FACULTY OF SCIENCES

Spatial Symmetries and Symmetry Breaking with Matrix Product States

DEWOLF NICOLAS
Student number: 01402529

Promotor: Prof. Dr. Verstraete Frank
Supervisors: M. Sc. Vanhove Robijn, M. Sc. Van Damme Maarten

A dissertation submitted to Ghent University in partial fulfilment of the requirements for the degree of Master of Science in Physics and Astronomy

Academic year: 2018 - 2019
Revision: 2024

GHENT UNIVERSITY

English abstract

This thesis focuses on the classification of symmetry-protected topological (SPT) phases in one-dimensional quantum many-body systems and the interplay with nontrivial lattice or space group symmetries. The general starting point is an injective matrix product state description of a symmetric quantum state. In this framework, we can easily derive an SPT classification based on projective representations and group cohomology. After a theoretical investigation, where we systematically identify the cohomological structure behind the SPT classification and try to unify the physical paradigm with the mathematical literature, we numerically determine the classification for (small) symmetry groups and compare them to the literature. At the same time, an explicit construction of symmetric systems in terms of a matrix product state ansatz is given for any SPT phase. We also show that the nontrivial spatial configurations fit in the cohomological framework and try to generalize the results for on-site symmetries by including nontrivial space group symmetries. For some general cases, a manifestly symmetric matrix product state is constructed. These constructions are relevant for the optimization of numerical methods for simulating quantum many-body problems.

Nederlandstalige samenvatting

Deze thesis richt zich op de classificatie van symmetrie-beschermde topologische (SPT[1]) fasen in één-dimensionale kwantumveeldeeltjessystemen en de interactie met niet-triviale rooster- of ruimtegroepsymmetrieën. Het algemene uitgangspunt is een injectieve matrix product toestand-beschrijving van een symmetrische kwantumtoestand. Binnen dit framework is het eenvoudig om een classificatie van de mogelijke SPT fasen in termen van projectieve representaties en groepscohomologie af te leiden. Naast een theoretische aanpak, waar we systematisch de achterliggende cohomologische structuur onderzoeken en waar we een link proberen te leggen tussen de wiskundige en fysische literatuur, geven we ook een numerieke methode waarmee de classificatie voor algemene symmetriegroepen kan bepaald worden. Verder geven we ook een expliciete constructie van kwantumsystemen die tot een gegeven SPT fase behoren in termen van een matrix product toestand. Na aan te tonen dat de niet-triviale roostersymmetrieën ook in een cohomologisch kader geplaatst kunnen worden, trachten we een systematische classificatie te vinden van de SPT fasen indien de symmetriegroep roostertransformaties bevat. Voor enkele belangrijke gevallen wordt een manifest symmetrische matrix product toestand geconstrueerd. Deze constructies zijn onder meer interessant voor het optimaliseren van numerieke methodes die gebruikt worden bij de simulatie van kwantumveeldeeltjesproblemen.

[1] Van het Engelse "symmetry-protected topological".

Acknowledgments

I would like to thank my supervisors, Robijn Vanhove and Maarten Van Damme, for their support and help during my thesis.

I also owe gratitude to my promotor Frank Verstraete. He not only made this thesis come to life by his ambitious suggestions, but he also never failed to motivate me by giving many enthusiastic talks about this and various other subjects. He has also been a great help with both the theoretical and numerical aspects of my thesis.

I also want to thank professor Jutho Haegeman for his help and support. He always had time to discuss the problems and results of my work.

This gratitude extends to the entire research group for helping with my thesis and for showing great interest. The dynamic atmosphere and weekly lunch talks were a huge motivation.

My friends, especially Kenneth Stoop and Elliot Blommaert, also deserve a word of appreciation. They always helped me even when I was clearly interfering with their work.

Finally, I want to thank my parents and girlfriend for their unconditional support. They have always encouraged me in my academic journey and they will always keep doing so.

Nicolas Dewolf,

2019 Gent

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Chapter 1

Introduction

1.1 Outline

Since the dawn of quantum mechanics, it has been clear that solving equations for many-body systems was an incredibly difficult task due to an exponential dependence of the dimension on the number of involved particles. However, in the last couple of decades, there was a strong influx of ideas from (quantum) information theory and this led people to believe that not all hope was lost. The entanglement structure of low-energy quantum states inspired researchers to come up with a new framework called tensor network states. These specifically target the relevant part of the Hilbert space of quantum states. Aside from their numerical advantage as a very efficient variational ansatz, they also contribute to theoretical insights in the universal properties of quantum many-body systems and even more exotic subjects such as conformal field theory.

Due to the local structure of tensor networks they are especially suited for describing topological order in quantum systems such as symmetry-protected topological phases. A nearly complete classification of symmetry-protected topological phases for on-site symmetries has already been constructed using tensor networks. However, the interplay with space group symmetries is not yet clear and this is what we hope to achieve: to give a unified description of ground state tensor works with both on-site and space group symmetries.

The structure of this thesis is as follows. In the first chapter, we start by giving a general introduction to the theory of tensor network states and, more specifically, matrix product states. Then, we introduce the concept of topological order and explain how symmetries of the physical system come into play. The classification of symmetry-protected topological phases is given in the second chapter, where we use methods based on group cohomology. We also explicitly construct for any solution to the relevant equations a matrix product state satisfying the given symmetries. In chapter three, we consider systems where the symmetry group is enlarged to allow for nontrivial lattice transformations. This generalization is placed within the existing framework, some explicit examples are considered and, for some relevant cases, we construct a manifestly symmetric normal form for the matrix product ansatz. In the first appendix, we give an introduction to some mathematical concepts from abstract algebra such as representation theory and group cohomology

in more detail. In the second appendix, we introduce the graphical calculus of tensor networks and we explain some relevant results from linear algebra.

1.2 Tensor network states

The introduction and study of **tensor networks states** (TNs) was motivated by the search for an efficient way to handle the immense complexity of quantum many-body systems. Consider for example a quantum mechanical system of N sites, where every site has as a local state space a d_i-dimensional Hilbert space $\mathcal{H}_i$ (as shown in Fig. 1.1).

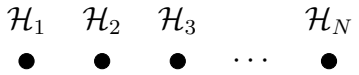


Figure 1.1: System with N sites.

A general wave function for the total system, which is an element of the tensor product space $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_N$, can be expanded as follows:

$$|\psi\rangle = \sum_{\{i_1,\ldots,i_N\}} \mathbf{C}_{i_1,\ldots,i_N} |i_1 \cdots i_N\rangle \,, \tag{1.1}$$

where the sum ranges over all possible combinations of the physical indices i_k. Because there are N Hilbert spaces $\mathcal{H}_i$, each with a dimension d_i, the total Hilbert space has the dimension $d_1 d_2 \cdots d_N$. In terms of the above expansion, this means that we have to specify $d_1 \cdots d_N$ complex numbers $\mathbf{C}_{i_1,\ldots,i_N}$, one for every combination of the indices, to give a full description of the wave function. This exponential growth of the necessary information with respect to the number of sites makes an exact numerical approach unfeasible for realistic physical systems, which typically have a number of sites of the order of the Avogadro constant ($\sim 10^{23}$).

However, it was found [19, 25] that the relevant quantum states for a system described by a local gapped[1] Hamiltonian satisfy an area law for the bipartite entanglement entropy

$$S = -\operatorname{tr}(\rho_A \ln \rho_A) \tag{1.2}$$

i.e. if we consider a subsystem A of the complete system, the entropy S only depends on the number of sites on the boudary ∂A. These states occupy an exponentially small subset of the total Hilbert space and hence it should be possible to find an efficient description of these states. A very efficient variational approach to this problem is given by tensor network states [44, 45]. As we are only concerned with one-dimensional systems in this thesis, we will limit ourselves to the description of one-dimensional tensor networks known as **matrix product states** (MPS). It is a well-known result that this ansatz can be used to approximate one-dimensional states to arbitrary precision [58].

1.2.1 Matrix product states

Consider a quantum state $|\psi\rangle$ for a 1D lattice with open boundary conditions described by a coefficient tensor $\mathbf{C}$. The Schmidt decomposition allows for a powerful decomposition

[1] This means that even in the thermodynamic limit ($N \to \infty$) there exists an energy gap between the groundstates and the first excitations.

of $\mathbf{C}$ in terms of tensor of lower rank due to Vidal [60]. We first make a cut between the first site and the rest. The associated Schmidt decomposition gives us:

$$|\psi\rangle = \sum_{i=1}^{d_1} \lambda_i[1]|\alpha_i[1]\rangle \otimes |\Phi_i[2,3,\ldots,N]\rangle \tag{1.3}$$

The states $|\alpha_i[1]\rangle$ can then be rewritten in terms of the local (physical) basis of site 1:

$$|\alpha_i[1]\rangle = \sum_{j=1}^{d_1} \Gamma_i^j[1]|s_j[1]\rangle \tag{1.4}$$

Similarly one can express the state $|\Phi_i[2,3,\ldots]\rangle$ in terms of the local basis of site 2:

$$|\Phi_i[2,3,\ldots,N]\rangle = \sum_{j=1}^{d_2} |s_j[2]\rangle \otimes |\chi_{i,j}[3,\ldots,N]\rangle \tag{1.5}$$

We now make a cut between sites 2 and 3 and express the states $|\chi_{i,j}\rangle$ in terms of the right Schmidt vectors associated to this cut:

$$|\chi_{i,j}[3,\ldots,N]\rangle = \sum_{k=1}^{d_1 d_2} \Gamma_{i,k}^j[2]\ \lambda_k[2]|\Phi_k[3,\ldots,N]\rangle \tag{1.6}$$

Inserting all these steps in the formula for $|\psi\rangle$ gives us:

$$|\psi\rangle = \sum_{i_1,i_2} \sum_{j,k} \left(\Gamma_j^{i_1}[1]\ \lambda_j[1]\ \Gamma_{j,k}^{i_2}[2]\ \lambda_k[2]\right) |s_{i_1}[1]\rangle \otimes |s_{i_2}[2]\rangle \otimes |\Phi_k[3,\ldots,N]\rangle \tag{1.7}$$

where the indices are bounded in the folowing way:

$$\begin{cases} 1 \leq i_1 \leq d_1 \\ 1 \leq i_2, j \leq d_2 \\ 1 \leq k \leq d_1 d_2 \end{cases} \tag{1.8}$$

This process can now be applied iteratively to obtain the following decomposition of $\mathbf{C}$:

$$\mathbf{C}_{i_1 i_2 \ldots i_N} = \sum_{\{i_k\}}^{\{d_k\}} \sum_{\{j_i\}} \Gamma_{j_1}^{i_1}[1]\ \lambda_{j_1}[1]\ \Gamma_{j_1,j_2}^{i_2}[2]\ \lambda_{j_2}[2]\ \Gamma_{j_2,j_3}^{i_3}[3]\ \cdots\ \Gamma_{j_{N-1}}^{i_N}[N] \tag{1.9}$$

where the j_i run from 1 to $\min\left(\dim(\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_i), \dim(\mathcal{H}_{i+1} \otimes \cdots \otimes \mathcal{H}_N)\right)$. To conclude, we can rewrite this decomposition by introducing the following tensors:

$$\begin{cases} A[1] = \Gamma[1]\,, \\ A_{m,n}^{i_k}[k] = \lambda_m[k-1]\Gamma_{m,n}^{i_k}[k]\,. \end{cases} \tag{1.10}$$

This way, we can graphically[2] represent the coefficient $\mathbf{C}_{i_1 i_2 \ldots i_N}$ as in Fig. 1.2.

From this construction, it should, however, still be clear that the complexity grows exponentially in the number of sites. The ability to solve this problem lies in the use of the Schmidt decomposition. First of all, not all Schmidt values will be nonzero, so there could arise a natural cut-off on the number of relevant degrees of freedom (e.g. due to

[2]See Section B.1 in the appendix for an introduction to the graphical calculus of tensor networks.

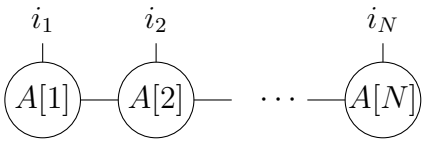


Figure 1.2: Graphical representation of a finite-size MPS.

the area law) and even if this was not the case one could impose an artificial cut-off by retaining only the D largest Schmidt values. This value D is called the *bond dimension*[3]. For a system with n sites, physical dimensions $\{d_i\}_{i\leq n}$ and bond dimensions $\{D_i\}_{i\leq n}$, the MPS state space $\mathbb{A}_{\mathrm{MPS}}$ has dimension

$$\dim(\mathbb{A}_{\mathrm{MPS}}) = \sum_{i=1}^{n} D_{i-1} d_i D_i \,, \tag{1.11}$$

which clearly scales only polynomially in the number of sites.

A different but equivalent construction uses maximally entangled pairs and is based on the valence bond construction. Between every neighbouring pair of sites, we place a maximally entangled pair

$$|\omega\rangle_i = \sum_{k=1}^{D} |k\rangle \otimes |k\rangle \in \mathcal{H}_i^R \otimes \mathcal{H}_{i+1}^L \,, \tag{1.12}$$

where we introduced the virtual Hilbert spaces $\mathcal{H}_i^L, \mathcal{H}_i^R$ for each site $i \leq N$. Then, we define MPS projectors[4] $\mathcal{P}_i : \mathcal{H}_i^L \otimes \mathcal{H}_i^R \to \mathcal{H}_i$:

$$\mathcal{P}_i = \sum_{k=1}^{d_i} \sum_{\alpha=1}^{D_{i-1}} \sum_{\beta=1}^{D_i} P_{\alpha,\beta}^k \, |k\rangle \otimes \langle\alpha| \otimes \langle\beta| \,, \tag{1.13}$$

where, in general, both the physical and virtual dimensions d, D depend on the site index i. The product operator $\otimes_{i\leq N}\mathcal{P}_i$ then maps the tensor product of all entangled pairs to a state in the physical many-body Hilbert space $\otimes_{i\leq N}\mathcal{H}_i$.

This construction is motivated by the well-known AKLT model [2], which was the first model proposed to describe the *Haldane phase* for a spin-1 chain. As the local two-site Hamiltonian, one takes the projector $\mathcal{P}^{(2)} : \mathbb{C}^3 \otimes \mathbb{C}^3 \to \mathbb{C}^5$ on the spin-2 subspace. The groundstate can then be constructed (Fig. 1.3) as the kernel of this projector by placing the maximally entangled singlet state

$$|\alpha\rangle \equiv \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \tag{1.14}$$

between every pair of neighbouring sites and, then, projecting onto the spin-1 subspace at every site.

From the maximally entangled pair construction, we can easily deduce the area law for entanglement entropy. First of all, we recall the so-called 'monogamy of entanglement' [15],

[3] In fact the upper limits of the indices j_i in Eq. (1.9) are also called the (local) bond dimensions.

[4] The name 'projector' should not be taken too seriously from a mathematical viewpoint as the operators do not satisfy $\mathcal{P}^2 = \mathcal{P}$.

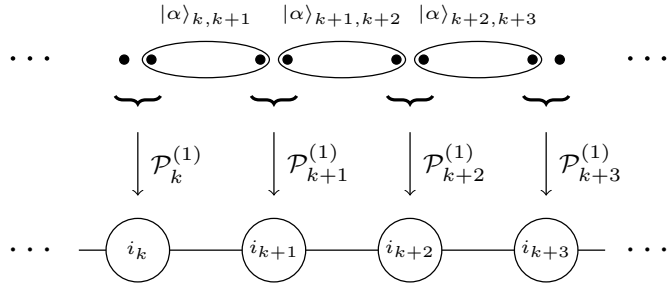


Figure 1.3: Ground state construction of AKLT model.

i.e. the constituents of a maximally entangled pair cannot be entangled to a third particle. This implies that an upper bound[5] to the entanglement entropy between a subregion and its environment can be calculated by assuming that the subregion is correlated to the rest of the system exclusively through the maximally entangled pairs. To calculate the entanglement entropy, we thus only have to look at how many entangled pairs are cut by the boundary of the region. The entanglement entropy of a single maximally entangled state of dimension D is:

$$\begin{aligned} S(\rho_{\mathrm{ME}}) &= -\operatorname{tr}\left(\rho_{\mathrm{ME}} \ln \rho_{\mathrm{ME}}\right) \\ &= -\sum_{i=1}^{D} \frac{1}{D} \ln\left(\frac{1}{D}\right) \\ &= \ln(D)\,, \end{aligned} \tag{1.15}$$

where $\rho_{\mathrm{ME}} = \sum_{i=1}^{D} \frac{1}{D} |i\rangle \langle i|$. Because the projected pair construction uses 2-site projectors, the maximal amount of pairs through which the subregion and environment are entangled is given by the length of the boundary L (see Fig. 1.4) and, if we have chosen a bond dimension D, the entanglement entropy is bounded as follows:

$$S(\rho) \leq \ln\left(D^L\right) = L \ln(D)\,. \tag{1.16}$$

For a 1D chain (the case of MPS), the boundary always consists of two sites and, hence, the upper bound of $S(\rho)$ is even independent of the system size.

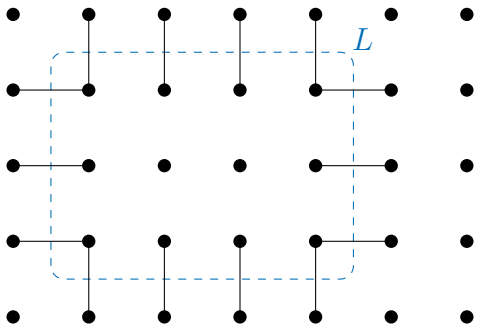


Figure 1.4: Subregion of lattice (in 2D) with boundary length $L = 14$.

Matrix product states have a long history. The translation-invariant case can be traced back to the work on *finitely correlated states* [20]. Eventually, they were also found to

[5]The local projectors cannot increase the entanglement.

constitute the underlying structure of the famous *density matrix renormalization group* algorithm [49, 64] which is still the most succesful method for simulating equilibrium properties of quantum systems (on a lattice). At the same time, they also form the backbone of an important algorithm for the time-evolution of quantum systems, the *time-evolving block decimation* (TEBD) algorithm [16]. Recently, they have even been applied to fermionic systems [7] and quantum gauge theories [9].

1.2.2 Injective MPS

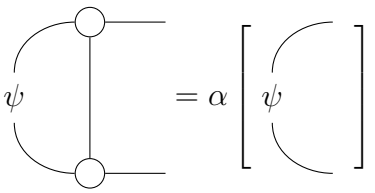
An important subclass of matrix product states is given by the injective matrix product states. Multiple equivalent definitions exist (see for example [47]), but here we will consider only the two most important ones.

Definition 1.1 (Injective MPS). An MPS A is said to be injective if there exists a number $n \in \mathbb{N}_0$, called the *injectivity length*, such that after blocking by n sites the (blocked) matrices $A^{i_1}[1] \cdots A^{i_n}[n]$, where i_k runs over the physical dimension, span the full matrix algebra $M_D(\mathbb{C})$.

Consider the operator $\mathbb{E}[A] = \sum_i^d A^i \otimes \overline{A^i}$, called the *transfer operator*[6]. An alternative definition of injective MPS is based on the spectrum of this operator:

Definition 1.2 (Injective MPS, bis). An MPS is said to be injective if the associated transfer operator has a unique maximal eigenvalue, i.e. $\mathbb{E}$ has a unique eigenvalue λ such that $|\lambda| = \rho(\mathbb{E})$. We will always assume that the spectral radius $\rho(\mathbb{E})$ is normalized.

So in graphical notation we have that A is injective if there exists only one eigenvector ψ such that:



with $|\alpha| = 1$. (1.17)

The injectivity of an MPS implies a couple of useful relations. Consider a matrix X which commutes with all the matrices A^i. Because the A^i span (potentially after blocking) all of $M_D(\mathbb{C})$, we know that X has to be an element of the center of the square complex matrices. It is known that the center $Z(M_D(\mathbb{C}))$ consists only of the scalar multiples of the identity and hence we obtain:

$$\Big(\forall i \leq d : [X, A^i] = 0\Big) \implies X = \lambda \mathbb{1}, \lambda \in \mathbb{C} \tag{1.18}$$

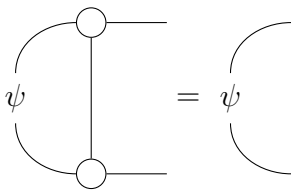
One can generalize this property by considering an equation of the form

$$XA^i = e^{i\varphi} A^i X \tag{1.19}$$

where X and φ are independent of the index $i \leq d$. For an injective MPS we know that,

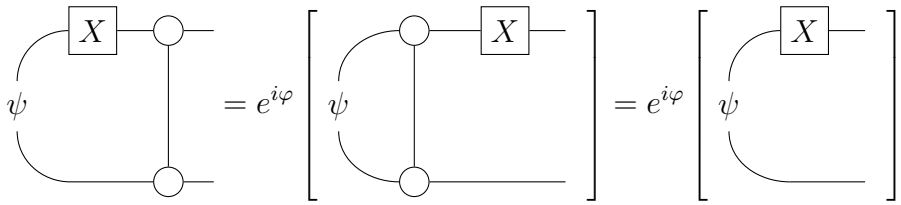
[6] See for example [24] for the definition and applications of the transfer operator and the relation to the structure of matrix product states.

by definition, Eq. (1.17) is valid:



(1.20)

Using Eq. (1.19), we can, however, show that the eigenvector ψ multiplied by X from the left is also an eigenvector of the transfer operator with an eigenvalue of modulus 1:



(1.21)

By injectivity, this is only possible if $\varphi = 0$ and $X = \lambda\mathbb{1}$. In a similar way, we can prove the following statement which will be a cornerstone of this thesis.

