

Tensor network states and topological quantum phases

Nick Bultinck

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Supervisors: Jutho Haegeman & Frank Verstraete



Doctoral Committee

Frank Verstraete (promotor)
Universiteit Gent, Belgium
Universität Wien, Austria

Jutho Haegeman (copromotor)
Universiteit Gent, Belgium

Jan Ryckebusch (chairman)
Universiteit Gent, Belgium

Karel Van Acoleyen(secretary)
Universiteit Gent, Belgium

Stijn De Baerdemacker
Universiteit Gent, Belgium

Norbert Schuch
Max-Planck-Institut für Quantenoptik, Germany

Simon Trebst
Universität Koeln, Germany

Joris Van der Jeugt
Universiteit Gent, Belgium

Voorwoord

Het werk dat in deze thesis neergeschreven staat heeft in totaal vier jaar in beslag genomen. Het is dus een lang en arbeidsintensief proces geweest om van laatstejaarsstudent fysica te komen tot het punt waarop ik deze thesis kan schrijven. Maar het was enorm leerrijk en het heeft me elke seconde van die vier jaar geboeid.

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Nederlandstalige samenvatting

Fases van materie zijn een centraal begrip in de fysica. Ze beschrijven hoe een grote hoeveelheid microscopische deeltjes (bijvoorbeeld atomen) zich collectief gedragen. Uit deze algemene beschrijving is het meteen duidelijk dat een fase van materie een universeel begrip is dat in enorm veel verschillende contexten toepassingen kent. Ook mensen die zich niet verdiepen in natuurkunde ondervinden dagelijks het verschil tussen vaste stoffen, vloeistoffen en gassen.

Hoewel het concept 'fase van materie' een alledaags gegeven is heeft het toch betrekkelijk lang geduurd voordat natuurkundigen er een systematische theorie voor hadden ontwikkeld. Pas in het midden van de twintigste eeuw realiseerde men zich dat de verschillende fases en de geassocieerde fasetransities nauw verbonden zijn met het begrip symmetrie. In een vaste stof zitten de atomen bijvoorbeeld op vaste posities in een rooster, waardoor enkel rotaties over bepaalde hoeken het rooster onveranderd laten. Voor een vloeistof is de situatie anders. Vloeistoffen zijn veel chaotischer en kunnen dus over elke hoek gerotereerd worden zonder dat je dit kan opmerken. Een vaste stof heeft dus minder symmetrie dan een vloeistof en deze observatie kan voor heel veel andere verschillende fases van materie gemaakt worden.

Met de ontwikkeling van de kwantum mechanica aan het begin van de twintigste eeuw nam het begrip van de microscopische wereld en de corresponderende natuurwetten toe. Hierdoor ontstond ook de mogelijkheid om nieuwe soorten materie te gaan bestuderen. Uit deze studies werd duidelijk dat sommige van deze *kwantum fases van materie* niet gerelateerd kunnen worden aan symmetrie eigenschappen, zoals voorheen wel altijd het geval was geweest. Aan het eind van de twintigste en het begin van de éérentwintigste eeuw werd duidelijk dat een nieuw wiskundig concept, namelijk topologie, nodig was om deze kwantum fases te begrijpen. Deze thesis bestudeert net deze topologische fases voor kwantum systemen in één en twee dimensies.

De belangrijkste theoretische methode die in deze thesis gebruikt wordt zijn de zogenaamde *tensor netwerk toestanden*. Deze methode is gebaseerd op recente inzichten in kwantumverstrengeling, een eigenschap die intrinsiek is aan kwantum mechanische systemen. Tensor netwerk toestanden laten ons toe om de lage energie eigenschappen van kwantum veeldeeltjes systemen op een efficiënte manier te modelleren. Er wordt in dit werk getracht om de connectie tussen topologische kwantum fases en kwantum verstrengeling concreet uit te werken. De motivatie voor dit werk is tweezijdig: enerzijds kan op deze manier een theoretische connectie gemaakt worden tussen fysische eigenschappen van kwantum systemen en concepten uit de wiskunde, en anderzijds laten de inzichten die hier ontwikkeld worden toe om deze fysische systemen beter numeriek te simuleren.

Concreet worden in dit werk volgende verschillende types kwantum veeldeeltjes systemen bestudeerd: elektron (fermion) systemen in één dimensie, magnetische (spin) systemen in twee dimensies en elektron systemen in twee dimensies. Voor de elektron systemen wordt een nieuw tensor netwerk formalisme ontwikkeld op basis van het wiskundig concept *super vector ruimtes*. Via dit nieuw formalisme wordt de volledige lijst van mogelijke topologische fases in één dimensie gereproduceerd en wordt ook hun onderlinge verhouding (i.e. de corresponderende *groepsstructuur*) blootgelegd. De link tussen verstrengelingseigenschappen en topologische fases komt heel natuurlijk tevoorschijn en geeft waardevolle informatie voor het identificeren van de fase van een bepaald elektron systeem.

Voor de twee dimensionale spin systemen worden twee verschillende klassen bestudeerd: systemen met een globale symmetrie en systemen met onconventionele lage-energie deeltjes. Wanneer een globale symmetrie aanwezig is concentreren we ons steeds op het geval waarbij deze niet spontaan gebroken is. In kwantum veeldeeltjes systemen kan de globale symmetrie op verschillende manieren gerealiseerd worden bij lage temperatuur. De tensor netwerk toestanden worden gebruikt om fysische gevolgen van deze verschillende symmetrie realisaties te onderzoeken. Voor de systemen met onconventionele excitaties (lage energie deeltjes) genaamd *anyonen*, die zich noch als een spin (boson) noch als een elektron (fermion) gedragen, wordt de connectie tussen kwantum verstrengeling en deze excitaties onderzocht. De topologische eigenschappen van de anyonen blijken volledig geëncodeerd te zijn in de verstrengelingsstructuur.

De twee dimensionale elektron systemen worden op analoge manier bestudeerd. Net als voor spin systemen blijkt opnieuw dat de topologische eigenschappen zich manifesteren in kwantum verstrengeling. Dit wordt gebruikt om een systematische theorie voor elektron kwantum fases te ontwikkelen, zowel voor systemen met een globale symmetrie als voor systemen met anyonen. Uit deze theorie volgt een expliciete tensor netwerk constructie voor al de verschillende fases. Gebruik makend van deze modellen worden de universele fysische eigenschappen van de topologische systemen bestudeerd en worden nieuwe numerieke simulatietechnieken mogelijk.

Het formalisme dat in deze thesis ontwikkeld wordt kan als startpunt dienen voor verdere theoretische en numerieke studies. Topologische fases zijn een nieuw begrip en er zal nog veel wetenschappelijk werk nodig zijn vooraleer het duidelijk wordt welke plaats ze gaan innemen in de fysica, en eventueel daarbuiten in ingenieurstoepassingen. Hopelijk kan deze thesis op korte of lange termijn een bijdrage leveren aan dit proces.

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Introduction

0.1 Quantum many-body physics

The theory of quantum mechanics has been developed for almost a century now. It tells us how particles at the microscopic level behave, which turns out to be very different from the macroscopic objects we see in the world around us. The fundamental principles underlying quantum mechanics are conceptually very intriguing, and sometimes subtle to interpret. Even experienced physicists still get confused about the precise statements of the theory in a particular situation. Quantum mechanics is not only conceptually appealing, but also of great scientific value because of its predictive power. One of the first instances where this was beautifully illustrated is the calculation of the energy spectrum of the hydrogen atom. In the past hundred years quantum mechanics has survived many non-trivial experimental tests, leaving no room for doubt that it is indeed the correct way to think about the microscopic world. For this reason it is without exaggeration that quantum mechanics can be called one of the greatest intellectual triumphs in physics.

The many successes of quantum mechanics do not mean that everything is solved. Most of the physically interesting situations involve not one, but many microscopic particles. Examples of this go from molecules to macroscopic materials and even potential quantum technologies. Quantum mechanics governs the laws according to which each individual particle behaves, but studying the collective behavior of a macroscopic amount of particles requires another level of understanding. Unfortunately it is inherent in the mathematical structure of quantum mechanics that the problem becomes exponentially harder to solve when the number of particles increases, ruling out the possibility (in most cases) of exactly solving the equations, or even doing it numerically on a computer.

In quantum many-body physics one looks for ways to approach a problem involving many microscopic particles in such a way that some interesting physical properties can be studied or relevant quantities can be calculated. Although quantum many-body systems are in principle exponentially hard to solve, it is often possible to identify the degrees of freedom that capture the relevant physical properties and find suitable approximations. Instead of trying to solve the complete equations, which bury the sought answers under all the complicated details of the problem, one often constructs an effective theory which contains only the relevant degrees of freedom. Identifying the physical essence of a system and finding manageable approximations, possibly in the form of an effective theory, is at the core of quantum many-body (and most other branches of) physics.

A first starting point in quantum many-body physics is often to work at zero temperature, which is also the regime of interest in this dissertation. In this case one is interested only in the ground state of the system. However, solving the problem at zero temperature generically already gives a great deal of information about the behavior of the system at low, non-zero temperatures. This is because the ground state structure contains a lot of information about the first excited states and the associated elementary quasi-particles. Quantum many-body physics is a rich branch of physics which is of course not confined to the study of low-temperature equilibrium systems. Other prominent topics of active research are disordered, many-body localised systems at high temperature, or open quantum systems.

0.2 Quantum phases of matter

Phases of matter and the transitions between them are central concepts in physics. They are very familiar even to non-physicists because our world consists of solids, liquids and gasses and we experience the differences between them on a daily basis. The corresponding phase transitions such as melting and boiling can also hardly be called exotic. Although phases of matter and phase transitions are so familiar, it took a long time before the correct physical language was developed to understand them. A phenomenological description of phase transitions has been around since the development of thermodynamics in the nineteenth century, but a detailed understanding of their universality and the underlying physical mechanisms only arose in the second half of the twentieth century.

The paradigm for describing phase transitions became known as the Landau-Ginzburg theory [1]. It associates a pattern of spontaneous symmetry breaking to every transition. This means that when a system goes from one phase to another, it becomes either more or less symmetrical. For example, when a solid melts, the atoms are no longer locked at fixed positions in the crystalline structure such that there is more translational and rotational symmetry in the liquid phase. This idea has a very broad applicability and

can also be used to describe for example phase transitions in magnets. It was also observed that near a phase transition systems with very different microscopic structure start behaving in similar ways. This universality of phase transitions gave rise to the intuitive understanding that near a critical point the system develops very large correlations, thereby forgetting its microscopic structure.

All examples of phase transitions we have given up to now are driven by thermal fluctuations. We can go from one phase to another by increasing or lowering the temperature until a non-zero critical temperature is reached at which the transition occurs. In the low-temperature region of quantum many-body systems, which is the focus of this thesis, not all transitions are related to a change in temperature. Even in the zero temperature limit phase transitions can occur by changing a parameter in the Hamiltonian governing the dynamics of the system. For quantum magnets this parameter could for example be the strength of an external magnetic field. In this case it are inherently quantum mechanical fluctuations that drive the transition. The Landau-Ginzburg theory is also applicable to zero-temperature quantum phase transitions. Well-known examples are quantum ferromagnets breaking spin rotation symmetry, Bose-Einstein condensation and the associated superfluids corresponding to breaking of particle number symmetry and gauge symmetry breaking in superconductors.

In the 1970s and 1980s new critical phenomena and unconventional phases of matter that were not predicted by Landau-Ginzburg theory started to appear. It was observed that the confinement-deconfinement transition in a simple lattice model of a \mathbb{Z}_2 gauge theory could not be related to any breaking of a global symmetry [2]. The same holds for the Kosterlitz-Thouless transition in the XY model, where the different phases are characterized by the long-distance correlations of vortices [3]. The integer quantum Hall system [4], discovered 1980, was the first observed phase which does not break any symmetries but has universal, robust properties that are not shared by conventional symmetric systems. Specifically, the Hall conductance was found to be quantized to extraordinary precision and along the boundary of the sample purely left- or right-moving currents appear [5]. Soon after the discovery of the integer quantum Hall effect also the fractional quantum Hall effect was experimentally observed [6], which has even more exotic features. The quasi-particles in the fractional quantum Hall states behave as a generalization of bosons and fermions, picking up arbitrary phases when they are interchanged [7]. Such quasi-particles are called anyons [8] and they always appear together with a robust ground state degeneracy depending on the boundary conditions of the system [9]. Around the same time resonating valence bond states were studied in the context of high T_c superconductivity [10]. It was realized that also these spin systems have anyonic excitations [11]. Next to the resonating valence bond states new featureless spin liquid states, such as the chiral spin liquids [12, 13], showing similar behavior to the fractional quantum Hall systems were put forward in theoretical studies.

The one-dimensional Heisenberg model of spin-1 moments was also found to share some interesting features with the quantum Hall effects: under open boundary conditions there appear gapless edge degrees of freedom in the form of ‘fractionalised’ spin-1/2 moments [14, 15].

After the first wave of discoveries beyond the Landau-Ginzburg paradigm, the study of quantum phases of matter received a second boost with the discovery of topological superconductors such as the Majorana chain [16] and the $p + ip$ superconductor [17], and the two-dimensional spin quantum Hall insulator [18]. These free fermion models show a lot of resemblances to the quantum Hall materials, but differ crucially in terms of their global symmetries. Particle number symmetry is obviously broken in superconductors, which prevents topological properties to be probed via external electromagnetic fields as in measurements of the Hall conductivity. A spin quantum Hall sample has gapless degrees of freedom on the boundary only when time reversal symmetry is preserved. This is in sharp contrast to the standard quantum Hall effects, where time reversal symmetry is explicitly broken by external magnetic fields. Soon after its theoretical prediction, the spin quantum Hall effect was experimentally realised in HgTe quantum wells [19, 20]. The physical principles of the two dimensional spin quantum Hall effect were shown to also be applicable to three dimensional materials with only slight modifications [21]. Together with the Majorana chain, the three dimensional spin quantum Hall effect generalised the physics of quantum Hall phases, which are confined to two spatial dimensions. The insights obtained from the topological superconductors and the spin quantum Hall effects were used to obtain a full classification of topological phases in free fermion systems based on the realisation of possible global anti-unitary symmetries such as time reversal or charge conjugation [22, 23]. The classification, going under the name of the periodic table for topological insulators and superconductors, not only unifies many known quantum phases such as the above mentioned topological superconductors, the spin quantum Hall effects and the integer quantum Hall effect, but also predicts new phases in higher dimensions.

As stressed above, global symmetries play a pivotal role in the periodic table of topological insulators and superconductors. Many of the non-trivial phases contained in the classification lose their non-trivial universal properties once the relevant global symmetry is allowed to be broken. This observation has led to the general concept of a Symmetry-Protected Topological (SPT) phase [24]. SPT phases are not confined to free fermions, but also appear in interacting spin or boson systems. In fact, the spin-1 Heisenberg model with fractionalised spin-1/2 moments on the edge mentioned previously, is a phase protected by global spin rotation symmetry. A first classification for SPT phases in spin systems protected by on-site symmetries was proposed in terms of group cohomology [24]. This classification is very successful, but it was shown that some phases protected by time reversal symmetry in three dimensions and higher were not captured. The generalisation

for fermions based on supercohomology [25] misses an important subclass of topological superconductors, even in two dimensions. Improvements on the cohomology classification using invertible topological field theories were formulated and relate the classification of SPT phases to cobordism theory [26–28]. Next to the work on classification of SPT phases, many insights about the physical characteristics of these phases were obtained. Although SPT phases seem featureless in the bulk, they respond in unconventional ways to external fields. This behavior of SPT phases is similar to observations made a long time ago for the quantum Hall effect, where an external magnetic flux piercing a quantum Hall sample acquires an electric charge [29, 30]. The gapless boundary degrees of freedom in SPT phases were shown to be related to quantum anomalies of the global symmetry. This connects the physics of SPT phases to many concepts developed in quantum field theory in the 1980s.

Next to the substantial progress made in the physics of SPT phases, people also developed a systematic understanding of bosonic quantum phases containing anyonic excitations in two dimensions [31, 32], which are in close spirit to the fractional quantum Hall effect. These phases are said to have intrinsic topological order. A lot of the interest in these phases comes from their potential for topological quantum computers [33]. Many subtleties occur when a system has topological order. A main example is how a global symmetry can be implemented on the low-energy states. Because of their special properties, anyons can intertwine with the global symmetry in a non-trivial way. The corresponding phases are called symmetry-enriched topological phases. They are of great interest since many of the spin liquids that can potentially be realised in experiments combine the anyonic excitations with global spin rotation or time reversal symmetry. The analogous theory of anyons and symmetry-enriched phases in fermionic systems and in higher dimensional boson systems is much less developed and still poses many interesting questions in contemporary quantum many-body physics.

0.3 Tensor network states

In recent years a new perspective on quantum many-body systems based on entanglement has been developed. A crucial observation was the entanglement area-law behavior in ground states of systems with a non-zero energy gap between the ground state and the first excited state. In such ground states the entanglement entropy associated to the reduced density matrix of a spatial region was found to scale with the boundary of the region, whereas generically one would expect this quantity to scale with the volume. This implies that for gapped systems, not only the correlations but also the entanglement pattern is local. This local entanglement structure leads to many new and useful tools in the study of quantum many-body systems. These tools can be both conceptual, like for instance the entanglement Hamiltonian,

or more applied. A prime example of the latter are tensor networks. Tensor networks represent a certain quantum many-body state as a contraction over many local tensors. In this way, the number of parameters describing the state is greatly reduced. Because of this special structure, tensor network states have the entanglement area law built-in, and therefore make up a powerful ansatz for studying the low-energy physics of gapped quantum many-body systems.

To make tensor networks more tangible, let us start by explaining Matrix Product States (MPS) [34–36], which are tensor networks for one-dimensional spin chains. The building block for MPS is a rank three tensor $A^i_{\alpha\beta}$, with $i = 1 \dots d$ and $\alpha, \beta = 1 \dots D$. d is called the physical dimension, and D is the virtual or bond dimension. If we fix the value of i , then we obtain a $D \times D$ matrix denoted by A^i . To construct a MPS for a chain of L spin- s moments with periodic boundary conditions we take matrices A^i with $d = 2s + 1$ and write the corresponding state $|\psi\rangle$ as

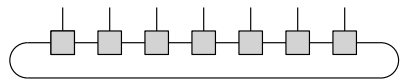
$$|\psi\rangle = \sum_{\{i\}} \text{tr} \left(A^{i_1} A^{i_2} \dots A^{i_L} \right) |i_1\rangle |i_2\rangle \dots |i_L\rangle,$$

from which we see that the coefficients of the many-body spin state are given by the trace of a product of matrices. All information about the quantum state should therefore be encoded in the matrices A^i . For example, for this state to have exponential decay of correlations A^i should span a simple $D \times D$ matrix algebra [34]. Also global symmetries of the system, like spin rotation symmetry, are reflected in local intertwining properties of the tensor [37]. These are two basic examples of one of the strengths of tensor network states: local tensors and their algebraic structure determine global, physical properties of the many-body state.

It is convenient to denote tensor network states in a graphical way. In this graphical notation every tensor is depicted by a planar object like a square, circle, triangle,... with a number of lines connected to it that represent its indices. For the MPS tensor $A^i_{\alpha\beta}$ this means we depict it as

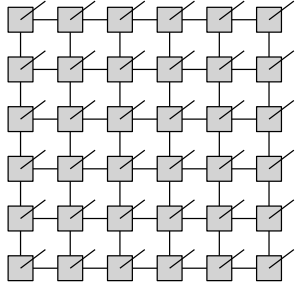
$$\begin{array}{c} i \\ | \\ \square \\ \hline \alpha \quad \beta \end{array} = A^i_{\alpha\beta}.$$

In the graphical notation tensor contraction corresponds to simply connecting the lines of those indices that are being contracted. We thus depict the MPS $|\psi\rangle$ as

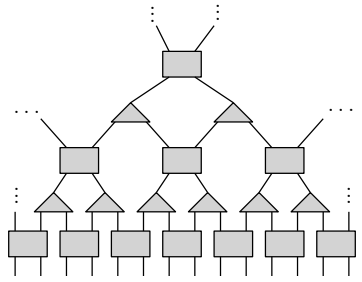


We can now generalise the construction of MPS to two dimensional spin systems. For this we associate a rank $C + 1$ tensor to every vertex of the lattice on which the spin system is defined, where C is the coordination number

of the vertex (i.e. the number of edges connected to it). We subsequently contract the C virtual indices with those of the neighboring tensors. The resulting tensor network states are called Projected Entangled-Pair States (PEPS) [38]. As an illustration, a PEPS on a 6×6 square lattice with open boundary conditions takes the form

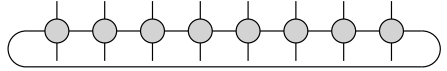


Up to now we have only used tensor networks to construct quantum many body states by contracting tensors as determined by the geometry of the underlying physical lattice. However, generalisations to this construction are possible. For example, one can also use Multiscale Entanglement Renormalisation (MERA) tensor networks [39] to study one-dimensional spin chains. MERA tensor networks are particularly useful for gapless spin systems as they mimic the scale-invariant behavior associated to infinite correlations lengths. A subregion of a MERA network looks like



where the lower indices correspond to the physical spins and we have only represented a finite subregion of the infinite chain. The open indices with dots should be contracted with the part of the MERA that is not represented in the figure, so they are in fact not really open indices. As shown in the figure, a MERA network consists of multiple layers, each layer consisting of rank 4 or rank 3 tensors. Going from one layer to another can be interpreted a renormalization step to a different length scale. To be truly scale-invariant it is clear that the number of layers should be infinite. However, similar to MPS, all information about the infinite network can be obtained by studying the local rank 4 and rank 3 tensors.

