# **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.<sup>1</sup> Soon after, a generalization of the spin quantum Hall effect to three dimensions was found.<sup>2</sup> By now, a comprehensive classification of noninteracting fermionic systems is available which describes various types of topological insulators and superconductors.<sup>3–6</sup> These results have been motivated by the symmetry classification of quadratic random Hamiltonians à la Altland and Zirnbauer.<sup>7,8</sup>

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 spectra9,10 which contain information about potential surface modes by introducing virtual interfaces into the system or from single-particle Green's functions.<sup>11</sup> The first systematic studies of topological phases of interacting fermions have been concerned with Majorana chains.<sup>12–14</sup> 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,<sup>17,18</sup> 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,<sup>18</sup> one has a bulk-boundary correspondence: open boundary

conditions imply massless edge modes carrying a topological quantum number,<sup>19</sup> the ground state leads to a characteristic entanglement spectrum,<sup>20,21</sup> and last but not least there exists a nonlocal string order parameter.<sup>22</sup>

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.<sup>27–29</sup> In all these examples, the matrix product (or valence bond) state formalism plays a crucial role.<sup>30–33</sup> 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.<sup>34–36</sup> 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<sup>35,37,38</sup> (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.<sup>34,35</sup> 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  $G/\Gamma$ . The group  $\Gamma$  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  $SO(N) = \text{Spin}(N)/\mathbb{Z}_2$  where two topological phases have been found.<sup>40</sup> 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  $\Gamma$ , which can also be interpreted as the fundamental group of  $G/\Gamma$  [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  $G/\Gamma$ . 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<sup>41,42</sup> 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.<sup>43–46</sup> 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.<sup>47</sup>

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 g and its various associated compact connected Lie groups, which can all be represented as a quotient  $G/\Gamma$  of a simply connected universal covering group G. We introduce the congruence class  $[\lambda]$  of an irreducible representation  $\lambda$  of 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  $G/\Gamma$  with their fundamental group  $\Gamma$ , 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 onedimensional (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 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  $H \in \operatorname{End}_{\mathfrak{g}}(\mathcal{H})$  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  $\mathbb{E}$  and II  $\mathbb{F}$  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.<sup>36</sup> 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

$$\omega(g_1, g_2)\,\omega(g_1g_2, g_3) \,=\, \omega(g_2, g_3)\,\omega(g_1, g_2g_3). \tag{1}$$

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

$$\omega(g_1, g_2) = f(g_1g_2)/f(g_1)f(g_2).$$
(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  $D: G \rightarrow U(N)$  satisfying

$$D(g_1)D(g_2) = \omega(g_1, g_2) D(g_1g_2).$$
(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  $D(g) \rightarrow f(g)D(g)$ .

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  $\Omega$ , this central extension  $\tilde{G}(\Omega)$  is defined as the set  $G \times U(1)$ 



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.

with group multiplication

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

One can check that cocycles  $\omega$  belonging to the same class  $\Omega$  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.<sup>34,35</sup> 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.<sup>20,21</sup> The two possibilities are sketched in Fig. 1.

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).<sup>34,35</sup> 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<sup>33</sup>

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

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.<sup>32,33</sup> 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 Gon  $\mathcal{H}_k$  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)

$$R^{[k]}(g) \cdot A^{[k]} = D^{[k]}(g)A^{[k]}D^{[k+1]}(g)^{-1}.$$
 (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  $\Omega$  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  $\Omega$  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.<sup>52</sup>

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.<sup>53–55</sup> 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.<sup>40,54,55</sup> 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  $\Omega$  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  $\overline{S}_k$  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).<sup>34</sup> The two central extensions [by U(1)] corresponding to these two classes are  $SO(3) \times U(1)$ and U(2).<sup>56</sup> 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  $\mathfrak{g}$ .<sup>57</sup> 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  $\lambda$ , 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.<sup>58</sup>



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<sup>59</sup> 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 g can be exponentiated to a compact connected Lie group. However, as we have just seen in Sec. IID, several distinct Lie groups might have the same underlying Lie algebra g. The Lie groups associated with g all look the same locally but they differ in their global topological properties, more precisely in their fundamental group.<sup>60</sup> To obtain a description of all Lie groups belonging to 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 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  $G_{\Gamma}$  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 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 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 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  $G_{\Gamma}$  (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 g and their associated compact connected simply connected Lie group G. The table also contains the congruence group P/Q of g and the center  $\mathcal{Z}(G)$  of G.