Theorem 1.1 (Fundamental theorem). *Let the rank-3 tensor A define an injective translation-invariant MPS. If for every physical index $i \leq d$, where d is the dimension of the physical Hilbert space, the condition*

$$e^{i\chi} Y A^i Y^{-1} = e^{i\varphi} X A^i X^{-1} \tag{1.22}$$

is satisfied, we can conclude two things:

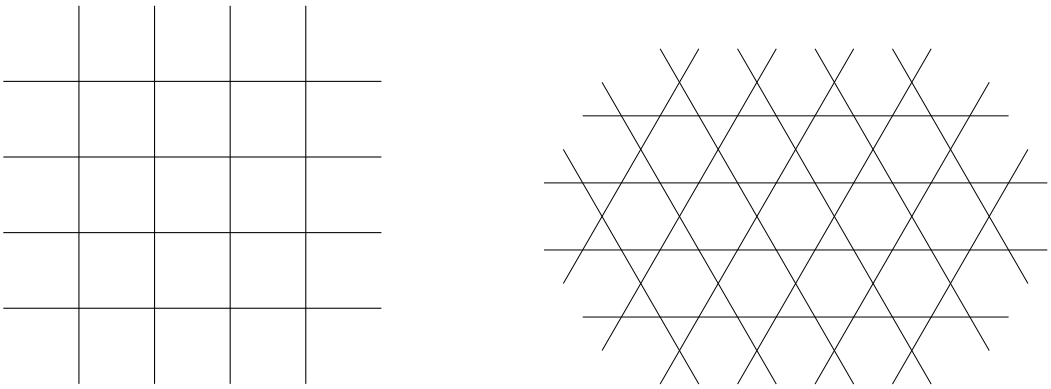
1. $\chi - \varphi = 0 \mod 2\pi$, *and*
2. $X^{-1}Y = e^{i\psi}\mathbb{1}$ *for some* $\psi \in \mathbb{R}$.

For a general statement and treatment, see [17, 24].

1.2.3 Higher dimensions

The maximally entangled pair construction can easily be generalized to higher dimensions and gives rise to so-called *projected-entangled pair states* (PEPS) [57, 59]. These form the immediate generalization of MPS in dimension 2 and higher. Because in 2D there exist nontrivial uniform tilings (see Fig. 1.5 for two examples), a richer theory emerges. However, the construction always proceeds in the same way.

This of course implies that, in general, PEPS have a lot of properties in common with matrix product states [45]. For example, they still satisfy an area law for the entanglement entropy and, if we allow a high enough bond dimension, they can approximate any state with arbitrary precision. However, there are important differences. While MPS cannot describe a critical system, i.e. a system with polynomial (algebraic) correlation functions, a higher-dimensional ($d \geq 2$) PEPS can. The numerical implementations are also different. For example, PEPS cannot be efficiently contracted without losing exactness nor does there exist a canonical (orthonormal) form. In general, one has to resort to approximations when computing expectation values and correlation functions with PEPS.



(a) Square lattice. (b) Kagome lattice.

Figure 1.5: Uniform tilings of 2D space.

In addition to the MPS-like tensor networks, which are the most relevant for the ideas explained in this thesis, there exists a variety of other structures. Important examples are the *multi-scale entanglement renormalization ansatz* (MERA) [61] and the *tree tensor networks* (TTN) [51]. The former is strongly related to entanglement renormalization methods and is especially suited for simulating critical systems (even in 1D), while the latter is useful for simulating systems with nonlocal interactions [43]. In contrast to PEPS, these tensor networks allow for efficient and exact calculations of expectation values.

1.3 Symmetries

In general, all physical systems we encounter in nature exhibit some kind of symmetry, be it a spatial symmetry like reflection symmetry or an internal symmetry like the spin rotation symmetry in the Heisenberg chain. Solving the dynamics of these systems often simplifies if we take the symmetries into account. The best example being an integrable systems where the solution can be constructed solely from the conserved quantities associated to the symmetries through Noether's theorem.

Likewise, in a variational approach to many-body problems, it is useful to start from an ansatz that already has the same symmetry group as the system we want to describe (or a subgroup thereof in the case of symmetry breaking) because this reduces the number of a priori possible solutions. Therefore, part of this thesis will be dedicated to finding certain constraints on the variational ansatz (MPS in this case), or even to construct a manifestly symmetric form that that can be used as a starting point for numerical methods.

1.3.1 Symmetry-protected topological order

Before the advent of topological phenomena in physics, the general framework for understanding phases and phase transitions was the Landau–Ginzburg paradigm. In this framework, the primary quantity is the *order parameter* ξ (or the Higgs field in field theories). This parameter can, for example, be used to give a distinction between the disordered symmetric phase ($\xi = 0$) and the ordered symmetry-broken phase ($\xi \neq 0$). From the group theory point of view one looks at the symmetry group G of a class of Hamiltonians describing the system. The different phases are then classified by the quotient groups G/H, where H is the symmetry group of the symmetry-broken state describing a

certain phase. The main example being the Bardeen–Cooper–Schrieffer (BCS) description of superconductivity [4], where the formation of Cooper pairs breaks the U(1) symmetry group to a discrete $\mathbb{Z}_2$ subgroup.

However, in the last couple of decades of the 20th century, physical phenomena were discovered in which different phases had the same symmetries and, hence, could not be explained by the Landau–Ginzburg paradigm. One of the most important examples is the fractional quantum Hall effect [39, 54]. To accompany these discoveries, the concept of topological order was introduced.

Definition 1.3 (Topological order). Two gapped quantum states $|\psi_{1,2}\rangle$ are said to be in the same phase if they can be realized as the ground state of two Hamiltonians $\hat{H}_{1,2}$ such that there exists a (smooth[7]) homotopy $\hat{H}(t)$ between $\hat{H}_1$ and $\hat{H}_2$, i.e. there exists a continuous path of gapped Hamiltonians between $\hat{H}_1$ and $\hat{H}_2$.

A different, but equivalent, definition is that two quantum states are in the same phase if there exists a local unitary (LU) transformation[8] (local quantum circuit) connecting the two states [12]. A state with trivial topological order is then a quantum state which can be transformed into a product state by such a quantum circuit.

In the above definitions, there was no mention of the possible symmetries of the system and accordingly this type of order is called *intrinsic* topological order. There also exists a notion of *symmetry-protected* topological (SPT) order which does take into account the symmetries of the system. These are the phases with which we are concerned in this thesis and they are defined slightly more general than the intrinsic case.

Definition 1.4 (SPT order). A quantum state belongs to a nontrivial SPT phase if it cannot be transformed to a product state by an LU tranformation that preserves the symmetry of the system. It should be noted that SPT phases are not truly intrinsic topological phases because it is possible to find an LU transformation which breaks the symmetry but maps the state to a product state.

In the case of injective MPSs, it has been shown [48] that a symmetry constraint on the physical level can be translated to a constraint on the virtual level. By using these relations together with the group structure of the symmetries, one can construct a classification of SPT phases. This classification is based on the algebraic framework of *group cohomology* [11, 14]. The whys and the hows of this cohomological approach are explained in detail in Chapter 2, but essentially one uses the content of Theorem 1.1 to extract topological indicators which follow from the conditions of group cohomology. It has been shown that this data only depends on the phase of the system and not on the specific state itself [13] and thus by finding all indicators we find a classification of all SPT phases.

The theory becomes even more interesting when we consider not only on-site symmetry groups, but also nontrivial lattice transformations (such as reflections or rotations) that leave the system invariant. In this thesis, we will limit ourselves to one spatial dimension

[7] Meaning that the energy gap does not close.

[8] This is defined as the finite time evolution generated by a local Hamitonian.

and, although there are not that many possibilities, it can serve as a good introduction to get acquainted with the nontrivial consequences of lattice symmetries before moving on to the more exotic cases in two dimensions and higher.

1.4 Cohomology theory

In general, (co)homology theories are used for obstruction and classification problems, both in physics and mathematics, by reducing problems in, for example, geometry to, often simpler, problems in algebra. This line of work started roughly around the middle of 19th century with the work of Riemann on the concept of *genus* [40]. This work was continued by people like Betti and Poincaré. They founded what would now be called simplicial homology. The first ideas leading up to the birth of cohomology can be traced back to the work of Poincaré on Poincaré duality (e.g. Analysis Situs, 1895)[9]. The relation with algebra was only formally made by Noether during her lectures in the 1920s, but until the 1940's (co)homology theory mostly remained a part of (algebraic) topology. However, around the time of World War II[10], these techniques were applied to problems in algebra, which brought about a revolution. Homological algebra [1] was born and (co)homology theories really started to arise everywhere, one example being group cohomology theory, which will be of interest in thesis.

Now, although the framework of cohomology theory might seem to be rather esoteric and abstract, it has a lot of applications in physics. For example, group cohomology, which we introduce in the next chapter, is used to classify both crystallographic groups and SPT phases (both in arbitrary dimensions). Other examples in the field of condensed matter theory are the classification of *topological insulators* and *superconductors* by Kitaev using *K-theory*[11] [38] or the classification of topologically ordered systems using *Chern numbers* as in the quantum Hall effect [3]. But even outside this field, cohomology theories pop up everywhere: in quantum field theory, both the *BRST quantization procedure* [5] and the framework of *gauge theories* (e.g. Yang–Mills theory) use cohomology theory. One does not even have to stroll this far into the world of theoretical physics to encounter cohomology. Even simple things such as the concept of mass in quantum mechanics [29], Maxwell's equations[12] or even Kirchhoff's laws of electrical currents[13] [63] can be understood in the context of cohomology theory.

[9] However, this paper was flawed (he and others corrected it later) and the true cohomological form of Poincaré duality was only introduced in 1930 by work of Čech and Whitney.

[10] One of the most important techniques (sheaf cohomology and spectral sequences) was introduced by Leray while he was detained in a prisoner-of-war camp.

[11] This is what algebraic topologists would call a *generalized* cohomology theory.

[12] This is closely related to cohomology theory behind Yang–Mills theories.

[13] Even as soon as 1923.

Chapter 2

Cohomological SPT classification

In general, when we start learning quantum mechanics, we are told that the space of possible states is a (*separable*) Hilbert space $\mathcal{H}$ (over the complex numbers) and the physical operations are implemented by linear operators in $\mathrm{GL}(\mathcal{H})$ or even in $\mathrm{U}(\mathcal{H})$. A representation of a symmetry group[1] G is then given by a representation of G, i.e. a group morphism $G \to \mathrm{GL}(\mathcal{H})$.

However, as is well-known, the state of a quantum system is only defined up to an arbitrary phase $e^{i\varphi} \in \mathrm{U}(1)$. So the correct setting to work in is not the Hilbert space $\mathcal{H}$ but its projectivization $\mathbb{P}(\mathcal{H}) = \mathcal{H}/\mathbb{C}^\times$, where $\mathbb{C}^\times$ denotes the invertible (nonzero) complex numbers. Due to this $\mathrm{U}(1)$-invariance, the requirement that symmetries are implemented by unitary operators is too strong as was shown by Wigner [65]. The correct notion is that of a *ray* or *projective* representation[2], i.e. a group morphism $G \to \mathrm{PGL}(\mathcal{H})$. The general property of a projective representation (when viewing it as a function into the general linear group) is:

$$V(gh) = e^{i\omega(g,h)}V(g)V(h) \tag{2.1}$$

for every two group elements g, h. In Section A.2 in the appendix, a more formal introduction to the relation between (projective) representations and group cohomology is given.

2.1 On-site symmetries

Consider a translation-invariant (TI) system on a 1D lattice Λ with an on-site symmetry group G. Given a representation[3] $\widehat{U} : G \to \mathrm{GL}(\mathcal{H}_1)$ on the single-site Hilbert space, a representation $G \to \mathrm{GL}(\mathcal{H})$ on the full lattice is constructed as $\widehat{U}(g) \otimes \cdots \otimes \widehat{U}(g)$. (We do not go into detail about how the tensor product $\mathcal{H} = \bigotimes_{i\in\Lambda} \mathcal{H}_1$ can be given the structure of a Hilbert space in a well-defined way.)

[1] See Section A.1.2 in the appendix for more information.

[2] In fact, his theorem also allows for antilinear operators, a fact which will become important for our story later on.

[3] The reason why the representation on the physical level is required to be linear instead of projective can be found in [13].

Because all MPS tensors are equal (see Section 3.2.1 below), the on-site symmetries are, taking into account the projective nature of the state space, implemented in the following way [48]:

$$\sum_j U_{ij}(g)A^j = \varphi(g)X(g)^{-1}A^iX(g) \tag{2.2}$$

for all $g \in G$. Here, $U : G \to \mathrm{GL}(\mathcal{H})$ is the linear representation of G on the physical single-site Hilbert space as constructed above and the morphism $\varphi : G \to \mathrm{U}(1) \subset \mathrm{GL}(\mathcal{H})$ forms a 1D linear representation of G.

Using the graphical notation, the equation above is visualised as in diagram 2.1 below. This way it is clearer that a symmetry operation $\widehat{U}_g$ on the physical level is equivalent to an operation X_g on the virtual level (up to a phase factor which was drawn in the diagram).

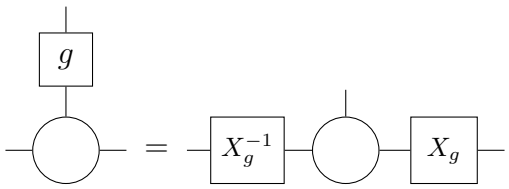


Figure 2.1: MPS symmetry.

If the operators $X(g)$ are required to satisfy the above relation, they do not have to form a linear representation, i.e. they do not have to satisfy $X(gh) = X(g)X(h)$. By the fundamental theorem 1.1, they are also allowed to form a projective representation: $X(gh) = e^{i\omega(g,h)}X(g)X(h)$ and, hence, this is entirely consistent with the discussion of Wigner's theorem in the introduction to this chapter.

One of the defining properties of a group is the associativity axiom and, because a (projective) representation is a group morphism, we obtain the following condition on the function $\omega : G \times G \to S^1 \cong \mathbb{R}/\mathbb{Z}$:

$$\omega(g_1g_2, g_3) + \omega(g_1, g_2) = \omega(g_1, g_2g_3) + \omega(g_2, g_3)\,, \tag{2.3}$$

where equality is understood up to a multiple of 2π.[4] This condition is called the **cocycle condition**. There is, however, some freedom in the choice of the function ω. We can rescale the representation ρ as $\rho'(g) = e^{i\varphi(g)}\rho(g)$ and this induces the rescaling $\omega'(g,h) = \omega(g,h) + \varphi(gh) - \varphi(g) - \varphi(h)$. The last three terms in ω' form a function which is known as a **coboundary**.

From Section A.2, it follows that the set of cocycles modulo the set of coboundaries forms a group $H^2(G; \mathrm{U}(1))$. Picking an element in this group is equivalent to picking a certain projective representation of G, so the different SPT phases corresponding to an on-site symmetry are partially classified by the cohomology group $H^2(G; \mathrm{U}(1))$ with trivial action.

These classes can also be given a more physical interpretation. Consider the entangled pair construction of an MPS given in Section 1.2.1, where every site is decomposed as a pair

[4] In the literature, one often encounters this formula in its multiplicative form where ω is then understood as a function $G \times G \to \mathrm{U}(1)$. However, due to the isomorphism $S^1 \cong \mathrm{U}(1)$ these two perspectives are equivalent.

of states. Now, consider a finite subchain of the 1D lattice (in the case of open boundary conditions one can take the whole lattice) as indicated by a yellow box in Fig. 2.2. In the bulk of the lattice, the phase factors $e^{i\omega}$ and $e^{-i\omega}$ cancel out, but on the boundaries they remain. For systems with open boundary conditions, these give rise to so-called *edge modes/states*.

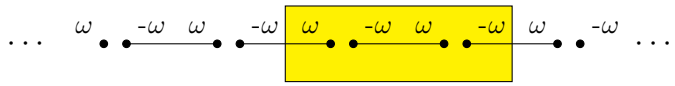


Figure 2.2: Finite chain.

The second part of the classification follows from the presence of the linear representation φ in Eq. (2.2). The defining relation of a 1D linear representation is:

$$\varphi(gh) = \varphi(g) + \varphi(h) \tag{2.4}$$

and this is exactly the same as Eq. (A.15) for a 1-cocycle (again with trivial action). Hence, the remaining part of the classification of SPT phases with on-site symmetry groups for TI systems is given by the first cohomology group $H^1(G; \mathrm{U}(1))$.

2.1.1 Gauge matrices

Here, we give some explanation on what the structure of the gauge matrices X is. Above, we only required them to be invertible, but, in fact, a stronger condition can be derived. For a general (injective) MPS, it can be proven [46] that there always exist a gauge transformation such that we obtain the following condition:

$$\sum_{i=1}^{d_m} \left(A^i[m]\right)^\dagger A^i[m] = \mathbb{1}\,, \tag{2.5}$$

where d_m is the physical dimension of the site m. This form is called the *left canonical form*[5]. Now, consider an on-site symmetry transformation

$$A^i \longrightarrow \tilde{A}^i = \sum_{j=1}^{d} U_{ij} A^j = e^{i\varphi} X^{-1} A^i X\,. \tag{2.6}$$

The formula above then changes accordingly:

$$\begin{aligned}
\sum_{i=1}(A^i)^\dagger A^i \longrightarrow \sum_{i=1}(\tilde{A}^i)^\dagger \tilde{A}^i &= \sum_{i=1}\sum_{k,l=1} \overline{U_{ik}} (A^k)^\dagger U_{il} A^l \\
&= \sum_{i=1}\sum_{k,l=1} U^\dagger_{ki} (A^k)^\dagger U_{il} A^l \\
&= \sum_{k,l=1} \delta_{kl} (A^k)^\dagger A^l \\
&= \sum_{k=1} (A^k)^\dagger A^k \\
&= \mathbb{1}
\end{aligned} \tag{2.7}$$

[5] or *left orthonormal form*

and, hence, the transformed MPS is still in the left canonical form. However, we could also expand it as follows:

$$\sum_{i=1}^{d}(A^i)^\dagger A^i \longrightarrow \sum_{i=1}^{d} X^\dagger (A^i)^\dagger (X^{-1})^\dagger X^{-1} A^i X \,. \tag{2.8}$$

Now, if these two expressions ought to be equal, we should have the following condition:

$$\sum_{i=1}^{d}(A^i)^\dagger (X^{-1})^\dagger X^{-1} A^i = (X^{-1})^\dagger X^{-1} \,. \tag{2.9}$$

This implies that X should be unitary.

With the following sections in mind, we will also consider the cases of time-reversal and reflection invariance. For time-reversal symmetry, we obtain the following transformation rule:

$$A^i \longrightarrow \tilde{A}^i = \sum_{j=1}^{d} U_{ij}\overline{A^j} = e^{i\varphi} X^{-1} A^i X \,. \tag{2.10}$$

We can then perform a calculation similar to the on-site case:

$$\begin{aligned}
\sum_{i=1}(A^i)^\dagger A^i \longrightarrow \sum_{i=1}(\tilde{A}^i)^\dagger \tilde{A}^i &= \sum_{i=1}\sum_{k,l=1} \overline{U_{ik}(A^k)^\dagger} U_{il}\overline{A^l} \\
&= \sum_{i=1}\sum_{k,l=1} U^\dagger_{ki}\overline{(A^k)^\dagger} U_{il}\overline{A^l} \\
&= \sum_{k,l=1} \delta_{kl}\overline{(A^k)^\dagger A^l} \\
&= \sum_{k=1} \overline{(A^k)^\dagger A^k} \\
&= \overline{\sum_{k=1}(A^k)^\dagger A^k} \\
&= \mathbb{1} \,.
\end{aligned} \tag{2.11}$$

So, a time-reversal operation leaves the MPS in left canonical form and we obtain that the gauge matrix in the case of time-reversal symmetries is also unitary.

The last case to consider is that of a reflection. Of course, nature will not stay kind to us and we will see that the gauge matrix for a reflection symmetry does not have to be unitary. For reflection symmetry, we get the following transformation rule:

$$A^i \longrightarrow \tilde{A}^i = \sum_{j=1}^{d} U_{ij}(A^j)^t = e^{i\varphi} X^{-1} A^i X \,. \tag{2.12}$$

We can now again check if the canonical form is left unchanged under this transformation:

$$\begin{aligned}
\sum_{i=1}(A^i)^\dagger A^i \longrightarrow \sum_{i=1}(\tilde{A}^i)^\dagger \tilde{A}^i &= \sum_{i=1}\sum_{k,l=1} \overline{U_{ik}A^k} U_{il}(A^l)^t \\
&= \sum_{i=1}\sum_{k,l=1} U^\dagger_{ki}\overline{A^k} U_{il}(A^l)^t \\
&= \sum_{k,l=1} \delta_{kl}\overline{A^k}(A^l)^t
\end{aligned}$$

$$= \sum_{k=1} \overline{A^k}(A^k)^t$$
$$= \sum_{k=1} \left(A^k(A^k)^\dagger\right)^t . \tag{2.13}$$

Now, by bringing the transpose outside of the summation, we do not get the expression of the left canonical form, but it is still very similar. This similarity is explained by noting that for an MPS there also exists a *right canonical form* given by following condition:

$$\sum_{i=1}^{d} A^i(A^i)^\dagger = \mathbb{1} . \tag{2.14}$$

So, we see that a reflection interchanges the left and right canonical forms. To derive that the gauge matrix for reflection symmetries is unitary, we should thus need that the MPS is both in left and right canonical form. Because not every MPS satisfies this strong condition, we will, in general, not assume the gauge matrices associated to a reflection symmetry to be unitary.

2.2 Time-reversal

For on-site symmetries, we obtained an SPT classification based on group cohomology with a trivial action. Including time-reversal as a symmetry operation will force us to work with cohomology with nontrivial actions. In this paragraph, we will determine the actions and generalize the classification to this more general setting. To this intent, we consider a general symmetry group G^T that contains a time-reversal generator of order 2. In particular, we will assume the form $G \times \mathbb{Z}_2$, where G is the on-site symmetry group. A general element can be written as $g_\pm$, where the subscript $-$ indicates that the element contains a time-reversal.

At this stage, we will not give a relation to projective representations. We will just start with a physically motivated relation on the gauge matrices $X(g)$ and in the last section of this chapter, we will clarify what kind of representation the gauge matrices form. If we denote by $\widehat{\mathcal{C}}_g$ the operation of taking the complex conjugate if $g = g_-$, the gauges ought to satisfy the following relation:

$$X(gh) = e^{i\omega(g,h)} X(g)\widehat{\mathcal{C}}_g\Big[X(h)\Big] , \tag{2.15}$$

where ω is still an arbitrary function $G \times G \to S^1$ at this point. This result can be derived if all symmetry operations are implemented as $U(g)\hat{\mathcal{C}}_g$ on the physical level.