A second generalisation to the tensor network constructions considered up to now is that the formalism is not restricted to states, but can also be used to construct linear operators. For example, an operator defined on the Hilbert space of a one-dimensional spin chain can be represented as



Written down explicitly, this operator takes the form

$$\sum_{\{i\}\{j\}} \text{tr} \left(B^{i_1, j_1} B^{i_2, j_2} \dots B^{i_L, j_L} \right) |i_1\rangle \langle j_1| |i_2\rangle \langle j_2| \dots |i_L\rangle \langle j_L|,$$

where $B^{i,j}$ are $D \times D$ matrices. In analogy to MPS, these operators are called Matrix Product Operators (MPO). Similar constructions of course also lead to operators acting on spins defined on higher dimensional lattices.

0.4 This dissertation

In the previous sections we have presented the broader context in which this dissertation is to be situated. In this section we discuss the general philosophy and the specific approach explored in chapters 1, 2, 3 and 4, which contain the main results. We also give an outline of the results per chapter.

0.4.1 Topological phases, entanglement and tensor networks

One of the hallmarks of topological quantum phases is that they cannot be distinguished via local order parameters. So an obvious question that raises itself is where to look for signatures of the non-trivial phase once we have obtained the ground state wave function for our system of interest. In recent years it was observed that non-trivial topological quantum phases leave clear imprints in the entanglement structure of the ground state wave function. For systems with intrinsic topological order, the entanglement entropy of a spatial region in the ground state scales as $S(L) = \alpha L - \gamma + \mathcal{O}(1/L)$, where L is the length of the boundary of the region. The coefficient α determines the area-law scaling as mentioned above and is non-universal. However, γ is observed to be constant for all wavefunctions that correspond to the same quantum phase; in particular it takes the value zero for systems without any anyonic excitations. It is therefore a robust and universal characteristic of non-trivial topological order [40, 41].

Many topological phases are characterised by gapless modes localised on the boundary of the system. Rather surprisingly, the ground state wave function and its local entanglement structure in a region far away from any

physical boundaries was found to contain information about these edge modes. To extract the relevant bulk entanglement properties we first define the entanglement Hamiltonian H_Σ associated to a spatial region Σ , where H_Σ is related to the reduced density matrix ρ_Σ of Σ as $\rho_\Sigma = \exp(-H_\Sigma)$. It was observed that the low-energy spectrum of H_Σ mimics the low-energy edge physics. This connection between bulk entanglement and edge modes was originally observed for fractional quantum Hall states in Ref. [42], but has since then been generalised to many other topological phases. In particular, the discovery of SPT phases in spin chains originated from studies of entanglement spectra [43].

Another connection between topological phases and entanglement manifests itself in the so-called minimally entangled states. For intrinsic topologically ordered systems on a torus the ground states with a definite anyon flux through one of the cycles were found to minimise the entanglement entropy for cuts along orthogonal cycles [44]. This identification of states with a definite anyon flux is particularly useful for numerical studies of topological phases since it allows one to calculate the T and S matrices, which contain universal information about the topological phase.

All these observations firmly established the deep and general connection between ground state entanglement and topological quantum phases. In chapters 1 to 4 this connection is studied from the perspective of tensor networks. The local structure of tensor networks gives direct access to the entanglement structure and in this way allows for a systematic study of all such possible structures. This naturally leads to mathematical concepts such as G -equivariant algebras, \mathbb{Z}_2 graded algebras and fusion categories. The main object of this dissertation is to connect these mathematical concepts to the physics of topological phases in one and two spatial dimensions.

0.4.2 Outline of the results

The four main chapters in this dissertation are integral reprints of research papers. Here we give an outline of the results contained in each chapter/research paper.

Chapter 1: Fermionic matrix product states and one-dimensional topological phases

In this chapter a framework for fermionic tensor networks based on super vector spaces is introduced. Although previous formulations of fermionic tensor network were available in the literature, the formalism using super vector space has the advantage that it is particularly well-suited for theoretical studies. We exploit this advantage to develop a complete theory for fermionic MPS. In particular, we identify two types of fermionic MPS corresponding to unique ground states of local Hamiltonians and relate these to two different types of quantum phases: the standard, trivial phase and

the topological phase, where Majorana edge states appear. Our fermionic MPS formalism naturally captures fermion systems with closed boundary conditions, both periodic and anti-periodic, which are difficult to study via a Jordan-Wigner transformation. In particular, we show that local tensor properties of the fMPS imply that the trivial and the Majorana phases respond very differently to anti-periodic boundary conditions. The fermionic MPS interpretation of the Majorana phase also provides a direct link between the Majorana edge modes and degeneracies in the entanglement spectrum, both for non-interacting and interacting fermion systems. The super vector space formalism gives rise to a clear generalisation of the concept of parent Hamiltonians, familiar from bosonic MPS. We show that the fermionic parent Hamiltonians have very similar features to bosonic parent Hamiltonians, and in particular, we show that each fermionic parent Hamiltonian has the corresponding fMPS as its unique ground state.

We further explore fermionic MPS with global symmetries, both unitary and anti-unitary. In this way we recover the classification of fermionic SPT phases in one dimension. Additionally, we also reveal the group structure of these phases under ‘stacking’, which is bringing two parallel fermionic chains in proximity of each other. One of the added values of our formalism is that it can also deal with spatial reflection symmetry and predict the correct classification and group structure of the associated topological phases, which relies crucially on the intrinsic fermionic formulation of our method.

The results presented in this work should be seen as a first step towards a more general and systematic understanding of fermionic tensor networks. The insights obtained in the one-dimensional case are crucial for the work in chapter 4, which concerns two-dimensional systems. The fMPS formalism can also be generalised to parafermion systems [45], where less is known about the possible quantum phases.

Chapter 2: Matrix product operators for symmetry-protected topological phases

The first general understanding of SPT phases in one-dimensional spin systems arose from studies of MPS [46–49]. Soon after, X. Chen and collaborators used similar tensor network techniques to study the CZX model, a specific two-dimensional SPT protected by \mathbb{Z}_2 symmetry [50]. From the insights obtained in MPS and the CZX model a general classification of bosonic SPT phases in all dimensions was proposed based on group cohomology. However, the findings in the CZX model were not generalised to a general theory of SPT phases in PEPS. This is exactly the goal of the work in chapter 2.

We start from a general PEPS with non-zero correlation length and identify the class of local tensors that lead to short-range entangled states. Restricting to short-range entangled PEPS we study how global symmetries can be implemented on the virtual level of the tensor network using MPOs.

Using the results of Chen on the CZX model we are then able to relate the group cohomology classification of SPTs to the properties of these virtual symmetry MPOs, which completes the framework within one can study SPT properties of PEPS associated to on-site symmetries.

From the general, abstract formalism we recover many characterising properties of SPT phases. We show how the group cohomology data reflects itself in non-trivial properties of symmetry defects. These defects can, and for non-trivial SPT phases in general will, carry fractional charges determined by the group cohomology data. We also apply the quantum state gauging procedure [51] to the class of SPT PEPS and establish rigorous connections between the PEPS before and after gauging. In particular, we show that the energy gap does not close under gauging and that the gauged PEPS has intrinsic topological order determined by a virtual symmetry MPO with identical group cohomology data as the SPT symmetry MPO. This establishes a precise tensor network formulation of the connection between topological properties of SPT phases and gauge theories with discrete gauge groups.

With this general understanding of SPT phases in PEPS one should be able to develop new algorithms to study these phases numerically. Having in mind the general theoretical framework allows one to identify the properties of the PEPS one wants to study numerically, i.e. it helps to ask the right questions to which the computer should give the answer.

Chapter 3: Anyons and matrix product operator algebras

The fundamental imprint of intrinsic topological order in PEPS is that the local tensors have a purely virtual symmetry. This was first exemplified for topological order corresponding to deconfined discrete gauge theories in the formalism of G -injectivity [52]. The virtual symmetry representation considered in G -injective PEPS consists of a tensor product of matrices, one for each virtual PEPS index, which form a representation of the discrete group G . The concept of G -injectivity was subsequently generalised to MPO-injectivity, where the virtual symmetries need not be tensor products of matrices, but can also be non-trivial MPOs.

In chapter 3 we start from the formalism of MPO-injectivity and we develop a general theory for the algebras of MPOs that can serve as symmetries of a PEPS. This results in an abstract and mathematical formalism which we show is intimately related to tensor fusion categories. The main goal is then to develop a method to extract physical properties from this abstract framework. In particular, we want to understand how one can calculate properties of the anyons present as low-energy excitations in these models. We solve this problem by identifying a second, larger algebra, which contains the symmetry MPO algebra as a subalgebra, and relate topological superselection sectors to the irreducible central idempotents of this algebra. This identification of the topological superselection sectors allows us to devise methods to obtain the topological spins of the anyons and the S matrix,

which also gives the fusion rules.

The theoretical methods are illustrated using numerous examples, both analytically for the twisted quantum double models, and numerically for the Fibonacci, Ising and $\text{Rep}(S_3)$ string-net PEPS. The anyons we obtain and their topological properties are shown to match with previous results, indicating the validity of our approach.

Chapter 4: Fermionic projected entangled-pair states and topological phases

In the fourth and final chapter we turn to fermionic tensor networks in two dimensions based on super vector spaces. Similar to the bosonic case considered in chapter 3, we study topological properties of fermionic PEPS by looking at the possible fermionic MPO (fMPO) symmetries on the virtual indices. From the results on fermionic MPS in chapter 1 it is clear that there are two types of fermionic symmetry MPO, characterised by the absence or presence of Majorana edge states. Leaving out the fMPOs with Majorana edge modes, the mathematical structure underlying the fMPO symmetry algebras is equivalent to the mathematical structure used to construct fermionic string nets, which are solvable fixed-point models for two-dimensional phases of fermions with intrinsic topological order [53, 54]. However, with inclusion of the Majorana-type symmetry MPOs we obtain a more general class of models.

From the algebraic data associated to a fMPO algebra we show how to construct a fermionic PEPS that has this algebra as a virtual symmetry. So the first part of chapter 4 consists of a bootstrap method: first we study the fMPO algebras and then we engineer a tensor network that has the relevant symmetries from the algebraic data. For the case without Majorana fMPOs our construction gives the tensor network representation of the ground state of fermionic string-nets. With Majorana fMPOs, the PEPS construction involves some additional subtleties. For this reason we treat this case separately at the end of chapter 4 and focus on a particular class of examples.

For the special case where the symmetry fMPOs form a group we also discuss the connection to short-range entangled symmetry-protected phases. Similar to the results of chapter 2 we argue that these fMPO group representations classify fermionic SPT phases associated to on-site unitary symmetries in two dimensions. We show how to modify the fermionic PEPS construction to obtain the short-range entangled PEPS intertwining the global on-site symmetry action to a particular fMPO group representation on the virtual indices. A large part of chapter 4 is devoted to showing that the general properties of fermionic MPOs reproduce the physical properties of fermionic SPT phases. For the non-Majorana fMPO group representations, corresponding to the supercohomology models [25], we study the group structure under stacking, fractionalization of symmetry defects and calculate the modular matrices of

twisted states on the torus.

Going beyond supercohomology, it is shown that including Majorana type fMPOs leads to symmetry defects that bind Majorana modes. For the case of \mathbb{Z}_2 fMPO symmetries we study the defects and stacking in more detail. We show how to recover the connection between spin structures and fermion parity of the local symmetry action on Majorana defects. In this way we relate the abstract algebraic data associated to a \mathbb{Z}_2 fMPO representation to universal physical properties of fermionic \mathbb{Z}_2 SPT phases. To obtain the \mathbb{Z}_8 group structure of the \mathbb{Z}_2 SPT phases under stacking we reveal its relation to the \mathbb{Z}_8 group structure of time reversal invariant Majorana chains.

Fermionic matrix product states and one-dimensional topological phases

Synopsis

We develop the formalism of fermionic matrix product states (fMPS) and show how irreducible fMPS fall in two different classes, related to the different types of simple \mathbb{Z}_2 graded algebras, which are physically distinguished by the absence or presence of Majorana edge modes. The local structure of fMPS with Majorana edge modes also implies that there is always a two-fold degeneracy in the entanglement spectrum. Using the fMPS formalism we make explicit the correspondence between the \mathbb{Z}_8 classification of time-reversal invariant spinless superconductors and the modulo 8 periodicity in the representation theory of real Clifford algebras. Studying fMPS with general on-site unitary and anti-unitary symmetries allows us to define invariants that label symmetry-protected phases of interacting fermions. The behavior of these invariants under stacking of fMPS is derived, which reveals the group structure of such interacting phases. We also consider spatial symmetries and show how the invariant phase factor in the partition function of reflection symmetric phases on an unorientable manifold appears in the fMPS framework.

Based on

‘Fermionic matrix product states and one-dimensional topological phases’
N. Bultinck, D.J. Williamson, J. Haegemant and F. Verstraete
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1.1 Introduction

Tensor network states form a natural ansatz for the ground state of gapped local Hamiltonians because of their local entanglement structure. In one spatial dimension, it can even be proven that every ground state of such a Hamiltonian can be approximated by a tensor network state to arbitrary precision [55]. Such one-dimensional tensor networks, called matrix product states (MPS), thus capture the relevant subspace in which the low energy physics of gapped local systems takes place. For this reason, MPS are not only useful to describe model-dependent microscopic properties of quantum many-body systems, but also for universal properties associated to an entire family of Hamiltonians in the same quantum phase. It was realized that the universal properties that are stable under renormalization and manifest themselves in the far infrared field theory descriptions of the system are encoded in the entanglement properties of the MPS [42]. This insight has led to a complete classification of bosonic quantum phases in one spatial dimension using tensor networks [46–49]. Although we will stick to one-dimensional systems in this work, we note for completeness that similar techniques applied to two-dimensional tensor network states have led to a systematic understanding of the entanglement structure in non-chiral topological order and the properties of the associated superselection sectors [56–58]. Also two-dimensional symmetry-protected phases [59, 60] and chiral phases [61–63] can be described using the tensor network language.

Extending the class of systems under consideration to also include fermionic degrees of freedom allows for a greater variety of quantum phases. For example, fermionic systems can have Majorana edge modes when defined on a lattice with boundary [16]. A complete classification of quantum phases for free fermion systems, known as the periodic table for topological insulators and superconductors, has been established through the use of tools such as Anderson localization and K -theory [22, 23]. However, when interactions are taken into account the classification can change drastically [64]. Recently it has been claimed that interacting symmetry-protected fermionic phases can be classified using cobordism theory [28, 65]. In one spatial dimension, the classification of interacting fermionic systems was considered in [66]. Building upon this work, we develop a tensor network approach towards symmetric fermionic phases. As a first step, in sections 1.3 and 1.4 we construct tensor networks that can carry fermionic degrees of freedom using the mathematical formalism of super vector spaces. We note that there already exist equivalent fermionic tensor network constructions in the literature using fermionic mode operators or Grassmann numbers [53, 67–70], but for our purposes we find it more convenient to adopt the language of super vector spaces. Furthermore, these proposals are aimed towards two-dimensional tensor networks, as one-dimensional fermion systems are typically mapped to spin systems using the Jordan-Wigner transformation in numerical studies. However, the intrinsically fermionic formalism has sev-

eral advantages. For example, periodic or antiperiodic boundary conditions are automatically incorporated and fermionic parent Hamiltonians can be constructed in a systematic way (see section 1.5).

In section 1.4 we identify two distinct classes of irreducible fermionic matrix product states (fMPS), which are characterised by the presence or absence of Majorana zero modes at the ends of open chains. Both classes of irreducible fMPS are shown to be the unique ground state or their associated fermionic parent Hamiltonian with periodic boundary conditions in section 1.5. The physical distinction between both types of fMPS has a clear signature in the algebraic structure of the local tensors constructing the fMPS and is related to the possible types of simple \mathbb{Z}_2 graded algebras over \mathbb{C} . This local tensor structure has a profound influence on the entanglement spectrum since it implies that Majorana edge modes are always accompanied by a two-fold degeneracy of the Schmidt values, as we show in section 1.6. In section 1.7 we include time-reversal symmetry, in the form of complex conjugation, and observe that the local structure of the fMPS tensors also provides an explicit link between the \mathbb{Z}_8 classification of time reversal symmetric spinless superconductors [64] and the 8-fold periodicity in the representations of real Clifford algebras. Using the fundamental theorem of MPS in section 1.8 enables us to go beyond just time reversal and study general on-site unitary and anti-unitary symmetries by identifying invariants associated to the possible symmetric phases. Similar to the bosonic case, these invariants are obtained by studying the entanglement degrees of freedom in the ground state wave function. In this way we recover the classification derived in Ref. [66], i.e. without Majorana edge modes a one-dimensional fermionic topological phase protected by the symmetry group G is characterized by $H^2(G, U(1))$, while a fermionic symmetry protected phase with Majorana modes can only occur when $G = \tilde{G} \times \{I, P\}$ and corresponds to an element of $H^2(\tilde{G}, U(1))$ and $H^1(\tilde{G}, \mathbb{Z}_2)$. Sections 1.6, 1.7, 1.8.1 and 1.8.2 are largely covered by Ref. [66] but we revisit them using the fMPS formalism to make this work self-contained. In section 1.8.3 it is explained how the fMPS formalism is a natural framework for calculating the group structure of fermionic symmetric phases by studying the behavior of the invariants under stacking, which was not considered in Ref. [66].

In section 1.9 we show that our method is not restricted to on-site symmetries and also recovers the \mathbb{Z}_8 group structure of reflection symmetric phases. This result relies heavily on the intrinsically fermionic nature of our formalism. To obtain the correct group structure we use the recently proposed method of partial reflection [71, 72] and show that it fits comfortably within the tensor network language.

Since the fMPS formalism is an extension of bosonic matrix product states, we first review some basic facts about them in section 1.2.

1.2 Bosonic matrix product states

A matrix product state (MPS) is defined in the Hilbert space $\mathcal{H}^1 \otimes \mathcal{H}^2 \otimes \dots \otimes \mathcal{H}^N$ of a one dimensional lattice of N finite-dimensional bosonic degrees of freedom. A general state is defined by the array of coefficients C^{i_1, i_2, \dots, i_N} with respect to the product basis $|i_1\rangle \otimes |i_2\rangle \otimes \dots \otimes |i_N\rangle$. To construct a MPS one associates a rank three array $A^i[j]_{\alpha\beta}$ to every site j , where the index i is associated with the basis $|i\rangle$ of the local physical Hilbert space \mathcal{H}^j and the so-called virtual indices α and β are of dimension D_j and D_{j+1} respectively. We also denote by $A^i[j]$ the $D_j \times D_{j+1}$ matrix obtained by fixing the index i . The MPS is then defined as

$$|\psi\rangle = \sum_{\{i_j\}} \text{tr} \left(A^{i_1}[1] A^{i_2}[2] \dots A^{i_N}[N] \right) |i_1\rangle |i_2\rangle \dots |i_N\rangle. \quad (1.1)$$

When all local Hilbert spaces $\mathcal{H}^j \equiv \mathbb{C}^d$ with constant physical dimension d , we can associate the same $A^i_{\alpha\beta}$ to every site in order to obtain translation invariant states¹. The dimension D of the virtual indices is then independent of the links and is referred to as the bond dimension. From the definition (1.1) it is clear that the resulting MPS is invariant under a similarity transformation of the matrices A^i , i.e. if we replace the d matrices A^i with $X A^i X^{-1}$ then the resulting state $|\psi\rangle$ remains the same. For this reason we call such a transformation of the tensor A a gauge transformation.

MPS of this form can be brought into a canonical form [73, 74]. In discussing this canonical form we will follow the presentation of Ref. [75]. Let us consider the situation where we decompose the identity on the virtual indices as a sum of two projectors P and $P^\perp = 1 - P$, where P corresponds to the orthogonal projector onto an invariant subspace of the matrices A^i , i.e.

$$A^i P = P A^i P \quad (1.2)$$

$$P^\perp A^i = P^\perp A^i P^\perp. \quad (1.3)$$

Using these relations one sees that the MPS

$$|\psi\rangle = \sum_{\{i_j\}} \text{tr} \left(A^{i_1} A^{i_2} \dots A^{i_N} \right) |i_1\rangle |i_2\rangle \dots |i_N\rangle \quad (1.4)$$

can equivalently be constructed by replacing the matrices A^i with \hat{A}^i , where

$$\hat{A}^i = P A^i P + P^\perp A^i P^\perp \equiv A_1^i \oplus A_2^i. \quad (1.5)$$

¹A translation invariant MPS is not necessarily of this form and can for example have an additional matrix B in the trace that commutes with all of the A^i . For an irreducible MPS (see below), such a B naturally satisfies $B \sim 1$, but in the case of fermionic MPS, a non-trivial B can arise.