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

In order to study this issue more systematically, let us consider an irreducible representation  $V_{\lambda}$  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,  $V_{\lambda}$  can be viewed as dim $(V_{\lambda})$  copies of one and the same one-dimensional representation  $[\lambda]$  of the Abelian group  $\mathcal{Z}(G)$ .<sup>62</sup> We call  $[\lambda]$ the *congruence class* of  $\lambda$ .  $[\lambda]$  can be interpreted as an element  $[\lambda] \in \text{Hom}(\mathcal{Z}(G), U(1))$  of the character group of  $\mathcal{Z}(G)$ . In our situation, with  $\mathcal{Z}(G)$  being finite, the character group  $\text{Hom}(\mathcal{Z}(G), U(1))$  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 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  $\lambda^+$  denotes the representation conjugate to  $\lambda$ , 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  $G_{\Gamma}$  admit an action on  $\mathfrak{g}$  by conjugation which is insensitive to the action of the center. Since the generators of 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  $P/Q \to \operatorname{Hom}(\mathcal{Z}(G), U(1))$ . A closer inspection shows that the homomorphism just constructed is actually an isomorphism (Ref. 63, Theorem 8.30).<sup>64</sup> Summarizing our previous discussion, we obtain an isomorphism

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

Any representation  $\lambda$  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  $[\cdot]_{\Gamma} : P \to \operatorname{Hom}(\Gamma, U(1))$ . Since all the groups involved are Abelian, one can regard the character group  $\operatorname{Hom}(\Gamma, U(1))$  of  $\Gamma$  as a quotient of the character group  $\operatorname{Hom}(\mathcal{Z}(G), U(1))$  [see also Eq. (35)] and hence as a sublattice of P/Q. If  $Q_{\Gamma}$  denotes the kernel of the map  $[\cdot]_{\Gamma}$ , we obviously obtain the isomorphisms

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

All linear representations  $\lambda$  of  $G_{\Gamma}$  satisfy  $[\lambda]_{\Gamma} \equiv [0]$ . If this equation is not satisfied,  $\lambda$  is a projective representation of  $G_{\Gamma}$ . 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  $\Gamma$  and  $\Gamma'$  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  $\pi_1(K)$ .<sup>65</sup>

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

$$H^{2}(K, U(1)) \cong \operatorname{Hom}(\pi_{1}(K), U(1)).$$
 (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 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  $G_{\Gamma}$  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  $G_{\Gamma}$  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

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

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  $G_{\Gamma}$  are just the representations of *G* (or g) themselves. Different projective classes correspond to different actions of the subgroup  $\Gamma$ . Indeed, due to Schur's lemma, the center  $\Gamma$  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  $G_{\Gamma}$ . 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  $G_{\Gamma}$ . 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:

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

In other words, the different topological phases of a spin chain with symmetry group  $G_{\Gamma}$  are in one-to-one correspondence with the elements of its fundamental group  $\Gamma$ . 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

$$H^2(PG, U(1)) \cong \operatorname{Hom}(\mathcal{Z}(G), U(1)) \cong \mathcal{Z}(G) \cong P/Q.$$
  
(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  $G_{\Gamma}$  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  $G_{\Gamma}$  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  $\lambda$  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  $\Omega \in \text{Hom}(\mathcal{Z}(G), U(1))$  labeling the topological phase.<sup>66</sup> 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.<sup>67</sup> 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 g similar to Eq. (13), then all the  $\lambda$  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  $\lambda$  of g.