Proof. To include time-reversal symmetry, we first have to modify Eq. (2.2):

$$\sum_j U_{ij}(g)\hat{\mathcal{C}}_g[A_j] = \varphi(g)X(g)^{-1}A^i X(g) . \tag{2.16}$$

Acting with a product $gh \in G^T$ (here, we choose h to be purely on-site) gives:

$$\varphi(gh)X(gh)^{-1}A^i X(gh) = \varphi(g)\hat{\mathcal{C}}_g\Big[\varphi(h)\Big]\hat{\mathcal{C}}_g\Big[X(h)^{-1}\Big]X(g)^{-1}A^i X(g)\hat{\mathcal{C}}_g\Big[X(h)\Big] . \tag{2.17}$$

Comparing both sides gives us Eq. (2.15) as desired (again by applying the fundamental theorem 1.1). A second consequence is that the phase factors $\varphi(g)$ do not form a 1D

linear representation anymore. They now satisfy a more general 1-cocyle condition:

$$\varphi(gh) = \varphi(g) + \beta(g)\varphi(h)\,, \tag{2.18}$$

where the action $\beta : G^T \to \mathbb{Z}_2 : g_\pm \mapsto \pm 1$ is induced by complex conjugation.

To find the generalization of the projective representations, we apply the same procedure as for on-site symmetries. If we act on the MPS tensor A^i with a triple product $ghk \in G^T$, we can expand it in two ways using the associativity property. By the defining equation 2.15, we obtain the following equality:

$$\begin{aligned} X(ghk) &= e^{i\omega(gh,k)} X(gh)\widehat{\mathcal{C}}_{gh}\Big[X(k)\Big] \\ &= e^{i\omega(gh,k)+i\omega(g,h)} X(g)\widehat{\mathcal{C}}_g\Big[X(h)\Big]\widehat{\mathcal{C}}_{gh}\Big[X(k)\Big]\,. \end{aligned} \tag{2.19}$$

On the other hand, associativity also requires this equation to be equal to:

$$\begin{aligned} X(ghk) &= e^{i\omega(g,hk)} X(g)\widehat{\mathcal{C}}_g\Big[X(hk)\Big] \\ &= e^{i\omega(g,hk)} X(g)\widehat{\mathcal{C}}_g\left[e^{i\omega(h,k)} X(h)\widehat{\mathcal{C}}_h\Big[X(k)\Big]\right]\,. \end{aligned} \tag{2.20}$$

We can combine the occurrences of the operation t in a general product $gh \in G^T$ such that $\widehat{\mathcal{C}}_g\widehat{\mathcal{C}}_h = \widehat{\mathcal{C}}_{gh}$ and, hence, the above two expressions are equal if and only if the following relation holds for all group elements $g, h, k \in G^T$:

$$\omega(gh,k) + \omega(g,h) = \omega(g,hk) + \alpha_T(g)\omega(h,k)\,. \tag{2.21}$$

This is a 2-cocycle condition with the action $\alpha_T : G^T \to \mathbb{Z}_2 : g_\pm \mapsto \pm 1$ induced by complex conjugation. □

We can conclude that the SPT classification (for TI systems) in the case of on-site symmetries together with time-reversal symmetry is characterized by an element in $H^2_{\alpha_T}(G^T; \mathrm{U}(1))$ and an element in $H^1_\beta(G^T; \mathrm{U}(1))$.

2.2.1 Physical representation

As in previous section on on-site symmetries we should also consider which representations are allowed on the physical level. By assumption, the time-reversal operator is of order 2, so to find the possible representations, we have to calculate $H^2_{\alpha_T}(\mathbb{Z}_2; \mathrm{U}(1))$. The cocycle equations in this case are:

$$\left\{\begin{array}{rcrcrcrcl} \alpha_T(e)\omega(e,e) & - & \omega(e,e) & + & \omega(e,e) & - & \omega(e,e) & = & 0 \\ \alpha_T(e)\omega(e,t) & - & \omega(e,t) & + & \omega(e,t) & - & \omega(e,e) & = & 0 \\ \alpha_T(e)\omega(t,e) & - & \omega(t,e) & + & \omega(e,t) & - & \omega(e,t) & = & 0 \\ \alpha_T(e)\omega(t,t) & - & \omega(t,t) & + & \omega(e,e) & - & \omega(e,t) & = & 0 \\ \alpha_T(t)\omega(e,e) & - & \omega(t,e) & + & \omega(t,e) & - & \omega(t,e) & = & 0 \\ \alpha_T(t)\omega(e,t) & - & \omega(t,t) & + & \omega(t,t) & - & \omega(t,e) & = & 0 \\ \alpha_T(t)\omega(t,e) & - & \omega(e,e) & + & \omega(t,t) & - & \omega(t,t) & = & 0 \\ \alpha_T(t)\omega(t,t) & - & \omega(e,t) & + & \omega(t,e) & - & \omega(t,t) & = & 0 \end{array}\right. \tag{2.22}$$

Using the normalization of the cocycles (see Section A.2.1 in the appendix), we see that only the last condition is nontrivial. Solving it gives us:

$$\omega(t,t) \in \{0,\pi\}\,. \tag{2.23}$$

We thus obtain that $H^2_{\alpha_T}(\mathbb{Z}_2;\mathrm{U}(1)) \cong \mathbb{Z}_2$, which in turn implies that the time-reversal subgroup has only two projective representations corresponding to $\widehat{T}^2 = \pm\mathbb{1}$ (with $\widehat{T}$ the physical representation of $t \in \mathbb{Z}_2$).

Now, let us check if both possibilities are physically realizable. The first case we should check is for a uniform MPS. In this case, we obtain:

$$\sum_j T_{ij}\overline{A^j} = e^{i\varphi}X^{-1}A^iX\,. \tag{2.24}$$

Performing a second time-reversal then gives:

$$(\pm 1)A^i = \overline{X^{-1}}X^{-1}A^iX\overline{X}\,. \tag{2.25}$$

From Theorem 1.1, it is immediately clear that only the $+1$ case is physically possible for an injective uniform MPS (cf. [13]). But what about a system which is only translation invariant up to a 2-site translation (this is relevant for the next chapter)? In this case, we obtain:

$$\begin{aligned}\sum_j T_{ij}\overline{A^j} &= e^{i\varphi_A}X_A^{-1}A^iX_B \quad ,\\ \sum_j T_{ij}\overline{B^j} &= e^{i\varphi_B}X_B^{-1}B^iX_A \quad ,\end{aligned} \tag{2.26}$$

or, after a second time-reversal:

$$\begin{aligned}(\pm 1)A^j &= \overline{X_A^{-1}}X_A^{-1}A^iX_B\overline{X_B}\,,\\ (\pm 1)B^j &= \overline{X_B^{-1}}X_B^{-1}B^iX_A\overline{X_A}\,.\end{aligned} \tag{2.27}$$

However, in this case Theorem 1.1 is not readily applicable. We first need to block the two distinct sites. But, by doing this, the phase factor of the physical projective representation $\widehat{T}$ will cancel out, i.e. $(\pm 1)^2 = 1$, and, hence, no obstruction can be obtained for the -1 case. This implies that for a system with a 2-site unit cell, we should also allow the case $\widehat{T}^2 = -\mathbb{1}$ (also cf. [13]).

2.3 Reflection symmetry

Analogous to the previous section, we can consider a symmetry group G^R that contains a spatial reflection operation. We will now perform a short calculation to derive a result similar to Eq. (2.15). As in the case of time-reversals, we will denote an element $g \in G^R$ containing a reflection operation by g^r. We will use the fact that in our framework reflections are implemented by taking transposes of MPS matrices. This result will be proven in the next chapter (see Eq. (3.21)).

Now, consider the product $gh \in G^R$ (we again choose h to be purely on-site). Acting with

this product on an MPS tensor A^i gives the following equation:

$$\sum_j U_{ij}(gh)\left(A^j\right)^{t_g} = \varphi(gh)X(gh)^{-1}A^iX(gh)\,, \tag{2.28}$$

where the parametric transposition operator $(\cdot)^{t_g}$ only tranposes its argument if $g \equiv g^r$. We could also first act with h and then with g:

$$\sum_j U_{kj}(h)A^j = \varphi(h)X(h)^{-1}A^kX(h) \tag{2.29}$$

$$\implies \sum_k U_{ik}(g)\left(\sum_j U_{kj}(h)A^j\right)^{t_g} = \varphi(g)\varphi(h)\hat{\mathcal{R}}_g\Big[X(h)^{-1}\Big]X(g)^{-1}A^iX(g)\hat{\mathcal{R}}_g\Big[X(h)\Big]\,,$$

where the operator $\hat{\mathcal{R}}_g$, induced by the parametric transposition operator, transposes and inverts its argument if $g \equiv g^r$. Combining these relations, we see that the gauge matrices associated to symmetries in G^R behave in the following way:

$$X(gh) = e^{i\omega(g,h)}X(g)\widehat{\mathcal{R}}_g\Big[X(h)\Big]\,. \tag{2.30}$$

Now, we can derive the cocycle conditions as in the case of time-reversal. Consider an arbitrary triple product $ghk \in G^R$. By associativity, we can expand this product in two ways:

$$\begin{aligned} X(ghk) &= e^{i\omega(gh,k)}X(gh)\hat{\mathcal{R}}_{gh}\Big[X(k)\Big] \\ &= e^{i\omega(gh,k)+i\omega(g,h)}X(g)\hat{\mathcal{R}}_g\Big[X(h)\Big]\hat{\mathcal{R}}_{gh}\Big[X(k)\Big] \end{aligned} \tag{2.31}$$

or

$$\begin{aligned} X(ghk) &= e^{i\omega(g,hk)}X(g)\hat{\mathcal{R}}_g\Big[X(hk)\Big] \\ &= e^{i\omega(gh,k)}X(g)\hat{\mathcal{R}}_g\left[e^{i\omega(g,h)}X(h)\hat{\mathcal{R}}_h\Big[X(k)\Big]\right]\,. \end{aligned} \tag{2.32}$$

Using the group relations of G^R, we can again deduce that $\hat{\mathcal{R}}_g\hat{\mathcal{R}}_h = \hat{\mathcal{R}}_{gh}$ and, hence, we obtain the same cocycle condition for ω as for G^T:

$$\omega(gh,k) + \omega(g,h) = \omega(g,hk) + \alpha_R(g)\omega(h,k)\,. \tag{2.33}$$

However, for the phase factors φ, it should be clear from the above calculations that in the case of reflections we do not obtain a nontrivial cocycle condition and, hence, these form an ordinary 1D linear representation:

$$\varphi(gh) = \varphi(g)\varphi(h) \tag{2.34}$$

for all $g, h \in G^T$.

We can conclude that the SPT classification (for TI systems) in the case of on-site symmetries together with reflection symmetry is characterized by an element in $H^2_{\alpha_R}(G^R;\mathrm{U}(1))$ and an element in $H^1(G^R;\mathrm{U}(1))$.

At last, we want to remark that for unitary gauges[6] taking the transpose inverse is the

[6]For on-site symmetries and time-reversal symmetry, we can always choose the gauge matrices to be unitary by working, for example, in the left canonical gauge. However, for reflections, which interchange

same as taking the complex conjugate and, hence, $\hat{\mathcal{R}}$ and $\hat{\mathcal{C}}$ coincide in these cases.

2.4 Time-reversal and reflection symmetry

We can now combine the results derived in the last two sections in a straightforward manner. Consider the symmetry group G^{TR} that contains both time-reversal and reflection operations. Because the derivations for G^T and G^R are completely independent, we can simply combine the obtained results.

For the gauge matrices X in (the generalization of) Eq. (2.2), we obtain the following 2-cocycle condition:

$$\omega(gh,k)+\omega(g,h)=\omega(g,hk)+\alpha_T(g)\alpha_R(g)\omega(h,k)\,, \tag{2.35}$$

where, as before, $\alpha_T : G^{TR} \to \{1,-1\}$ is -1 if g contains a time-reversal and $\alpha_R : G^{TR} \to \{1,-1\}$ is -1 if g contains a reflection. These two morphisms can be combined into one as follows:

$$\alpha(g)=\begin{cases}+1 & g \text{ is purely on-site}\\ -1 & g \text{ contains either a time-reversal or reflection}\\ +1 & g \text{ contains both a time-reversal and reflection}\end{cases} \tag{2.36}$$

For the phase factors φ, we obtain the following 1-cocycle condition (which we again state in the additive form, i.e. $\varphi = e^{i\chi}$):

$$\chi(gh)=\chi(g)+\beta(g)\chi(h)\,, \tag{2.37}$$

where β is the same morphism as in the case of time-reversal.

We can conclude that the SPT classification (for TI systems) in the case of on-site symmetries together with reflection and time-reversal symmetry is characterized by an element in $H^2_\alpha(G^{TR};\mathrm{U}(1))$ and an element in $H^1_\beta(G^{TR};\mathrm{U}(1))$.

2.5 Projective representations

For the above considerations, we did not really explain what the full structure of the symmetry group was and how the 2-cocycle solutions where related to (projective) representations. The only restriction on the symmetry group under consideration is that, if they contain a time-reversal or reflection, then these generate $\mathbb{Z}_2$ subgroups.

Now, the best way to look at the problem is by considering how the gauge matrices change under the action of a symmetry element. We assume w.l.o.g. that the MPS matrix is of the form $Z^{-1}AZ$, where Z can be a gauge matrix of a previous symmetry operation. Then, three elementary possibilities occur:

an MPS in the left (resp. right) canonical gauge by one in the right (resp. left) canonical gauge, this choice is not generally possible.

- g is an on-site symmetry operation:

$$Z \mapsto X(g)Z\,, \tag{2.38}$$

- t is a time-reversal:

$$Z \mapsto X(t)\overline{Z}\,, \tag{2.39}$$

- r is a reflection:

$$Z \mapsto X(r)Z^{\dagger t} \tag{2.40}$$

So, now, define a map Υ_g that acts on the gauge matrices in the following way:

$$\Upsilon_g : Z \mapsto X(g)\hat{\mathcal{C}}_g\hat{\mathcal{R}}_g[Z]\,. \tag{2.41}$$

This is a combination of the above three fundamental operations. Now, we can act with a product $gh \in G$ and play the same game as in the foregoing sections. We first act by h and then by g:

$$\begin{aligned}\Upsilon_g\Upsilon_h(Z) &= \Upsilon_g\left(X(h)\hat{\mathcal{C}}_h\hat{\mathcal{R}}_h[Z]\right)\\ &= X(g)\hat{\mathcal{C}}_g\hat{\mathcal{R}}_g\Big[X(h)\hat{\mathcal{C}}_h\hat{\mathcal{R}}_h[Z]\Big]\\ &= X(g)\hat{\mathcal{C}}_g\hat{\mathcal{R}}_g\Big[X(h)\Big]\hat{\mathcal{C}}_{gh}\hat{\mathcal{R}}_{gh}[Z]\,.\end{aligned} \tag{2.42}$$

We can also act directly with the product:

$$\Upsilon_{gh}(Z) = X(gh)\hat{\mathcal{C}}_{gh}\hat{\mathcal{R}}_{gh}[Z]\,. \tag{2.43}$$

If both results have to give rise to the same MPS, the fundamental theorem 1.1 says that:

$$\Upsilon_{gh} = e^{i\omega(g,h)}\Upsilon_g\Upsilon_h \tag{2.44}$$

and for the gauge matrices:

$$X(gh) = e^{i\omega(g,h)}X(g)\hat{\mathcal{C}}_g\hat{\mathcal{R}}_g\Big[X(h)\Big]\,. \tag{2.45}$$

By completely analogous calculations as in the foregoing sections, we can show that the function ω satisfies the 2-cocycle condition (Eq. (A.16) in the appendix). So although the gauge matrices $X(g)$ do not form a projective representation anymore, the action of the symmetry group on these matrices does.

On the other hand, we could also consider the structure on the gauge matrices as a generalization of a representation. This gives rise to so-called unitary-antiunitary (UA) representations as shown in Section A.2.4 in the appendix. Because time-reversal is implemented by an antiunitary operation, we should not be surprised that this is passed down to the virtual level. However, there is one important caveat. Although the gauge matrices behave as a UA representation (Eq. (2.45)), they are still represented by matrices (linear operators).

So, how do we reconcile these statements? First, we assume that all gauge matrices are

represented (anti)unitarily, even in the case of reflection symmetry.[7] This is only necessary to obtain an exact mathematical correspondence, otherwise the correspondence is more of an analogy. Then, we can assume that we really do have a (projective) UA representation $\widehat{X}$ such that:

$$\begin{cases} \widehat{X}(g) \text{ is antiunitary} & g \text{ contains a time-reversal or}^{8} \text{ reflection}\,, \\ \widehat{X}(g) \text{ is unitary} & \text{otherwise}\,. \end{cases} \tag{2.46}$$

It is not hard to check that the elements that do not contain a time-reversal nor reflection together with those that contain both, form an order-2 subgroup of the complete symmetry group. So, this is consistent with the definition in the appendix. Now, a projective UA representation satisfies by definition:

$$\widehat{X}(gh) = e^{i\omega(g,h)}\widehat{X}(g)\widehat{X}(h)\,. \tag{2.47}$$

This is the same equation as for projective unitary representations, but now the operators $\widehat{X}$ can be antiunitary operators. Every antiunitary operator A can be written[9] as the composition of a unitary operator U and a complex conjugation operator $\mathcal{K}$ (in some basis):

$$A = U\mathcal{K}\,. \tag{2.48}$$

So, the projectivity condition above can be rewritten as follows:

$$X(gh)\mathcal{K}(gh) = e^{i\omega(g,h)}X(g)\mathcal{K}(g)X(h)\mathcal{K}(h)\,, \tag{2.49}$$

where the parametric complex conjugation operator is defined as follows:

$$\mathcal{K}(g) = \begin{cases} \mathcal{K} & g \text{ contains a time-reversal or}^{10} \text{ reflection}\,, \\ \mathbb{1} & \text{otherwise}\,. \end{cases} \tag{2.50}$$

Using the properties of the operator $\mathcal{K}$, we can rewrite the equations above as:

$$X(gh)\mathcal{K}(gh) = e^{i\omega(g,h)}X(g)\hat{\mathcal{C}}_g\hat{\mathcal{R}}_g\Big[X(h)\Big]\mathcal{K}(gh)\,, \tag{2.51}$$

where the operator $\hat{\mathcal{R}}$ now also performs a complex conjugation if g contains a reflection operation, since all gauge matrices are supposed to be unitary. If we drop the complex conjugation operator, we obtain:

$$X(gh) = e^{i\omega(g,h)}X(g)\hat{\mathcal{C}}_g\hat{\mathcal{R}}_g\Big[X(h)\Big]\,. \tag{2.52}$$

We see that this equation is exactly the same as Eq. (2.45) and, hence, we obtain the behaviour obeyed by the gauge matrices of a symmetric MPS. We conclude that the generalization of systems with on-site symmetries to systems with both on-site, time-reversal and reflection symmetries is given as follows:

SPT phases for systems with on-site symmetries are (partially) classified by

[7] This is, for example, the case in the AKLT model.

[8] exclusive or

[9] Equation (A.10) and onwards in the appendix.

[10] exclusive or

projective unitary representations living on the boundary sites.

$$\Downarrow$$

SPT phases with ***on-site, time-reversal and reflection*** *symmetries are (partially) classified by projective* ***unitary-antiunitary*** *representations of the pair (G, H), where H is the subgroup of elements containing either no time-reversal or reflection or containing both, living on the boundary sites.*

A similar statement holds for the phase factors $e^{i\varphi(g)}$ where the function $\varphi(g)$ satisfies the 1-cocycle condition (2.18). For on-site symmetries and reflection symmetries, we have shown that these phases form a 1D unitary representation (cf. [14]). Like the generalization of the projective representations above, we can regard the phase factors in the case of time-reversal symmetries as a 1D unitary-antiunitary representation:

$$\begin{aligned} e^{i\varphi(gh)}\mathcal{K}(gh) &= e^{i\varphi(g)}\tilde{\mathcal{K}}(g)e^{i\varphi(h)}\tilde{\mathcal{K}}(h) \\ &= e^{i\varphi(g)}\hat{\mathcal{C}}_g\left[e^{i\varphi(h)}\right]\tilde{\mathcal{K}}(gh) \\ &= e^{i\varphi(g)}e^{i\beta(g)\varphi(h)}\tilde{\mathcal{K}}(gh)\,, \end{aligned} \tag{2.53}$$

where the parametric conjugation operator $\tilde{\mathcal{K}}$ is now defined as:

$$\tilde{\mathcal{K}}(g) = \begin{cases} \mathcal{K} & g \text{ contains a time-reversal}\,, \\ \mathbb{1} & \text{otherwise}\,. \end{cases} \tag{2.54}$$

After dropping the complex conjugation operator, we indeed get the 1-cocycle condition Eq. (2.18) and so we obtain the following conclusion (for systems that are not translation-invariant, only the the projective representations on the boundary spins are relevant):

SPT phases for TI systems with on-site symmetries are classified by:

- *A projective unitary representation of G living on the boundary sites.*
- *A 1D unitary representation of G characterizing the symmetry of each site.*

$$\Downarrow$$

SPT phases for TI systems with ***on-site, time-reversal and reflection*** *symmetries are classified by:*

- *A projective* ***unitary-antiunitary*** *representation of the pair (G, H), where H is the subgroup of elements containing* ***either no time-reversal/reflection or containing both****, living on the boundary sites.*
- *A 1D* ***unitary-antiunitary*** *representatons of the pair $(G, \tilde{H})$, where $\tilde{H}$ is the subgroup of elements containing* ***a reflection****, characterizing the symmetry of each site.*

2.5.1 Projective commutation relations

From the rules above, we can build more complicated operations. For example, we can consider the action of both a time-reversal and reflection. We could first act by the time-reversal and then by the reflection:

$$Z \mapsto X(r)X(t)^{-t}Z\,, \tag{2.55}$$

or we could do it the other way around:

$$Z \mapsto X(t)\overline{X(r)}Z\,. \tag{2.56}$$

As these operations are symmetry operations, we know from the fundamental theorem 1.1 that

$$X(r)\overline{X(t)} = e^{i\theta}X(t)\overline{X(r)}\,. \tag{2.57}$$

After absorbing the phase $e^{i\theta/2}$ in either $X(r)$ or $X(t)$, we obtain the relation

$$X(t)\overline{X(r)} = X(r)\overline{X(t)}\,. \tag{2.58}$$

So, the representations of time-reversals and reflections commute. By a similar reasoning, we can show that for time-reversals (and reflections), the following equality is satisfied for all on-site symmetry operations g:

$$X(t,r)\overline{X(g)} = e^{i\theta(g)}X(g)X(t,r)\,. \tag{2.59}$$

Hence, we see that the representations of on-site symmetries commute in a projective way, i.e. up to a phase, with the representations of time-reversals and reflections. Consider the gauge map Υ defined in Eq. (2.41). If we act with an on-site symmetry g and a time-reversal t (the same relation can be obtained for reflections), we obtain:

$$\begin{aligned}\Upsilon_{gt}(Z) &= e^{i\omega(g,t)}\Upsilon_g X(t)\overline{Z}\\ &= e^{i\omega(g,t)}X(g)X(t)\overline{Z}\\ &= e^{i\omega(g,t)-i\theta(g)}X(t)\overline{X(g)Z}\\ &= e^{i\omega(g,t)-i\theta(g)-i\omega(t,g)}\Upsilon_{tg}(Z)\,,\end{aligned} \tag{2.60}$$

where we used Eq. (2.59) in the third line. Now, because on-site symmetries and time-reversals are supposed to commute, Υ_{gt} and Υ_{tg} are equal and, thus, we obtain an expression for the projective commutation phase $e^{i\theta(g)}$ in terms of the 2-cocycles:

$$\theta(g) = \omega(g,t) - \omega(t,g)\,. \tag{2.61}$$

Now, we can check that this implies that $\theta(g)$ forms a 1D representation up to a square in the 2-cocycles (cf. [14]):

$$\begin{aligned}\theta(gh) &= \omega(gh,t) - \omega(t,gh)\\ &= \omega(h,t) + \omega(g,ht) - \omega(g,h) - \omega(g,h) - \omega(tg,h) - \omega(t,g)\\ &= \omega(h,t) + \omega(g,ht) - 2\omega(g,h) - \omega(gt,h) - \omega(t,g)\\ &= \omega(h,t) + \omega(g,ht) - 2\omega(g,h) - \Big(\omega(t,h) + \omega(g,th) - \omega(g,t)\Big) - \omega(t,g)\\ &= \omega(h,t) + \omega(g,ht) - 2\omega(g,h) - \omega(t,h) - \omega(g,ht) + \omega(g,t) - \omega(t,g)\end{aligned}$$

$$
\begin{aligned}
&= \omega(h,t) - 2\omega(g,h) - \omega(t,h) + \omega(g,t) - \omega(t,g) \\
&= \theta(g) + \theta(h) - 2\omega(g,h)\,,
\end{aligned} \tag{2.62}
$$

where we used the direct product structure of the total symmetry group in lines 3 and 5.

