different non-local/hidden manners. Moreover, the NL-UT maps boundary modes occurring in systems residing in an SPT phase to bulk degrees of freedom responsible for the ground state degeneracy of systems residing in an SSB phase. SPT phases can thus be understood in complete analogy with Landau symmetry breaking phases. Where in the latter case, order parameters are used to detect symmetry breaking, in the former case *string* order parameters can be used to detect *hidden* symmetry breaking. Using the above point, we conclude that SPT phases occurring in spin chains with a symmetry described by a connected compact simple Lie group G_Γ (with the exception of $PSO(4N)$) can also be understood to arise due to a hidden symmetry breaking.

Discussion

In the introduction I emphasized the characteristic boundary physics that occurs in gapped systems residing in a topologically non-trivial phase. Indeed, both the integer/fractional quantum Hall effect [5, 7] and the 2D/3D time reversal invariant topological insulators [17, 19] give rise to gapless boundary modes which are not present in the bulk. Additionally, topological invariants can be defined which take on a non-trivial value in the bulk of systems residing in a topological phase. The effect that at the boundary of a topological insulator, where a topological invariant jumps from a non-trivial to a trivial value (in vacuum), where gapless boundary modes necessarily exist, is called the bulk-boundary correspondence.

The SPT phases of gapped quantum spin chains are characterized in a very similar way. However, the presence of boundary modes alone does not guarantee an SPT phase. The boundary modes are only protected against G invariant perturbations (where G is the symmetry group of the spin chain) when the representation according to which the boundary modes transform is projective. This is similar to the time-reversal invariant topological insulators in both two and three dimensions [17, 19]. In a similar way the presence of boundary modes does not guarantee an SPT phase for these systems. They only reside in an SPT phase when an odd number of boundary modes are present. Since these can only be gapped out in pairs, one boundary mode is always protected against time-reversal invariant perturbations when an odd number of boundary modes are present.

A remarkable property of a 3D topological insulator is that its boundary surface is characterized by a single Dirac cone [19]. Single Dirac cones do not appear in conventional 2D conducting surfaces due to the fermion doubling theorem [60]. Thus we are dealing with a boundary described by physics which is emergent and cannot be present without the non-trivial topology of the bulk. This effect can be put into connection with the Majorana wire [9] which is discussed in the introduction. The boundary mode of this system is described by an emergent particle which does not occur in the bulk. The boundary modes of spin chains are also described by different physics when compared to the bulk. The representation according to which the boundary modes transform is a representation of a different group than the group G which describes the bulk symmetries of the spin chain.

The entanglement spectrum as a tool to measure boundary modes was mentioned during the introduction. Indeed it has been shown that the Haldane phase in $SO(3)$ spin 1 chains is characterized by an entanglement spectrum whose eigenvalues are even-fold degenerate [16]. This degeneracy is most easily understood when comparing it to the entanglement spectrum of the AKLT state. It consist of just a single double-degenerate level, reflecting the spin 1/2 (half-integer, projective) edge mode. In light of the entanglement spectrum, our non-local unitary transformation introduced in

Eq. (5.25) can be understood as a complete disentangler. It removes the N-fold degeneracy observed in the entanglement spectrum of spin chains with $\mathbb{Z}_N \times \mathbb{Z}_N$ symmetry residing in an SPT phase. This has been shown to be the case for $N = 2$ numerically [58] and I give analytical arguments why this statement holds for all N.

Finally, I would like to touch on the Haldane conjecture [2, 3] which was also discussed in the introduction. Our work suggests a natural generalization of this conjecture to spin chains with a symmetry described by a connected compact simple Lie group G_Γ [DQ1]: If G_Γ is a proper quotient of its universal cover G, then such spin chains allow for gapped G_Γ invariant translationally invariant Hamiltonians with a symmetry preserving ground state. A gap was explicitly shown for $PSU(N)$ models [61] and is explained by confinement of elementary excitations (spinons). Confinement means that the energy of a pair of elementary excitations depends linearly on the distance between the excitations. Spinon confinement was also observed in spin chains with $SU(N)/\mathbb{Z}_q$ symmetry where $q \neq 1$. These two examples support our generalization since both $PSU(N)$ and $SU(N)/\mathbb{Z}_q$ are proper quotients of their universal cover $SU(N)$. Also, our suggested generalization is consistent with the original conjecture which states that the Heisenberg Hamiltonian is gapped on integer/$SO(3)$ spin chains and gappless on half-integer/$SU(2)$ spin chains. The group $SO(3)$ has $SU(2)$ as its universal cover whereas the group $SU(2)$ is simply connected and is thus its own universal cover. The main difference between the Haldane conjecture and our suggested generalization thereof is that the original conjecture is a statement about a specific Hamiltonian whereas our generalization only states when gapped G_Γ invariant models exist.

Outlook

The study of SPT phases in spin chains has some obvious restrictions. Of course it only includes systems in 1-dimension. Attempts to classify SPT phases using group cohomology in higher dimensions have already been made [53]. Also in other works the techniques of MPSs have been generalized to incorporate interacting fermionic systems [62, 63]. It remains an open problem whether a topological invariant, which characterizes the SPT phases appearing in higher dimensional systems, can be detected by making use of some generalization of a string order parameter.

MPS techniques are tuned to study gapped quantum phases. They can be used to study critical phases. However, their bond dimensions will scale polynomially with system size to approximate the ground state with the same precision. Infinite matrix product states make use of an infinite dimensional auxiliary space and are suitable to study critical systems [64]. It is interesting to investigate whether similar techniques, such as the study of the entanglement spectrum [65], can be used to classify critical systems.

Our non-local transformation mapping SPT phases to SSB phases is explained to remove entanglement. This is closely related to quantum teleportation in which entanglement is replaced in order to simultaneously teleport quantum information [66]. How these two topics are precisely connected is still unclear and is left open for further studies.

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Statement of contribution

I contributed to obtaining the conceptual ideas and working out statements and proofs in all three papers. I contributed in increasing manner to the writing of the three papers. The first paper [DQ1] was written by Thomas Quella, I contributed substantially in writing the second paper [DQ2] and the last paper was written for most part by myself [DQ3]. I contributed to the revision of all three papers.

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