We can now apply the same argument to further decompose the A_1^i and A_2^i blocks under the presence of possible invariant subspaces. After a finite number of iterations we can write the matrices as

$$\hat{A}^i = \bigoplus_{k=1}^r A_k^i, \quad (1.6)$$

where none of the blocks A_k^i contains an invariant subspace. This form of the matrices implies that we can decompose $|\psi\rangle$ as a sum of multiple MPS: $|\psi\rangle = \sum_{k=1}^r |\psi\rangle_k$, where $|\psi\rangle_k$ is a MPS constructed from the matrices A_k^i . The existence of the canonical form implies that without loss of generality we can restrict to matrices \hat{A}^i that span a semisimple algebra. If the A^i span a simple $D \times D$ matrix algebra we see that the corresponding MPS is irreducible, i.e. it cannot be decomposed as a sum of multiple MPS. This class of irreducible MPS is commonly referred to as injective MPS because they satisfy the property that there exists a $p \in \mathbb{N}$, such that for all $q > p$ we have that $(A^{i_1} A^{i_2} \dots A^{i_q})_{\alpha\beta}$, interpreted as a map from α, β to i_1, i_2, \dots, i_q , is injective.

To every such MPS we can also associate a so-called parent Hamiltonian [73]. It consists of a sum of local terms acting on $q > p$ neighbouring sites. To define the local terms we again consider the map $(A^{i_1} A^{i_2} \dots A^{i_q})_{\alpha\beta}$. The local Hamiltonian terms are then projectors onto the space orthogonal to the image of this map. Because the image is D^2 dimensional and the total physical space corresponding to q site is d^q , this space orthogonal to the image is always non-zero for large enough q . By construction, the parent Hamiltonian of a MPS is frustration free and has the MPS as its ground state. If the MPS is irreducible, one can even show that the parent Hamiltonian is gapped and that its ground state is unique. If the MPS is reducible, i.e. $|\psi\rangle = \sum_{k=1}^r |\psi\rangle_k$, then every state $|\psi\rangle_k$ is by itself a ground state of the parent Hamiltonian.

1.3 Super vector spaces

To construct fermionic matrix product states we will make use of super vector spaces. In this section we introduce the relevant concepts and present the notation to be used in following sections. A super vector space V has a natural direct sum decomposition

$$V = V^0 \oplus V^1, \quad (1.7)$$

where we refer to vectors in $V^0(V^1)$ as even (odd) parity vectors. Vectors that have a definite parity are called homogeneous. We denote the parity of a homogeneous basis state $|i\rangle$ by $|i| \in \{0, 1\}$. The tensor product of two homogeneous vectors $|i\rangle$ and $|j\rangle$ is again a homogeneous vector, and its parity is given by $|i| + |j| \bmod 2$. In other words, V and the associated

operation of taking tensor products is \mathbb{Z}_2 graded. We will denote the graded tensor product as

$$|i\rangle \otimes_{\mathfrak{g}} |j\rangle \in V \otimes_{\mathfrak{g}} V. \quad (1.8)$$

The key relation between super vector spaces and fermionic degrees of freedom is the following canonical graded tensor product isomorphism

$$\begin{aligned} \mathcal{F} : V \otimes_{\mathfrak{g}} W &\rightarrow W \otimes_{\mathfrak{g}} V \\ |i\rangle \otimes_{\mathfrak{g}} |j\rangle &\rightarrow (-1)^{|i||j|} |j\rangle \otimes_{\mathfrak{g}} |i\rangle \end{aligned} \quad (1.9)$$

The canonical isomorphism \mathcal{F} is the crucial ingredient of super vector spaces and it shows why even (odd) parity vectors can be interpreted as having even (odd) fermion number.

The dual space V^* , defined via its linear action on V , has a canonical basis $\langle i|$ satisfying $\langle i|j\rangle = \delta_{i,j}$ that inherits the \mathbb{Z}_2 grading of V . In particular, the definition of \mathcal{F} has a natural extension to also include the action on the relevant dual spaces. For example, if we replace V with its dual space V^* , then \mathcal{F} acts as

$$\begin{aligned} \mathcal{F} : V^* \otimes_{\mathfrak{g}} W &\rightarrow W \otimes_{\mathfrak{g}} V^* \\ \langle i| \otimes_{\mathfrak{g}} |j\rangle &\rightarrow (-1)^{|i||j|} |j\rangle \otimes_{\mathfrak{g}} \langle i|, \end{aligned} \quad (1.10)$$

and similarly for the other cases $V \otimes_{\mathfrak{g}} W^*$ and $V^* \otimes_{\mathfrak{g}} W^*$. We will often refer to \mathcal{F} as fermionic reordering and use the notation \mathcal{F} very loosely, i.e. every isomorphism between graded tensor products of super vector spaces that corresponds to multiple applications of \mathcal{F} as defined above will actually be denoted with the same symbol, and clearly the precise order of such subsequent applications is irrelevant.

A tensor in $V^* \otimes_{\mathfrak{g}} V$ can be mapped to \mathbb{C} by using the natural action of the dual space. We denote this homomorphism as a contraction \mathcal{C}

$$\mathcal{C} : V^* \otimes_{\mathfrak{g}} V \rightarrow \mathbb{C} : \langle \psi| \otimes_{\mathfrak{g}} |\phi\rangle \rightarrow \langle \psi|\phi\rangle, \quad (1.11)$$

and in particular $\mathcal{C}(\langle j| \otimes_{\mathfrak{g}} |i\rangle) = \delta_{i,j}$. Applying the contraction of V^* and V in a more general tensor product involving several super vector spaces requires that we first apply \mathcal{F} so as to isolate $V^* \otimes_{\mathfrak{g}} V$. Still denoting this combined reordering and contraction as \mathcal{C} , we obtain for example the famous supertrace

$$\mathcal{C}(|i\rangle \otimes_{\mathfrak{g}} \langle j|) = (-1)^{|i||j|} \mathcal{C}(\langle j| \otimes_{\mathfrak{g}} |i\rangle) = (-1)^{|i|} \delta_{i,j}. \quad (1.12)$$

To obtain the normal trace, we need to include the fermion parity operator $\sum_k (-1)^{|k|} |k\rangle \otimes_{\mathfrak{g}} \langle k|$ so that we indeed obtain

$$\mathcal{C}\left(\sum_k (-1)^{|k|} |k\rangle \otimes_{\mathfrak{g}} \langle k| \otimes_{\mathfrak{g}} |i\rangle \otimes_{\mathfrak{g}} \langle j|\right) = (-1)^{|i|} \mathcal{C}(|i\rangle \otimes_{\mathfrak{g}} \langle j|) = \delta_{i,j}. \quad (1.13)$$

The contraction map also defines the canonical isomorphism $(V \otimes_{\mathfrak{g}} W)^* \simeq W^* \otimes_{\mathfrak{g}} V^*$, as indeed we have $\mathcal{C}(\langle j' | \otimes_{\mathfrak{g}} \langle i' | \otimes_{\mathfrak{g}} | i \rangle \otimes_{\mathfrak{g}} | j \rangle) = \delta_{i',i} \delta_{j',j}$.

The grading of the super vector space V carries over to the algebra of (anti-)linear operators acting on V , as linear operators on V are naturally represented as tensors in $V \otimes_{\mathfrak{g}} V^*$ as

$$M = \sum_{i,j} M_{ij} |i\rangle \otimes_{\mathfrak{g}} \langle j| \in V \otimes_{\mathfrak{g}} V^*. \quad (1.14)$$

The algebra of operators on V thus becomes a superalgebra, whose homogeneous elements are represented by tensors M with a well defined parity, henceforth denoted as $|M|$, i.e. $|i| + |j| \pmod{2} = |M|$ is equal for all contributions to the sum (1.14). The algebra multiplication rule \cdot is obtained by applying the contraction map \mathcal{C} , which involves the fermionic reordering \mathcal{F} . For the algebra of operators on $V \otimes_{\mathfrak{g}} W$, this results in the multiplication rule

$$(M \otimes_{\mathfrak{g}} N) \cdot (O \otimes_{\mathfrak{g}} P) = (-1)^{|N||O|} (M \cdot O) \otimes_{\mathfrak{g}} (N \cdot P), \quad (1.15)$$

with $M, O \in V \otimes_{\mathfrak{g}} V^*$ and $N, P \in W \otimes_{\mathfrak{g}} W^*$.

1.4 Fermionic matrix product states

In this section we introduce the general formalism of fermionic matrix product states (fMPS). We obtain two distinct classes, one leading to even parity states with periodic boundary conditions, and one to odd parity states. But firstly, we introduce the general notion of fermionic tensor networks using super vector spaces.

1.4.1 Fermionic tensor networks

We start by providing a more abstract definition of the bosonic MPS. We therefore promote the rank three arrays $A_{\alpha,\beta}^i$ to tensors

$$A[j] = \sum_{i,\alpha,\beta} A[j]_{\alpha,\beta}^i |\alpha\rangle_{j-1} \otimes |i\rangle_j \otimes \langle \beta|_j \in V^j \otimes \mathcal{H}^j \otimes (V^{j+1})^*, \quad (1.16)$$

where round bras and kets correspond to the basis of the virtual spaces $V^j \simeq \mathbb{C}^{D_j}$ (and its duals). The MPS $|\psi\rangle$ from Eq. (1.1) is then obtained as

$$|\psi\rangle = \mathcal{C}_v(A[1] \otimes A[2] \otimes \cdots \otimes A[N]) \quad (1.17)$$

where \mathcal{C}_v denotes the contraction of all the virtual indices and the different tensor product orders are trivially isomorphic in the bosonic case (reordering does not introduce signs).

A natural definition of a fMPS follows from this construction by starting from tensors $A[j] \in V^j \otimes_{\mathfrak{g}} \mathcal{H}^j \otimes_{\mathfrak{g}} (V^{j+1})^*$ where both the physical Hilbert space \mathcal{H}^j and the virtual spaces V^j are super vector spaces. The fMPS is then obtained as

$$|\psi\rangle = C_v(A[1] \otimes_{\mathfrak{g}} A[2] \otimes_{\mathfrak{g}} \cdots \otimes_{\mathfrak{g}} A[N]) \quad (1.18)$$

where the contraction C_v over the virtual indices now involves the fermionic reordering isomorphism \mathcal{F} . This construction extends to fermionic tensor networks in general. If all of the individual tensors have a well defined parity $|A[j]|$, then so does the resulting state and a different initial order of the tensors in the graded tensor product will at most result in a global sign difference of the state. In particular, if at most one of the tensors is odd, the definition of the fermionic tensor network is independent of the order of the individual tensors. As the ability to manipulate tensor networks locally is of paramount importance both for numerical as well as theoretical applications, we will always impose this constraint as a consistency condition.

As an illustration, let us define following fermionic tensors

$$C = \sum_{\alpha\beta\gamma} C_{\alpha\beta\gamma} |\alpha\rangle |\beta\rangle \langle \gamma|$$

$$D = \sum_{\lambda\kappa} D_{\lambda\kappa} |\lambda\rangle \langle \kappa|$$

Suppose we wish to contract the β index of C with the κ index of D . As explained above, we first take the graded tensor product of C and D :

$$C \otimes_{\mathfrak{g}} D = \sum_{\alpha\beta\gamma\lambda\kappa} C_{\alpha\beta\gamma} D_{\lambda\kappa} |\alpha\rangle |\beta\rangle \langle \gamma| \otimes_{\mathfrak{g}} |\lambda\rangle \langle \kappa|.$$

Next, we bring the κ bra next to the β ket using fermionic reordering

$$\mathcal{F}(C \otimes_{\mathfrak{g}} D) = \sum_{\alpha\beta\gamma\lambda\kappa} C_{\alpha\beta\gamma} D_{\lambda\kappa} (-1)^{|\kappa|(|\lambda|+|\gamma|+|\beta|)} |\alpha\rangle \langle \kappa| |\beta\rangle \langle \gamma| |\lambda\rangle.$$

If the tensors C and D are even, this is equivalent to

$$\mathcal{F}(C \otimes_{\mathfrak{g}} D) = \sum_{\alpha\beta\gamma\lambda\kappa} C_{\alpha\beta\gamma} D_{\lambda\kappa} (-1)^{|\kappa|+|\kappa||\alpha|} |\alpha\rangle \langle \kappa| |\beta\rangle \langle \gamma| |\lambda\rangle.$$

Now we apply the contraction to obtain the final tensor:

$$F \equiv \sum_{\alpha\gamma\lambda} \left(\sum_{\beta} C_{\alpha\beta\gamma} D_{\lambda\beta} (-1)^{|\beta|+|\beta||\alpha|} \right) |\alpha\rangle \langle \gamma| |\lambda\rangle.$$

Note that also in the definition of the contracted tensor F we have to include an internal ordering. Different internal orderings give additional minus signs to the tensor components. It therefore only makes sense to compare tensors that have the same internal ordering. Let us now use this formalism to study the two different classes of fMPS.

1.4.2 Even parity states

To build translation invariant fMPS on chains of every length, we start from even tensors $A = \sum_{i\alpha\beta} A_{\alpha,\beta}^i |\alpha\rangle \otimes_{\mathfrak{g}} |i\rangle \otimes_{\mathfrak{g}} |\beta\rangle$. As in the bosonic case, we will denote by A^i the matrices obtained by fixing the superscript i in the array $A_{\alpha,\beta}^i$. Evenness of the tensors requires these matrices to take the following form

$$\begin{aligned} A^i &= \begin{pmatrix} B^i & 0 \\ 0 & C^i \end{pmatrix} & \text{if } |i| = 0 \\ A^i &= \begin{pmatrix} 0 & D^i \\ F^i & 0 \end{pmatrix} & \text{if } |i| = 1, \end{aligned} \quad (1.19)$$

in a standard basis of the virtual space where $|\alpha| = 0$ for $\alpha = 1, \dots, D_e$ and $|\alpha| = 1$ for $\alpha = D_e + 1, \dots, D_e + D_o = D$. Note that D_e and D_o can be different. By the chosen internal order of the tensors A , the contraction of the virtual indices on the bonds 1 to $N - 1$ is trivial and gives rise to

$$|\psi\rangle_e = \mathcal{C}_N \left(\sum_{\{i\}} \sum_{\alpha\beta} \left(A^{i_1} A^{i_2} \dots A^{i_N} \right)_{\alpha\beta} |\alpha\rangle_N |i_1\rangle |i_2\rangle \dots |i_N\rangle (\beta|_N \right).$$

where no minus signs have been generated and only the virtual index on bond N remains to be contracted. Using that all tensors are even, we can apply fermionic reordering to obtain

$$|\psi\rangle_e = \mathcal{C}_N \left(\sum_{\{i\}} \sum_{\alpha\beta} \left(A^{i_1} A^{i_2} \dots A^{i_N} \right)_{\alpha\beta} (-1)^{|\beta|} (\beta| |\alpha\rangle |i_1\rangle |i_2\rangle \dots |i_N\rangle \right),$$

where we can apply the contraction trivially in order to obtain

$$|\psi\rangle_e = \sum_{\{i\}} \text{tr} \left(\mathcal{P} A^{i_1} A^{i_2} \dots A^{i_N} \right) |i_1\rangle |i_2\rangle \dots |i_N\rangle. \quad (1.20)$$

Here, we introduced the parity matrix \mathcal{P}

$$\mathcal{P} = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} \quad (1.21)$$

which has the defining property

$$\mathcal{P} A^i = (-1)^{|i|} A^i \mathcal{P}, \quad (1.22)$$

because we started from even tensors A . The resulting fMPS $|\psi\rangle_e$, being the contraction of these even tensors, has even fermion parity, as indicated by the subscript. One sees that the coefficients of the fMPS satisfy

$$\text{tr} \left(\mathcal{P} A_e^{i_1} A_e^{i_2} \dots A_e^{i_N} \right) = (-1)^{|i_1|} \text{tr} \left(\mathcal{P} A_e^{i_2} A_e^{i_3} \dots A_e^{i_1} \right),$$

which is indeed the correct behaviour for translationally invariant fermionic states with even fermion parity, as shown in appendix 1.A.

1.4.3 Odd parity states

Because the fMPS tensors A are even, a fMPS with odd fermion parity is obtained by adding one additional tensor with odd parity and no physical component to the tensor network. We choose $Y = \sum_{\alpha,\beta} Y_{\alpha,\beta} |\alpha\rangle_N \otimes_{\mathfrak{g}} (\beta|_1$ with $Y_{\alpha,\beta} = 0$ if $|\alpha| + |\beta| \pmod{2} = 0$. Evaluating

$$|\psi\rangle_o = \mathcal{C}_v \left(Y \otimes_{\mathfrak{g}} A[1] \otimes_{\mathfrak{g}} A[2] \otimes_{\mathfrak{g}} \cdots \otimes_{\mathfrak{g}} A[N] \right) \quad (1.23)$$

using the same steps as in the previous subsection results in

$$|\psi\rangle_o = \sum_{\{i\}} \text{tr} \left(Y A^{i_1} A^{i_2} \cdots A^{i_N} \right) |i_1\rangle |i_2\rangle \cdots |i_N\rangle. \quad (1.24)$$

If we require this state to be invariant under translations then, as shown in appendix 1.A, it should hold that

$$\text{tr} \left(Y A^{i_1} A^{i_2} \cdots A^{i_N} \right) = \text{tr} \left(Y A^{i_2} A^{i_3} \cdots A^{i_1} \right),$$

implying that Y has to commute with all A^i . To satisfy these requirements we choose $D_e = D_o$ and take the tensors to be of the form

$$\begin{aligned} A^i &= \begin{pmatrix} B^i & 0 \\ 0 & B^i \end{pmatrix} = \mathbb{1} \otimes B^i & \text{if } |i| = 0 \\ A^i &= \begin{pmatrix} 0 & B^i \\ -B^i & 0 \end{pmatrix} = y \otimes B^i & \text{if } |i| = 1, \end{aligned} \quad (1.25a)$$

with

$$y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (1.25b)$$

The odd matrix commuting with A^i is then simply

$$Y = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix} = y \otimes \mathbb{1}. \quad (1.25c)$$

We will comment on the generality of this choice in the next section.

Let us now look at what happens when we define the fMPS with odd fermion parity on a chain with open boundary conditions. We will do this by looking at a particular example, namely the Kitaev chain for spinless fermions, which is described by the Hamiltonian [16]

$$H_{\text{Kitaev}} = -i \sum_{j=1}^N \gamma_{2j} \gamma_{2j+1}, \quad (1.26)$$

where

$$\gamma_{2j-1} = -i(a_j - a_j^\dagger) \quad (1.27)$$

$$\gamma_{2j} = a_j + a_j^\dagger \quad (1.28)$$

are Majorana operators satisfying $\gamma_j^\dagger = \gamma_j$ and $\{\gamma_j, \gamma_k\} = 2\delta_{jk}$. We can easily obtain the exact fMPS description of the ground state with periodic boundary conditions by applying the projectors

$$P_j = \frac{1}{2} (\mathbb{1} + i\gamma_{2j}\gamma_{2j+1}) = \frac{1}{2} \left(\mathbb{1} - (a_j^\dagger + a_j)(a_{j+1}^\dagger - a_{j+1}) \right) \quad (1.29)$$

to an arbitrary state with odd fermion parity (acting with these projectors on an even parity state gives zero). The matrices of the fMPS ground state are:

$$A^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (1.30)$$

$$A^1 = Y = y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad (1.31)$$

which is indeed a special case of the general structure given in equations (1.25). Starting from the expression

$$\sum_{\{i\}} \left(A^{i_1} A^{i_2} \dots A^{i_N} \right)_{\alpha\beta} |\alpha\rangle |i_1\rangle |i_2\rangle \dots |i_N\rangle \langle \beta| \quad (1.32)$$

we can now obtain four ground states on a chain with open boundary conditions by closing the virtual indices at the boundaries with either $(0|$ ($|0\rangle$) or $(1|$ ($|1\rangle$)). However, because of the special structure of the tensor, the two states with even fermion parity, obtained by closing the virtual indices diagonally with either $(0| \otimes_g |0\rangle$ or $(1| \otimes_g |1\rangle$ are equal. Also the two odd parity states obtained by closing off-diagonally with $(0| \otimes_g |1\rangle$ or $(1| \otimes_g |0\rangle$ are equal up to a minus sign. So on a chain with open boundary conditions we have only two different ground states, one with even and one with odd parity. The information about which ground state we pick is shared between the two edges; i.e. it is encoded in the way the fMPS was closed, either diagonally or off-diagonally. Because there is no local way to detect this difference, there is no local term that can be added to the Hamiltonian to split the degeneracy for large system sizes. This is the fMPS manifestation of the appearance of Majorana edge modes [16].