2.6 Explicit construction

In the following sections, we try to construct a system (and associated MPS tensor) invariant under a symmetry group G (possibly containing time-reversals or reflections) given an SPT phase classified by a 1-cocycle $\varphi \in H^1_\beta(G;\mathrm{U}(1))$ and 2-cocycle $\omega \in H^2_\alpha(G;\mathrm{U}(1))$. We will by no means try to give a physical interpretation of the obtained MPS. We only show that it is, in theory, possible to construct a system (described by an MPS) that belongs to the given SPT phase.

We will use a different notation in the remainder of this chapter to reduce the number of parentheses. The gauge matrices will be denoted by V^g where $g \in G$ is the symmetry element. As before, we know that requiring symmetry of an MPS matrix A^i is equivalent to stating the following two conditions (injectivity and projectivity constraints):

$$V^g \sum_j u(g)^{ij} A^j = e^{i\varphi(g)} A^i V^g\,, \tag{2.63}$$

$$V^g V^h = e^{i\omega(g,h)} V^{gh}\,. \tag{2.64}$$

To find a representative of the SPT phase fixed by φ and ω, we are inspired by the associated cocycle conditions and we will explicitly use them during the construction.

2.6.1 On-site

For on-site symmetries, we will show that the following ansatz satisfies the required conditions:

$$(V^g)_{a,b} = \begin{cases} e^{i\omega(a,g)} & b = ag \\ 0 & \text{otherwise} \end{cases} \tag{2.65}$$

$$(A^{h,m})_{a,b} = \begin{cases} e^{i\omega(h,a)+i\varphi(m)} & b = ha \\ 0 & \text{otherwise} \end{cases} \tag{2.66}$$

We choose the physical action $\widehat{U}(g)$ to map $A^{h,m}$ to $A^{h,mg}$. From this construction, it is immediately clear that the dimensions of the physical and virtual spaces are given by respectively $|G|^2$ and $|G|$.

Proof of soundness.

$$
\begin{aligned}
(V^g)_{a,ag}(V^h)_{ag,agh} &= e^{i\omega(a,g)+i\omega(ag,h)} \\
e^{i\omega(g,h)}(V^{gh})_{a,agh} &= e^{i\omega(g,h)+i\omega(a,gh)}
\end{aligned}
$$

By the 2-cocycle condition for ω, the two expressions are equal and so the projectivity

condition (2.64) is satisfied. In the same way, we obtain:

$$(V^g)_{a,ag}(A^{h,mg})_{ag,hag} = e^{i\omega(a,g)+\left[i\omega(h,ag)+i\varphi(mg)\right]}$$
$$e^{i\varphi(g)}(A^{h,m})_{a,ha}(V^g)_{ha,hag} = e^{i\varphi(g)+\left[i\omega(h,a)+i\varphi(m)\right]+i\omega(ha,g)} .$$

By the 1- and 2-cocycle conditions for φ and ω, the two lines are equal and so the injectivity condition (2.63) is satisfied. □

2.6.2 Time-reversal

For symmetry groups with time-reversal included, we have to modify the above construction, because the cocycle conditions contain a nontrivial action. The function ω is now an element of $H^2_\alpha(G;\mathrm{U}(1))$, where $\alpha(g) = -1$ if and only if g contains a time-reversal operation. The same holds for $\varphi \in H^1_\beta(G;\mathrm{U}(1))$ with α replaced by β.

The direct modifications of the ansatz in previous section are:

$$(V^g)_{a,b} = \begin{cases} e^{i\alpha(a)\omega(a,g)} & b = ag \\ 0 & \text{otherwise} \end{cases} \tag{2.67}$$

$$(A^{h,m})_{a,b} = \begin{cases} e^{i\alpha(ha)\omega(h,a)+i\beta(m)\varphi(m)} & b = ha \\ 0 & \text{otherwise} \end{cases} \tag{2.68}$$

with the physical action $\widehat{U}(g)$ again mapping $A^{h,m}$ to $A^{h,mg}$.

Proof of soundness.

$$(V^g)_{a,ag}\overline{(V^h)_{ag,agh}}^{\,g} = e^{i\alpha(a)\omega(a,g)+i\alpha(g)\alpha(ag)\omega(ag,h)}$$
$$e^{i\omega(g,h)}(V^{gh})_{a,agh} = e^{i\omega(g,h)+\alpha(a)i\omega(a,gh)} ,$$

where, in the first line, the bar with subscript g indicates the fact that we only take the complex conjugate if g contains a time-reversal operation (similar to the operator $\hat{\mathcal{C}}_g$ in previous sections). This parametrized complex conjugation is the reason for the appearance of an extra factor $\alpha(g)$ in the exponent on the right-hand side. Because α is a G-action, we can simplify the product $\alpha(g)\alpha(ag)$ as $\alpha(a)$.

To apply the 2-cocycle condition (with nontrivial action α) for ω, we should normally have the factor $\alpha(a)$ in the term $i\omega(g,h)$. However, this factor does not appear in that term, but it does in all other terms. Because α takes its values in $\mathbb{Z}_2$, we can just multiply all terms in the exponents by $\alpha(a)$ to fix this, since changing the sign of all terms in an equation does not change its validity. We see that the two lines are equal and, hence, condition (2.64) is satisfied.

In the same way, we obtain:

$$(V^g)_{a,ag}\overline{(A^{h,mg})_{ag,hag}}^{\,g} = e^{i\alpha(a)\omega(a,g)+\beta(g)\left[i\alpha(hag)\omega(h,ag)+i\beta(mg)\varphi(mg)\right]}$$
$$e^{i\varphi(g)}(A^{h,m})_{a,ha}(V^g)_{ha,hag} = e^{i\varphi(g)+\left[i\alpha(ha)\omega(h,a)+i\beta(m)\varphi(m)\right]+i\alpha(ha)\omega(ha,g)}$$

By the same reasoning as above and by noting that for time-reversals $\alpha = \beta$, we see that the two lines are equal and condition (2.63) is satisfied.

2.6.3 Reflection

For symmetry groups with reflection symmetry included, we have to modify the above constructions even more. The function ω is still an element of $H^2_\alpha(G; \mathrm{U}(1))$, where $\alpha(g) = -1$ if and only if g contains a reflection, but now, the function φ is again an element of the first cohomology group with trivial action.

The modifications of the ansatz found in previous section are:

$$(V^g)_{a,b} = \begin{cases} e^{i\alpha(a)\omega(a,g)} & b = ag \\ 0 & \text{otherwise} \end{cases} \tag{2.69}$$

$$(A^{h,m})_{a,b} = \begin{cases} e^{i\alpha(ha)\omega(h,a)+i\varphi(m)} & b = ha \\ 0 & \text{otherwise} \end{cases} \tag{2.70}$$

with the physical action $\widehat{U}(g)$ mapping $A^{h,m}$ to $A^{h^{-1},mg}$ if g contains a time-reversal (this odd-looking feature will be explained below) and mapping $A^{h,m}$ to $A^{h,mg}$ if it does not (as before).

Proof of soundness. To ease the notation, we will only consider the case where g contains a reflection (the other case is trivial and belongs to the first section).

$$\begin{aligned} (V^g)_{a,ag}\overline{(V^h)_{ag,agh}} &= e^{i\alpha(a)\omega(a,g)+i\alpha(g)\alpha(ag)\omega(ag,h)} \\ e^{i\omega(g,h)}(V^{gh})_{a,agh} &= e^{i\omega(g,h)+\alpha(a)i\omega(a,gh)} \end{aligned}$$

The reason why we used complex conjugation in the first line instead of a transpose inverse is that we can assume the gauge matrices of on-site symmetries to be unitary as shown in Section 2.1.1. Then, by the exact same reasoning as in the previous section, we see that Eq. (2.64) is satisfied.

In the same way, we obtain:

$$\begin{aligned} (V^g)_{a,ag}(A^{h^{-1},mg})^t_{ag,hag} &= e^{i\alpha(a)\omega(a,g)+\left[i\alpha(ag)\omega(h^{-1},hag)+i\varphi(mg)\right]} \\ e^{i\varphi(g)}(A^{h,m})_{a,ha}(V^g)_{ha,hag} &= e^{i\varphi(g)+\left[i\alpha(ha)\omega(h,a)+i\varphi(m)\right]+i\alpha(ha)\omega(ha,g)} \end{aligned}$$

The reason for the peculiar physical action is the following. For reflections, we have to take the transpose of the MPS matrices and, by definition of a transpose, $B^t_{i,j} = B_{j,i}$. For our choice of MPS matrices this becomes:

$$(A^{h,m})^t_{a,b} = (A^{h,m})_{b,a} = \begin{cases} e^{i\alpha(hb)\omega(h,b)+i\varphi(m)} & a = hb\,, \\ 0 & \text{otherwise}\,. \end{cases} \tag{2.71}$$

Now, if the incoming bond carries an index a, the outgoing one will carry the index $h^{-1}a$. (This property, that the matrix indices satisfy a one-to-one relationship, follows from the

fact that left multiplication is a group isomorphism.) It follows that, if we want our transformed matrix to take an index ag to an index hag, we need the physical action to replace the matrix $A^{h,m}$ by $A^{h^{-1},m}$.

To obtain the desired result, we show that $\omega(h^{-1}, hag) \sim \omega(ha, g)$. We first write out the 2-cocycle condition:

$$\omega(h^{-1}, hag) - \omega(e, ag) + \alpha(h)\omega(h, ag) - \omega(h^{-1}, h) = 0\,, \tag{2.72}$$

where we used that $\alpha(h^{-1}) = \alpha(h)$, which follows from the fact that the reflection operation generates a $\mathbb{Z}_2$ subgroup of the total symmetry group. It is exactly the third term that we need so we still have to show that both the second and the last term vanish. This can be derived from the general structure of $H^2_\alpha(G; \mathrm{U}(1))$.

- As shown in Section A.2.1 in the appendix, we can always normalize the cocycles:

  $$\omega(e, g) = \omega(g, e) = 0$$

  for all $g \in G$.

- From the 2-cocycle condition we obtain:

  $$\alpha(x)\omega(x^{-1}, x) - \omega(xx^{-1}, x) + \omega(x, x^{-1}x) - \omega(x, x^{-1}) = 0\,.$$

  The second and third term vanish due to the statement above and so we get:

  $$\omega(x, x^{-1}) = \alpha(x)\omega(x^{-1}, x)\,. \tag{2.73}$$

  We now use this equality and the remaining 'gauge freedom' to set these values to 0. By adding a coboundary κ, we perform the transformation

  $$\omega(x, x^{-1}) \to \omega(x, x^{-1}) + \kappa(e) - \alpha(x)\kappa(x^{-1}) - \kappa(x)\,.$$

  We make the following choice:

  $$\kappa(x) = \frac{\omega(x, x^{-1})}{2}\,. \tag{2.74}$$

  This transformation leaves the choice $\omega(e, e) = 0$ unchanged, so the second term vanishes. The third and last term are equal because of Eq. (2.73) above and together give a contribution $-\omega(x, x^{-1})$, which cancels the first term. We thus obtain the desired transformation $\omega(x, x^{-1}) \to 0$.

After making these 'gauge transformations', Eq. (2.72) gives:

$$\omega(h^{-1}, hag) = -\alpha(h)\omega(h, ag)\,. \tag{2.75}$$

Inserting this in the MPS transformation equations leads to:

$$(V^g)_{a,ag}(A^{h^{-1},mg})^t_{ag,hag} = e^{i\alpha(a)\omega(a,g)+\left[-i\alpha(hag)\omega(h,ag)+i\varphi(mg)\right]}\,,$$
$$e^{i\varphi(g)}(A^{h,m})_{a,ha}(V^g)_{ha,hag} = e^{i\varphi(g)+\left[i\alpha(ha)\omega(h,a)+i\varphi(m)\right]+i\alpha(ha)\omega(ha,g)}\,.$$

Because we looked at the situation where g contains a reflection, we know that $\alpha(g) = -1$

and, hence, the term $-i\alpha(hag)\omega(h, ag)$ in the exponent on the first line can be rewritten as $\alpha(ha)\omega(h, ag)$. From here, we have to apply the same reasoning as in previous section to complete the proof that Eq. (2.63) is satisfied. □

2.6.4 Everything together

The results obtained in the previous section can be combined almost verbatim to construct symmetric MPS ansätze for more general symmetry groups.

2.7 Numerical results

Here, we list some results obtained from numerical computations for on-site symmetries, on-site symmetries combined with a time-reversal symmmetry and on-site symmetries combined with both time-reversal and reflection symmetry. To obtain these results, we used the *Smith normal form* to efficiently solve the cocycle conditions. We do not explain how this algorithm works at this point. For the sake of continuity, we defer this explanation until the next chapter.

For systems that are not translation-invariant, different choices of 1-cocycles do not lead to distinct phases [13] and, hence, the columns $|H^1(G; \mathrm{U}(1))|$ can be ignored in this case.

For on-site symmetries (with translation invariance):

G	$\lvert H^1\rvert$	$\lvert H^2\rvert$
$\{e\}$	1	1
$\mathbb{Z}_2$	2	1
$\mathbb{Z}_3$	3	1
$\mathbb{Z}_8$	8	1
$\mathbb{Z}_2 \times \mathbb{Z}_3$	6	1
$\mathbb{Z}_4 \times \mathbb{Z}_6$	2×12	2
D_2	2^2	2
D_3	2	1
D_4	2^2	2

In these tables, the case $G = \{e\}$ means that the on-site symmetry group is trivial.

For combined on-site and time-reversal symmetries (with translation invariance):

G	$\lvert H^1\rvert$	$\lvert H^2\rvert$
$\{e\}$	1	2
$\mathbb{Z}_2$	2	2^2
$\mathbb{Z}_3$	1	2
$\mathbb{Z}_8$	2	2^2
$\mathbb{Z}_2 \times \mathbb{Z}_3$	2	2^2
$\mathbb{Z}_4 \times \mathbb{Z}_6$	2^2	/
D_2	2^2	2^4
D_3	2	2^2
D_4	2^2	2^4

For combined on-site, time-reversal and reflection symmetries (with translation invariance):

G	$\lvert H^1\rvert$	$\lvert H^2\rvert$
$\{e\}$	2	2^2
$\mathbb{Z}_2$	2^2	2^4
$\mathbb{Z}_3$	2	2^2
$\mathbb{Z}_8$	2^2	/
$\mathbb{Z}_2 \times \mathbb{Z}_3$	2^2	2^4
$\mathbb{Z}_4 \times \mathbb{Z}_6$	/	/
D_2	2^3	2^7
D_3	2^2	2^4
D_4	2^3	/

Remark: Entries with a slash '/' indicate that the computation time exceeded reasonable bounds. However, it should be noted that the algorithm was not fine-tuned for an optimal execution time and that the calculation was run on a small laptop. So, this result is not very representative. On the other hand, it is well-known that the calculation of the Smith normal form is an expensive task and so it could be useful to run the calculations using a more specialized algorithm [35, 30].

Comparing these results with the ones listed in [14, 11] shows that the systematic classification based on the first and second cohomology groups is consistent with the literature and, hence, provides a viable numerical tool for the classification of SPT phases. If we compare the cohomology that we compute (our symmetry group explicitly includes time-reversal and/or reflection symmetries) with the results in [14], we see that we obtain the following systematic way of classifying SPT phases:

Separate classification of the parity of the system under a reflection and 1D representations of the on-site symmetry group.

$\Downarrow$

Single calculation of 1-cocycles of the total symmetry group (with nontrivial action).

Separate classification of reflection and time-reversal parity of the boundary spin, projective representations of the on-site symmetry group and projective commutation relations.

$\Downarrow$

Single calculation of 2-cocycles of the total symmetry group (with nontrivial action).

The first conclusion is completely consistent with the result obtained in Section 2.5 above. By including time-reversal and reflection symmetries in the total symmetry group, we can consider the 1D phase representation of the on-site symmetry group and the reflection parity of the system as one and the same thing. The second conclusion is also not totally surprising. By using the fact that the total symmetry group is a direct product (by assumption) and the projective behaviour of the gauge matrices, we have determined in Section 2.5.1 that the representation of the total symmetry group satisfies a (projective) commutation relation and we have expressed this in terms of the 2-cocycles. This way, the projective commutation relations are automatically classified if the 2-cocyles are found.

However, the algorithm not only gives the structure of the cohomology groups, it also gives explicit solutions for the cocycles and coboundaries. This is very useful in combination with the explicit MPS construction from the previous section. So, given a symmetry group, we cannot only numerically find all possible SPT phase, we can also construct, for a given SPT phase, a representative MPS in one go.

Chapter 3

Introducing space groups

In a homogeneous Euclidean space, we can perform any rotation, translation or reflection and obtain the same Euclidean space again. Now, consider a *lattice* in this Euclidean space, i.e. a discrete subgroup of $\mathbb{R}^n$ isomorphic to $\mathbb{Z}^n$ that spans the Euclidean space. If we require that the allowed transformations leave the lattice unchanged, it is immediately obvious that not all transformations are allowed anymore. For example, if the lattice spacing is λ, then a translation over $\lambda/3$ will not leave the lattice unchanged. This leads to the classification of space group symmetries, i.e. groups which a certain kind of ordered lattice invariant.

In general, there are multiple facets to this classification. First of all, we should classify the so-called point groups. These are the symmetry groups that leave a certain point (generally the origin) fixed. So, translations will never be a part of the point group. The point groups are the symmetry groups of the unit cell. If we consider a regular lattice, not all point groups are admissable anymore as they should leave the complete lattice invariant. So, the number of relevant point groups when working with a lattice is generally reduced after this additional restriction. On the other hand, we should also classify the Bravais lattices which give the ordering of the lattice. A Bravais lattice is defined as a lattice in Euclidean space that is compatible with one of the (reduced) point groups found before. The combination of point groups and Bravais lattices gives the space groups. For example, in 3 dimensions there are 7 point groups and 14 Bravais lattices. However, there are 230 distinct space groups, which is clearly more than $7 \times 14 = 98$. This follows from the fact that there exist so-called *glide reflections* and *screw axes*, which are combinations of reflections, rotations and translations.

3.1 One-dimensional classification

As mentioned above, it is well known that there exist 230 different space groups for three-dimensional lattices. In 1 dimension[1], this number is greatly reduced (for example, there clearly exists only one Bravais lattice) and only 7 symmetry groups remain. These are the so-called *frieze groups*. Formally, they are defined as follows:

Definition 3.1. Consider the strip $\mathbb{S} = \mathbb{R} \times I$, where I is a finite interval, and denote

[1]For a truly one-dimensional system, only 3 possibilities arise (see [42]).

its group of isometries by Isom(𝕊). The discrete subgroups of Isom(𝕊) that contain a translation generator are called the frieze groups.

The 7 frieze groups are generated by 5 different elements:

1. T: translation (by a unit cell)
2. H: reflection across y-axis
3. V: reflection across x-axis
4. G: glide reflection (translation by half a cell followed by V)
5. R: rotation over 180° (this generator is equal to the product HV)

Using these elements, we can construct (see e.g. [53]) the discrete subgroups of Isom(𝕊).

Theorem 3.1 (Classification of frieze groups). *Up to conjugation, the following 7 groups are the only discrete isometry (sub)groups of the one-dimensional strip:*

1. $F_0 = \langle T \mid \emptyset \rangle$,
2. $F_V = \langle T, V \mid V^2 = e, V^{-1}TV = T \rangle$,
3. $F_H = \langle T, H \mid H^2 = e, H^{-1}TH = T^{-1} \rangle$,
4. $F_G = \langle T, G \mid G^2 = T, G^{-1}TG = T \rangle$,
5. $F_R = \langle T, R \mid R^2 = e, R^{-1}TR = T^{-1} \rangle$,
6. $F_{VH} = \langle T, R, H \mid R^2 = H^2 = (HR)^2 = e, R^{-1}TR = T^{-1}, H^{-1}TH = T \rangle$, *and*
7. $F_{RG} = \langle T, R, G \mid R^2 = (RG)^2 = e, G^2 = T, R^{-1}TR = T^{-1}, G^{-1}TG = T \rangle$.