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

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

where the congruence vectors v 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) $v$     | 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 (v, 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  $N \ge 2$  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 *N*th 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

$$H^{2}(PSU(N), U(1)) \cong \mathbb{Z}_{N}.$$
(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  $\lambda = (\lambda_1, \dots, \lambda_{N-1})$  as above or, alternatively, in terms of Young tableaux  $\lambda = \{l_1; \dots; l_{N-1}\}$ . In terms of the weight, the partition of the associated Young tableau is specified by the numbers

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

By definition, the number  $l_i$  determines the number of boxes in the *i*th row of the tableau.

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

$$[\lambda] \equiv \sum_{k=1}^{N-1} k \lambda_k \mod N.$$
 (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  $\rho : SU(N) \rightarrow U(V_{\lambda})$  denotes the irreducible representation with highest weight  $\lambda$ , 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  $\lambda_2$ .

This equation is evident for the trivial representation and for the fundamental representation  $\lambda = (1, 0, ..., 0)$  (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  $\lambda$  just corresponds to the number of boxes  $|\lambda|$  modulo *N*. Indeed, a simple rewriting of Eq. (17) using the identity (16) yields

$$[\lambda] \equiv \sum_{i=1}^{N-1} l_i \mod N \equiv |\lambda| \mod N.$$
(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 *N*th 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  $N \ge 3$  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

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

Surprisingly, the groups 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 ( $n \ge 1$ ), 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 Spin(*N*) symmetric spin chains are thus given by

$$H^{2}(SO(2n+1), U(1)) \cong \mathbb{Z}_{2},$$
  

$$H^{2}(SO(2n)/\mathbb{Z}_{2}, U(1)) \cong \begin{cases} \mathbb{Z}_{4}, & n \text{ odd} \\ \mathbb{Z}_{2} \oplus \mathbb{Z}_{2}, & n \text{ even.} \end{cases}$$
(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 ( $n \ge 1$ ), 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  $\lambda = (\lambda_1, \dots, \lambda_n)$ ,

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

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

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

Accordingly, the situation is very similar to that of SU(2). Representations with  $[\lambda] \equiv 0$  are linear representations of Spin(N) and of SO(N). On the other hand, representations with  $[\lambda] \equiv 1$  are spinorial, i.e., they are linear representations of 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  $(n \ge 2)$ becomes slightly more involved but also more interesting. In this case, the center of Spin(*N*) is  $\mathbb{Z}_2 \times \mathbb{Z}_2$  for even *n* and  $\mathbb{Z}_4$  for odd n.<sup>69</sup> This observation in particular implies that the groups  $SO(N) = \text{Spin}(N)/\mathbb{Z}_2$  have a center  $\mathbb{Z}_2$ themselves such that one also needs to consider the group  $PSO(2n) = SO(2n)/\mathbb{Z}_2$ .<sup>70</sup> In order to determine the class of a representation  $\lambda = (\lambda_1, \dots, \lambda_n)$ , we have to calculate the  $\mathbb{Z}_2 \oplus \mathbb{Z}_4$ -valued quantity

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  $\mathcal{Z}(\text{Spin}(2n))$  and it is relevant when it comes to determining whether  $\lambda$  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,

$$[0,0], [0,2], [1,0], [1,2],$$
 (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  $\mathbb{Z}_2 \subset \text{Spin}(2n)$ , their action on an irreducible representation  $\rho : \text{Spin}(2n) \to U(V_\lambda)$  of highest weight  $\lambda$  is given by

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

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

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,

$$[0,0], [1,1], [0,2], [1,3],$$
(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  $\rho$  : Spin(2*n*)  $\rightarrow U(V_{\lambda})$  of highest weight  $\lambda$ , the center acts as

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

The generator  $\eta^2$  of the subgroup  $\mathbb{Z}_2 \subset \mathbb{Z}_4 \subset \text{Spin}(2n)$  which needs to be used to descend from Spin(2n) to SO(2n) is mapped to  $\pm \mathbb{I}$  under  $\rho$ , depending on whether  $[\lambda]_2$  is even or odd. We thus obtain the following three-level hierarchy: representations of 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.<sup>68</sup> 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

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

We thus have two distinct topological phases. Given any weight  $\lambda = (\lambda_1, \dots, \lambda_N)$ , the associated congruence class is determined by the number<sup>71</sup>

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

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  $V_{\lambda}$  of highest weight  $\lambda$ , 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  $SP(2N)/\mathbb{Z}_2$ .