1.4.4 Irreducibility

At this point the structure of the tensors we used to construct fMPS with odd parity (1.25) can be seen as a special case of the structure of tensors for even parity fMPS (1.19). Furthermore, interpreting the matrices A^i as those specifying a bosonic MPS, the existence of a matrix Y commuting with all A^i in the case of the odd parity states would point towards a reducible representation and hence symmetry breaking. We therefore need to redevelop the concept of irreducibility for fMPS from the ground up, using the notion of invariant subspaces. We thus start from the matrices A^i with

the general structure of Eq. (1.4.2), whose defining signature is the existence of the parity matrix $\mathcal{P} = \mathcal{P}^{-1}$ satisfying Eq. (1.22). If the matrices A^i have a non-trivial invariant subspace with corresponding orthogonal projector P satisfying

$$A^i P = P A^i P$$

then necessarily

$$\mathcal{P} A^i \mathcal{P} P = P \mathcal{P} A^i \mathcal{P} P$$

and thus

$$A^i \mathcal{P} P P = \mathcal{P} P \mathcal{P} A^i \mathcal{P} P P$$

so that $Q = \mathcal{P} P P$ is also an orthogonal projector onto an invariant subspace. If P was already associated to an irreducible invariant subspace (containing no smaller non-trivial invariant subspaces), then either $Q = P$ or $PQ = QP = 0$. Otherwise, the intersection of the invariant subspaces of Q and P would be an invariant subspace of its own, thus leading to a contradiction.

The case $Q = P$ corresponds to $[P, \mathcal{P}] = 0$ and allows one to decompose the invariant subspace (and its orthogonal complement) into an even and odd part using the projectors $P_{\pm} = (1 \pm \mathcal{P})/2$ as $P = P_+ P P_+ + P_- P P_-$. Consequently, we can replace A^i by $\hat{A}^i = P A^i P + P^{\perp} A^i P^{\perp}$ where both $P A^i P$ and $P^{\perp} A^i P^{\perp}$ individually have the structure of Eq. (1.22) and thus correspond to even fermionic tensors specifying a fMPS.

If the matrices A^i have no more non-trivial invariant subspaces satisfying $[P, \mathcal{P}] = 0$, we can try to reduce them further using invariant subspaces where $PQ = QP = 0$. Note, firstly, that $P + Q$ is an invariant subspace projector that does commute with \mathcal{P} and thus, by the previous assumption, is equal to the identity. This imposes the following structure on P and $Q = P^{\perp} = 1 - P = \mathcal{P} P \mathcal{P}$

$$P = \frac{1}{2} \begin{bmatrix} \mathbf{1} & U \\ U^{\dagger} & \mathbf{1} \end{bmatrix}, \quad Q = \frac{1}{2} \begin{bmatrix} \mathbf{1} & -U \\ -U^{\dagger} & \mathbf{1} \end{bmatrix}, \quad (1.33)$$

where idempotence requires $UU^{\dagger} = U^{\dagger}U = \mathbf{1}$. Hence, this is only possible if $D_e = D_o$ and U is a unitary matrix. This implies the matrices A^i are of the following form

$$A^i = \begin{pmatrix} B^i & 0 \\ 0 & U^{\dagger} B^i U \end{pmatrix} \quad \text{if } |z| = 0$$

$$A^i = \begin{pmatrix} 0 & B^i \\ U^{\dagger} B^i U^{\dagger} & 0 \end{pmatrix} \quad \text{if } |z| = 1. \quad (1.34)$$

An even-parity gauge transform of the form $\mathbf{1} \oplus iU$ will map this to the standard form of Eq. (1.25), which we will employ for the remainder of the discussion.

So why, despite the presence of non-trivial invariant subspaces, is this fMPS irreducible? So far, our irreducibility discussion has not distinguished between fermionic MPS or bosonic MPS with a \mathbb{Z}_2 symmetry. In the bosonic case, the latter form can be further reduced using P and P^\perp into two MPS, which will be irreducible if the B^i span a simple matrix algebra of dimension $D_e = D_o = D/2$. These individual MPS break the \mathbb{Z}_2 symmetry. The even and odd superposition on the periodic chain are obtained by closing the MPS with either the identity or with Y . In the fermionic case, the new matrices obtained by reducing A^i with P and P^\perp do not make sense as fermionic tensors, as they do not have well defined parity. Indeed, fermion parity cannot be broken. On the periodic chain, we can again try to create the symmetric and antisymmetric linear combinations corresponding to even and odd fermion parity. To close the fMPS, we also have to start at the level of the fermionic tensors, where we can thus try to add either the identity or the non-trivial element Y , giving rise to the two states $C_v(A^{\otimes_s N})$ and $C_v(Y \otimes A^{\otimes_s N})$. However, unlike in the bosonic case, upon applying the fermionic contraction and reordering, the first state evaluates to zero because an extra factor \mathcal{P} is introduced at the level of the matrices, as discussed in Section 1.4.2. So only the odd parity state survives as a translation invariant state.

We thus want to conclude that fermionic tensors A associated with the matrices $A^i = y^{|i|} \otimes B^i$ define an irreducible fMPS if the B^i span a simple $D/2 \times D/2$ dimensional matrix algebra. However, this is not sufficient as there is an extra condition hidden in the fact that A^i also doesn't have an invariant subspace that commutes with \mathcal{P} . Suppose indeed that $A^i = y^{|i|} \otimes B^i$ has a non-trivial invariant subspace $A^i P = P A^i P$ with P of the form

$$P = \begin{bmatrix} P_e & 0 \\ 0 & P_o \end{bmatrix}, \quad (1.35)$$

and $P_o = \mathbf{1}_{D/2} - P_e$. The condition $A^i P = P A^i P$ then implies that

$$\begin{aligned} B^i P_e &= P_e B^i P_e, \forall |i| = 0, & B^i P_o &= P_o B^i P_o, \forall |i| = 0, \\ B^i P_e &= P_o B^i P_e, \forall |i| = 1, & B^i P_o &= P_e B^i P_o, \forall |i| = 1. \end{aligned} \quad (1.36)$$

This type of invariant subspace is consistent with the requirement that the matrices B^i span a simple $D/2 \times D/2$ matrix algebra. However, when properties (1.36) hold we can conclude that the even subalgebra, spanned by $B^{i_1} \dots B^{i_p}$ with $p \in \mathbb{N}$ and $\sum_{j=1}^p |i_j| = 0 \pmod{2}$ has P_e and P_o as non-trivial invariant subspaces. A sufficient condition for the odd parity fMPS to be irreducible is thus that the even subalgebra spanned by $y^{|i|} \otimes B^i$ should be a simple $D/2 \times D/2$ matrix algebra. This is also a necessary condition, as an irreducible algebra B^i with a reducible even subalgebra automatically leads to the existence of a P_e and $P_o = P_e^\perp$ and thus to an invariant subspace projector P satisfying $[P, \mathcal{P}] = 0$ for the A^i . The physical reason for excluding this case is that the above structure of the B^i 's, in combination with the fact

that the resulting state has an odd fermion parity and thus an odd number of B^i factors with $|i| = 1$ automatically makes the state zero, as can readily be verified.

In summary, an fMPS is irreducible in the following two cases. In the standard basis where $\mathcal{P} = \mathbb{1}_{D_e} \oplus -\mathbb{1}_{D_o}$, the matrices A^i either

- take the form of Eq. (1.19) and span a simple $D \times D$ matrix algebra; the center is trivial and resulting translation invariant fMPS on the periodic chain have even fermion parity.
- take the form of Eq. (1.34), which can be gauge transformed into the canonical form of Eq. (1.25) where $A^i = y^{|i|} \otimes B^i$, and the even subalgebra of the B^i is a simple $D/2 \times D/2$ matrix algebra. The resulting translation invariant fMPS on a periodic chain has odd fermion parity.

The above two notions of irreducibility for even and odd parity fMPS correspond to the two possibilities for simple \mathbb{Z}_2 graded algebras [66, 76]. An even simple \mathbb{Z}_2 graded algebra is simple as an ungraded algebra, which implies that its center consists only of multiples of the identity. An odd simple \mathbb{Z}_2 graded algebra $\mathcal{A} = \mathcal{A}_0 \oplus \mathcal{A}_1$, where \mathcal{A}_0 consists of the even parity elements and \mathcal{A}_1 of the odd parity elements, has the property that \mathcal{A}_0 is simple and $\mathcal{A}_1 = Y\mathcal{A}_0$, with Y an odd element satisfying $Y^2 \propto \mathbb{1}$. The graded center of an odd simple algebra consists only of multiples of $\mathbb{1}$ and Y . So we see that the bosonic statement of irreducibility:

$$A \text{ MPS is irreducible} \Leftrightarrow A^i \text{ span a simple algebra}$$

has an elegant generalization to the fermionic case:

$$A \text{ fMPS is irreducible} \Leftrightarrow A^i \text{ span a simple } \mathbb{Z}_2 \text{ graded algebra}$$

The two types of simple \mathbb{Z}_2 graded algebras, which are called even and odd type, correspond to fMPS with even or odd fermion parity respectively under periodic boundary conditions. For this reason we henceforth refer to these two types of irreducible fMPS as even algebra and odd algebra fMPS respectively. As explained in the previous section, odd algebra fMPS have the physical property of Majorana edge modes on a chain with open boundary conditions.

1.4.5 \mathbb{Z}_2 group structure

Taking the graded tensor product of two fMPS with odd fermion parity under periodic boundary conditions obviously gives an fMPS with even fermion parity. In the previous section we related the global fermion parity of the fMPS to the type of simple \mathbb{Z}_2 graded algebra spanned by the matrices A^i . In this section we calculate how the type of simple graded algebra changes under the graded tensor product of two odd fMPS. We start by taking the

graded tensor product of two fMPS tensors, and applying the fermionic reordering to obtain the tensor of the new fMPS:

$$\begin{aligned}
 & \mathcal{F} \left(\left(\sum_{i\alpha\beta} A_{\alpha\beta}^i |\alpha\rangle |i\rangle \langle \beta| \right) \otimes_{\mathfrak{g}} \left(\sum_{j\gamma\delta} A_{\gamma\delta}^{j'} |\gamma\rangle |j\rangle \langle \delta| \right) \right) \\
 &= \sum_{ij\alpha\beta\gamma\delta} A_{\alpha\beta}^i A_{\gamma\delta}^{j'} \mathcal{F} (|\alpha\rangle |i\rangle \langle \beta| \otimes_{\mathfrak{g}} |\gamma\rangle |j\rangle \langle \delta|) \\
 &= \sum_{ij\alpha\beta\gamma\delta} A_{\alpha\beta}^i A_{\gamma\delta}^{j'} (-1)^{|\gamma||i|} |\alpha\rangle |\gamma\rangle |i\rangle |j\rangle \langle \delta| \langle \beta|
 \end{aligned}$$

From this we see that the tensor components of the fMPS describing the graded tensor product of the individual fMPS are

$$A_{(\alpha\gamma)(\beta\delta)}^{ij} = A_{\alpha\beta}^i A_{\gamma\delta}^{j'} (-1)^{|\gamma||i|} \quad (1.37)$$

As the tensor product of two simple matrix algebras over \mathbb{C} again forms a simple algebra, it is sufficient to start from the matrices $A^i = y^{|i|}$, i.e. those of the Kitaev chain (1.30). We also use a relabeling (permutation) for the virtual bases of the new fMPS tensors in which the even parity states come before the odd parity states, i.e. so that the parity matrix \mathcal{P} takes the standard form. We thus obtain:

$$\begin{aligned}
 A^{00} &= \mathbb{1} \otimes \mathbb{1}, & A^{11} &= \mathbb{1} \otimes y \\
 A^{01} &= y \otimes z, & A^{10} &= y \otimes x,
 \end{aligned}$$

with $y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, $z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and $x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. The Kitaev chain fMPS with periodic boundary conditions also contains an additional matrix y in the trace defining the coefficients. The reordered graded tensor product $\mathcal{F}(y \otimes_{\mathfrak{g}} y)$ expressed in the new basis given is by $-z \otimes y$. As the total fermion parity of the tensor product of two odd chains is even, the final fermion contraction induces an extra factor $\mathcal{P} = z \otimes \mathbb{1}$. We thus see that the coefficients of the new fMPS are of the form

$$\begin{aligned}
 & \text{tr} \left((\mathbb{1} \otimes y) A^{i_1 j_1} A^{i_2 j_2} \dots A^{i_N j_N} \right) \\
 & \equiv -\text{tr} \left(i\Lambda A^{i_1 j_1} A^{i_2 j_2} \dots A^{i_N j_N} \right).
 \end{aligned} \quad (1.38)$$

The matrices A^{ij} are of the form $y^{|i|+|j|} \otimes B^{i,j}$ where the even subalgebra of the B matrices is spanned by $\mathbb{1}$ and y and is thus reducible. This implies the existence of a parity preserving projector $Q = (1 + iy)/2 \oplus (1 - iy)/2$ and its complement $Q^\perp = (1 - iy)/2 \oplus (1 + iy)/2$. The non-trivial closure $i\Lambda = -\mathbb{1} \otimes y$ makes this state nonzero. The following gauge transform makes

this form explicit

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0 & i \\ 0 & 1 & 0 & 1 \\ i & 0 & -i & 0 \\ 1 & 0 & 1 & 0 \end{bmatrix}$$

and transforms the matrices into

$$\begin{aligned} A^{00} &= \mathbb{1} \oplus \mathbb{1}, & A^{11} &= (-iz) \oplus (-iz), \\ A^{01} &= (-ix) \oplus (ix), & A^{10} &= (y) \oplus (-y), \\ \mathcal{P} &= z \oplus z, & i\Lambda &= (iz) \oplus (iz) = i\mathcal{P}. \end{aligned}$$

Although the two individual fMPS tensors in the direct sum decomposition have a different sign in case of odd $|i|$, this sign is irrelevant as the odd matrices appear an even number of times. Hence, up to a global factor $-2i$, the tensor product of two Kitaev chain fMPS takes the standard form of an even fMPS [Eq. (1.19)] with matrices

$$\begin{aligned} A^{00} &= \mathbb{1}, & A^{11} &= (-iz), \\ A^{01} &= -ix, & A^{10} &= y. \end{aligned}$$

These matrices clearly span an even simple \mathbb{Z}_2 graded algebra. However, we notice that under time reversal for spinless fermions the matrices of the new fMPS transform as

$$\bar{A}^{ij} = y^T A^{ij} y \tag{1.39}$$

$$-i\mathcal{P} = y^T (i\mathcal{P}) y, \tag{1.40}$$

which implies that there will be Kramers pairs at the ends of an open chain because the global action of time reversal on the chain gets intertwined to an action of y on the virtual indices at the ends and $y^2 = -\mathbb{1}$ [64, 77]. We come back to this point in more detail in section 1.7.

1.5 Parent Hamiltonian and ground state uniqueness

In section 1.2 we explained how every bosonic MPS has a parent Hamiltonian associated to it. We show that this construction carries over directly to the fMPS framework and that the resulting parent Hamiltonian, both for even and odd algebra fMPS, has a unique ground state on a closed chain with periodic boundary conditions. The parent Hamiltonian construction is most cleanly expressed using fermionic tensors, such that the resulting Hamiltonian terms are fermionic operators by construction. The reason for this is that the framework of fermionic tensor networks was set up in such

a way (the use of even tensors and at most one odd tensor) that applying the fermionic reordering isomorphism \mathcal{F} before contracting the tensors, as well as the order in which the various contractions are evaluated, has no effect on the outcome. This is precisely what warrants the validity of the popular graphical notation used for bosonic tensor networks, and is thus still valid in the current fermionic context. Even at the level of a single tensor we can apply \mathcal{F} in order to choose a different internal ordering with respect to which the tensor coefficients are defined. This information is not encoded in the graphical notation, but does again not influence the end result, if the tensor coefficients are correctly transformed when going from one particular ordering to another. As such, boxes in the graphical tensor network notation do not denote a single tensor A , but the whole equivalence class $[A]$ of tensors related by the reordering isomorphism \mathcal{F} .

We first construct the parent Hamiltonian for the case of an irreducible even algebra fMPS and start by blocking the physical sites such that the tensors become injective at the single site level, i.e. $A^i_{\alpha,\beta}$ as a map from the D^2 -dimensional space corresponding to α and β to the d -dimensional space of i is injective. If $(A^+)^i_{\alpha,\beta}$ denotes the Moore-Penrose pseudo-inverse of $A^i_{\alpha,\beta}$, interpreted as matrix with rows i and columns α, β , then it actually is a left inverse, i.e.

$$\sum_i (A^+)^i_{\alpha,\beta} A^i_{\alpha',\beta'} = \delta_{\alpha,\alpha'} \delta_{\beta,\beta'} \quad (1.41)$$

Generically, the left inverse is not unique, but the Moore-Penrose pseudo-inverse is singled out by the condition that, acting on the right, it gives rise to a hermitian projector

$$\sum_{\alpha,\beta} A^i_{\alpha,\beta} (A^+)^{i'}_{\alpha,\beta} = (P_1)_{i,i'} \quad (1.42)$$

We now lift this definition to a fermionic tensor A^+ as

$$A^+ = \sum_{i,\alpha,\beta} (-1)^{|\alpha|} (A^+)^i_{\alpha,\beta} |\beta\rangle \otimes_{\mathfrak{g}} \langle i| \otimes_{\mathfrak{g}} |\alpha\rangle. \quad (1.43)$$

The reason for the additional sign $(-1)^{|\alpha|}$ becomes clear when we contract $A^+ \otimes_{\mathfrak{g}} A$ over the physical index and use a fermionic reordering to obtain

$$\begin{aligned} \mathcal{C}(A^+ \otimes_{\mathfrak{g}} A) &= \mathcal{C} \left(\sum_{i,\alpha,\alpha',\beta,\beta'} (-1)^{|\alpha|} (A^+)^i_{\alpha,\beta} A^i_{\alpha',\beta'} |\beta\rangle \otimes_{\mathfrak{g}} \langle i| \right. \\ &\quad \left. \otimes_{\mathfrak{g}} |\alpha\rangle \otimes_{\mathfrak{g}} |\alpha'\rangle \otimes_{\mathfrak{g}} |i\rangle \otimes_{\mathfrak{g}} |\beta'\rangle \right) \\ &\xrightarrow{\mathcal{F}} \mathcal{C} \left(\sum_{i,\alpha,\alpha',\beta,\beta'} (A^+)^i_{\alpha,\beta} A^i_{\alpha',\beta'} |\alpha'\rangle \otimes_{\mathfrak{g}} |\alpha\rangle \otimes_{\mathfrak{g}} |\beta\rangle \otimes_{\mathfrak{g}} \langle i| \otimes_{\mathfrak{g}} |i\rangle \otimes_{\mathfrak{g}} |\beta'\rangle \right) \\ &= \left(\sum_{\alpha} |\alpha\rangle \langle \alpha| \right) \otimes_{\mathfrak{g}} \left(\sum_{\beta} |\beta\rangle \langle \beta| \right) = \mathbf{1}. \end{aligned}$$

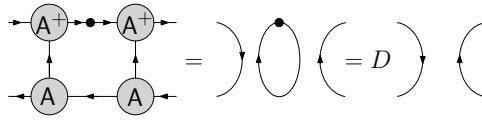


Figure 1.1: Stability of the injectivity property under contraction of tensors. The figure represents $\mathcal{C}(A_2^{(-1)} \otimes_{\mathfrak{g}} A_2) = D \mathbb{1} \otimes_{\mathfrak{g}} \mathbb{1}$, with D the bond dimension. The black dot represents the matrix $\sum_{\alpha} (-1)^{|\alpha|} |\alpha\rangle\langle\alpha|$. The arrows in the diagrammatic notation denote which indices correspond to bra's and which indices correspond to kets in the corresponding super vector spaces.

Hence, A^+ is a left inverse of A , i.e. in any tensor network diagram, we can cancel A^+ and A when contracted along the physical index.

However, upon applying several neighbouring A^+ to the MPS, we cannot simply contract the inner virtual degrees of freedom, as we will get supertraces (as discussed in Section 1.3) which are not merely traces of the identity. This is resolved by simply inserting additional parity operators when concatenating A^+ tensors. Consider hereto the MPS tensor A_2 of a two-site block, which is defined by contracting a single bond between two MPS tensors $A \otimes_{\mathfrak{g}} A$

$$A_2 = \mathcal{C}(A \otimes_{\mathfrak{g}} A) = \sum_{\alpha, \beta, \gamma, i, j} A_{\alpha, \beta}^i A_{\beta, \gamma}^j |\alpha\rangle\langle i| |j\rangle\langle\gamma|. \quad (1.44)$$

By constructing a left inverse $A_2^{(-1)}$ of A_2 as

$$\begin{aligned} A_2^{(-1)} &= \mathcal{C}(A^+ \otimes_{\mathfrak{g}} (\sum_{\beta} (-1)^{|\beta|} |\beta\rangle\langle\beta|) \otimes_{\mathfrak{g}} A^+) \\ &= \sum_{i, j, \alpha, \beta, \gamma} (-1)^{|\alpha|} (A^+)_{\alpha, \beta}^i (A^+)_{\beta, \gamma}^j \\ &\quad |\gamma\rangle \otimes_{\mathfrak{g}} \langle j| \otimes_{\mathfrak{g}} \langle i| \otimes_{\mathfrak{g}} |\alpha\rangle \end{aligned}$$

one can show stability of the injectivity property under contraction of tensors. This is illustrated in figure 1.1 using a diagrammatic notation.