Here, we used the presentation notation defined in the appendix (see Definition A.5). As this is a rather abstract way of defining these groups, we have given a graphical example of each of the frieze groups in Fig. 3.1. In architecture, these decorations are often called *friezes* (what's in a name).

From a mathematical point of view, this classification can also be carried out similar to the way we classified SPT phases in the previous chapter. The systematic approach is again based on the framework of group cohomology (see Section A.2 in the appendix) and gives a classification [26, 42] in terms of $H^1(G_0, \mathrm{U}(1)) \cong H^2(G_0, \mathbb{Z})$. Here, $G_0 = G/T$ is the point group obtained by quotienting out the translations from the total symmetry group. The isomorphism is the result of the long exact sequence in cohomology as explained in the appendix (see Eq. (A.37)).

Intuitively, we could, however, expect a different outcome. For example, all operations can be constructed using vertical reflections, horizontal reflections and glide reflections, all of which have order 2 (up to translation). Hence, we could expect that the frieze groups are given by the subgroups of $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$. However, there are 16 (and not 7) of

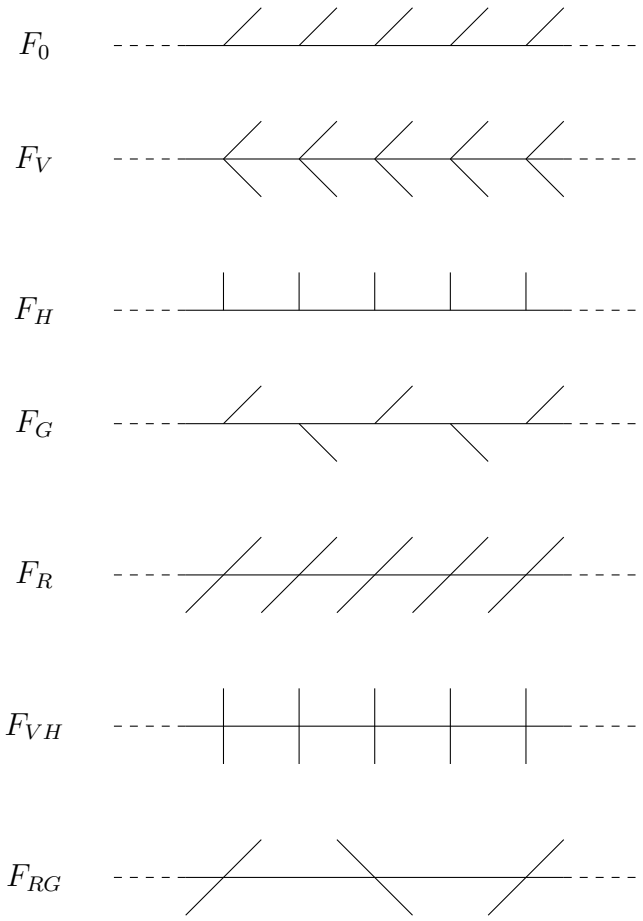


Figure 3.1: Friezes

these subgroups and this is exactly where the part '*up to conjugation*' in the classifying theorem 3.1 becomes important.

As an example, we will consider the frieze in Fig. 3.2. At first sight, this figure seems to have a symmetry group not listed above. However, according to the frieze group classification, this coincides with the case of F_R!

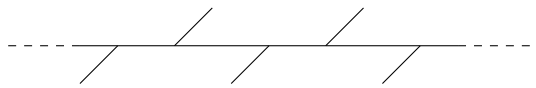


Figure 3.2: Another one?

Proof. A general planar isometry can be parametrized as $A\vec{x}+\vec{\omega}$ where $A \in \mathrm{O}(2)$, i.e. they are elements of the Euclidean group (a subgroup of the *affine group*). Because we look at the isometries of a strip, which has an upper and lower boundary, the translation vector $\vec{\omega}$ cannot have a vertical component and is, hence, of the form $\begin{pmatrix} x_1 \\ 0 \end{pmatrix}$. For the same reason,

the matrix A is of the form $\begin{pmatrix} \pm 1 & 0 \\ 0 & \pm 1 \end{pmatrix}$. The group multiplication is defined as follows:

$$\big(A_1, \vec{\omega}_1\big)\big(A_2, \vec{\omega}_2\big) = \big(A_1 A_2, A_1\vec{\omega}_2 + \vec{\omega}_1\big) \tag{3.1}$$

Both the symmetry group of Fig. 3.2 and the symmetry group F_R have 2 elements. The nontrivial element of these groups is, respectively, given by[2]:

$$\left(-\mathbb{1}, \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}\right) \qquad\qquad (-\mathbb{1}, 0)\ . \tag{3.2}$$

Both are easily checked to be of order 2 (when modding out by $\mathbb{Z}$ in the second argument) as required. If these groups are to be equal up to conjugation, there should exist an element $(A, \vec{\omega})$ in $\mathrm{Isom}(\mathbb{S})$ such that

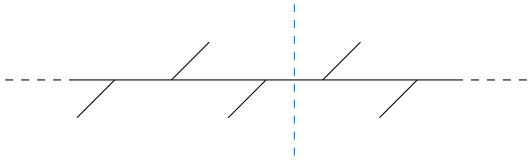
$$\big(A, \vec{\omega}\big)\left(-\mathbb{1}, \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}\right) = \big(-\mathbb{1}, 0\big)\big(A, \vec{\omega}\big)\,. \tag{3.3}$$

This can also be rewritten by working out the group multiplication:

$$\left(-A, A\begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} + \vec{\omega}\right) = \big(-A, -\vec{\omega}\big)\,. \tag{3.4}$$

It follows that, for any matrix A, we should be able to find a vector $\vec{\omega}$ satisfying the condition. For simplicity's sake, we will choose A to be the identity. Inserting this in the condition on $\vec{\omega}$, we obtain $\frac{1}{2} + \omega_1 = -\omega_1$ or, equivalently, $\omega_1 = -\frac{1}{4}$. Hence, the two symmetry groups are related by a shift over a quarter of a unit cell.

To make this visually clear, we will redraw Fig. 3.2 with an extra line indicating the position of the axis of reflection:



If we reflect about the dashed line instead of the site-centered axis, we indeed see that the symmetry group is isomorphic to F_R. □

3.1.1 On a lattice

Now, we have to ask ourselves the question what we really want. Consider for example a system on a one-dimensional chain as in the previous section. The F_R case would correspond to a translation-invariant chain with the additionial property that the particles at every site have some kind of rotational symmetry. The case depicted in Fig. 3.2, however, would correspond to a chain with sites alternating between two types A, B with the additional property that the A and B sites are related through a rotation. But this does not at all mean that the A and B sites are equal.

[2]We work in the convention where the distance between two consecutive upward pointing legs is 1.

The reason for this discrepancy is that in the above classification, every site contains exactly the same information. The upward and downward pointing legs in Fig. 3.2 are the same (except for their orientation). And indeed, blocking the two-site unit cell to a one-site unit cell and requiring some kind of symmetry is equivalent to starting with a one-site unit cell with that same symmetry. But we do not want the tensor networks to be exactly the same under a lattice transformation, we only want the resulting physics to be the same. So the frieze group classification is not exactly what we want.

However, we can easily remediate this problem. A first observation is that we will have to explicitly specify the periodicity of the lattice or, equivalently, the number of distinct sites within a single unit cell. This implies that a general transformation can still be written as an affine transformation $A\vec{x} + \vec{\omega}$, where A is still of the form

$$\begin{pmatrix} \pm 1 & 0 \\ 0 & \pm 1 \end{pmatrix}, \tag{3.5}$$

but where $\vec{\omega}$ is now of the form

$$\begin{pmatrix} k \\ 0 \end{pmatrix} \tag{3.6}$$

for some $k \in \mathbb{Z}_n$. The reason for this is that we mod out translations over unit cells. So, for a unit cell with n distinct sites, a translation over n sites is equivalent to no translation at all.

The composition law is still given by Eq. (3.1) and, hence, the closure property of the group implies that

$$A_{g_1}\vec{\omega}_{g_2} + \vec{\omega}_{g_1} = \vec{\omega}_{g_1 \cdot g_2} \tag{3.7}$$

for all $g_1, g_2 \in G$. Because only the first component of $\vec{\omega}_g$ is nonzero for all $g \in G$, this equation can be rewritten as a scalar equation:

$$\beta(g_1)\omega_{g_2} + \omega_{g_1} = \omega_{g_1 \cdot g_2} \mod n\,, \tag{3.8}$$

where $\beta(g)$ is ± 1 depending on the sign of the first element of A_g. This is exactly the cocycle condition for the first group cohomology $H^1_\beta(G; \mathbb{Z}_n)$ with nontrivial action β. For small symmetry groups, this set of $N^2 \times N$ conditions can be solved by hand, but it quickly becomes unmanageable.

As an example, we will consider the symmetry group given by an on-site $\mathbb{Z}_3$-symmetry on a periodicity-3 lattice. Because there is no reflection symmetry, the action $\beta : \mathbb{Z}_3 \to \{1, -1\}$ will be trivial, i.e. $\beta \equiv 1$. If we label the three elements of $\mathbb{Z}_3$ by $1, 2$ and 3, we obtain the following Cayley table:

	1	2	3
1	1	2	3
2	2	3	1
3	3	1	2

We can now insert these results in the system of conditions (3.8) (we remove all trivial

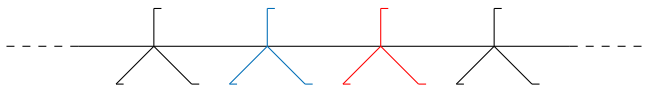
equations and all terms ω_1 as these are 0 due to the normalization[3]):

$$\begin{aligned}\omega_2 + \omega_3 &= 0\\ \omega_2 + \omega_2 &= \omega_3\\ \omega_3 + \omega_3 &= \omega_2\,.\end{aligned}$$

Solving this system (over $\mathbb{Z}_3$), gives us three solutions:

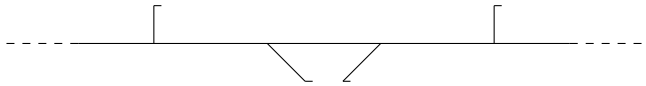
$$\begin{aligned}\omega_2 &= 0,\ \omega_3 = 0\\ \omega_2 &= 1,\ \omega_3 = 2\\ \omega_2 &= 2,\ \omega_3 = 1\,.\end{aligned}$$

The first one is the trivial solution, where every site is fully symmetric under $G = \mathbb{Z}_3$ (the three different colors emphasize that all three sites in the unit cell are different). The two nontrivial solutions correspond to situations where the different sites of a unit cell are related by the $\mathbb{Z}_3$ symmetry. All three solutions can easily be visualised (the small horizontal lines at the tips are added to break reflection symmetry):



(a) Fully symmetric (trivial case).

(b) Left chirality.



(c) Right chirality.

These three configurations are indeed, up to changes in the decoration of the sites which are irrelevant, the only possible configurations with a $\mathbb{Z}_3$-symmetry and lattice periodicity 3.

3.1.2 Smith normal form

To solve the cocycle conditions for larger symmetry groups, we can use a method based on the *Smith normal form* of a matrix. The following construction can also be used for the calculation of the cohomology groups from the previous chapter, even though the SPT classification was given in terms of coefficients in U(1) instead of $\mathbb{Z}_n$. However, thanks to the theorems of group cohomology, we can use the isomorphism in Eq. (A.37) to reformulate statements from cohomology with coefficients in U(1) as statements from cohomology with coefficients in $\mathbb{Z}$. On the other hand, since all coefficients in the cocycle conditions are ± 1 and $\mathrm{U}(1) \cong \mathbb{R}/\mathbb{Z}$, we do not even have to use the isomorphism (A.37) and just work modulo 1 at the end. This way we see that we can use the exact same algorithm without problem.

[3]See Section A.2.1 in the appendix.

Definition 3.2 (Smith normal form). A matrix A over a *principal ideal domain*[4] (PID) of dimension $m \times n$ is said to be in Smith normal form if it can be written in the following form:

$$A = \left(\begin{array}{c|c} \mathrm{diag}(a_1, a_2, \ldots, a_r) & 0 \\ \hline 0 & 0 \end{array}, \right) \tag{3.9}$$

where the coefficients a_i satisfy the condition that a_i divides a_{i+1} for all $i \leq r$.

Theorem 3.2. *Every matrix with coefficients in a PID can be brought to Smith normal form by invertible matrices U, V.*

We will not give a complete proof of this theorem, but we will give a sketch of how a matrix is brought to Smith normal form (based on the exposition in [34]). We do not consider the most efficient algorithm, but it is the simplest one to describe since it is a variation on the Gaussian elimination algorithm.

Sketch of proof. Let us start with an important remark. The rank of the matrix should not be altered since this is one of the important quantities when computing (co)homology data. Accordingly, we must ensure that all operations in the algorithm leave the rank invariant. As in the Guassian elimination algorithm, these are the elementary row/column operations:

- Type I: Exchanging rows or columns.
- Type II: Multiplying a row or column by a nonzero number.
- Type III: Adding a multiple of a row/column to another row/column.

The algorithm proceeds iteratively. The procedure at every iteration goes as follows:

1. We look for the smallest entry (in absolute value) and, by type-I moves, bring it to the upper left corner of the matrix. This entry will be called the *pivot*.
2. By type-III moves, we try to set all entries below and to the right of the pivot to 0. If this is not possible, we reduce the magnitude of the entries below and to the right of the pivot and start anew (potentially changing the pivot) until the zero entries are obtained.
3. Then, we check if the pivot divides all other entries. If so, we can proceed. If not, we use type-III moves to make the first entry that is not divisible by the pivot divisible and start anew until all entries are divisible by the pivot.
4. After satisfying the divisibility condition, we check if the pivot is negative. If not, we use a type-II move (with factor -1) to make it positive.

The next iteration proceeds by working in the submatrix obtained by removing the first row and column. □

Using this theorem and the underlying construction (see [18, 34]), we can find a numerical

[4]The exact definition is not important. Relevant examples are any field or the ring of integers $\mathbb{Z}$.

way to solve the system of cocycle conditions

$$A\vec{\omega} = 0\,.$$

We will explain the construction in the case of the classifcation of (generalized) space groups. Because, in this case, the matrix A associated to the system of cocycle conditions is technically not a matrix over a principal ideal domain[5] but over some cyclic group $\mathbb{Z}_n$, we will have to use some modified methods. Generally, we can still work with matrices over the integers and use the Smith normal form, with the exception that we mod out by the order n in the end (or even during intermediate steps if we are careful). This way, we still obtain a decomposition UDV over the integers with D in Smith normal form.

Because $A\vec{\omega} = 0$ and U is invertible, we have $DV\vec{\omega} = 0$. All diagonal elements D_i that are 0 correspond to coboundaries and, hence, can be discarded. At this point, we should make a distinction between the different use cases. Depending on the choice of module in the construction of our cohomology groups, we can discard even more diagonal elements. For example, we know that in the current case we are working over some cyclic group $\mathbb{Z}_n$ and, hence, (at the end) we will mod out by n. So, diagonal elements D_i that are multiples of n can already be discarded in this step. Now, let I denote the set of row or column indices corresponding to the diagonal elements that were not discarded. To find the corresponding $\vec{\omega}$, we will use the linearity of the cocycle conditions. To this intent, we select an index $i \in I$ and set $(V\omega)_j = \delta_{ij}(n/D_i)$. Multiplying this equation by the inverse matrix V^{-1} gives $\omega_k = V^{-1}_{ki}(n/D_i)$ and, so, the nontrivial cocycles $\vec{\omega}$ are given by the (scaled) columns $V^{-1}_{li}(n/D_i)$ for all $i \in I$.

Every step in the algorithm is linear as we already noted and, hence, a linear combination of solutions is also a solution. For example, consider an internal $\mathbb{Z}_3$-symmetry on a periodicity-3 lattice as above. If the algorithm gives us the solution $\vec{\omega} = (0\ 1\ 2)$, we can find another cocycle, namely $2\vec{\omega} = (0\ 2\ 1)$, which is exactly the solution corresponding to the other chirality.

3.2 Frieze groups

In this section, we will consider (some) symmetry groups corresponding to the friezes in Fig. 3.1. Our basic tool will be the fundamental theorem 1.1. Using this theorem, we will derive the classification of SPT phases and, for each phase, we will give a generic MPS representation.

3.2.1 F_0-group

This is the symmetry group of a translation-invariant system. This system does not have any symmetries aside from the translation invariance and, hence, does not admit nontrivial SPT phases. Because translation invariance will be an important property for all systems under consideration, we will first show that every TI system admits a description by a uniform MPS, i.e. an MPS for which $A[n] \equiv A$ for every site index n.

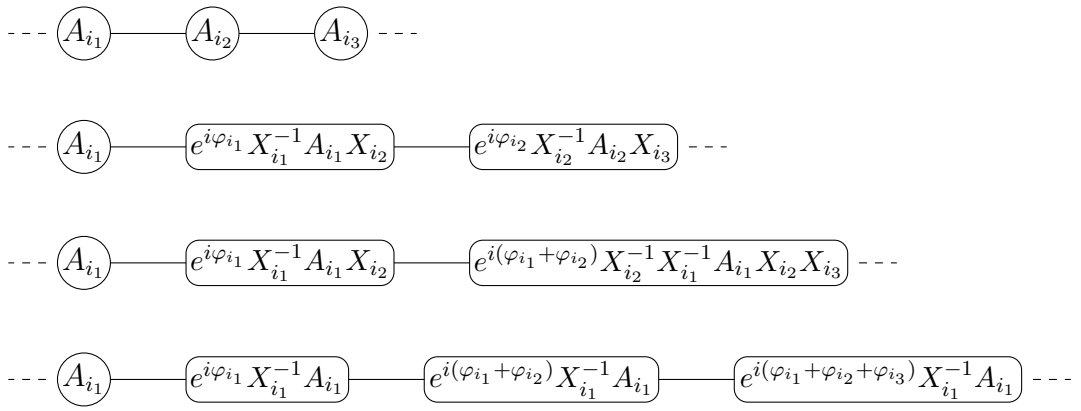
Assume that we start with a general MPS described by tensors $\{A[n]\}_{n\in\Lambda}$, where Λ

[5] A general property of PIDs is that there are no nontrivial zero divisors, i.e. for every element a, the equality $ab = 0$ implies that $b = 0$. However, for cyclic groups it is obvious that this property fails.

denotes the one-dimensional lattice on which we work. For notational simplicity, we will henceforth write A_n instead of $A[n]$. When requiring translation invariance, Theorem 1.1 implies the following condition for all site indices $i \in \Lambda$:

$$A_{i+1}^k = e^{i\varphi_i} X_i^{-1} A_i^k X_{i+1} \,. \tag{3.10}$$

This relation can now be inserted in the general MPS formula to express all MPS tensors relative to a given site index $i_1 \in \Lambda$. The MPS tensors associated to sites to the left of i_1 can be rewritten in a similar way by solving Eq. (3.10) for A_i^k and replacing i by $i-1$. Graphically, this then gives us:



It is impossible to remove all the phase factors, but because every quantum state is defined up to an arbitrary phase, we can simply ignore this global phase. Hence, by a redefinition $X_{i_1}^{-1} A_{i_1} \longrightarrow A_{i_1}$, we can always choose a uniform MPS discription for a TI system:

$$|\psi\rangle_{TI} = \sum_{\{s_i\}} \mathrm{tr}\left(\prod_{i=1}^{N} A^{s_i}\right) |s_1 s_2 \cdots s_N\rangle \,, \tag{3.11}$$

where the tensors A^i are now site-independent.

3.2.2 SWAP: F_V-group

In this case, the state is not only translation-invariant, but it is also invariant under a reflection about the horizontal axis (a 'swap'). As in the previous case, we will start from an MPS with the same tensor C at every site but with the generalization that the tensor has two physical indices: $C \equiv C^{ij}$ (see Fig. 3.4).

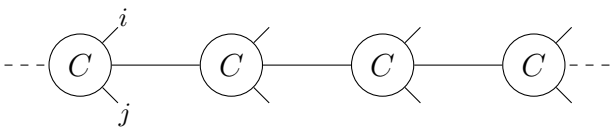


Figure 3.4: Two-legged MPS.

Invariance under the swap-operation implies that

$$C^{ji} = e^{i\varphi} X^{-1} C^{ij} X \,. \tag{3.12}$$

Applying this operation a second time gives:

$$C^{ij} = e^{2i\varphi} X^{-2} C^{ij} X^2 \,. \tag{3.13}$$

From Theorem 1.1, we can conclude that $\varphi \in \{0, \pi\}$ and that

$$X^2 = e^{i\chi} \mathbb{1} \,. \tag{3.14}$$

No further restrictions on the constant χ arise and we can absorb this phase in X. It follows that the gauge matrices in the case of a swap-symmetry are *involutory*. However, it is not very difficult to check that the analysis in Section 2.1.1 generalizes to this case and, hence, that X can be assumed to be unitary. Combining this with the above condition, we obtain that X is also Hermitian, i.e. $X^\dagger = X$. Now, we will prove that matrices that are both unitary and Hermitian are unitarily equivalent to matrices of the form

$$Z = \begin{pmatrix} \mathbb{1}_m & 0 \\ 0 & -\mathbb{1}_n \end{pmatrix} . \tag{3.15}$$

Proof. Since unitary/Hermitian matrices are unitarily diagonalizable we obtain a decomposition of the form

$$X = UDU^\dagger$$

with D diagonal and U unitary. Because X is unitary we immediately find that $D^{-1} = D^\dagger$ or equivalently that the diagonal elements of D lie on the complex unit circle: $\overline{D_i} = \frac{1}{D_i}$. On the other hand we can immediately see that because X is Hermitian all eigenvalues are real. So the diagonal elements should be both real and and lie on the complex unit circle. The only numbers that satisfy these conditions are ± 1 and this completes the proof. □

Inserting this into the symmetry condition gives us:

$$C^{ji} = \pm (UZU^\dagger) C^{ij} (UZU^\dagger) \,, \tag{3.16}$$

where we used that $Z = Z^{-1}$. This equation can also be rewritten as:

$$U^\dagger C^{ji} U = \pm Z (U^\dagger C^{ij} U) Z \,. \tag{3.17}$$

After the redefinition $U^\dagger C^{ij} U \longrightarrow D^{ij}$, we obtain:

$$D^{ji} = \pm Z D^{ij} Z \,. \tag{3.18}$$

So, up to a conjugation by a matrix of the form (3.15), we obtain (anti)symmetric MPS tensors with respect to the swap-operation. This also implies that in the case of swap-symmetry the number of degrees of freedom in the variational ansatz are greatly reduced. Up to the signature[6] of Z the matrices D^{ij} completely determine the 'swapped' matrices D^{ji}.