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

$$H^{2}(E_{6}/\mathbb{Z}_{3}, U(1)) \cong \mathbb{Z}_{3},$$
  
 $H^{2}(E_{7}/\mathbb{Z}_{2}, U(1)) \cong \mathbb{Z}_{2}.$  (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

 $\lambda$  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  $\lambda$  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  $G_{\Gamma}$  associated with  $\mathfrak{g}$ . In this section, we will analyze which of the possible Lie groups  $G_{\Gamma}$  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  $G_{\Gamma}$  and  $G_{\Gamma'}$ where  $\Gamma$  and  $\Gamma'$  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 g and a Hamiltonian that commutes with all elements of g. Furthermore, we assume the action of g on the total Hilbert space to be faithful and the existence of a unique and 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  $\mathcal{H}_k$ .<sup>72</sup> 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  $\Gamma_k$ . Whenever 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  $\Gamma_A = \bigcap_k \Gamma_k$  being the intersection of all kernels  $\Gamma_k$ , 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  $\Gamma$  with the kernel of G that arises when acting on the total Hilbert space  $\mathcal{H} = \bigotimes_k \mathcal{H}_k$ .<sup>73</sup> 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  $G_{\Gamma}$ , 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  $G_{\Gamma}$  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  $G_{\Gamma}$ , 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  $\Gamma$  which is contained in  $\Gamma_A$  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  $G_{\Gamma}$ , the topological phases are described by

$$H^{2}(G_{A}, U(1)) \cong \operatorname{Hom}(\Gamma_{A}, U(1)),$$
  

$$H^{2}(G_{\Gamma}, U(1)) \cong \operatorname{Hom}(\Gamma, U(1)).$$
(34)

We expect that  $G_A$  provides a finer resolution of topological phases than  $G_{\Gamma}$ . In other words, from the perspective of  $G_{\Gamma}$ , 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  $\Gamma_A/\Gamma$  which measures to which extent  $\Gamma_A$  is larger than  $\Gamma$ . 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

$$\operatorname{Hom}(\Gamma, U(1)) \cong \operatorname{Hom}(\Gamma_A/(\Gamma_A/\Gamma), U(1))$$
  
$$\cong \operatorname{Hom}(\Gamma_A, U(1))/(\Gamma_A/\Gamma).$$
(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  $G_{\Gamma}$  with  $\Gamma \subset \Gamma_A$  and then back from  $G_{\Gamma}$  to  $G_A$ . In many situations, however, it is even possible to change the perspective from  $G_A$  to a smaller group  $G_{\Gamma}$ right away. In this case, the latter is obtained from a central subgroup  $\Gamma$  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  $G_{\Gamma}$ ). 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  $G_{\Gamma}$  since the individual projective classes (with respect to  $\Gamma$ ) 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  $\mathcal{H}_{block} = \mathcal{H} \otimes \mathcal{H}^*$  which resides in the trivial class  $[\mathcal{H}_{block}] \equiv [\mathcal{H}] + [\mathcal{H}^*] \equiv [0]$  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:<sup>41,42</sup> 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  $\sigma$  models with or without  $\Theta$ term.<sup>41,42</sup> 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.<sup>75,76</sup> 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<sup>18</sup>) 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<sup>23,77</sup> (see Ref. 47 for some older work). In particular, the authors of Refs. 23 and 77 claimed that SU(N) chains with twosite interactions possess a Haldane-type gap due to spinon confinement if the physical sites are described by an irreducible representation  $\lambda$  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 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  $\lambda$  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  $G_{\Gamma}$ , 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.<sup>33,51</sup> 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  $n \neq 2$ ].<sup>60</sup> 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



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

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  $\Gamma$ . 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  $[SU(6)/\mathbb{Z}_3]/\mathbb{Z}_2 = PSU(6)$ , the phases of PSU(6) can be identified with the phases of  $SU(6)/\mathbb{Z}_3$  up to the identifications  $[0] \sim [3], [1] \sim [4], \text{ and } [2] \sim [5], \text{ thus } [\mathcal{B}]_{\mathbb{Z}_3} \equiv$  $[\mathcal{B}] \mod 3$ . 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. 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 <sup>87</sup>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.<sup>44,46</sup> 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  $\lambda$  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,  $\lambda$  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 AKLTtype 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.<sup>46</sup>