A different left inverse

$$A_2^+ = \sum_{i, j, \alpha, \beta, \gamma} (-1)^{|\alpha|} (A_2^+)_{\alpha, \gamma}^{i, j} |\gamma\rangle \otimes_{\mathfrak{g}} \langle j| \otimes_{\mathfrak{g}} \langle i| \otimes_{\mathfrak{g}} |\alpha\rangle. \quad (1.45)$$

can be constructed from the pseudo-inverse $(A_2^+)_{\alpha, \gamma}^{i, j}$ of the coefficients $(A_2)_{\alpha, \gamma}^{i, j} = \sum_{\beta} A_{\alpha, \beta}^i A_{\beta, \gamma}^j$, interpreted as matrix with rows (i, j) and columns (α, β) . While $A_2^{(-1)}$ can be used to prove the ground state uniqueness (see below), we need to use A_2^+ in the construction of the parent Hamiltonian, in order to obtain a hermitian operator. By contracting $A_2 \otimes_{\mathfrak{g}} A_2^+$ along

the virtual bonds α and γ , we obtain the orthogonal projector P_2 onto the physical support on two sites as

$$\begin{aligned} P_2 &= \mathcal{C}(A_2 \otimes_{\mathfrak{g}} A_2^+) \\ &= \sum_{i,i',j,j',\alpha,\gamma} (A_2)_{\alpha,\gamma}^{i'j'} (A_2^+)_{\alpha,\gamma}^{ij} |i'\rangle |j'\rangle \langle j| \langle i|. \end{aligned} \quad (1.46)$$

The extra factor $(-1)^{|\alpha|}$ was cancelled by the factor picked up from reordering the $(\alpha|$ before contracting it with $|\alpha\rangle$. The resulting fermion operator P_2 is a hermitian projector, as can be verified from the properties of the pseudo-inverse $(A_2^+)_{\alpha,\gamma}^{i,j}$. The parent Hamiltonian is then simply

$$H = \sum_{i=1}^N (\mathbb{1} - P_2)_i, \quad (1.47)$$

where $(1 - P_2)_i$ acts on two consecutive sites i and $i + 1 \pmod N$. It clearly annihilates the fMPS. Vice versa, when showing uniqueness, we use that the ground subspace of the local terms is of the form $\mathcal{C}(A \otimes_{\mathfrak{g}} A \otimes X)$ with X an arbitrary tensor with well-defined parity (we try even and odd separately) on the other sites. That the intersection of all these local ground states only contains the translation invariant even parity fMPS containing only A tensors follows from proving the intersection and closure property from Ref. [56]. These proofs can be completely expressed in terms of tensor network diagrams of the type shown in figure 1.1 (using the left inverse $A_2^{(-1)}$) and are therefore equally valid for the bosonic and fermionic case.

For the odd algebra $A^i = y^{|i|} \otimes B^i$, we first block sites to the point where $B_{a,b}^i$ with $|i| = 0$ provides an injective mapping from the $(D/2)^2$ dimensional space labeled by a and b to the d_e -dimensional space of $|i| = 0$, and separately for $B_{a,b}^i$ with $|i| = 1$ ². We here used the notation $\alpha = (|\alpha|, a)$ where $a = 1, \dots, D/2$ spans the space in which the matrices B live and does not carry any information of the parity. Let us denote B^+ as the pseudo-inverse of B in the two parity sectors individually, i.e. $\sum_{|i|=0} (B^+)_{a,b}^i B_{a',b'}^i = \delta_{a,a'} \delta_{b,b'}$ and similarly for the sum over $|i| = 1$, whereas $\sum_{a,b} B_{a,b}^i (B^+)_{a,b}^{i'}$ is a hermitian projector in the block corresponding to $|i| = |i'| = 0$, as well as when restricted to the block $|i| = |i'| = 1$. The Moore-Read pseudo-inverse of A can then be verified to be given by $(A^+)_{\alpha,\beta}^i = \frac{1}{2} (y^{|i|})_{|\alpha|,|\beta|} (B^+)_{a,b}^i$. It indeed

²Note that under blocking two sites n times, we have $d_e^{(n)} = (d_e^{(n-1)})^2 + (d_o^{(n-1)})^2$ and $d_o^{(n)} = 2d_e^{(n-1)}d_o^{(n-1)}$, so that the ratio $x^{(n)} = d_e^{(n)}/d_o^{(n)} = x^{(n-1)}/2 + 1/2x^{(n-1)}$ converges to 1 and thus $d_{e,o}^{(n)} \rightarrow d^{(n)}/2 = d^{2^n}/2$.

satisfies

$$\begin{aligned}
 \sum_{\alpha,\beta} A_{\alpha,\beta}^i (A^+)^{i'}_{\alpha,\beta} &= \sum_{\alpha,\beta} \frac{1}{2} (y^{|\alpha|})_{|\alpha|,|\beta|} (y^{|\beta'|})_{|\alpha|,|\beta|} B_{a,b}^i (B^+)^{i'}_{a,b} \\
 &= \delta_{|\alpha|,|\beta'|} \sum_{a,b} B_{a,b}^i (B^+)^{i'}_{a,b} \\
 &= (P_1)_{i,i'}
 \end{aligned}$$

with P_1 a hermitian projector. Note that the restriction to $|i| = |\beta'|$ follows from the y part in A and A^+ . Acting on the left, by evaluating the sum over $|i| = 0$ and $|i| = 1$ separately, it results in

$$\begin{aligned}
 \sum_i (A^+)^i_{\alpha',\beta'} A_{\alpha,\beta}^i &= \frac{1}{2} [\delta_{|\alpha|,|\beta|} \delta_{|\alpha'|,|\beta'|} + y_{|\alpha|,|\beta|} y_{|\alpha'|,|\beta'|}] \delta_{a,a'} \delta_{b,b'} \\
 &= \frac{1}{2} [\delta_{|\alpha|,|\alpha'|} \delta_{|\beta|,|\beta'|} + y_{|\alpha|,|\alpha'|} y_{|\beta|,|\beta'|}] \delta_{a,a'} \delta_{b,b'}
 \end{aligned}$$

Again defining the fermionic tensor A^+ using Eq. (1.43), we obtain

$$\begin{aligned}
 \mathcal{C}(A^+ \otimes_{\mathfrak{g}} A) &\xrightarrow{\mathcal{F}} \sum_{\alpha,\beta,\alpha',\beta'} \frac{1}{2} [\delta_{|\alpha|,|\alpha'|} \delta_{|\beta|,|\beta'|} + y_{|\alpha|,|\alpha'|} y_{|\beta|,|\beta'|}] \delta_{a,a'} \delta_{b,b'} |\alpha'\rangle \langle \alpha| \otimes_{\mathfrak{g}} |\beta\rangle \langle \beta'| \\
 &= \frac{1}{2} [\mathbb{1} \otimes_{\mathfrak{g}} \mathbb{1} - Y \otimes_{\mathfrak{g}} Y],
 \end{aligned}$$

where the minus sign in the second term originates from $y = -y^T$. Hence, A^+ acts as a left pseudo-inverse onto the subspace where the tensor is injective. As in the even algebra case, we obtain a left pseudo-inverse $A_2^{(-1)}$ on two sites by combining $A^+ \otimes_{\mathfrak{g}} A^+$ with a parity operator on the internal virtual bond. The latter gives rise to a normal trace, so that we obtain

$$\begin{aligned}
 \mathcal{C}(A_2^{-1} \otimes_{\mathfrak{g}} A_2) &\sim \mathbb{1} \otimes_{\mathfrak{g}} \text{tr}(\mathbb{1}) \otimes_{\mathfrak{g}} \mathbb{1} - Y \otimes_{\mathfrak{g}} \text{tr}(Y) \otimes_{\mathfrak{g}} \mathbb{1} \\
 &\quad - \mathbb{1} \otimes_{\mathfrak{g}} \text{tr}(Y) \otimes_{\mathfrak{g}} Y + Y \otimes_{\mathfrak{g}} \text{tr}(YY) \otimes_{\mathfrak{g}} Y \\
 &\sim \mathbb{1} \otimes_{\mathfrak{g}} \mathbb{1} - Y \otimes_{\mathfrak{g}} Y,
 \end{aligned}$$

i.e. the left inverse property is stable under blocking. The parent Hamiltonian is constructed in the same way as in the even case using the pseudo-inverse A_2^+ . Let us make the explicit exercise for the fermionic MPS representing the Kitaev chain, with tensor $A^i = y^{|\alpha|}$ and thus $B^0 = B^1 = 1$. On a single site, this tensor already satisfies the injectivity condition, so no extra blocking is needed. We obtain $B_2^{00} = B_2^{01} = B_2^{10} = -B_2^{11} = 1$. The pseudo-inverse B_2^+ is constructed using the parts of even and odd $|i| + |j|$ separately, so we obtain $(B_2^+)^{00} = -(B_2^+)^{11} = 1/2$ for the even part and $(B_2^+)^{01} = (B_2^+)^{10} = 1/2$

for the odd part. We then find $(A_2^+)^{00} = -(A_2^+)^{11} = \mathbb{1}/4$ and $(A_2^+)^{01} = (A_2^+)^{10} = y/4$. The projector onto the physical support on two sites is then given by

$$P_2 = \frac{1}{2}(|00\rangle - |11\rangle)(\langle 00| - \langle 11|) + \frac{1}{2}(|01\rangle + |10\rangle)(\langle 01| + \langle 10|)$$

and by rewriting it in terms of creation and annihilation operators, we obtain the projector P_j defined for the Kitaev Hamiltonian in Eq. (1.29), up to a constant.

To prove uniqueness of the ground state, we recycle the intersection and closure property of \mathbb{Z}_2 -injective MPS, as discussed in Ref. [56]. These are proven diagrammatically and are thus equally valid in the fermionic case. The only difference is in the final conclusion. We find again that the most general fermionic tensor that can be used to close the fMPS with periodic boundary conditions is a two-dimensional linear combination, namely of $\mathbb{1}$ and Y . However, when investigating the linear independence of these two closures, the first one turns out to give rise to a zero state, as already discussed in the previous section. So we end up with a unique ground state for the parent Hamiltonian (1.47) corresponding to the closure Y , and thus to a state with odd fermion parity.

Let us now discuss the odd algebra fMPS case in more physical terms. To recapitulate, after evaluating the contraction of the virtual bonds, the odd algebra fMPS takes the form

$$|\psi\rangle = \sum_{\{i_j\}} \text{tr} \left(Y A^{i_1} A^{i_2} \dots A^{i_N} \right) |i_1\rangle |i_2\rangle \dots |i_N\rangle, \quad (1.48)$$

with $Y = y \otimes \mathbb{1}$ and $A^i = y^{|i|} \otimes B^i$. In the bosonic case, the state

$$|\varphi\rangle = \sum_{\{i_j\}} \text{tr} \left(A^{i_1} A^{i_2} \dots A^{i_N} \right) |i_1\rangle |i_2\rangle \dots |i_N\rangle. \quad (1.49)$$

would be another ground state. However, if we close the fMPS with an fermionic identity $\sum_{\alpha} |\alpha\rangle_N \langle \alpha|_1$ and evaluate the virtual contractions, we pick up an additional matrix \mathcal{P} which renders the state zero, as discussed above. Vice versa, we can try to obtain the state $|\varphi\rangle$ as a fermionic state with even fermion parity. This requires that we start from a fermionic tensor network that is closed with an extra $\sum_{\alpha} (-1)^{|\alpha|} |\alpha\rangle_N \langle \alpha|_1$ factor. However, this factor is not in the center and can therefore not be moved to other positions. Indeed, an even fermionic state $|\varphi\rangle$ is not translation invariant (see appendix 1.A) and the position of this factor will be detected by the parent Hamiltonian and cost energy. Hence, $|\varphi\rangle$ is not a ground state of the parent Hamiltonian. We note, however, that $|\varphi\rangle$ is invariant under T_{AP} (see appendix 1.A for the definition of T_{AP}). Hence, $|\varphi\rangle$ would be the ground state of the Hamiltonian obtained after inserting a π -flux. Indeed, Majorana chains on a ring change their ground state parity under insertion of a π -flux, which is the characterizing topological bulk response.

1.6 Entanglement spectrum and Majorana modes

It was shown in Ref. [78] that within the mean-field BCS description of superconductors the presence of Majorana zero modes leads to a two-fold degeneracy in the entanglement spectrum of the ground state wave function. We will use the fMPS description of Majorana chains to show why this remains true beyond the mean-field approximation. We note that the two-fold degeneracy in the entanglement spectrum of interacting Majorana chains was also discussed in Ref. [77]. Let us first define the transfer matrix

$$\mathbb{E}_{(\alpha\gamma)(\beta\delta)} = \sum_i A_{\alpha\beta}^i \bar{A}_{\gamma\delta}^i, \quad (1.50)$$

which is a $D^2 \times D^2$ matrix. It is an important object since it appears in every calculation of expectation values with (f)MPS. Normalization of the (f)MPS implies that the largest eigenvalue of \mathbb{E} has norm one. If the A^i span a simple $D \times D$ matrix algebra, one can show that this largest eigenvalue is unique and that the associated left and right fixed points are positive matrices. Given this fact, one can always perform a gauge transformation such that one of the two fixed points, say the left fixed point, is the identity matrix and the other, right, fixed point a positive diagonal matrix [73, 74]. For an odd algebra fMPS the matrices are of the form $A^i = y^{|i|} \otimes B^i$. Let us first consider

$$\mathbb{E}'_{(\alpha\gamma)(\beta\delta)} = \sum_i B_{\alpha\beta}^i \bar{B}_{\gamma\delta}^i. \quad (1.51)$$

If the odd algebra fMPS is irreducible then we can work in the gauge described above such that the $(D/2)^2 \times (D/2)^2$ matrix \mathbb{E}' has a unique left fixed point given by the identity and a unique right fixed point given by a diagonal positive matrix Λ . The fixed points of the full transfer matrix \mathbb{E} will of course not be unique since $A^i = y^{|i|} \otimes B^i$ do not span a simple matrix algebra. As it turns out, the eigenspace corresponding to eigenvalue 1 is two-dimensional. Using Λ we can easily find two orthogonal right fixed points of \mathbb{E} :

$$R_e = \mathbb{1} \otimes \Lambda \quad (1.52)$$

$$R_o = y \otimes \Lambda. \quad (1.53)$$

Similarly, two orthogonal left fixed points of \mathbb{E} are given by

$$L_e = \mathbb{1} \otimes \mathbb{1} \quad (1.54)$$

$$L_o = y \otimes \mathbb{1}. \quad (1.55)$$

Let us now consider an odd algebra fMPS defined on a chain of length N with open boundaries

$$|\psi\rangle = \sum_{\{i\}} v_L^T A^{i_1} A^{i_2} \dots A^{i_N} v_R |i_1\rangle |i_2\rangle \dots |i_N\rangle, \quad (1.56)$$

where v_L and v_R are two D -dimensional vectors used to close the virtual indices on the boundary. The Hermitian conjugate of $|\psi\rangle$ is given by

$$\langle\psi| = \sum_{\{i\}} \bar{v}_L^T \bar{A}^{i_1} \bar{A}^{i_2} \dots \bar{A}^{i_N} \bar{v}_R \langle i_N | \dots \langle i_2 | \langle i_1 |. \quad (1.57)$$

We will now divide the chain in two, where the first $N/2$ sites are in subsystem A and the $N/2$ sites on the right constitute subsystem B . The reduced density matrix of subsystem A is then defined as³

$$\begin{aligned} \rho_A \equiv & \sum_{i_1 \dots i_{N/2}, i'_1 \dots i'_{N/2}} \left(\sum_{i_{N/2+1} \dots i_N} (v_L^T A^{i_1} \dots A^{i_{N/2}} A^{i_{N/2+1}} \dots A^{i_N} v_R) \right. \\ & \left. (\bar{v}_L^T \bar{A}^{i'_1} \dots \bar{A}^{i'_{N/2}} \bar{A}^{i_{N/2+1}} \dots \bar{A}^{i_N} \bar{v}_R) \right) |i_1\rangle \dots |i_{N/2}\rangle \langle i'_{N/2}| \dots \langle i'_1|. \end{aligned} \quad (1.58)$$

In the expression for ρ_A we recognize $N/2$ times the application of \mathbb{E} to $v_R \otimes \bar{v}_R$. Since v_R has a well-defined fermion parity, $v_R \otimes \bar{v}_R$ is even such that for N going to infinity we get

$$\lim_{N \rightarrow \infty} \sum_{\beta\delta} \left(\mathbb{E}^{N/2} \right)_{(\alpha\gamma)(\beta\delta)} (v_R)_\beta (\bar{v}_R)_\delta = \mathbf{1} \otimes \Lambda = R_e. \quad (1.59)$$

Because we are only interested in this limit we can rewrite the reduced density matrix of subsystem A as

$$\begin{aligned} \rho_A = & \sum_{i_1 \dots i_{N/2}, i'_1 \dots i'_{N/2}} \left(\sum_{\alpha\beta} (v_L^T A^{i_1} \dots A^{i_{N/2}})_\alpha (R_e)_{\alpha\beta} (\bar{v}_L^T \bar{A}^{i'_1} \dots \bar{A}^{i'_{N/2}})_\beta \right) \\ & |i_1\rangle \dots |i_{N/2}\rangle \langle i'_{N/2}| \dots \langle i'_1|. \end{aligned} \quad (1.60)$$

Using the fact that the spectra of AB and BA for two matrices A and B are the same, we see that the eigenvalues of ρ_A are the same as the eigenvalues of the matrix

$$E_{\alpha\beta} = \sum_{\gamma} \left(\sum_{i_1 \dots i_{N/2}} (v_L^T A^{i_1} \dots A^{i_{N/2}})_\gamma (\bar{v}_L^T \bar{A}^{i_1} \dots \bar{A}^{i_{N/2}})_\alpha \right) (R_e)_{\gamma\beta}, \quad (1.61)$$

where we again recognize multiple applications of the transfer matrix. Using

$$\lim_{N \rightarrow \infty} \sum_{\kappa\lambda} (v_L^T)_\kappa (\bar{v}_L^T)_\lambda \left(\mathbb{E}^{N/2} \right)_{(\kappa\lambda)(\gamma\alpha)} = (\mathbf{1} \otimes \mathbf{1})_{\gamma\alpha} = (L_e)_{\gamma\alpha} \quad (1.62)$$

³ ρ_A is a positive matrix obtained from tracing out the degrees of freedom in region B , starting from $|\psi\rangle\langle\psi|$. Note that in this fermionic setting, tracing is not obtained by simply contracting using \mathcal{C} , as the latter gives rise to the supertrace as discussed in Section 1.3. Instead, we first have to apply the corresponding parity operator.

we find that in the large N limit

$$\text{spec}(\rho_A) = \text{spec}(L_e^T R_e). \quad (1.63)$$

Since $L_e^T R_e = \mathbb{1} \otimes \Lambda$, we indeed see that the entanglement spectrum is two-fold degenerate.

1.7 Time reversal symmetry and the \mathbb{Z}_8 classification

In section 1.4.5 we saw that the graded tensor product of two Kitaev chains is non-trivial when time reversal is included because of the appearance of Kramers pairs at the ends of open chains. To recapitulate, we showed that the tensors describing the graded tensor product of the ground states of two Kitaev chains satisfy

$$\bar{A}^{ij} = \mathcal{T}^{-1} A^{ij} \mathcal{T}, \quad (1.64)$$

with $\mathcal{T} = y$ and $\mathcal{P} = z$. This relation will also hold for the tensors describing the ground state of n Kitaev chains, but with different expressions for \mathcal{T} . Just as in the MPS description of symmetry-protected phases in spin chains, we can extract discrete invariants from \mathcal{T} . For an even algebra fMPS these invariants are $\kappa \in \{0, 1\}$ and $\mu \in \{0, 1\}$, defined via

$$\mathcal{T}\bar{\mathcal{T}} = (-1)^\kappa \mathbb{1} \quad (1.65)$$

$$\mathcal{T}\mathcal{P} = (-1)^\mu \mathcal{P}\mathcal{T}. \quad (1.66)$$

The first requirement stems from the fact that time reversal for spinless fermions squares to the identity. Because time reversal is anti-unitary $(-1)^\kappa$ cannot be absorbed in a redefinition of \mathcal{T} . The invariant μ denotes whether \mathcal{T} has even or odd fermion parity. So for $n = 2$ we see that $\kappa = \mu = 1$.