[6]The number of 1's and -1's on the diagonal.

3.2.3 Reflections: F_H-group

In this case the system is invariant under reflections across a vertical axis. In the MPS formalism this operation is implemented by taking the transpose of all matrices. This can be proven as follows:

$$\begin{aligned} |\psi\rangle &= \sum_{\{s_i\}} \mathrm{tr}\Big(A^{s_1}A^{s_2}A^{s_3}\dots A^{s_N}\Big)|s_1 s_2 \dots s_N\rangle \\ \mathcal{R}|\psi\rangle &= \sum_{\{s_i\}} \mathrm{tr}\Big(A^{s_1}A^{s_2}A^{s_3}\dots A^{s_N}\Big)|s_N \dots s_2 s_1\rangle \end{aligned} \tag{3.19}$$

Using the invariance of the trace under taking transposes we can rewrite the second equation as:

$$\mathcal{R}|\psi\rangle = \sum_{\{s_i\}} \mathrm{tr}\Big((A^{s_N})^t \dots (A^{s_2})^t (A^{s_1})^t\Big)|s_N \dots s_2 s_1\rangle \tag{3.20}$$

Relabeling all indices ($s_k \longrightarrow s_{N-k+1}$) gives us what we wanted:

$$\mathcal{R}|\psi\rangle = \sum_{\{s_i\}} \mathrm{tr}\Big((A^{s_1})^t (A^{s_2})^t \dots (A^{s_N})^t\Big)|s_1 s_2 \dots s_N\rangle \tag{3.21}$$

□

We can now consider a system symmetric under reflections. Requiring invariance of the MPS under a reflection $\mathcal{R}$ gives us the following condition:

$$\sum_j R_{ij}(A^j)^t = e^{i\varphi} X^{-1} A^i X\,, \tag{3.22}$$

where R is aunitary matrix satisfying $R^2 = \mathbb{1}$. Applying a second reflection, gives:

$$\begin{aligned} A^i &= e^{2i\varphi} X^t X^{-1} A^i X X^{-t} \\ &= e^{2i\varphi} (X X^{-t})^{-1} A^i X X^{-t}\,. \end{aligned} \tag{3.23}$$

Using the injectivity of A^i to apply Theorem 1.1 gives us two conditions:

- $\varphi \in \{0, \pi\}$, and
- $X X^{-t} = e^{i\chi}\mathbb{1}$.

The second condition can be rewritten as follows:

$$X = e^{i\chi} X^t\,. \tag{3.24}$$

This equation gives rise to two possibilities:

- $\mathrm{tr}(X) \neq 0$: Because $\mathrm{tr}(X) = \mathrm{tr}(X^t)$, we obtain that $\chi = 0$ and, hence, that X is symmetric.
- $\mathrm{tr}(X) = 0$: Here, we cannot use an argument based on the trace. However, iterating Eq. (3.24) shows that the phase factor squares to 1 or, equivalently, that $\chi \in \{0, \pi\}$. This tells us that X is symmetric or skew-symmetric[7].

[7]For odd bond dimensions, only the symmetric case is possible since skew-symmetric matrices are not

Due to the discrete character of the indicators φ and χ, we get 3 nontrivial SPT phases, i.e. we obtain a $\mathbb{Z}_2 \times \mathbb{Z}_2$ classification. This is completely consistent with numerical results from the Smith normal form algorithm and with the literature [14].

A reflection symmetric MPS can also be brought to a kind of normal form. First, we will consider the symmetric case $X = X^t$. Using the Autonne–Takagi factorization (see Section B.2 in the appendix), we can write every complex symmetric matrix in the following form:

$$X = UU^t \tag{3.25}$$

for some complex matrix U. Inserting this expression in condition (3.22) gives:

$$\begin{aligned} \sum_j R_{ij}(A^j)^t &= \pm U^{-t}U^{-1}A^iUU^t \\ \iff \sum_j R_{ij}U^t(A^j)^tU^{-t} &= \pm U^{-1}A^iU \\ \iff \sum_j R_{ij}\left(U^{-1}A^jU\right)^t &= \pm U^{-1}A^iU\,. \end{aligned}$$

Starting from a uniform MPS with tensor A, inserting the unit matrix $\mathbb{1} = UU^{-1}$ between all sites and defining $C \equiv U^{-1}AU$, we see that we can obtain a manifestly (anti)symmetric MPS with respect to reflections.

For the skew-symmetric case ($X = -X^t$), we can use a similar trick. Every complex skew-symmetric matrix can be written in the following way (see Section B.3 in the appendix):

$$X = U(\mathbb{1}_n \otimes i\sigma_y)U^t\,, \tag{3.26}$$

where U is some complex matrix and σ_y is the Pauli y-matrix:

$$\sigma_y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{3.27}$$

From here on, we will denote the matrix $\mathbb{1}_n \otimes i\sigma_y$ by Γ to ease the notation. We can now perform a similar calculation as before to obtain the equation

$$-\sum_j R_{ij}(U^{-1}A^jU\Gamma)^t = \pm U^{-1}A^iU\Gamma \tag{3.28}$$

in which we used that $\Gamma^t = -\Gamma = \Gamma^{-1}$. This could also be written more symmetrically by introducing the square root $\sqrt{\Gamma}$:

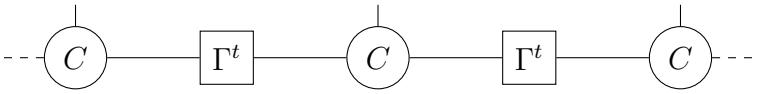
$$-\sum_j R_{ij}(\sqrt{\Gamma}U^{-1}A^jU\sqrt{\Gamma})^t = \pm\sqrt{\Gamma}U^{-1}A^iU\sqrt{\Gamma}\,. \tag{3.29}$$

We can again get MPS tensors that are reflection-(anti)symmetric as before, but there is a little twist to the story. The new tensors would be obtained by defining $C = \sqrt{\Gamma}U^{-1}AU\sqrt{\Gamma}$:

$$-\sum_j R_{ij}(C^j)^t = \pm C^i\,. \tag{3.30}$$

invertible in odd dimensions.

However, for this to work we should, instead of inserting the identity in the form of $\mathbb{1} = UU^{-1}$ between the tensors A, insert the identity in the form of $\mathbb{1} = U\sqrt{\Gamma}(-\Gamma)\sqrt{\Gamma}U^{-1}$ between the tensors (where we used that $\Gamma^2 = -\mathbb{1}$). Although this results in MPS tensors that are manifestly (anti)symmetric under reflections, we obtain a new feature. Nontrivial bond tensors Γ arise because only one matrix Γ is used in the definition of the new MPS tensors C. This nontrivial structure is most easily visualized using the graphical notation:



The presence of these matrices Γ is very similar to the bond tensors that appear in [32] for symmetric 2D PEPS. They are also used as a means to make the on-site and lattice symmetries work together in a consistent way. The extra minus sign that appears on the left-hand side in the transformation formula (3.30) is cancelled by the bond tensors, since these too give rise to a minus sign under transposition ($\Gamma^t = -\Gamma$). In general, we see that, given a physical system that is (anti)symmetric under reflections, we can start from (anti)symmetric variational ansätze without loss of generality (possibly with the inclusion of the bond tensors Γ).

3.2.4 Glide reflections: F_G-group

We again consider a system with two-legged MPS tensors, labeled C^{ij} and D^{ij}, but this time we only require the swap-symmetry up to a shift over one site.

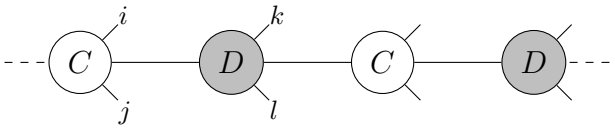


Figure 3.5: General system with two distinct two-legged tensors.

The glide reflection symmetry then gives:

$$\begin{aligned} C^{ji} &= e^{i\theta} Y^{-1} D^{ij} X\,, \\ D^{ji} &= e^{i\varphi} X^{-1} C^{ij} Y\,. \end{aligned} \tag{3.31}$$

where we chose different gauges on the C-D and D-C bonds. Performing a second glide reflection gives:

$$\begin{aligned} C^{ij} &= e^{i(\theta+\varphi)} (XY)^{-1} C^{ij} YX\,, \\ D^{ij} &= e^{i(\varphi+\theta)} (YX)^{-1} D^{ij} XY\,. \end{aligned} \tag{3.32}$$

To find a condition on φ, θ, X and Y, we cannot readily apply Theorem 1.1. However, by multiplying both equations (blocking two sites), we obtain the correct form for the fundamental theorem. For the phases, we get the following condition:

$$2(\varphi + \theta) = 0 \mod 2\pi \implies \varphi + \theta = 0 \mod \pi\,. \tag{3.33}$$

So, within the constraint $\varphi + \theta = 0 \mod \pi$, we can make an arbitrary choice for one of the phases. For the gauge matrices X, Y, we obtain:

$$XY = e^{i\chi}\mathbb{1}\,. \tag{3.34}$$

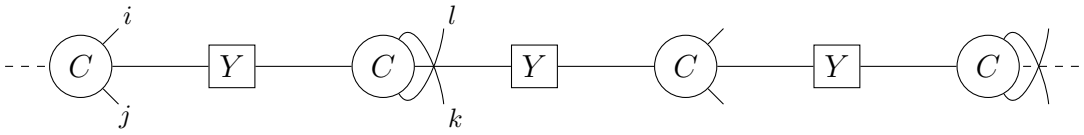
We conclude that the gauges X and Y are (proportional to[8]) each other's inverses. However, if we insert this into the relations above, we obtain:

$$\begin{aligned} C^{ij} &= e^{i(\varphi+\theta)} C^{ij} \\ D^{ij} &= e^{i(\varphi+\theta)} D^{ij} \end{aligned} \tag{3.35}$$

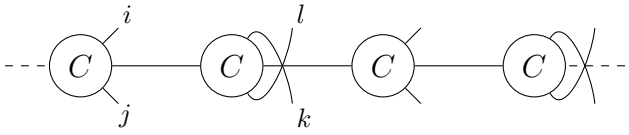
with $e^{i(\varphi+\theta)} = \pm 1$. If this phase would be -1, both tensors C, D would have to be identically zero and this is not possible. We conclude that only $\varphi + \theta = 0 \mod 2\pi$ is physically relevant. After making the choice $\theta = 0$, we can rewrite Eq. (3.31) as follows:

$$D^{ji} = Y C^{ij} Y \,. \tag{3.36}$$

Inserting this in the MPS in Fig. 3.5 gives:



By redefining $C^{ij}Y \longrightarrow C^{ij}$, we obtain the following generic glide reflection-invariant MPS:



We can also conclude that, due to the remark made above, there exists no nontrivial SPT phase for glide reflection symmetries.

3.2.5 Rotations: F_R-group

In this case, the system is invariant under a rotation over π. This is equivalent to the invariance under the combination of a swap and a reflection. As in the swap and glide-reflection cases, we use an MPS tensor with two physical indices: $C \equiv C^{ij}$. Requiring invariance under F_R gives:

$$(C^{ji})^t = e^{i\varphi} X^{-1} C^{ij} X \,. \tag{3.37}$$

Applying a second rotation gives:

$$C^{ij} = e^{2i\varphi} (X X^{-t})^{-1} C^{ij} X X^{-t} \,. \tag{3.38}$$

Using the fundamental theorem 1.1 we get exactly the same conditions as for reflections (F_H-group) and, hence, we obtain a nontrivial SPT classification.

Figure 3.6: Reflection with a shift.

3.3 Beyond frieze

3.3.1 Reflection with a shift

Let us consider a system that is invariant under a reflection up to a shift over 1 site. If we denote the MPS tensors at the two different sites by, respectively, A and B, we obtain the following set of equations for the only nontrivial element in the symmetry group (which is isomorphic to $\mathbb{Z}_2$):

$$\begin{aligned} \sum_j R_{ij}(A^j)^t &= e^{i\varphi_A} X^{-1} B^i Y \,, \\ \sum_j R_{ij}(B^j)^t &= e^{i\varphi_B} Y^{-1} A^i X \,, \end{aligned} \tag{3.39}$$

where R is a unitary matrix satisfying $R^2 = \mathbb{1}$. Repeating this transformation a second time gives us:

$$\begin{aligned} A^i &= e^{i(\varphi_A+\varphi_B)} Y^t Y^{-1} A^i X X^{-t} \,, \\ B^i &= e^{i(\varphi_A+\varphi_B)} X^t X^{-1} B^i Y Y^{-t} \,. \end{aligned} \tag{3.40}$$

Applying theorem 1.1 to the products A^iB^j and B^iA^j gives us:

- $2(\varphi_A + \varphi_B) = 0 \mod 2\pi \implies \varphi_A + \varphi_B \in \{0, \pi\}$,
- $X^t X^{-1} = e^{i\chi_X}\mathbb{1} \implies X^t = \pm X$, and
- $Y^t Y^{-1} = e^{i\chi_Y}\mathbb{1} \implies Y^t = \pm Y$.

By inserting these relations in Eq. (3.40), we obtain[9]:

$$\varphi_A + \varphi_B \pm \chi_X \pm \chi_Y = 0 \,. \tag{3.41}$$

Hence, if we have made a choice for $\varphi_A + \varphi_B$ and either χ_X or χ_Y, the other one is fixed. This again gives us a $\mathbb{Z}_2 \times \mathbb{Z}_2$ SPT classification.

We can now proceed by making the general form of this MPS more explicit. First, we consider the case where both X and Y are symmetric. As in Section 3.2.3, we will use the Autonne–Takagi factorization for complex symmetric matrices (Section B.2 in the appendix). This way, we can rewrite the symmetry condition of the MPS tensors as follows:

$$\sum_j (R_{ij}A^j)^t = e^{i\varphi_A}(UU^t)^{-1} B^i (VV^t) \,, \tag{3.42}$$

[8]The proportionality constant can be absorbed in the matrices.

[9]The $\pm$-sign is, in fact, not relevant since the phases χ are equal to 0 or π and, hence, equivalent to their negation.

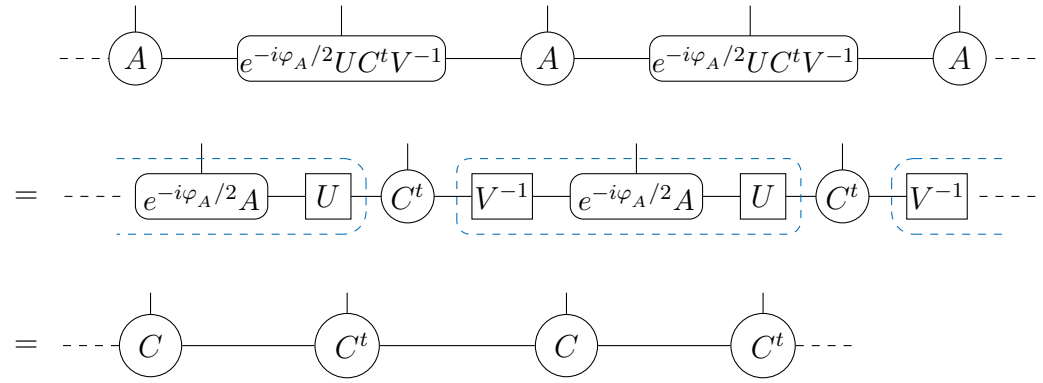
or equivalently:

$$\sum_j e^{-i\varphi_A} U \left[V^{-1}(R_{ij}A^j)U\right]^t V^{-1} = B^i \,. \tag{3.43}$$

Now, assume that $R = \mathbb{1}$ (this is merely for ease of notation, the general case will recovered at the end). After substituting this in the generic MPS and defining

$$C^i = e^{-i\varphi_A/2} V^{-1} A^i U \,, \tag{3.44}$$

we obtain the following MPS:



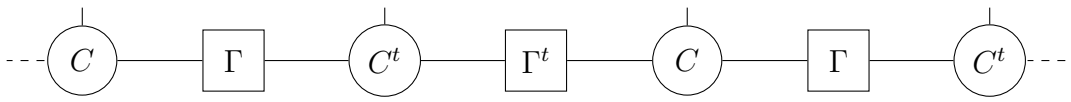
Now, we consider the case where both X and Y are skew-symmetric. Here, we again use the factorization for complex skew-symmetric matrices (Section B.3 in the appendix):

$$X = U\Gamma U^t$$

where

$$\Gamma = \mathbb{1} \otimes i\sigma_y = \mathbb{1} \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} . \tag{3.45}$$

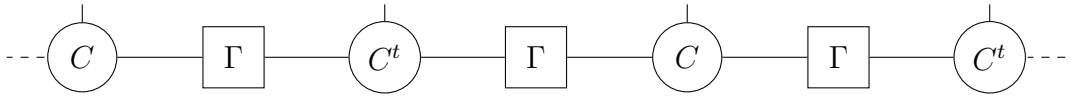
By the exact same reasoning as in the symmetric case, we obtain the following MPS:



where we used that

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}^{-1} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{3.46}$$

to write Γ^{-1} as $-\Gamma$. By absorbing a factor $\sqrt{-1}$ in every tensor, we can rewrite the MPS as:



The cases with one symmetric and one skew-symmetric gauge matrix are similar to the one above, but where the matrices Γ at every second bond are replaced by the identity.

Before redefining the MPS matrices we assumed that $R = \mathbb{1}$ which allowed us to forget about these physical actions and obtain a nice alternating pattern in the MPS. To obtain the general case where R is nontrivial, we simply have to apply the operator R to the C^t-sites. Since the physical action R is not a part of the variational ansatz, this does not increase the number of degrees of freedom. In general, we see that under this symmetry the information in one MPS tensor completely fixes the other ones.

3.3.2 Time-reversal

Although this case does not contain a nontrivial lattice symmetry, we will include it for the sake of completeness. We again start from a uniform MPS representation. Invariance under a time-reversal operation (without a lattice shift) gives the following condition:

$$\sum_j T_{ij}\overline{A^j} = e^{i\varphi} X^{-1} A^i X \,, \tag{3.47}$$

where the unitary matrix T must satisfy $T\overline{T} = \mathbb{1}$ as shown in Section 2.2.1 of the previous chapter. A second time-reversal then gives:

$$A^i = \overline{X^{-1}} X^{-1} A^i X \overline{X} \,. \tag{3.48}$$

The fact that the phase factor $e^{i\varphi}$ drops out of the equation and, accordingly, that we cannot find a constraint on this factor, is consistent with the fact that in condition (3.47) we can absorb the phase factor in the MPS tensor without loss of generality by the transformation

$$e^{i\varphi/2} A^i \longrightarrow A^i \,. \tag{3.49}$$

The fundamental theorem 1.1 gives us the following condition on the matrix X:

$$X\overline{X} = e^{i\chi}\mathbb{1} \,. \tag{3.50}$$

As shown in Section 2.1.1, we can assume the matrix X to be unitary. This implies that $\overline{X} = X^{-t}$ and, by insertion in the above condition, we get:

$$X = e^{i\chi} X^t \,. \tag{3.51}$$

As in the case of reflection symmetry, this relation tells us that $e^{i\chi} = \pm 1$ or, equivalently, that X is (skew)symmetric. In representation theory this phase, which is called the *Frobenius–Schur indicator*, is very important. It classifies the real irreducible representations. Below we will see this classification in action.

We will perform similar calculations as before to bring the time-reversal symmetric MPS in normal form. First, we consider the symmetric case $X = X^t$. Using the Autonne–Takagi factorization we obtain an invertible matrix U such that $X = UU^t$. However, because X is unitary, we have the extra property that U is also unitary. Condition (3.47) can then be rewritten as follows:

$$\begin{aligned} \sum_j T_{ij}\overline{A^j} \quad &= U^{-t}U^{-1}A^i U U^t \\ \iff \sum_j T_{ij} U^t \overline{A^j} U^{-t} \quad &= U^{-1} A^i U \end{aligned}$$

$$\iff \sum_j T_{ij}\overline{U^{-1}A^jU} = U^{-1}A^iU\,.$$

So, by inserting the identity $\mathbb{1} = UU^{-1}$ between all sites and defining $C \equiv U^{-1}A^iU$, we obtain a manifestly time-reversal symmetric MPS tensor, i.e. $\sum_j T_{ij}\overline{C^j} = C^i$. So, up to the mixing by T, we find that the MPS tensors can be chosen to be real. Coincidentally, the real self-conjugate representations are exactly those for which the Frobenius–Schur indicator is $+1$.

For the case $X = -X^t$ we can again use the factorization $X = U\Gamma U^t$ with $\Gamma = \mathbb{1}\otimes i\sigma_y$ and U unitary. Similar to the case of reflection symmetry, we can try to obtain a manifestly symmetric form. However, the closest we get is:

$$\sum_j T_{ij}\overline{\sqrt{\Gamma}U^{-1}A^jU\sqrt{\Gamma}^t} = \sqrt{\Gamma}^t U^{-1}A^iU\sqrt{\Gamma}\,. \tag{3.52}$$

We are not so lucky as in the reflection symmetric case as the matrices $\sqrt{\Gamma}$ and $\sqrt{\Gamma}^t$ are located on the wrong side. A more natural form of the above relation is:

$$\sum_j T_{ij}\overline{U^{-1}A^jU} = \Gamma^{-1}U^{-1}A^iU\Gamma\,. \tag{3.53}$$

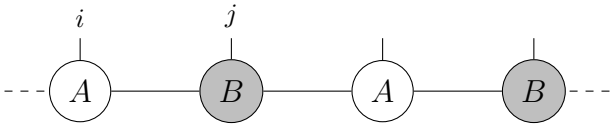
This is also the relation (up to the mixing by T) that characterizes the so-called self-conjugate representations of *quaternionic type*. These are representations ρ for which there exists a unitary matrix W such that

$$\overline{\rho} = W^\dagger \rho W \tag{3.54}$$

but that are not real. The best-known example is the Spin(3)-representation given by the Pauli matrices. These quaternionic representations are exactly the representations for which the Frobenius–Schur indicator is -1, as is the case here.