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.<sup>55</sup> 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  $H^2(G_{\Gamma}, U(1))$  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<sup>41,42</sup> 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  $\lambda$  is a linear representation of *any* of the groups  $G_{\Gamma}$  (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.<sup>23</sup> We believe that their analysis can be carried over to groups of type Spin(2*N*), 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<sup>22</sup> (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,<sup>55</sup> 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.<sup>34,36</sup> 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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- <sup>52</sup>For the S = 1 spin chain in the Haldane phase, the previous paragraph amounts to the following statements: The system is invariant under SU(2) as well as under SO(3). If one restricts oneself to deformations which preserve the SO(3) symmetry, the system is in a topologically nontrivial phase. However, it is in the topologically trivial phase with regard to deformations which only need to preserve SU(2). An intuitive way of understanding this is the observation that the emerging  $S = \frac{1}{2}$  boundary spins are not stable against the explicit addition of extra  $S = \frac{1}{2}$  boundary spins. On the other hand, this addition is not allowed if we wish to preserve SO(3) invariance locally since  $S = \frac{1}{2}$  is a representation of SU(2)but not of SO(3).
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- <sup>56</sup>Note that U(2) is *not* a central extension of SU(2) since U(2)/U(1) = SO(3). Indeed, the subgroup  $\mathbb{Z}_2 \subset SU(2)$  is contained in  $U(1) \subset U(2)$ . In other words,  $U(2) = [SU(2) \times U(1)]/\mathbb{Z}_2$ .
- <sup>57</sup>The background on Lie theory needed for this section can for instance be found in Refs. 60,63, and 80.
- <sup>58</sup>We note the amusing fact that the order |P/Q| coincides with the determinant of the Cartan matrix of g.
- <sup>59</sup>Recall that the su(2) weights are twice the integral or half-integral magnetic quantum numbers used in physics.
- <sup>60</sup>M. Mimura and H. Toda, *Topology of Lie Groups. I, II* (American Mathematical Society, Providence, RI, 1991), Vol. 91.
- <sup>61</sup>Elsewhere this group is also called the adjoint group Ad(G) (Ref. 63).
- <sup>62</sup>For an Abelian group, all irreducible representations are one dimensional.
- <sup>63</sup>B. C. Hall, *Lie Groups, Lie Algebras, and Representations* (Springer, New York, 2003), Vol. 222.
- <sup>64</sup>Basically, this statement amounts to the fact that the root lattice can be defined as the kernel of the exponential map from g to G.
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- <sup>66</sup>This condition can be violated if the boundary Hilbert space  $\mathcal{B}$  describing the gapless edge mode at one boundary is not an irreducible representation.
- <sup>67</sup>The assignment of  $\Omega$  to the left edge is by convention only and represents no loss of generality. We could equally well flip the orientation of the whole system. In any case, the edges need to transform in opposite classes since the action of the symmetry group *PG* on the total chain should correspond to the trivial class [0], i.e., to a linear representation.
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- <sup>70</sup>For odd *n*, there exist three choices of subgroups  $\mathbb{Z}_2 \subset \mathbb{Z}_2 \times \mathbb{Z}_2$ . One of them leads to SO(2n), while the other two lead to isomorphic groups which are known as *semispinor* groups (Ref. 60). The semispinor groups SS(2n) are isomorphic to SO(2n) for n = 4but not for n > 4.
- <sup>71</sup>For N = 2, the second contribution involving  $\lambda_3$  is omitted.
- <sup>72</sup>We note in passing the following important facts: When the symmetries are restricted to groups of type  $G_{\Gamma}$ , 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  $G_{\Gamma}$  are a subset of irreducible representations of  $\mathfrak{g}$ . Similarly, if the ground state is  $\mathfrak{g}$  invariant, it will also automatically be  $G_{\Gamma}$  invariant.

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