For an odd algebra fMPS we have to define different invariants. Let us for example consider the case $n = 1$, i.e. a single Kitaev chain described by the matrices $A^0 = \mathbb{1}$ and $A^1 = y$. We easily see that

$$\bar{A}^i = A^i, \quad (1.67)$$

so $\mathcal{T} = \mathbb{1}$. However, for an odd algebra fMPS the graded algebra spanned by the A^i has a graded center consisting of multiples of $\mathbb{1}$ and $Y (= y)$. So we could equivalently choose $\mathcal{T} = y$. Since $y^2 = -\mathbb{1}$ this ambiguity makes the invariants as defined for an even algebra fMPS ill-defined for an odd algebra fMPS. However, we can use this ambiguity to always make \mathcal{T} even, i.e. of the two choices for \mathcal{T} given by \mathcal{T}_e and $\mathcal{T}_o = Y\mathcal{T}_e$ we always pick \mathcal{T}_e and then define κ as

$$\mathcal{T}_e \bar{\mathcal{T}}_e = (-1)^\kappa \mathbb{1}. \quad (1.68)$$

To define the μ invariant we note that for the odd algebra fMPS with periodic boundary conditions to be invariant under time reversal it should hold that:

$$\mathcal{T}\bar{Y} = (-1)^\mu Y\mathcal{T}. \quad (1.69)$$

Note that we could change μ by redefining $Y \rightarrow iY$. For this reason equation (1.69) should be considered together with the requirement $Y^2 = -\mathbb{1}$ for μ to be a true invariant. So we see that $\mu = \kappa = 0$ for $n = 1$. The invariants obtained for the even and odd algebra fMPS give rise eight different possibilities, implying that there are eight different spinless superconductors under the protection of time reversal. In the remainder of this section we will study these invariants for the tensors describing the graded tensor product of n copies of the Kitaev chain ground state. In this way we obtain the group structure of time reversal symmetric fMPS under stacking. Let us start with $n = 3$.

$n = 3$

The matrices of the fMPS ground state of 3 copies of the Kitaev chain are

$$\begin{aligned} A &= \mathbb{1} \otimes \mathbb{1} & B &= \mathbb{1} \otimes y & C &= -iz \otimes x & D &= -iz \otimes z \\ E &= y \otimes x & F &= y \otimes z & G &= -ix \otimes \mathbb{1} & H &= -ix \otimes y \end{aligned} \quad (1.70)$$

The extra matrix in the trace expression for the fMPS coefficients (1.24) becomes

$$\mathcal{F}(y \otimes_{\mathfrak{q}} i\mathbb{1}) = ix \otimes y = -H. \quad (1.71)$$

As expected, these matrices span an odd graded algebra because its graded center contains the odd element H . However, these matrices do not take on the standard form $y^{|i|} \otimes A^i$ for an odd graded algebra. To make the odd algebra structure explicit we note that the fMPS coefficients are fully determined by the following properties of the traceless matrices:

$$A^2 = H^2 = \mathbb{1} \quad (1.72)$$

$$B^2 = C^2 = D^2 = E^2 = F^2 = G^2 = -\mathbb{1} \quad (1.73)$$

$$[B, G] = [C, F] = [D, E] = 0 \quad (1.74)$$

$$[A, X] = [H, X] = 0 \quad \forall X \in \{A, B, \dots, H\}, \quad (1.75)$$

and all other elements anti-commuting with each other. We can use a different representation of this algebra by choosing the matrices

$$\begin{aligned} A &= \mathbb{1} \otimes \mathbb{1} & B &= \mathbb{1} \otimes y & C &= \mathbb{1} \otimes iz & D &= \mathbb{1} \otimes ix \\ E &= y \otimes x & F &= y \otimes z & G &= y \otimes iy & H &= y \otimes i\mathbb{1}, \end{aligned} \quad (1.76)$$

which are of the standard form $y^{|i|} \otimes A^i$. Indeed, these representations are related by the following gauge transformation

$$G = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -y \end{bmatrix} \times \left(\mathbb{1} \otimes \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \right).$$

We will not do this step for the other cases below since it is not required to find the invariants associated to time reversal. One can now easily check that the even virtual time reversal action is of the form

$$\mathcal{T}_e = z \otimes y, \quad (1.77)$$

implying that for $n = 3$

$$\mathcal{T}_e \bar{\mathcal{T}}_e = -\mathbb{1} \quad \text{and} \quad \mathcal{T} \bar{Y} = -Y \mathcal{T}, \quad (1.78)$$

with $Y = y \otimes \mathbb{1}$.

$n = 4$

We can obtain the fMPS tensor for the ground state of four copies of the Kitaev chain by taking the graded tensor product of the tensors corresponding to the $n = 2$ case. In this way we find the matrices

$$\begin{array}{cccc} \mathbb{1} \otimes \mathbb{1} & -i\mathbb{1} \otimes z & -iy \otimes y & y \otimes x \\ -iz \otimes z & -z \otimes \mathbb{1} & -x \otimes x & -ix \otimes y \\ -ix \otimes \mathbb{1} & -x \otimes z & -z \otimes y & -iz \otimes x \\ y \otimes z & -iy \otimes \mathbb{1} & -i\mathbb{1} \otimes x & \mathbb{1} \otimes y \end{array} \quad (1.79)$$

These span an even simple graded algebra and the virtual time reversal action is

$$\mathcal{T} = z \otimes y. \quad (1.80)$$

So the invariants are

$$\mathcal{T} \bar{\mathcal{T}} = -\mathbb{1} \quad \text{and} \quad \mathcal{T} \mathcal{P} = \mathcal{P} \mathcal{T} \quad (1.81)$$

$n = 5$

For $n = 5$ we combine the tensors of the $n = 2$ and $n = 3$ case and find following matrices

$$\begin{array}{cccc} \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} & -iy \otimes y \otimes \mathbb{1} & -i\mathbb{1} \otimes z \otimes \mathbb{1} & y \otimes x \otimes \mathbb{1} \\ -iz \otimes z \otimes x & -x \otimes x \otimes x & -z \otimes \mathbb{1} \otimes x & -ix \otimes y \otimes x \\ y \otimes z \otimes x & -i\mathbb{1} \otimes x \otimes x & -iy \otimes \mathbb{1} \otimes x & \mathbb{1} \otimes y \otimes x \\ -ix \otimes \mathbb{1} \otimes \mathbb{1} & -z \otimes y \otimes \mathbb{1} & -x \otimes z \otimes \mathbb{1} & -iz \otimes x \otimes \mathbb{1}, \end{array} \quad (1.82)$$

and all elements obtained by right multiplication with $\mathbb{1} \otimes \mathbb{1} \otimes y$. We thus find that the even virtual symmetry action \mathcal{T}_e and the central odd element Y are given by

$$\mathcal{T}_e = z \otimes y \otimes \mathbb{1} \quad (1.83)$$

$$Y = x \otimes z \otimes y. \quad (1.84)$$

So the invariants are given by

$$\mathcal{T}_e \bar{\mathcal{T}}_e = -\mathbb{1} \quad \text{and} \quad \mathcal{T} \bar{Y} = Y \mathcal{T}. \quad (1.85)$$

$n = 6$

By combining the matrices of $n = 2$ and $n = 4$ we find that the matrices for $n = 6$ are generated by following elements

$$\begin{aligned}
 & -ix \otimes \mathbb{1} \otimes \mathbb{1} & -iz \otimes z \otimes z \\
 & -i\mathbb{1} \otimes \mathbb{1} \otimes z & y \otimes x \otimes \mathbb{1} \\
 & -iy \otimes z \otimes y & i\mathbb{1} \otimes z \otimes \mathbb{1}
 \end{aligned} \tag{1.86}$$

We thus see that the virtual time reversal symmetry action \mathcal{T} is given by

$$\mathcal{T} = y \otimes x \otimes y, \tag{1.87}$$

leading to the invariants

$$\mathcal{T}\bar{\mathcal{T}} = 1 \quad \text{and} \quad \mathcal{T}\mathcal{P} = -\mathcal{P}\mathcal{T}. \tag{1.88}$$

$n = 7$

Taking the graded tensor product of $n = 1$ and $n = 6$ we find that the matrices of the ground state fMPS of seven copies of the Kitaev chain are generated by

$$\begin{aligned}
 & -ix \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} & y \otimes x \otimes \mathbb{1} \otimes \mathbb{1} \\
 & -i\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes z & -iy \otimes z \otimes z \otimes y \\
 & y \otimes z \otimes x \otimes \mathbb{1} & i\mathbb{1} \otimes \mathbb{1} \otimes z \otimes \mathbb{1} \\
 & \mathbb{1} \otimes \mathbb{1} \otimes y \otimes z &
 \end{aligned} \tag{1.89}$$

The even virtual time reversal action and odd central element corresponding to this odd graded simple algebra are

$$\mathcal{T}_e = z \otimes y \otimes x \otimes y \tag{1.90}$$

$$Y = x \otimes y \otimes \mathbb{1} \otimes \mathbb{1}, \tag{1.91}$$

giving the invariants

$$\mathcal{T}_e \bar{\mathcal{T}}_e = \mathbb{1} \quad \text{and} \quad \mathcal{T}_e \bar{Y} = -Y \mathcal{T}_e. \tag{1.92}$$

$n = 8$

For $n = 8$ we find by combining $n = 4$ and $n = 4$ that the fMPS matrices are generated by

$$\begin{aligned}
 & iz \otimes z \otimes \mathbb{1} \otimes z & i\mathbb{1} \otimes z \otimes z \otimes \mathbb{1} \\
 & ix \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} & iy \otimes y \otimes \mathbb{1} \otimes \mathbb{1} \\
 & i\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes z & i\mathbb{1} \otimes \mathbb{1} \otimes z \otimes \mathbb{1} \\
 & iy \otimes z \otimes \mathbb{1} \otimes y & iy \otimes x \otimes y \otimes \mathbb{1}.
 \end{aligned} \tag{1.93}$$

We thus see that

$$\mathcal{T} = z \otimes \mathbb{1} \otimes y \otimes y, \tag{1.94}$$

such that

$$\mathcal{T}\bar{\mathcal{T}} = 1 \quad \text{and} \quad \mathcal{T}\mathcal{P} = \mathcal{P}\mathcal{T}. \tag{1.95}$$

So for $n = 8$ we obtain an even algebra fMPS with $\kappa = \mu = 0$. From this we conclude that taking eight copies of the Kitaev chain ground state results in a trivial time reversal symmetric state, implying that the time reversal invariant one-dimensional spinless superconductors form a \mathbb{Z}_8 group under stacking [64, 66, 77].

In section 1.4.4 we mentioned that any odd algebra fMPS can be gauge transformed into the form $A^i = y^{|i|} \otimes B^i$ and is thus trivially time-reversal invariant ($\mathcal{T}_e = \mathbb{1}$ and thus $\kappa = 0$) if all the matrices B^i are real. The Kitaev fMPS, which has $B^i = 1$, was the simplest starting point to generate the \mathbb{Z}_8 group of time-reversal invariant fMPS by stacking. However, also if B^i is real for $|i| = 0$ and purely imaginary for $|i| = 1$ we obtain a state that is trivially time-reversal invariant. This is most easily observed by writing $A^j = (iy)^{|j|} \otimes C^j$ with all the C^j real and performing a unitary gauge transform $u \otimes \mathbb{1}$ to a different standard form $A^j = x^{|j|} \otimes C^j$ where all the matrices are again completely real. The simplest case is obtained with $C^j = 1$, which would provide an equally simple starting point (i.e. fMPS with $D = 2$) to build the \mathbb{Z}_8 group table. We therefore dub this fMPS the type 2 Majorana chain (and refer to the original Kitaev chain as the type 1 Majorana chain). In this type 2 standard form $A^i = x^{|i|} \otimes C^i$, the odd central element is given by ix , where the imaginary factor is included to have $(ix)^2 = -1$. As mentioned above, this was required in order to obtain μ as an invariant. With $\mathcal{T}_e = \mathbb{1}$, we thus obtain

$$\mathcal{T}_e \bar{\mathcal{T}}_e = \mathbb{1} \quad \text{and} \quad \mathcal{T}(ix) = -ix\mathcal{T}. \quad (1.96)$$

and thus $\kappa = 0$ and $\mu = 1$. We can now do the same steps as for the type 1 (Kitaev) chain and calculate the invariants for n' copies of the type 2 chain. The result of these calculations, together with the invariants for n copies of the Kitaev chain are presented in Table 1.1, where $\epsilon \in \{0, 1\}$ denotes whether n copies of the Kitaev chain ground state correspond to an even or odd algebra fMPS.

The matrices that build up the ground state of n Kitaev chains form a representation of the real Clifford algebra $Cl_{n,0}$. This can easily be seen by explicitly identifying the anti-commuting generators that square to $-\mathbb{1}$, as explicitly denoted in Table 1.2. If we consider n' type 2 chains one can similarly check that the ground state matrices correspond to the real Clifford algebra $Cl_{0,n'}$. Using following relations

$$Cl_{p+1,q+1} \simeq Cl_{p,q} \otimes \mathbb{R}(2) \quad (1.97)$$

$$Cl_{p+8,q} \simeq Cl_{p,q+8} \simeq Cl_{p,q} \otimes \mathbb{R}(16), \quad (1.98)$$

where $\mathbb{R}(n)$ denotes the algebra of real n by n matrices, one can then give an alternative explanation for the mod 8 periodicity under stacking. It also shows the equivalence of $n = 7$ and $n' = 1$.

# Type 1 (Kitaev) chains ($A^1 = y$)	ϵ	κ	μ	# Type 2 chains ($A^1 = x$)
$n = 1$	1	0	0	$n' = 7$
$n = 2$	0	1	1	$n' = 6$
$n = 3$	1	1	1	$n' = 5$
$n = 4$	0	1	0	$n' = 4$
$n = 5$	1	1	0	$n' = 3$
$n = 6$	0	0	1	$n' = 2$
$n = 7$	1	0	1	$n' = 1$
$n = 8$	0	0	0	$n' = 8$

Table 1.1: Invariants for n copies of the type 1 or n' copies of the type 2 Majorana chain. ϵ denotes the simple \mathbb{Z}_2 graded algebra type of the fMPS tensor. κ and μ are related to time reversal.

$n = 1$	y	$Cl_{1,0}$
$n = 2$	iz, ix	$Cl_{2,0}$
$n = 3$	$\mathbb{1} \otimes y, \mathbb{1} \otimes iz, y \otimes x$	$Cl_{3,0}$
$n = 4$	$i\mathbb{1} \otimes z, iy \otimes y, z \otimes y, i\mathbb{1} \otimes x$	$Cl_{4,0}$
$n = 5$	$i\mathbb{1} \otimes z \otimes \mathbb{1}, y \otimes x \otimes \mathbb{1}, \mathbb{1} \otimes y \otimes x$ $iz \otimes x \otimes \mathbb{1}, \mathbb{1} \otimes y \otimes z$	$Cl_{5,0}$
$n = 6$	$iy \otimes z \otimes y, ix \otimes \mathbb{1} \otimes \mathbb{1}, iz \otimes \mathbb{1} \otimes \mathbb{1}$ $y \otimes x \otimes \mathbb{1}, y \otimes z \otimes x, y \otimes z \otimes z$	$Cl_{6,0}$
$n = 7$	$ix \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1}, y \otimes z \otimes x \otimes \mathbb{1}, y \otimes x \otimes \mathbb{1} \otimes \mathbb{1}, iy \otimes z \otimes z \otimes y$ $iz \otimes x \otimes z \otimes z, iz \otimes x \otimes z \otimes z, z \otimes x \otimes y \otimes \mathbb{1}$	$Cl_{7,0}$
$n = 8$	$iy \otimes z \otimes \mathbb{1} \otimes y, iy \otimes x \otimes y \otimes \mathbb{1}, iy \otimes y \otimes \mathbb{1} \otimes \mathbb{1}, ix \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1}$ $y \otimes z \otimes \mathbb{1} \otimes x, y \otimes x \otimes x \otimes \mathbb{1}, y \otimes x \otimes z \otimes \mathbb{1}, y \otimes z \otimes \mathbb{1} \otimes z$	$Cl_{8,0}$

Table 1.2: Anti-commuting generators that square to -1 for n copies of the Kitaev chain, thus providing a representation of the real Clifford algebra $Cl_{n,0}$.

1.8 General on-site symmetries

After having studied time-reversal for spinless fermions in the previous section we will now turn to general on-site symmetries. The goal is to find the invariants and group structure of symmetric phases. For fermionic systems the on-site symmetry group G always contains the central \mathbb{Z}_2 subgroup $\{I, P\}$, where I is the trivial group element and P is fermion parity. We denote the on-site symmetry representation as $U(g)$. Note that $U(g)P = PU(g), \forall g \in G$. Acting with the symmetry on the MPS should leave it invariant, possibly up to a phase. The fundamental theorem of MPS [74, 75, 79] can also be used in the fermionic case and states that two MPS are the same for every length of the lattice on which they are defined iff their tensors are related by a gauge transformation. Concretely, this implies that the invariance of a MPS under a unitary on-site symmetry is translated into the following local tensor relation:

$$\sum_j U(g)_{ij} A^j = e^{i\theta(g)} V(g)^{-1} A^i V(g). \quad (1.99)$$

For an anti-unitary symmetry we get a similar condition:

$$\sum_j U(g)_{ij} \bar{A}^j = e^{i\theta(g)} V(g)^{-1} A^i V(g). \quad (1.100)$$

In appendix 1.B we show that without loss of generality one can assume that $V(g)$ has a well-defined parity, i.e. $\mathcal{P}V(g)\mathcal{P} = \pm V(g)$.

1.8.1 Classification

We start by considering unitary on-site symmetries, and treat the case of even and odd algebra fMPS separately.

Even algebra:

For an even algebra fMPS one can show using similar techniques as in the bosonic case [79] that the virtual symmetry matrices $V(g)$ should satisfy

$$V(g)\mathcal{P} = (-1)^{\mu(g)}\mathcal{P}V(g) \quad (1.101)$$

$$V(g)V(h) = \omega(g, h)V(gh), \quad (1.102)$$

with $\omega(g, h) \in \mathbb{C}$ and $\mu(g) \in \{0, 1\}$ a homomorphism from G to \mathbb{Z}_2 with the restriction that $\mu(P) = 0$. Note that $(-1)^{\mu(g)}$ is incorporated in $\omega(g, h)$ but we treat it on a separate level because it has a distinguished physical meaning, namely, it is the sign picked up by the fMPS with periodic boundary conditions under the symmetry action. Stated otherwise, on a ring with periodic boundary conditions the system transforms according the one-dimensional representation given by $\mu(g)$. It also has a distinct role in the group structure under stacking of phases as we will explain later on.

Associativity of the product of virtual symmetry matrices implies that $\omega(g, h)$ satisfies

$$\omega(g, h)\omega(gh, k) = \omega(g, hk)\omega(h, k), \quad (1.103)$$

which means it is a 2-cocycle. Note that every $V(g)$ is only defined up to a complex number $\beta(g)$, implying that $\omega(g, h)$ has the same ambiguity:

$$\omega(g, h) \rightarrow \omega(g, h) \frac{\beta(g)\beta(h)}{\beta(gh)}, \quad (1.104)$$

where the ratio of betas appearing in the redefinition of ω is called a coboundary. So just as in the bosonic case, symmetric even algebra fMPS are classified by the different classes of $\omega(g, h)$ under the above equivalence relation. Mathematically, these classes are described by the second cohomology group $H^2(G, \mathbb{C}^*)$, or, since $H^2(G, \mathbb{R}^+)$ is trivial, by $H^2(G, U(1))$.

Odd algebra:

In an odd algebra fMPS the parity of $V(g)$ is ambiguous since we can always multiply $V(g)$ by Y , which commutes with all the fMPS tensors. We make use of this freedom to make $V(g) = V_e(g)$ even for all $g \in G$. However, for an odd fMPS with periodic boundary conditions (1.24) to be invariant under the symmetry action we see that $V(g)$ has to commute or anti-commute with Y . This implies following properties of $V(g)$:

$$V(g)Y = (-1)^{\mu(g)}YV(g) \quad (1.105)$$

$$V_e(g)V_e(h) = \omega(g, h)V_e(gh). \quad (1.106)$$

Here, $\mu(g) \in \{0, 1\}$ is again a homomorphism from G to \mathbb{Z}_2 , but this time it is not included in ω and we have $\mu(P) = 1$. It has the same physical meaning as in the even algebra case, i.e. it is the one dimensional representation under which the fMPS with periodic boundary conditions transforms. $\omega(g, h) \in \mathbb{C}$ again has to satisfy equation (2.61) and has the same ambiguity (1.104) under multiplication of $V(g)$ by a complex number.