3.3.3 Time-reversal with a shift

We will again start from an MPS with two a priori different tensors:



Requiring invariance under a time-reversal operation up to a one-site shift gives the following set of equations:

$$\begin{aligned}\sum_j T_{ij}\overline{A^j} &= e^{i\varphi_A}X^{-1}B^iY\,,\\ \sum_j T_{ij}\overline{B^j} &= e^{i\varphi_B}Y^{-1}A^iX\,,\end{aligned} \tag{3.55}$$

where T is a unitary matrix satisfying $T\overline{T} = \mathbb{1}$. Repeating this transformation a second time gives us:

$$\begin{aligned} A^i &= e^{i(\varphi_B - \varphi_A)}\overline{X^{-1}}Y^{-1}A^iX\overline{Y}\,, \\ B^i &= e^{i(\varphi_A - \varphi_B)}\overline{Y^{-1}}X^{-1}B^iY\overline{X}\,. \end{aligned} \tag{3.56}$$

Applying the fundamental theorem 1.1 to the products A^iB^j and B^iA^j gives us $X\overline{Y} = e^{i\chi}\mathbb{1}$ and, as in the case of time-reversal without a shift, the phases φ_A, φ_B are unconstrained. If we want to remove these phases by absorbing them in the MPS tensors as we did in the previous section, we could, for example, absorb a phase $e^{i\varphi_A/2}$ in both A and B. But to consistently cancel the phase $e^{i\varphi_B}$ in the second symmetry condition, we should have that $\varphi_A - \varphi_B = 0$.

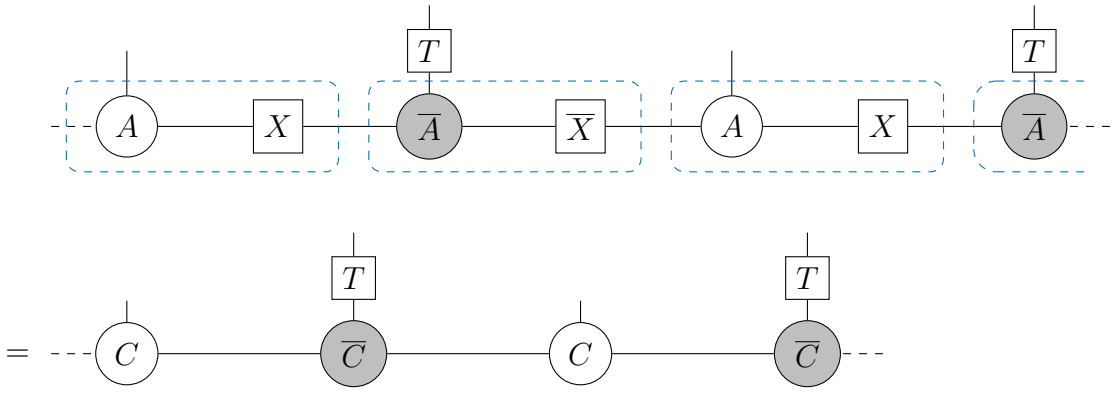
By inserting the relation on the gauge matrices in Eq. (3.56), we obtain the condition:

$$\varphi_B - \varphi_A + 2\chi = 0\,. \tag{3.57}$$

This relation does not really give us a topological indicator as the phase $e^{i\chi}$ can be consistently absorbed in the gauge matrices, but it agrees with the condition obtained if we want to consistently absorb the phases φ_A, φ_B in the MPS tensors, so everything matches nicely. For the classification of SPT phases, we see that we only obtain the trivial phase. However, as before, we can use the symmetry conditions above to find a symmetric normal form. First, we use our results to rewrite the conditions as follows:

$$\begin{aligned} \sum_j T_{ij}\overline{A^j} &= X^{-1}B^iY \\ &= X^{-1}B^i\overline{X^{-1}}\,. \end{aligned} \tag{3.58}$$

By defining $C^i = A^iX$, we obtain the following MPS representation:



Chapter 4

Conclusion and outlook

4.1 Results

We started out with the rather ambitious goal of obtaining a general and numerically easy-to-implement method to classify SPT phases in 1D bosonic systems in the case of nontrivial space group symmetries. For all symmetries in one dimension (on-site, time-reversal, reflection), we obtained a purely cohomological classification by generalizing the way we look at the projective representations and phase factors obtained from the fundamental theorem of matrix product states. These results were compared to the literature [11, 14] using numerical methods and were found to be consistent. We also gave an interpretation of the group cocycles by generalizing the classification in terms of projective unitary representations to a classification in terms of projective unitary-antiunitary representations. An explicit construction of a representative in each SPT phase was given, but a concrete interpretation in terms of physically realizable systems is still lacking.

For the inclusion of nontrivial lattice transformations, we argued that the classical space groups were not sufficient, although the distinction on what are physically distinct systems is not completely unambiguous. For the relevant spatial symmetry groups, we constructed a cohomological method which gave plausible results. However, further research on this topic will be necessary. At the same time, the generalization of the cohomological classification from fully translation-invariant systems to systems with nontrivial space group symmetries is also not completely clear. It was expected that the number of SPT phases (at least in one dimension) would remain the same. However, certain cases such as systems with a swap or glide reflection symmetry or time-reversal symmetric systems, which are related by a 1-site shift, showed that this is not true. This difficulty in interpreting the results could be a consequence of the unclear view on which systems are physically distinct.

4.2 Outlook

In the future, it should be possible to generalize the methods in a couple of different ways, even in the case of one-dimensional systems. For example, one could try to include

continuous on-site symmetries which are described by (compact) Lie groups. A problem with this generalization is that Lie groups have an infinite number of elements, but for numerical purposes there should only be a finite number of variables. At the same time, Lie groups also carry topological information, so one should replace the ordinary group cohomology by a complex that also takes into account that topological information. Lie algebra cohomology (e.g. *Chevalley–Eilenberg* cohomology) could be a possibility. This is numerically feasible, since the relevant Lie algebras have a finite number of generators and Lie algebras are inherently linear, although they only contain information about the group elements connected to the identity (so this might not always suffice). According to [11], the right choice would be *Borel cohomology*, based on *measurable functions*, but it is not (yet) clear how to compute this numerically. A good understanding of the various approaches and their relations (for example [52]) will be a good start for further investigation.

A second possible generalization is the inclusion of fermionic matrix product states. It has been shown that these are classified by so-called group supercohomology [8, 22, 62]. This generalization from cohomology to supercohomology arises from the fermionic particle statistics which induce $\mathbb{Z}_2$-graded algebraic structures. The existence of these structures even gives rise to topological order in the case of symmetries which for bosonic systems do not admit SPT phases and, hence, it would be interesting to know if their interplay with space group symmetries gives an even richer phase classification.

Another type of generalization would be to go to higher dimensions (e.g. PEPS). In higher dimensions, SPT phases are still (partially) classified by group cohomology. However, because the spatial structure of physical systems in 2 and more dimensions can be more exotic, the inclusion of space group symmetries will be more intricate. Some cases were already considered in the literature [32], but this was not done in a systematic way. If this method could be reformulated in a systematic and easily carried out approach, this would be a major step forward.

Another aspect that only arises in dimension 2 and higher is the occurence of *matrix product operator* (MPO) symmetries [24]. These can be used to describe both intrinsic topological order and SPT order, but it is still not fully clear what the exact relation between SPT order and MPO symmetries is and, especially, how the MPO symmetry algebra relates to the cohomological approach used in this thesis.

Several other directions exist. For example Kapustin et al. [36, 37] reformulated the framework of SPT phases and tensor networks in the context of *topological quantum field theory* (TQFT). It could be interesting to see how the space group symmetries translate to the geometric language of TQFT. While residing in the world of geometry, it could also be interesting to study how the presence of symmetries is reflected in the manifold and fibre bundle structure of MPSs introduced in [23].

A completely different idea would be to include explicit symmetry breaking. In [50], it was shown that for systems with a degenerate groundstate the symmetries are described by *induced representations*. It is still not completely clear how all these concepts relate to our results and to each other.

Finding a complete and satisfying answer to all of these open research questions is a

very ambitious task. However, based on the current research and literature, this is not impossible and studying these problems could lead to important insights in both the theoretical and numerical nature of tensor networks states.

Appendix A

Algebra

A.1 Group theory

A.1.1 Abstract group theory

Definition A.1 (Order). The order $|G|$ of a finite group G is defined as the number of elements in the group. The order of an element $g \in G$ is defined as the smallest (positive) integer n such that:

$$g^n = e\,, \tag{A.1}$$

where e is the identity element in G. The order of a subgroup $H \subset G$ is defined as the ratio $|G|/|H|$.

Definition A.2 (Normal subgroup). Let G be a group. A subgroup $H \subset G$ is said to be normal if

$$gHg^{-1} = H \tag{A.2}$$

for all $g \in G$.

Definition A.3 (Direct product). Let G, H be two groups. The underlysing set of the direct product $G \times H$ is defined as the Cartesian product of G and H:

$$G \times H = \{(g, h) \mid g \in G, h \in H\}\,. \tag{A.3}$$

The group structure on $G \times H$ is defined by pairwise multiplication:

$$(g_1, h_1) \cdot (g_2, h_2) = (g_1 g_2, h_1 h_2)\,. \tag{A.4}$$

Definition A.4 (Free group). Consider a set S, which will be called the set of *generators*. The free group F_S on S is defined as the set of all *words* on S, i.e. all finite sequences of elements of S. The multiplication in this group is given by concatenation of words.

Definition A.5 (Presentation). Consider a group G. A presentation of G is a tuple (S, R), often denoted by $\langle S|R\rangle$, where:

- S is a set of generators, and

- R is a set of relations among the generators (generally these are products of elements which equal the identity)

such that G is isomorphic to the quotient of the free group F_S by the set of relations R. An element of this quotient is also called a reduced word.

A.1.2 Representation theory

Definition A.6 (Representation). A (linear) representation of a group G on a vector space V is a group morphism $\rho : G \to \mathrm{GL}(V)$. This definition is equivalent to stating that the following equation holds for all $g, h \in G$:

$$\rho(g)\rho(h) = \rho(gh)\,. \tag{A.5}$$

This equation implies the following two important properties:

- $\rho(e) = \mathbb{1}_V$ for e the identity in G, and
- $\rho(g^{-1}) = \rho(g)^{-1}$ for all $g \in G$.

Definition A.7 (Projective representation). A projective representation of a group G on a vector space V is a group morphism $\rho : G \to \mathrm{PGL}(V)$. Here $\mathrm{PGL}(V)$ denotes the projective linear group, i.e. the quotient group $\mathrm{GL}(V)/\mathbb{C}^\times$ of the general linear group by the invertible complex numbers.

Equivalently (see for example [6]), a projective representation is a function $\hat{\rho} : G \to \mathrm{GL}(V)$ such that the following relation holds for all $g, h \in G$:

$$\hat{\rho}(g)\hat{\rho}(h) = e^{i\omega(g,h)}\hat{\rho}(gh) \tag{A.6}$$

for some function $e^{i\omega} : G \times G \to \mathrm{U}(1)$.

Definition A.8 (Unitary representation). Let $\mathcal{H}$ be a (finite-dimensional) Hilbert space[1]. A representation $\rho : G \to \mathrm{GL}(\mathcal{H})$ is said to be unitary if for every element $g \in G$, the corresponding operator $\rho(g)$ is a unitary operator.

There is an important theorem stating that every representation of a finite or compact Lie group G is equivalent to a unitary representation. For finite groups, this is easily proven by defining a G-invariant inner product obtained by averaging over the group elements. For Lie groups, the averaging process is not so simple since one cannot simply sum over all elements. For this one needs an appropriate integration measure. It can be proven that for compact Lie groups the existence of such a measure, called the *Haar measure*, is always guaranteed.

In quantum mechanics, phases are not relevant and, hence, the important structure is the projectivization of the Hilbert space $\mathbb{P}(\mathcal{H})$. The inner product $\langle\cdot|\cdot\rangle$ on $\mathcal{H}$ induces a mapping on $\mathbb{P}(\mathcal{H}) \times \mathbb{P}(\mathcal{H})$ by taking the modulus:

$$(\Psi, \Phi) = \frac{|\langle\Psi|\Phi\rangle|}{|\langle\Psi|\Psi\rangle||\langle\Phi|\Phi\rangle|}\,. \tag{A.7}$$

[1] The existence of an inner product suffices.

Although only the unitary operators on $\mathcal{H}$ leave the inner product $\langle\cdot|\cdot\rangle$ invariant, the product on $\mathbb{P}(\mathcal{H})$ is also left invariant by the antiunitary operators, i.e. operators T that satisfy

$$\langle T\Psi|T\Phi\rangle = \overline{\langle\Psi|\Phi\rangle} = \langle\Phi|\Psi\rangle \ . \tag{A.8}$$

This relation, among other things, implies that every antiunitary operator is, in particular, antilinear[2]:

$$T(a\Psi + \Phi) = \overline{a}\, T(\Psi) + T(\Phi)\,. \tag{A.9}$$

It is also easy to see that the antiunitary operators do not form a group as the product of two antiunitary opertors is a unitary operator. This property, however, implies that the union of the set of unitary operators and the set of antiunitary operators can be given the structure of a group. This group is sometimes called the *unitary-antiunitary* (UA) group.

Now, by Wigner's theorem [65], every isometry of $\langle\cdot|\cdot\rangle$ is induced by either a unitary or an antiunitary operator. With this in mind, we can define a generalization of unitary representations.

Definition A.9 (UA representation). Let (G, H) be a pair of groups such that H is a subgroup of G of order at most 2. A projective unitary-antiunitary representation[3] of G on $\mathcal{H}$ is a function $\rho : G \to \mathrm{UA}(\mathcal{H})$ such that the following conditions are satisfied:

- $\rho(g)\rho(h) = e^{i\omega(g,h)}\rho(gh)$, and
- $\begin{cases} \rho(g) \in \mathrm{U}(\mathcal{H}) & g \in H\,, \\ \rho(g) \notin \mathrm{U}(\mathcal{H}) & g \in G\backslash H\,. \end{cases}$

Similar to the case of projective representations, the first property is equivalent to stating that ρ is a group morphism from G to the automorphism group of $\mathbb{P}(\mathcal{H})$.

This definition is rather general. The ordinary UA-representations are obtained by considering the case $\omega \equiv 1$. The ordinary unitary representations are obtained by taking $H = G$.

For completeness' sake, we mention an important property that is relevant for this thesis. Every antilinear operator $\mathcal{A}$ can be written as the composition of a linear operator A and a complex conjugation operator $\mathcal{K}$ (with respect to a certain basis) [55]:

$$\mathcal{A} = A\mathcal{K} \tag{A.10}$$

The complex conjugation operator $\mathcal{K}$ is defined a follows. Let $\mathcal{B} = \{|e_i\rangle\}$ be a given basis for a complex vector space. The complex conjugation operator $\mathcal{K}_\mathcal{B}$ associated to this basis is defined by the following two properties:

- $\mathcal{K}_\mathcal{B}\,|e_i\rangle = |e_i\rangle$, and

[2]Because of this, these operators do not admit a matrix representation [55].

[3]Linear-antilinear representations are obtained by replacing (anti)unitary operators by (anti)linear operators.

- $\mathcal{K}_{\mathcal{B}}\left(c\left|\psi\right\rangle\right) = \overline{c}\left(\mathcal{K}_{\mathcal{B}}\left|\psi\right\rangle\right)$

where c is an arbitrary scalar and $|\psi\rangle$ an arbitrary vector. This construction is, in particular, valid for antiunitary operators where the linear operator A is now a unitary operator.

From its definition, we can conclude that the complex conjugation operator has the following properties:

- $\mathcal{K}U = \overline{U}\mathcal{K}$ for every linear map U, and
- $\mathcal{K}^2 = \mathbb{1}$.

A.2 Group cohomology

The cocycle condition from Chapter 2 was a very important relation. It implied that the function ω is a 2-cocycle for the group cohomology of G. But what does this mean?

Definition A.10 (G-module). Consider a group G. A (left) G-module A is as an Abelian group together with a function $\lambda : G \times A \to A$ satisfying the following conditions:

1. $\lambda(e, a) = a$,
2. $\lambda(gh, a) = \lambda(g, \lambda(h, a))$, and
3. $\lambda(g, a + b) = \lambda(g, a) + \lambda(g, b)$.

These say that λ is a left G-action compatible with the group structure on A, i.e. λ is a group morphism $G \to \mathrm{Aut}(A)$.

This definition can also be reformulated in the language of linear algebra. Let $\mathbb{Z}G$ be the group ring of G over $\mathbb{Z}$, i.e. the ring defined by all formal linear combinations of elements of G (over $\mathbb{Z}$) with the multiplication induced by the multiplications in G and $\mathbb{Z}$. A G-module as defined above is then equivalent to a $\mathbb{Z}G$-module in the sense of modules over a ring. This second definition is the preferred way when dealing with tensor products of group modules.

Now, let us define the cohomology of a group G with respect to a G-module A. Let $C^k(G; A)$ denote the Abelian group of (set-theoretic) functions $f : G^k \to A$, where the multiplication is defined pointwise. The elements of this group are called *k-cochains*. Just like in the case of singular cohomology in algebraic topology or de Rham cohomology in differential geometry, we construct the *coboundary operators*[4]:

$$d_k : C^k(G; A) \to C^{k+1}(G; A)\,. \tag{A.11}$$

Their defining relation is:

$$d_{k+1} \circ d_k = 0\,. \tag{A.12}$$

[4]When the degree can be deduced from the context, one often calls all of these 'the coboundary operator' and one drops the subscript k.

For group cohomology, the degree-k operator is a group morphism, explicitly defined as follows[5]:

$$d_k f(g_1,\dots,g_k,g_{k+1}) = g_1\cdot f(g_2,\dots,g_{k+1}) + \sum_{i=1}^{k}(-1)^i f(g_1,\dots,g_{i-1}g_i,\dots,g_{k+1}) + (-1)^{k+1} f(g_1,\dots,g_k)\,, \tag{A.13}$$

where the symbol $\cdot$ in the first term denotes the action λ of G on A. The kernel of the coboundary operator is called the group of *cocycles*, often denoted by $Z^k_\lambda(G;A)$. Below, we list the cocycle conditions relevant for this thesis:

1. 0-cocycle:

$$g\cdot\kappa-\kappa=0\,, \tag{A.14}$$

   where κ is a constant element in A.

2. 1-cocycle:

$$g_1\cdot f(g_2)-f(g_1g_2)+f(g_1)=0 \tag{A.15}$$

3. 2-cocycle:

$$g_1\cdot f(g_2,g_3)-f(g_1g_2,g_3)+f(g_1,g_2g_3)-f(g_1,g_2)=0 \tag{A.16}$$

These cocycle conditions are the ones we found in Chapter 2. The action λ for on-site symmetries was trivial, but if one included symmetries such as time-reversal of reflection symmetry, then this action became important.

Aside from the k-cocycles, we can also define the group $B^k(G;A)$ of k-*coboundaries* as the set of cochains that are obtained by acting with the coboundary operator on a $(k-1)$-cochain:

$$B^k(G;A) := \left\{\omega\in C^k(G;A) : \omega = d_k\varphi\ ,\ \varphi\in C^{k-1}(G;A)\right\}\,. \tag{A.17}$$

From the property $d^2=0$ it follows that B^k is a subgroup of Z^k and, hence, we can define their quotient. This brings us to the definition of the cohomology groups $H^k_\lambda(G;A)$ of the group G with coefficients in A and nontrivial action λ:

$$H^k_\lambda(G;A) := Z^k_\lambda(G;A)/B^k_\lambda(H;A) = \frac{\ker\, d_k}{\mathrm{im}\, d_{k-1}}\,. \tag{A.18}$$

The fact that we mod out the group $B^k_\lambda(G;A)\equiv \mathrm{im}(d_{k-1})$ should remind us of the conditions that we obtained for the function ω in Chapter 2, which followed from the invariance under phase transformations. Hence, we conclude that the functions ω in the definition of a projective representation are not merely 2-cocycles, but in fact they are elements of the cohomology group $H^2(G;\mathrm{U}(1))$. This statement is a well-known fact in group theory: the projective representations of a group G are classified by the elements

[5] In homological algebra, this construction is generally known as the **(normalized) bar resolution (in inhomogeneous form)**. See for example [27].

of the second cohomology group $H^2(G;\mathrm{U}(1))$, which in this context is sometimes called the Schur multiplier. (We come back to this classification in a later section.)

We here state a property (without proof) relevant for our story. For finite groups, it can be shown that all cohomology groups H^k with $k \geq 1$ are *torsion* and *finitely generated*, i.e. they are of the form $\mathbb{Z}_{i_1} \times \cdots \times \mathbb{Z}_{i_n}$ for some $n \in \mathbb{N}$. Applying this property to the classification of SPT phases shows that for any finite symmetry group, the number of distinct SPT phases is also finite.

A.2.1 Normalized complex

The construction of group cohomology above is sometimes called the *normalized standard resolution*[6] in homological algebra. The reason for this name stems from the property that every k-cocycle is cohomologous to a *normalized cocycle*, i.e. for all $k \in \mathbb{N}$ one can choose coboundaries such that for all $\omega \in H^k(G;A)$:

$$\omega(g_1, ..., g_k) = e \tag{A.19}$$

if any of the g_i is the identity e.

Proof. We will prove the statement for $k = 2$ as this is the case we will use the most. First consider the elements $g_1 = e, g_2 = x, g_3 = y$:

$$\begin{aligned} 0 &= e \cdot \omega(x,y) - \omega(ex,y) + \omega(e,xy) - \omega(e,x) \\ &= \omega(x,y) - \omega(x,y) + \omega(e,xy) - \omega(e,x) \\ &= \omega(e,xy) - \omega(e,x) \end{aligned} \tag{A.20}$$

However this is valid for all $y \in G$ and hence $\omega(e,x)$ is invariant under right translation of x. Because right translation induces a group isomorphism, every $x \in G$ can be obtained by right translating the identity and hence

$$\omega(e,x) = \omega(e,e) \tag{A.21}$$

for all $x \in G$. A similar reasoning shows that $\omega(x,e) = \omega(e,e)$ for all $x \in G$.