The fact that $\mu(P) = 1$ has a big implication. Suppose that $g^2 = P$. Then $V_e(g)^2 = \omega(g, g)\mathcal{P}$. But $\mathcal{P}Y = -Y\mathcal{P}$, which is inconsistent with the fact that $V_e(g)$ should commute or anti-commute with Y . In general, we can multiply all group elements with $\mu(g) = -1$ with P . Because P commutes with everything the redefined group elements all have $\mu(g) = 0$ and form a subgroup of G . This implies that $G \simeq \tilde{G} \times \{I, P\}$ [66]. So systems with particle number conservation cannot be written as an odd algebra fMPS, or physically, these systems cannot have Majorana edge modes. We give an alternative proof of this fact, based directly on the algebraic structure of the fMPS tensors, in appendix 1.C. We can also conclude that symmetric odd algebra fMPS are classified by $H^2(\tilde{G}, U(1))$ and $H^1(\tilde{G}, \mathbb{Z}_2)$, where H^1 denotes the homomorphism μ [66].

1.8.2 Anti-unitary symmetries

To incorporate anti-unitary symmetries we now introduce a new homomorphism $\gamma : G \rightarrow \mathbb{Z}_2$, where γ denotes whether g is unitary or anti-unitary. A straightforward generalization shows that the virtual symmetry matrices now have to satisfy

$$V(g)[V(h)]^{\gamma(g)} = \omega(g, h)V(gh), \quad (1.107)$$

where we introduced the notation

$$[X]^{\gamma(g)} = \begin{cases} X & \text{if } \gamma(g) = 0 \\ \bar{X} & \text{if } \gamma(g) = 1 \end{cases}. \quad (1.108)$$

The complex numbers, or, without loss of generality, phases $\omega(g, h)$ have the following property due to associativity

$$\omega(g, h)\omega(gh, k) = \omega(g, hk)[\omega(h, k)]^{\gamma(g)}, \quad (1.109)$$

and are again ambiguous under a redefinition of $V(g)$ with scalars $\beta(g)$:

$$\omega(g, h) \rightarrow \omega(g, h) \frac{\beta(g)[\beta(h)]^{\gamma(g)}}{\beta(gh)}. \quad (1.110)$$

So for non-trivial γ , symmetric fMPS are characterized by the homomorphism $\mu(g)$ and classes of $\omega(g, h)$ satisfying (1.109) under the equivalence relation given in Eq. (1.110). One can show using similar arguments as above that, if $\mu(P) = 1$, then $G \simeq \tilde{G} \times \{I, P\}$ also for non-trivial γ . This implies for example that Majorana edge states also do not appear in systems where $T^2 = P$.

We conclude the classification with a comment on the role of the phase factors $e^{i\theta(g)}$ in equations (1.99, 1.100). These phase factors have to satisfy

$$e^{i\theta(g)} [e^{i\theta(h)}]^{\gamma(g)} = e^{i\theta(gh)}. \quad (1.111)$$

However, they are not stable under a redefinition of the unit cell, i.e. under blocking of n MPS tensors the new phase factors become $e^{in\theta(g)}$. So for quantum phases that do not require strict translational symmetry on the original lattice, which is the case we concentrate on, no additional invariants can be derived from these phase factors.

1.8.3 Group structure

We now look at the group structure of phases protected by on-site symmetries under stacking. We start with the stacking of two even algebra fMPS.

Even - even:

If we take the graded tensor product of two even fMPS, each symmetric under the symmetry group G and with respective virtual symmetry actions

$V_1(g)$ and $V_2(g)$, then the virtual symmetry of the new fMPS is given by $\tilde{V}(g) = V_1(g) \otimes_{\mathfrak{g}} V_2(g)$. If a representative cocycle for $V_1(g)$ is given by $\omega_1(g, h)$ and for $V_2(g)$ by $\omega_2(g, h)$, then we see that multiplication of the new virtual symmetry action is given by

$$\begin{aligned} \tilde{V}(g)[\tilde{V}(h)]^{\gamma(g)} &= (V_1(g) \otimes_{\mathfrak{g}} V_2(g)) \left([V_1(h)]^{\gamma(g)} \otimes_{\mathfrak{g}} [V_2(h)]^{\gamma(g)} \right) \quad (1.112) \\ &= (-1)^{\mu_1(h)\mu_2(g)} \omega_1(g, h) \omega_2(g, h) (V_1(gh) \otimes_{\mathfrak{g}} V_2(gh)) , \quad (1.113) \end{aligned}$$

where $\mu_{1(2)}(g)$ denotes the parity of $V_{1(2)}(g)$. So the symmetry-protected phase of the stacked fMPS is captured by following algebraic data:

$$\tilde{\mu}_{ee}(g) = \mu_1(g) + \mu_2(g) \pmod{2} \quad (1.114)$$

$$\tilde{\omega}_{ee}(g, h) = (-1)^{\mu_1(h)\mu_2(g)} \omega_1(g, h) \omega_2(g, h) . \quad (1.115)$$

Note that this expression is symmetric since $\mu_1(h)\mu_2(g) + \mu_2(h)\mu_1(g) = \mu_1(gh)\mu_2(gh) + \mu_1(g)\mu_2(g) + \mu_1(h)\mu_2(h)$ can be absorbed by a redefinition of the virtual symmetry actions.

Even - odd:

To expose the behaviour of the invariants under stacking of an even and odd algebra fMPS we first note that the virtual symmetry action for an odd algebra fMPS takes the form

$$V_e(g) = \mathbb{1} \otimes V'(g) \quad \text{if} \quad \mu(g) = 0 \quad (1.116)$$

$$V_e(g) = z \otimes V'(g) \quad \text{if} \quad \mu(g) = 1 . \quad (1.117)$$

The virtual symmetry of the stacked fMPS is again the graded tensor product of $V_{1e}(g) = z^{\mu_1(g)} \otimes V'_1(g)$ and $V_2(g)$, corresponding to the odd and even algebra fMPS respectively. This graded tensor product takes on the parity of $V_2(g)$. However, the stacked fMPS is again of odd algebra type so to expose the invariants all virtual symmetry actions should be even. To accomplish this we multiply all $V_{1e}(g) \otimes_{\mathfrak{g}} V_2(g)$ for which $\mu_2(g) = 1$ with $Y \otimes_{\mathfrak{g}} \mathbb{1}$, the odd central element of the tensors of the stacked fMPS. This leads to the following expression for the even virtual symmetry actions of the stacked fMPS:

$$\tilde{V}_e(g) = z^{\mu_1(g)} y^{\mu_2(g)} \otimes V'_1(g) \otimes_{\mathfrak{g}} V_2(g) \quad (1.118)$$

We can now extract the new $\tilde{\mu}$ invariant

$$\begin{aligned} \tilde{V}_e(g)Y &= \left(z^{\mu_1(g)} y^{\mu_2(g)} \otimes V'_1(g) \otimes_{\mathfrak{g}} V_2(g) \right) (y \otimes \mathbb{1} \otimes_{\mathfrak{g}} \mathbb{1}) \\ &= (-1)^{\mu_2(g)} z^{\mu_1(g)} y^{\mu_2(g)} y \otimes V'_1(g) \otimes_{\mathfrak{g}} V_2(g) \\ &= (-1)^{\mu_1(g)+\mu_2(g)} y z^{\mu_1(g)} y^{\mu_2(g)} \otimes V'_1(g) \otimes_{\mathfrak{g}} V_2(g) \\ &= (-1)^{\mu_1(g)+\mu_2(g)} Y \tilde{V}_e(g) \quad (1.119) \end{aligned}$$

In a similar way we can obtain a representative 2-cocycle for the stacked fMPS:

$$\begin{aligned} \tilde{V}_e(g)\tilde{V}_e(h) &= \left(z^{\mu_1(g)} y^{\mu_2(g)} \otimes V'_1(g) \otimes_{\mathfrak{g}} V_2(g) \right) \times \\ &\quad \left(z^{\mu_1(h)} y^{\mu_2(h)} \otimes [V'_1(h)]^{\gamma(g)} \otimes_{\mathfrak{g}} [V_2(h)]^{\gamma(g)} \right) \end{aligned} \quad (1.120)$$

$$\begin{aligned} &= (-1)^{\mu_2(h)\mu_2(g)} z^{\mu_1(g)} y^{\mu_2(g)} z^{\mu_1(h)} y^{\mu_2(h)} \otimes V'_1(g) [V'_1(h)]^{\gamma(g)} \\ &\quad \otimes_{\mathfrak{g}} V'_2(g) [V'_2(h)]^{\gamma(g)} \end{aligned} \quad (1.121)$$

$$\begin{aligned} &= (-1)^{\mu_2(g)(\mu_1(h)+\mu_2(h))} \omega_1(g, h) \omega_2(g, h) \\ &\quad z^{\mu_1(g)+\mu_1(h)} y^{\mu_2(g)+\mu_2(h)} \otimes V'_1(gh) \otimes_{\mathfrak{g}} V'_2(gh) \end{aligned} \quad (1.122)$$

Using the fact that μ_1 and μ_2 are homomorphisms, and that $y^2 = -1$ we find

$$\tilde{V}_e(g)\tilde{V}_e(h) = (-1)^{\mu_2(g)(\mu_1(h)+\mu_2(h))} \omega_1(g, h) \omega_2(g, h) i^{\mu_2(g)+\mu_2(h)-\mu_2(gh)} \quad (1.123)$$

$$z^{\mu_1(gh)} y^{\mu_2(gh)} \otimes V'_1(gh) \otimes_{\mathfrak{g}} V'_2(gh) \quad (1.124)$$

So, putting everything together, we conclude that the stacked odd algebra fMPS has invariants described by the data

$$\tilde{\mu}_{eo}(g) = \mu_e(g) + \mu_o(g) \pmod{2} \quad (1.125)$$

$$\tilde{\omega}_{eo}(g, h) = (-1)^{\mu_e(g)\mu_o(h)} \omega_e(g, h) \omega_o(g, h), \quad (1.126)$$

where we replaced the subscripts 1 and 2 with o and e to denote the odd and even fMPS that are being stacked.

Odd - odd:

Before we derive the behaviour of the invariants in symmetric odd algebra fMPS under stacking we first make a few observations. Since $U(g)P = PU(g)$

we have $U(g) = \begin{pmatrix} U^0(g) & 0 \\ 0 & U^1(g) \end{pmatrix}$ and we can write the local condition for the fMPS to be invariant under the symmetry as

$$\begin{aligned} &\sum_{j:|j|=|i|} \left(U^{|i|}(g) \right)_{ij} \left(y^{|j|} \otimes [B^j]^{\gamma(g)} \right) \\ &= \left(z^{\mu(g)} \otimes V'(g)^{-1} \right) \left(y^{|i|} \otimes B^i \right) \left(z^{\mu(g)} \otimes V'(g) \right) \\ &= (-1)^{|i|\mu(g)} \left(\mathbb{1} \otimes V'(g)^{-1} \right) \left(y^{|i|} \otimes B^i \right) \left(\mathbb{1} \otimes V'(g) \right) \end{aligned} \quad (1.127)$$

From this we see that

$$\sum_{j:|j|=|i|} \left(U^{|i|}(g) \right)_{ij} [B^j]^{\gamma(g)} = (-1)^{|i|\mu(g)} V'(g)^{-1} B^i V'(g) \quad (1.128)$$

In section 1.4.5 we also learned that the fMPS tensors for the stacked state take the form

$$\begin{aligned}
 \tilde{A}^{ij} &= \mathbf{1} \otimes B_1^i \otimes B_2^j && \text{if } |i| = |j| = 0 \\
 \tilde{A}^{ij} &= -ix \otimes B_1^i \otimes B_2^j && \text{if } |i| = 0 \text{ and } |j| = 1 \\
 \tilde{A}^{ij} &= y \otimes B_1^i \otimes B_2^j && \text{if } |i| = 1 \text{ and } |j| = 0 \\
 \tilde{A}^{ij} &= -iz \otimes B_1^i \otimes B_2^j && \text{if } |i| = |j| = 1.
 \end{aligned} \tag{1.129}$$

Combining this expression for the fMPS tensors with equation (1.128) one sees that the virtual symmetry actions of the stacked even algebra fMPS are

$$\tilde{V}(g) = x^{\mu_1(g)} y^{[\mu_2(g) + \gamma(g)]} \otimes V_1'(g) \otimes V_2'(g), \tag{1.130}$$

where $[\cdot] \in \{0, 1\}$ denotes modulo 2. The parity of this matrix is $\mu_1(g) + \mu_2(g) + \gamma(g) \bmod 2$.

Multiplication of these virtual symmetry actions also gives us a representative 2-cocycle and we see that the invariants of the stacked fMPS are described by

$$\tilde{\mu}_{oo}(g) = \mu_1(g) + \mu_2(g) + \gamma(g) \bmod 2 \tag{1.131}$$

$$\begin{aligned}
 \tilde{\omega}_{oo}(g, h) &= (-1)^{\mu_1(h)(\mu_2(g) + \gamma(g))} i^{[\mu_2(g) + \gamma(g)] + [\mu_2(h) + \gamma(h)] - [\mu_2(gh) + \gamma(gh)]} \\
 &\quad \times \omega_1(g, h) \omega_2(g, h)
 \end{aligned} \tag{1.132}$$

We note that this expression at first sight does not look symmetric in μ_1 and μ_2 . However, the symmetry can be understood from the fact that the stacked fMPS tensors of $|\psi\rangle_1 \otimes_{\mathfrak{g}} |\psi\rangle_2$ and $|\psi\rangle_2 \otimes_{\mathfrak{g}} |\psi\rangle_1$ are related by a unitary gauge transformation $U = u \otimes \mathbf{1} \otimes \mathbf{1}$, where u transforms $-ix$ into y and vice versa. The virtual symmetry matrices then transform as $U\tilde{V}(g)U^\dagger$, if $\gamma(g) = 0$ and as $U\tilde{V}(g)U^T$ if $\gamma(g) = 1$, effectively interchanging μ_1 and μ_2 and possibly adding some phase factors to the $\tilde{V}(g)$.

1.9 Reflection symmetry

Up to now we have studied the classification and group structure of on-site unitary and anti-unitary symmetries. In this last section we study a spatial symmetry, namely reflection symmetry. To perform a spatial reflection we need to contract the tensors in a different order. For this we first reorder the left and right virtual modes in a single fMPS tensor, resulting in:

$$\sum_{i\alpha\beta} A_{\alpha\beta}^i |\alpha\rangle |i\rangle \langle \beta| \rightarrow \sum_{i\alpha\beta} A_{\alpha\beta}^i (-1)^{|i||\alpha| + |\beta|} \langle \beta| |i\rangle |\alpha\rangle \tag{1.133}$$

Because the roles of virtual bras and kets are switched, the contraction of the virtual bonds in the fMPS is of the form $\mathcal{C}(|\alpha\rangle \otimes_{\mathfrak{g}} \langle \alpha|)$, i.e. a supertrace,

and an extra factor \mathcal{P} is picked up on every bond. Alternatively, we can interchange the bras and the kets between subsequent fMPS tensors in order to recover normal fMPS tensors where the left virtual mode is a ket and the right virtual mode is a bra. This yields the same sign factor, and we thus obtain:

$$\sum_{i\alpha\beta} A_{\alpha\beta}^i (-1)^{||i||\alpha|} |\beta\rangle |i\rangle \langle \alpha| = \sum_{i\alpha\beta} A_{\beta\alpha}^i (-1)^{||i||\beta|} |\alpha\rangle |i\rangle \langle \beta| \quad (1.134)$$

Apart from this change in contraction order, reflection can additionally involve an onsite unitary U_R , with $U_R P = P U_R$. If the transformed fMPS tensors represents the same state then we know they should be related to the original tensors via a gauge transformation \mathcal{R} . So the local condition for a reflection symmetric fMPS becomes

$$\sum_j (U_R)_{ij} \left(A^j \right)^T \mathcal{P}^{|j|} = \mathcal{R} A^i \mathcal{R}^{-1} \quad (1.135)$$

In the remainder of this section we will study the situation where $U_R^2 = P$. The case $U_R^2 = \mathbb{1}$ can be worked out similarly. If we apply reflection twice then we get following condition:

$$P_{ii} A^i = (-1)^{|i|\mu(R)} \mathcal{P}^{|i|} (\mathcal{R}^{-1 T} \mathcal{R}) A^i (\mathcal{R}^{-1} \mathcal{R}^T) \mathcal{P}^{|i|}, \quad (1.136)$$

where $\mu(R) \in \{0, 1\}$ denotes the parity of \mathcal{R} , i.e. $\mathcal{R} \mathcal{P} = (-1)^{\mu(R)} \mathcal{P} \mathcal{R}$. Using $P_{ii} = (-1)^{|i|}$ and $\mathcal{P}^{|i|} A^i \mathcal{P}^{|i|} = \mathcal{P} A^i \mathcal{P} = (-1)^{|i|} A^i$, Eq. (1.136) can be rewritten as

$$P_{ii}^{\mu(R)} A^i = (\mathcal{R}^{-1 T} \mathcal{R}) A^i (\mathcal{R}^{-1} \mathcal{R}^T). \quad (1.137)$$

1.9.1 Classification

To extract the discrete invariants that label different reflection symmetric phases we again consider the cases of even and odd graded algebras separately.

Even algebra:

If $\mu(R) = 0$ then we see from equation (1.137) that

$$\mathcal{R} = \alpha \mathcal{R}^T, \quad (1.138)$$

with $\alpha \in \mathbb{C}$. However, by taking the transpose of this expression one learns that $\alpha^2 = 1$. So we obtain the invariant $\rho \in \{0, 1\}$, which denotes whether \mathcal{R} is symmetric or anti-symmetric:

$$\mathcal{R} = (-1)^\rho \mathcal{R}^T. \quad (1.139)$$

If $\mu(R) = 1$ then equation (1.137) implies that

$$\mathcal{R} = \alpha \mathcal{R}^T \mathcal{P}. \quad (1.140)$$

Again taking the transpose of this expression we can obtain a similar condition on \mathcal{R} :

$$\mathcal{R} = -\alpha^{-1} \mathcal{R}^T \mathcal{P}. \quad (1.141)$$

So for $\mu(R) = 1$ the invariant ρ carries the following information about \mathcal{R} :

$$\mathcal{R} = (-1)^\rho i \mathcal{R}^T \mathcal{P}. \quad (1.142)$$

In total we thus obtain four possible reflection symmetric phases in even algebra fMPS, labeled by the invariants $\mu(R)$ and ρ .

Odd algebra:

For an odd algebra fMPS we can choose $\mathcal{R} \equiv \mathcal{R}_e$ in equation (1.135) to be even, i.e. $\mu(R) = 0$. Just as in the even algebra case this gives rise to an invariant $\rho_1 \in \{0, 1\}$:

$$\mathcal{R}_e = (-1)^{\rho_1} \mathcal{R}_e^T. \quad (1.143)$$

However, $\mathcal{R}_o \equiv \mathcal{R}_e Y$ can also serve as \mathcal{R} in equation (1.135). Because \mathcal{R}_o is odd, we can define a second invariant $\rho_2 \in \{0, 1\}$ by doing the same steps as in the even algebra case above:

$$\mathcal{R}_o = (-1)^{\rho_2} i \mathcal{R}_o^T \mathcal{P} \quad (1.144)$$

One can check that the conditions on \mathcal{R}_e and \mathcal{R}_o are independent and imply that \mathcal{R}_e is of the form

$$\mathcal{R}_e = \begin{pmatrix} (-1)^{\rho_1 + \rho_2} & 0 \\ 0 & 1 \end{pmatrix} \otimes \mathcal{R}' \quad \text{with} \quad \mathcal{R}'^T = (-1)^{\rho_1} \mathcal{R}'. \quad (1.145)$$

We thus again obtain four possibilities labeled by ρ_1 and ρ_2 , leading to a total of 8 different reflection symmetric phases. Note that \mathcal{R}_e does not commute or anti-commute with Y . This is also not required because reflection symmetry cannot be defined on a chain with periodic boundary conditions. If we would have used a different convention to define the odd gauge transformation, i.e. $\mathcal{R}'_o \equiv Y \mathcal{R}_e$, then we would obtain an equivalent invariant ρ'_2 , which is related to ρ_2 via $\rho'_2 = \rho_2 + 1 \pmod{2}$.

1.9.2 Partial reflection

To expose the group structure of the eight reflection symmetric phases we will use a different approach than in section 1.8. It was argued in Refs. [26, 65, 80–84] that the phase of the partition function of reflection symmetric phases on an unorientable spacetime is an invariant. It was shown in Refs. [71, 72] that this invariant phase on $\mathbb{R}P^2$ can be obtained from the ground state wave function. The approach is similar to the bosonic case [85, 86], and is based on the calculation of the ground state expectation value of a non-local operator R_{part} , called partial reflection.

We focus on the Kitaev chain described by Hamiltonian (1.26). This Hamiltonian has reflection symmetry given by

$$a_j \rightarrow ia_{-j} \quad (1.146)$$

So we see that

$$U_R = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}, \quad (1.147)$$

and $U_R^2 = P$. The MPS tensors of the Kitaev chain ground state satisfy Eq. (1.135), with

$$\mathcal{R} \equiv \mathcal{R}_e = \begin{pmatrix} e^{i\pi/4} & 0 \\ 0 & e^{-i\pi/4} \end{pmatrix} \quad (1.148)$$

To define the partial reflection operator we divide up the chain with periodic boundary conditions into two connected intervals I_1 and I_2 of length N_1 and N_2 . Partial reflection then acts as normal reflection, but only on one of the two intervals, which we take to be I_1 .