Now consider a transformation of $\omega(e,e)$ under the addition of a coboundary Φ:

$$\omega(e,e) \longrightarrow \omega(e,e) + \Phi(ee) - e \cdot \Phi(e) + \Phi(e) = \omega(e,e) + \Phi(e)\,. \tag{A.22}$$

By choosing $\Phi(e) = -\omega(e,e)$ and using the normalization condition (A.21), we obtain:

$$\omega(e,x) = e \tag{A.23}$$

for all $x \in G$. □

This result also corresponds to our intuition. The identity element corresponds physically to doing nothing and doing nothing twice should not generate a phase, so $e^{i\omega(e,e)} = 1$. Similarly, performing an operation corresponding to the symmetry element $g \in G$ first and then doing nothing should not give an extra phase next to the symmetry operation, so

[6] Or any other of a vast plethora of names (see also previous footnote).

$e^{i\omega(g,e)} = 1$. (This normalization is of course a consequence of the choice that the identity element $e \in G$ is still represented by the identity matrix.)

We can also show that every normalized coboundary is the coboundary of a normalized cochain and, hence, the normalization carries over to the quotient, i.e. to cohomology. So, when working with cohomology, we can always assume that the cochains are normalized.

A.2.2 Applications

Here, we want to give a bit of background on why group cohomology is also relevant outside the field of topological phases of matter and physics in general. In mathematics, the cohomology groups are used to find (algebraic) solutions to obstruction or classification problems in group theory.

As a simple example, we start by the zeroth cohomology group $H^0_\varphi(G; A)$. From Eq. (A.14) it is clear that these are exactly the fixed points of the action φ. For a trivial action, for example, this is obviously all of A. This group is generally known as the *invariant subgroup* of A (with respect to G), denoted by A^G.

A second, more important, example is the second cohomology group. In Chapter 2, it was shown to be useful in the classification of the projective representations of a finite group, but in group theory, it can also used to classify all *group extensions* (the relation between these two is given later).

Definition A.11 (Group extension). An extension of a group G by an Abelian group A is defined as a group E such that:

- $E/A \cong G$, and
- A is (isomorphic to) a normal subgroup of E.

Now, given a *section* of the projection map $\pi : E \to G$, i.e. function s such that $\pi \circ s = \mathrm{id}_G$, there exists an induced action of G on A defined by the following formula [6]:

$$g \cdot a = \iota^{-1}\left(s(g) a s(g)^{-1}\right) , \tag{A.24}$$

where ι denotes the inclusion $A \hookrightarrow E$.

The importance of the second cohomology group $H^2_\varphi(G; A)$ is that it classifies the equivalence classes of group extensions for which the above induced action is equivalent to the action $\varphi : G \to \mathrm{Aut}(A)$.

This classification also gives rise to a constructive procedure. Given an action $\varphi : G \to \mathrm{Aut}(A)$ and a 2-cocycle $f \in H^2_\varphi(G; A)$, one can construct a group extension E_f of G by A by taking the underlying set to be the Cartesian product[7] $G \times A$ and defining the group multiplication to be:

$$(g, a) \cdot (h, b) = (gh, a + \varphi(g)b + f(g, h)) . \tag{A.25}$$

[7]It can be shown that the underlying set of every group extension is always such a Cartesian product.

We will not show that this construction is well-defined, i.e. independent of the specific representative f of the cohomology class in $H^2_\varphi(G;A)$, but we will show that the multiplication as defined is consistent by virtue of the cocycle condition.

Proof. Applying the multiplication defined above, we obtain:

$$\begin{aligned}(g,a)\cdot\Big[(h,b)\cdot(k,c)\Big] &= (g,a)\cdot\Big(hk, b+\varphi(h)c+f(h,k)\Big)\\ &= \Big(ghk, a+\varphi(g)b+\varphi(g)\varphi(h)c+\varphi(g)f(h,k)+f(g,hk)\Big)\\ &= \Big(ghk, a+\varphi(g)b+\varphi(gh)c+\varphi(g)f(h,k)+f(g,hk)\Big)\,.\end{aligned}$$

If associativity holds, this should be equal to:

$$\begin{aligned}\Big[(g,a)\cdot(h,b)\Big]\cdot(k,c) &= \Big(gh, a+\varphi(g)b+f(g,h)\Big)\cdot(k,c)\\ &= \Big(ghk, a+\varphi(g)b+f(g,h)+\varphi(gh)c+f(gh,k)\Big)\,.\end{aligned}$$

By the cocycle condition on f, these two expressions are the same and, hence, associativity holds. □

From Eq. (A.25), it is also clear that semidirect product groups $G\ltimes_\varphi A$ are exactly those corresponding to the trivial cocycle in $H^2_\varphi(G;A)$. A special type of group extensions is obtained by considering cohomology with a trivial action. These are the so-called *central extensions*, i.e. those for which A is isomorphic to a subgroup of the center $Z(E)$. In this case, the trivial cocycle corresponds to the direct product $G\times A$.

A.2.3 Projective representations

Now, we could of course wonder whether there exists a relation between projective representations (see Section A.1.2 above for a quick recap) and (central) extensions of a finite group G by U(1), since both of these appear to be classified by the same object: the second group cohomology with trivial coefficients $H^2(G;\mathrm{U}(1))$. The relation between projective representations as group morphisms into $\mathrm{PGL}(V)$ and Eq. (A.6) (where the representations are viewed as functions into $\mathrm{GL}(V)$) is where the concept of group extension pops up. The general linear group $\mathrm{GL}(V)$ is a central extension of the projective linear group $\mathrm{PGL}(V)$ by the invertible complex numbers $\mathbb{C}^\times$.

We will now explain how one obtains projective representations from central extensions without going into too much detail. Given a projective representation $\rho: G\to\mathrm{PGL}(V)$ and any function $s:\mathrm{PGL}(V)\to\mathrm{GL}(V)$ such that $s(\tilde g)$ maps to $\tilde g$ under the quotient map

$$\pi:\mathrm{GL}(V)\longrightarrow\mathrm{PGL}(V)\cong\mathrm{GL}(V)/\mathbb{C}^\times \tag{A.26}$$

for all $\tilde g\in\mathrm{PGL}(V)$, we can construct a function $\psi: G\to\mathrm{GL}(V)$ which projects onto ρ. Using this function, we can reconstruct a linear representation of a central extension of G by $\mathbb{C}^\times$ from any projective representation of G in the following way:

> *Consider the map $\psi := s\circ\rho: G\to GL(V)$ where ρ is a projective representation of G on V determined by the 2-cocycle ω. A linear representation of the central extension of G by $\mathbb{C}^\times$ determined by the same 2-cocycle ω is then constructed*

as follows:

$$\sigma : (g, a) \mapsto e^{ia}\psi(g)\,. \tag{A.27}$$

This construction implies that every projective representation of G induces a linear representation of a central extension of G by $\mathbb{C}^\times$.

Using Eq. (A.25) (with the trivial G-action), this construction gives the following multiplication rule:

$$\begin{aligned}\sigma\Big((g,a)\cdot(h,b)\Big) &= \sigma\Big(gh, a+b+\omega(g,h)\Big)\\ &= e^{i(a+b+\omega(g,h))}\psi(gh)\,,\end{aligned} \tag{A.28}$$

where f is the 2-cocycle defining the central extension of G. Because σ is supposed to be a linear representation this should be equal to:

$$\sigma(g,a)\sigma(h,b) = e^{ia}\psi(g).e^{ib}\psi(h) = e^{i(a+b)}\psi(g)\psi(h)\,, \tag{A.29}$$

where the last equality is valid because ψ takes values in the group of linear maps and hence commutes with scalar multiplication (something which will be important in the next section). These two expressions are equal since one can show that $\psi(g)\psi(h)\psi(gh)^{-1}$ defines the same 2-cocycle as the projective representation ρ (see [6, 41] for the proofs).

Conversely every linear representation of the central extension induces a projective representation and these constructions are inverses [56]. This result was originally proven by Schur (in 1904) and he even proved the existence of a central extension[8] such that every projective representation of G lifts to a linear representation of this extension[9], i.e. every projective representation of G can be obtained from a linear representation of its representation group. This specific extension is referred to as the *Schur cover* of G. Furthermore, what we referred to as the second cohomology $H^2(G;\mathrm{U}(1))$ is (up to isomorphism) the Abelian group that extends G and is called the *Schur multiplier* in this context. It should be noted that in Schur's original work the Schur multiplier was given by the homology[10] group $H_2(G;\mathbb{Z})$. For finite groups, with which he was concerned, this group is isomorphic to the one we considered. However for general groups this is not true and the right group for the classification of projective representations is the second cohomology group $H^2(G;\mathrm{U}(1))$.

A.2.4 Generalized representations

Now, we can try to generalize the preceding section to cohomology with a nontrivial G-action on the coefficients. In this case, we have to take the action in Eq. (A.25) into account. If we still require the map σ to be a linear representation, we obtain the following equality:

$$e^{i(a+\varphi(g)b+f(g,h))}\psi(gh) = e^{i(a+b)}\psi(g)\psi(h)\,. \tag{A.30}$$

[8] However, not by $\mathbb{C}^\times$.

[9] Such groups are generally known as *representation groups* (see [41]).

[10] The exact definition of group homology is not relevant.

The above formula certainly works out if:

$$\psi(g)e^{ib} = e^{i\varphi(g)b}\psi(g)\,. \tag{A.31}$$

With the application to physics in mind, we will make a crucial assumption (and, thereby, lose some generality). We will only consider cases for which the action φ is of order 2, i.e. $\varphi^2 \equiv 1$. In this case, we can consider the linear-antilinear representations as presented in Section A.1.2 above. From the definition of an antilinear operator T, it readily follows that

$$Te^{i\chi} = e^{-i\chi}T\,. \tag{A.32}$$

If we compare this with the condition that ψ is induced by a linear representation above, we can see that these conditions are identical. Hence, we obtain the following relation:

> *The group extensions of G by $\mathrm{U}(1)$ with nontrivial action φ for which there exists an order 2 subgroup $H \subset G$ such that*
>
> $$\begin{cases} \varphi(g) = 1 & g \in H \\ \varphi(g) = -1 & g \in G\backslash H \end{cases} \tag{A.33}$$
>
> *are in bijection with the projective linear-antilinear representations of (G, H).*

A rigorous analysis of this construction can be found in [10, 31], where the authors also show that, as Schur did for ordinary projective representations, there exists for every finite group G a representation group $\tilde{G}$ such that every projective UA representation of (G, H) lifts to a UA representation of $\tilde{G}$. Although these papers are mainly concerned with unitary-antiunitary representations, the classification is also valid for linear-antilinear representations (at least in the case where G is finite). This can be seen by analyzing the reasoning in [31], where it is clear that one does not need the operators to be (anti)unitary. This should remind us of the fact that for finite groups (and compact Lie groups), all representations are equivalent to unitary representations (again, see Section A.1.2 above).

A.2.5 Some useful methods

In this section, we give, for the sake of completeness, some of the most relevant theoretical tools for working with group cohomology[11]. The first of these is the famous *Künneth formula*.

Theorem A.1 (Künneth formula). *Consider two groups G, K that act, respectively, on $\mathbb{Z}$-free modules[12] A, B. The group cohomology of the direct product $G \times K$ with coefficients in $A \otimes_{\mathbb{Z}} B$ is related to the group cohomologies of G and K in the following way:*

$$H^k(G \times K; A \otimes_{\mathbb{Z}} B) \cong \bigoplus_{p=0}^{k} \left[H^p(G; A) \otimes_{\mathbb{Z}} H^{k-p}(K; B)\right] \times \bigoplus_{p=0}^{k+1} \mathrm{Tor}(H^p(G; A), H^{k-p+1}(K; B))\,, \tag{A.34}$$

[11] And, in fact, for most cohomology theories (see [27] for more on this).

[12] These are modules that admit a basis over the ring of integers $\mathbb{Z}$.

where the operator Tor*, which is called the torsion product, has the following properties*[13]*:*

- $\mathrm{Tor}(A, B) = \mathrm{Tor}(B, A)$,
- $\mathrm{Tor}(\mathbb{Z}, A) = 0$,
- $\mathrm{Tor}(\mathbb{Z}_m, \mathbb{Z}_n) = \mathbb{Z}_{\gcd(m,n)}$,
- $\mathrm{Tor}(A \times B, M) = \mathrm{Tor}(A, M) \times \mathrm{Tor}(B, M)$*, and*
- $\mathrm{Tor}(A, M \times N) = \mathrm{Tor}(A, M) \times \mathrm{Tor}(A, N)$.

In this thesis, we assumed that we can always decompose the symmetry groups as $G_{\text{on-site}} \times G_{RT}$ where $G_{\text{on-site}}$ represents the on-site symmetry group and $G_{RT} \cong \mathbb{Z}_2 \times \mathbb{Z}_2$ represents the reflection/time-reversal symmetry group. The on-site symmetries act trivially, so $A = \mathbb{Z}$ and, hence, $A \otimes_{\mathbb{Z}} B \cong B$, which explains why we always work over the same coefficients, no matter what the structure of the symmetry group is.

The second theorem is related to the *long exact sequence* in (group) cohomology. For the sake of simplicity, we will only consider specific cases. Let G be a finite group and consider the groups $\mathbb{R}, \mathbb{Z}$ and $\mathrm{U}(1)$ as G-modules. These fit in a so-called (short) exact sequence:

$$0 \longrightarrow \mathbb{Z} \xrightarrow{\iota} \mathbb{R} \xrightarrow{\exp} \mathrm{U}(1) \longrightarrow 0\,. \tag{A.35}$$

This means that the kernel of one morphism (arrow) is equal to the image of the previous morphism (arrow). For the specific sequence above, this is easily seen. The inclusion morphism $\iota : \mathbb{Z} \to \mathbb{R}$ maps an integer to itself (but as an element of the reals) and, under the exponential map $\exp : r \mapsto e^{i2\pi r}$, these are exactly the elements mapped to the unit in $\mathrm{U}(1)$. The theorem now says that this sequence induces a (long) exact sequence of the form:

$$\cdots \longrightarrow H^k(G;\mathbb{Z}) \longrightarrow H^k(G;\mathbb{R}) \longrightarrow H^k(G;\mathrm{U}(1)) \longrightarrow H^{k+1}(G;\mathbb{Z}) \longrightarrow \cdots \tag{A.36}$$

for any group G. This theorem has an important corollary. Namely, it can be shown that the cohomology groups $H^k(G;\mathbb{R})$ vanish for all values of k and, by the definition of an exact sequence, this implies that there exists an isomorphism

$$H^k(G;\mathrm{U}(1)) \cong H^{k+1}(G;\mathbb{Z})\,. \tag{A.37}$$

A similar relation based on the short exact sequence

$$0 \longrightarrow \mathrm{U}(1) \longrightarrow \mathbb{C}^\times \longrightarrow \mathbb{R}^\times \longrightarrow 0 \tag{A.38}$$

can be used to extract an induced long exact sequence which, by the vanishing of chomology with coefficients in $\mathbb{R}$, implies the following isomorphism:

$$H^2(G;\mathrm{U}(1)) \cong H^2(G;\mathbb{C}^\times)\,. \tag{A.39}$$

This explains why we could use $\mathrm{U}(1)$ coefficients when working with group cohomology, while the theory of Schur, as explained in the previous sections, gave expression in terms

[13] A formal definition of this product is not relevant for this thesis.

of $\mathbb{C}^\times$.

Of course, there exist many more important theorems and formulae, for example the theory of spectral sequences as introduced by Leray (see footnote 10 in the introduction). In the context of group cohomology, this is given by the *Lyndon–Hochschild–Serre spectral sequence*. See [27] for a formal exposition or [11] for an application to the classification of SPT phases.

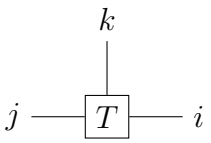
Appendix B

Linear algebra

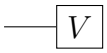
B.1 Graphical calculus

In this section, we will give a short introduction to the graphical calculus of tensor networks. For a more general and formal treatment, see for example [33].

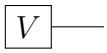
We will denote a tensor (multilinear map) of rank n by a circle or square (generally a vertex) with n wires attached to it. If we want to specify the indices of the tensor, these will be placed at the end of a wire (see Fig. B.1a). Furthermore, we will not be concerned with issues of raising/lowering indices as we are working with nonrelativistic theories. The distinction between vectors and dual vectors is induced by an orientation of the diagram as shown in Figs. B.1b and B.1c.



(a) Rank-3 tensor T^i_{jk}.



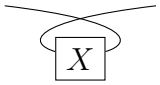
(b) Vector.



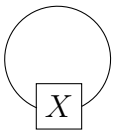
(c) Dual vector.

Figure B.1: Graphical representation of tensor networks.

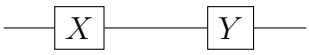
The contraction of two tensors is implemented by connecting a wire from one tensor to a wire from the other tensor. For example, the trace of a linear map is obtained by connecting the two wires of the same vertex and, hence, making a closed loop (see Fig. B.2b). In the same way, we obtain the composition of two linear maps by connecting one from the first map to a wire from the second map (see Fig. B.2c). Since the transpose of a linear map $X : V \to W$ is a map $X^t : W^* \to V^*$ between the dual spaces, hence, because of how (dual) vectors are implemented, we can graphically represent the transpose as in Fig. B.2a.



(a) Transpose of a linear map.



(b) Trace of a linear map X.



(c) Composite of two linear maps $X \circ Y$.

Figure B.2: Graphical manipulation of tensor networks.

B.2 Takagi factorization

For a complex symmetric matrix M, i.e. $M \in M_n(\mathbb{C})$ and $M^t = M$, there exists a decomposition

$$M = UDU^t\,, \tag{B.1}$$

where U is a unitary matrix and D is a real, diagonal, skew-symmetric matrix. This decomposition is called the Takagi factorization or Autonne–Takagi factorization. For the proof, we follow a paper by Hua [28].

Proof. Consider the matrix $M\overline{M}$ which is a positive-definite Hermitian matrix and, hence, can be brought to a diagonal form $\mathrm{diag}(a_1^2, a_2^2, \ldots, a_n^2)$ by conjugation with a unitary matrix W:

$$X\overline{X} = WM\overline{M}W^\dagger = \mathrm{diag}\left(a_1^2, a_2^2, \ldots, a_n^2\right)\,,$$

where $X := WMW^t$ and a_i real for all $i \leq n$. The matrix $X_0 = \mathrm{diag}(a_1, a_2, \ldots, a_n)$ also satisfies this equation and, hence, we can write $X\overline{X} = X_0\overline{X_0}$ or equivalently:

$$(X_0^{-1}X)\overline{(XX_0^{-1})} = \mathbb{1}\,.$$

By the choice of X_0 and the definition of X, these matrices are symmetric and, hence, this can also be rewritten as:

$$(X_0^{-1}X)(X_0^{-1}X)^\dagger = \mathbb{1}$$

and so we obtain a unitary matrix $A := X_0^{-1}X$. By diagonalizing A, we obtain the square root $\sqrt{A}$ and, hence:

$$X = X_0A = X_0\sqrt{A}^2\,.$$

Because both X and X_0 are symmetric, we have $X_0A = A^tX_0$, which implies $X_0\sqrt{A} = \sqrt{A}^tX_0$. After inserting this in the above equation, we obtain:

$$X = \sqrt{A}^tX_0\sqrt{A}$$

or, by $X = WMW^t$:

$$\left[\overline{\sqrt{A}}W\right] M \left[\overline{\sqrt{A}}W\right]^t = X_0 = \mathrm{diag}(a_1, a_2, \ldots, a_n)\,.$$

So, we obtain a diagonal matrix through congruence by a unitary matrix. □

If we start from the Autonne–Takagi factorization, it is immediately clear that M can also be written in the form

$$M = VV^t \tag{B.2}$$

by defining $V = U\sqrt{D}$. However, now, the matrix V is not required to be unitary anymore.

If the initial symmetric matrix M was also unitary, then we can show that the matrix V above is unitary. Because $M = UDU^t$ with U unitary, we see easily that the unitarity of M implies the unitarity of D. Now, consider the square root $\sqrt{D}$. Because D is unitary, this square root is also unitary and thus we find:

$$\begin{aligned} V^\dagger &= (U\sqrt{D})^\dagger \\ &= \sqrt{D}^\dagger U^\dagger \\ &= \sqrt{D}^{-1} U^{-1} \\ &= (U\sqrt{D})^{-1} \\ &= V^{-1}\,. \end{aligned} \tag{B.3}$$

B.3 Factorization of skew-symmetric matrices

The Autonne–Takagi factorization above can also be proven, starting from the Youla normal form [21], which is a general normal form based on unitary congruence UXU^t. Starting from this normal form one can prove that any complex skew-symmetric matrix M, i.e $M \in M_{2n}(\mathbb{C})$ and $M^t = -M$, can be written as follows:

$$M = U\Lambda U^t\,, \tag{B.4}$$

where U is unitary and Λ is block diagonal such that every block is of the form

$$\begin{pmatrix} 0 & \alpha \\ -\alpha & 0 \end{pmatrix} \tag{B.5}$$

for $\alpha \geq 0$. Equivalently, we can write M as follows:

$$M = U\left(\mathrm{diag}(\alpha_1, \ldots, \alpha_n) \otimes \varepsilon\right) U^t\,, \tag{B.6}$$

where $\alpha_i \geq 0$ for all $i \leq n$ and

$$\varepsilon := i\sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\,. \tag{B.7}$$

By using the property $(A \otimes B)(C \otimes D) = (AB) \otimes (CD)$, we can rewrite the matrix Λ as follows:

$$\begin{aligned}\Lambda &= \mathrm{diag}(\alpha_1, \ldots, \alpha_n) \otimes \varepsilon \\ &= \left[\sqrt{\mathrm{diag}(\alpha_1, \ldots, \alpha_n)}\sqrt{\mathrm{diag}(\alpha_1, \ldots, \alpha_n)}\right] \otimes \varepsilon \\ &= \left[\sqrt{\mathrm{diag}(\alpha_1, \ldots, \alpha_n)} \otimes \mathbb{1}_2\right] (\mathbb{1}_n \otimes \varepsilon) \left[\sqrt{\mathrm{diag}(\alpha_1, \ldots, \alpha_n)} \otimes \mathbb{1}_2\right] . \end{aligned} \tag{B.8}$$

The outer factors are diagonal, and in particular symmetric, and can thus be absorbed in the unitary matrices U to obtain a decomposition of the form

$$M = V(\mathbb{1}_n \otimes \varepsilon)V^t . \tag{B.9}$$

Again, when using this form, we should pay attention to the fact that the matrix V is not required to be unitary anymore. However, if M is unitary, we can show that V is also unitary by an argument similar to the one given in the previous section.

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