To apply R_{part} in the fMPS formalism we first perform step (1.133) and (1.134) on the MPS tensors in I_1 , together with the on-site unitary U_R . Note that we can only interchange virtual kets and bras between subsequent tensors [i.e. Eq. (1.134)] in the bulk of I_1 but not at the end points. Using Eq. (1.135) this gives the following concatenated tensor corresponding to I_1 :

$$\sum_{i_1, \dots, i_{N_1}} \left(\mathcal{R}_e A^{i_{N_1}} \dots A^{i_1} \mathcal{R}_e^{-1} \right)_{\alpha\beta} (-1)^{|\alpha|} (\alpha | i_{N_1} \rangle \dots | i_1 \rangle | \beta \rangle. \quad (1.149)$$

For I_2 we have the usual concatenated tensor

$$\sum_{i_{N_1+1}, \dots, i_{N_1+N_2}} \left(A^{i_{N_1+1}} \dots A^{i_{N_1+N_2}} y \right)_{\alpha\beta} |\alpha\rangle |i_{N_1+1}\rangle \dots |i_{N_1+N_2}\rangle \langle\beta|. \quad (1.150)$$

To obtain the total wavefunction we have to contract the virtual α and β indices. The final expression for $R_{\text{part}}|\psi\rangle$ is then

$$R_{\text{part}}|\psi\rangle = \sum_{i_1 \dots i_{N_1+N_2}} \sum_{\alpha\beta} \left(\mathcal{R}_e A^{i_{N_1}} \dots A^{i_1} \mathcal{R}_e^{-1} \right)_{\alpha\beta} \left(A^{i_{N_1+1}} \dots A^{i_{N_1+N_2}} y \right)_{\alpha\beta} (-1)^{|\beta|(|\alpha|+|\beta|)} |i_{N_1}\rangle \dots |i_1\rangle |i_{N_1+1}\rangle \dots |i_{N_1+N_2}\rangle \quad (1.151)$$

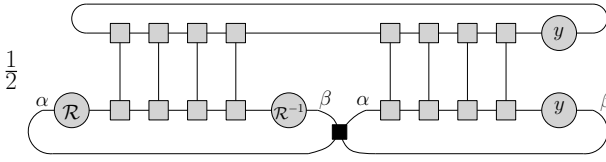
To calculate the expectation value we note that $\langle\psi|$ is given by

$$\langle\psi| = \sum_{i_1 \dots i_{N_1+N_2}} \text{tr} \left(\bar{A}^{i_{N_1}} \dots \bar{A}^{i_1} \bar{A}^{i_{N_1+1}} \dots \bar{A}^{i_{N_1+N_2}} y \right) \langle i_{N_1+N_2} | \dots \langle i_{N_1+1} | \langle i_1 | \dots \langle i_{N_1} | \quad (1.152)$$

We introduce following graphical notation for the transfer matrix (note that without arrows, the graphical notation denotes the tensor components):

$$\begin{array}{c} \alpha \\ \square \\ | \\ i \\ \square \\ \gamma \end{array} \begin{array}{c} \beta \\ \\ \\ \\ \delta \end{array} = \sum_i A_{\gamma\delta}^i \bar{A}_{\alpha\beta}^i = \frac{1}{2} (\mathbb{1}_{\gamma\delta} \mathbb{1}_{\alpha\beta} + y_{\gamma\delta} y_{\alpha\beta}) \quad , \quad (1.153)$$

where the normalization factor $1/2$ has been inserted to ensure that the transfer matrix is a projector (which is the fMPS manifestation of the fixed point character of the model). With this notation we can represent $\langle \psi | R_{part} | \psi \rangle$ as



$$\frac{1}{2} \quad (1.154)$$

The global factor $1/2$ comes from the normalization of $|\psi\rangle$ and the black square denotes the non-local sign $(-1)^{|\beta|(|\alpha|+|\beta|)}$. Putting everything together we easily obtain following result

$$\begin{aligned} \langle \psi | R_{part} | \psi \rangle &= \frac{1}{8} \left(\text{tr}(yy) \text{tr}(\mathcal{R} \mathcal{R}^{-1} y^T y^T) + \text{tr}(yy) \text{tr}(\mathcal{R} y \mathcal{R}^{-1} z y^T) \right) \\ &= \frac{1+i}{2} = \frac{e^{i\pi/4}}{\sqrt{2}} . \end{aligned} \quad (1.155)$$

This agrees with the previous studies of reflection symmetric phases on $\mathbb{R}P^2$. We see that in order to obtain a trivial phase factor one needs eight copies of the Majorana chain, which shows that reflection symmetric phases in one spatial dimension form a \mathbb{Z}_8 group.

1.10 Discussion

We have shown that the formalism of fermionic matrix product states captures all phases of interacting fermions in one dimension, both for general on-site and spatial symmetries. All universal information about the quantum phase, including the presence or absence of Majorana zero modes, can be extracted in a local fashion from the tensor building up the ground state wave function. This local encoding of the information allows for a straightforward analysis of the group structure of symmetric phases under stacking. An advantage of the framework is that it provides a physical interpretation for the invariants labeling the different phases, both in terms of the entanglement spectrum and quantum numbers of the ground state without or with a background gauge field. The latter case can be studied analogously to the

bosonic case [87].

Fermionic tensor network states, and particularly fermionic MPOs, can also be used to describe topological phases in higher dimensions [54, 61–63, 88–95]. In this way the observations made in this work should be relevant for a systematic understanding of how universal topological properties of two and three-dimensional systems, such as the binding of Majorana modes to symmetry defects, are connected to the entanglement structure of the ground state wave function. We hope that this work may pave the way to a more detailed understanding of higher dimensional topological fermionic tensor networks.

1.A Translation symmetry for fermionic systems

At the single particle level, the translation operator T_P with periodic boundary conditions is defined as

$$T_P a_j T_P^{-1} = a_{j+1} \quad (1.156)$$

Translation with a π -flux inserted through the system, or equivalently, with anti-periodic boundary conditions is defined as

$$T_{AP} a_j T_{AP}^{-1} = a_{j+1} \quad \text{for } j \neq N \quad (1.157)$$

$$T_{AP} a_N T_{AP}^{-1} = -a_1, \quad (1.158)$$

where N is the number of sites in the system. One obviously has

$$T_P^N = \mathbb{1} \quad (1.159)$$

$$T_{AP}^N = -\mathbb{1}, \quad (1.160)$$

so the eigenvalues e^{ik} of T_P have momenta $k = \frac{2\pi}{N}n$ with $n \in \{0, 1, \dots, N-1\}$ while those of T_{AP} have momenta $k = \frac{\pi}{N}(2n+1)$ with $n \in \{0, 1, \dots, N-1\}$. We would now like to implement T_P and T_{AP} on states in the fermionic many-body Hilbert space. We start with a general even state $|\psi_e\rangle$:

$$|\psi\rangle_e = \sum_{\{i\}=0}^1 \psi_{i_1 i_2 \dots i_N}^e |i_1\rangle_1 |i_2\rangle_2 \dots |i_N\rangle_N \in \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N, \quad (1.161)$$

where $\sum_{j=1}^N |i_j| = 0 \pmod{2}$. Applying T_P on $|\psi\rangle_e$ gives following state:

$$T_P |\psi\rangle_e = \sum_{\{i\}=0}^1 \psi_{i_1 i_2 \dots i_N}^e |i_1\rangle_2 |i_2\rangle_3 \dots |i_N\rangle_1 \in \mathcal{H}_2 \otimes \mathcal{H}_3 \otimes \dots \otimes \mathcal{H}_1 \quad (1.162)$$

To compare $T_P|\psi\rangle_e$ with $|\psi\rangle_e$ with need to use the fermionic tensor product isomorphism to map the translated state into the same Hilbert space as the original state. Using the fact that $\sum_{j=1}^{N-1} |i_j| = |i_N| \pmod 2$ we find

$$\begin{aligned} \mathcal{F}(T_P|\psi\rangle_e) &= \sum_{\{i\}=0}^1 \psi_{i_1 i_2 \dots i_N}^e (-1)^{|i_N|} |i_N\rangle_1 |i_1\rangle_2 \dots |i_{N-1}\rangle_N \\ &\quad \in \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N \\ &= \sum_{\{i\}=0}^1 \psi_{i_2 i_3 \dots i_1}^e (-1)^{|i_1|} |i_1\rangle_1 |i_2\rangle_2 \dots |i_N\rangle_N \end{aligned} \quad (1.163)$$

So the condition that $|\psi\rangle_e$ is an eigenstate of T_P becomes

$$\mathcal{F}(T_P|\psi\rangle_e) = e^{ik} |\psi\rangle_e \Rightarrow \psi_{i_1 i_2 \dots i_N}^e = e^{-ik} \psi_{i_2 i_3 \dots i_1}^e (-1)^{|i_1|} \quad (1.164)$$

Similarly, one can check that the condition for $|\psi\rangle_e$ to be an eigenstate of T_{AP} is

$$\mathcal{F}(T_{AP}|\psi\rangle_e) = e^{ik} |\psi\rangle_e \Rightarrow \psi_{i_1 i_2 \dots i_N}^e = e^{-ik} \psi_{i_2 i_3 \dots i_1}^e \quad (1.165)$$

For odd states $|\psi\rangle_o$, i.e. states with $\sum_{j=1}^N |i_j| = 1 \pmod 2$, we find

$$\mathcal{F}(T_P|\psi\rangle_o) = e^{ik} |\psi\rangle_o \Rightarrow \psi_{i_1 i_2 \dots i_N}^o = e^{-ik} \psi_{i_2 i_3 \dots i_1}^o \quad (1.166)$$

$$\mathcal{F}(T_{AP}|\psi\rangle_o) = e^{ik} |\psi\rangle_o \Rightarrow \psi_{i_1 i_2 \dots i_N}^o = e^{-ik} \psi_{i_2 i_3 \dots i_1}^o (-1)^{|i_1|} \quad (1.167)$$

We close this appendix by noting that for the classification of topological phases we consider in the main text, strict translational symmetry is not required. However, if one was to incorporate translational symmetry in the classification the number of phases would (at least) double because the fMPS tensors can be even or odd. We always assumed the fMPS tensors to be even, which can be done by a redefinition of the unit cell and blocking two tensors.

1.B Parity of gauge transformations

Gauge transformations correspond to different choices of basis in the virtual spaces of the tensor network. For fermionic tensor networks where the virtual spaces also have a \mathbb{Z}_2 grading, it is only sensible to work with a basis where the grading is explicit, and thus where \mathcal{P} takes the standard form $\mathbb{1}_{D_e} \oplus -\mathbb{1}_{D_o}$ before and after the transformation. In particular, we require that A^i and its gauge transformed version $A'^i = M A^i M^{-1}$ are even tensors with respect to the same \mathcal{P} , so we have that

$$\mathcal{P} M A^i M^{-1} \mathcal{P} = M \mathcal{P} A^i \mathcal{P} M^{-1} \quad (1.168)$$

This relation implies that

$$\mathcal{P}M = M\mathcal{P}X^{-1}, \quad (1.169)$$

where X is an invertible matrix in the center of the algebra spanned by the tensors A^i .

If the graded algebra is of even type this implies that

$$\mathcal{P}M = \pm M\mathcal{P}, \quad (1.170)$$

so the gauge transformation M has a well-defined parity. Note that an odd invertible matrix M (which interchanges the even and the odd basis vectors of the virtual space) can only exist if $D_e = D_o$.

If A^i span an odd algebra then we have

$$\mathcal{P}M = M\mathcal{P}(\alpha\mathbb{1} + \beta Y)^{-1}, \quad (1.171)$$

with $\alpha \neq \pm i\beta$. We split up M into its even and odd part, $M = M_e + M_o$, and obtain from the equation above

$$(1 - \alpha)M_e = +\beta M_o Y \quad (1.172)$$

$$(1 + \alpha)M_o = -\beta M_e Y \quad (1.173)$$

We first consider some special cases. If $\alpha = 1$, then the above equations imply that $\beta = 0$ and $M_o = 0$. If $\alpha = -1$, then $\beta = 0$ and $M_e = 0$. So in both cases M has a well-defined parity. We exclude $\alpha = \pm 1$ and $\beta = 0$ in the following steps. From equations (1.172) and (1.173) we find that

$$M_e = \frac{\beta}{1 - \alpha} M_o Y = \frac{1 + \alpha}{\beta} M_o Y, \quad (1.174)$$

which implies that $\alpha^2 + \beta^2 = 1$. We can now write M as

$$M = M_o \left(\mathbb{1} \pm \sqrt{\frac{1 + \alpha}{1 - \alpha}} Y \right) \equiv M_o X, \quad (1.175)$$

where X is invertible. Because X is in the center of the odd algebra spanned by A^i , the gauge transformation M_o also relates $A^{i'}$ to A^i :

$$A^{i'} = M_o A^i M_o^{-1}. \quad (1.176)$$

This shows that also in the case where A^i span an odd algebra we can without loss of generality restrict to gauge transformations that have a well-defined parity.

1.C Majorana modes and superconductivity

In this appendix we show that the structure of the tensors in an odd algebra fMPS is incompatible with a $U(1)$ charge conservation symmetry. This implies that Majorana edge modes can only appear in superconductors. The local condition for the fMPS to be symmetric under the global $U(1)$ symmetry is

$$\sum_j U(\theta)_{ij} A^j = e^{ip\theta} V(\theta) A^i V(\theta)^\dagger, \quad (1.177)$$

with $p \in \mathbb{Z}$. We also assume that the fMPS is irreducible. If we write $U(\theta) = \exp(iq\theta)$ and $V(\theta) = \exp(iQ\theta)$ and take the derivative of the above equation with respect to θ evaluated at $\theta = 0$, then we get

$$\sum_j (q - p\mathbb{1})_{ij} A^j = [Q, A^i]. \quad (1.178)$$

We continue to work in the basis for the local physical Hilbert space in which q is diagonal. Because $U(1)$ corresponds to charge conservation, q is of the form

$$q = \begin{pmatrix} e_1 & & & & \\ & \ddots & & & \\ & & e_r & & \\ & & & o_1 & \\ & & & & \ddots & \\ & & & & & o_s \end{pmatrix} \quad \text{with } r + s = d, \quad (1.179)$$

where d is the dimension of the local Hilbert space and e_i , the eigenvalues of states with even fermion parity, are even integers, while o_i are odd integers corresponding to eigenstates with odd fermion parity. Without loss of generality, we take Q to be an even matrix:

$$Q = \begin{pmatrix} Q_1 & 0 \\ 0 & Q_2 \end{pmatrix} \quad (1.180)$$

We recall that the tensors of an odd algebra fMPS take the form

$$\begin{pmatrix} B^i & 0 \\ 0 & B^i \end{pmatrix} \quad \text{if } |i| = 0 \quad (1.181)$$

$$\begin{pmatrix} 0 & C^i \\ -C^i & 0 \end{pmatrix} \quad \text{if } |i| = 1 \quad (1.182)$$

From this we see that equation (1.178) is equivalent to

$$\begin{aligned} [Q_1, B^i] &= [Q_2, B^i] = (e_i - p)B^i \\ \{Q_1, C^i\} &= \{Q_2, C^i\} \\ Q_1 C^i - C^i Q_2 &= (o_i - p)C^i, \end{aligned} \quad (1.183)$$

which implies that $[Q_1 - Q_2, B^i] = \{Q_1 - Q_2, C^i\} = 0$. However, because of the irreducibility of the fMPS we know that products of B^i and C^i span a full $D/2 \times D/2$ matrix algebra, where D is the bond dimension of the fMPS. This allows us to conclude that $Q_1 = Q_2$. Therefore, equations (1.183) reduce to

$$\begin{aligned} [Q_1, B^i] &= (e_i - p)B^i \\ [Q_1, C^i] &= (o_i - p)C^i \end{aligned} \quad (1.184)$$

We now work in the basis in which Q_1 takes following diagonal form

$$Q_1 = \begin{pmatrix} \lambda_{e_1} & & & & & \\ & \ddots & & & & \\ & & \lambda_{e_t} & & & \\ & & & \lambda_{o_1} & & \\ & & & & \ddots & \\ & & & & & \lambda_{o_u} \end{pmatrix} \quad \text{with } t + u = D/2, \quad (1.185)$$

where $\lambda_{e_i} \in 2\mathbb{Z}$ and $\lambda_{o_i} \in 2\mathbb{Z} + 1$. In this basis, equations (1.184) can be written as

$$(\lambda_j - \lambda_k)B_{jk}^i = (e_i - p)B_{jk}^i \quad (1.186)$$

$$(\lambda_j - \lambda_k)C_{jk}^i = (o_i - p)C_{jk}^i \quad (1.187)$$

If p is even, this implies that the B^i are block diagonal and the C^i are block off-diagonal. If p is odd, then the B^i are block off-diagonal and the C^i are block diagonal. The situations with p odd and p even clearly become equivalent after blocking two tensors. However, this structure of the B^i and C^i is in contradiction with the irreducibility of the fMPS, which requires the even subalgebra spanned by the fMPS matrices to be simple (see section 1.4.4). If the fMPS were not irreducible we could write it as a sum of multiple irreducible fMPS, each of which should have $U(1)$ charge symmetry (because $U(1)$ is continuous and connected it cannot permute the different irreducible fMPS), thus again leading to a contradiction. This shows that fMPS with an odd algebra structure cannot have charge conservation. Since fMPS represent the ground state of gapped local Hamiltonians, this does not exclude the possibility of having Majorana edge modes in gapless systems with particle number conservation. Indeed, explicit examples of such systems have been constructed in the literature [96–99].

Matrix product operators for symmetry protected-topological phases

Synopsis

Projected entangled pair states (PEPS) provide a natural description of the ground states of gapped, local Hamiltonians in which global characteristics of a quantum state are encoded in properties of local tensors. We show that on-site symmetries, as occurring in systems exhibiting symmetry-protected topological (SPT) quantum order, can be captured by a virtual symmetry of the tensors expressed as a set of matrix product operators labelled by the different group elements. A classification of SPT phases can hence be obtained by studying the topological obstructions to continuously deforming one set of matrix product operators into another. This leads to the classification of bosonic SPT states in terms of group cohomology, as originally derived by Chen et al. [24]. Our formalism accommodates perturbations away from fixed point models, and hence opens up the possibility of studying phase transitions between different SPT phases. We furthermore show how the global symmetries of SPT PEPS can be promoted into a set of local gauge constraints by introducing bosonic degrees of freedom on the links of the PEPS lattice, thereby providing a natural and general mapping between PEPS in SPT phases and topologically ordered phases.

Based on

‘Matrix product operators for symmetry-protected topological phases: gauging and edge theories’

D. Williamson, N. Bultinck, M. Mariën, M. Sahinoglu, J. Haegemand and F. Verstraete

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Contributions of the author: The author has contributed to both the main conceptual formalism developed in this work and also many of the technical calculations. However, the results in appendices 2.B, 2.F, 2.G, 2.G, 2.H and 2.I, are mainly due to collaborating authors.

2.1 Introduction

The phase diagrams of quantum many-body systems become much richer when global symmetries are imposed. It has become clear of late that in the presence of a global symmetry there exist distinct phases which cannot be distinguished via local order parameters. These phases are referred to as *symmetry-protected topological* (SPT) phases [24]. In contrast to topologically ordered systems [100], all SPT phases become trivial if the symmetry is allowed to be explicitly broken. While this implies that SPT ground states possess only short-range entanglement, they cannot be adiabatically connected to a product state without breaking the symmetry. Furthermore they exhibit interesting edge properties when defined on a finite system with nontrivial boundary.

In recent years there has been a growing interplay between the theory of quantum many-body systems and quantum information. This has led to the development of tensor network ansatz for the ground states of local, gapped Hamiltonians [34, 101–103]. Tensor network methods have proven particularly useful in understanding the emergence of topological phenomena in quantum many-body ground states. In one dimension, Matrix Product States were used to completely classify SPT phases via the second cohomology group of their symmetry group [43, 104, 105]. In two dimensions, Projected-Entangled Pair States (PEPS) have been used to characterize systems with intrinsic topological order [106–110], symmetry-protected topological order [111] and chiral topological insulators [112–114].

The first goal of this work is to present a general framework for the description of on-site symmetries within the PEPS formalism. The framework includes symmetry actions on states with topological order and thus provides a natural setting for the study of symmetry-enriched topological phases [115–124] with PEPS [125]. We then restrict to PEPS without topological order and provide a complete characterization of bosonic SPT order by formulating sufficient conditions to be satisfied by the individual PEPS tensors. Previously some powerful results for renormalization group (RG) fixed-point states with SPT order were presented by Chen *et al.* [24, 111], the present work extends these results to systems with a finite correlation length. Furthermore, application of the quantum state gauging procedure of Ref. [51] within the framework presented here illuminates the correspondence between SPT phases and certain topologically ordered phases in the language of PEPS, providing a complementary description to the Hamiltonian gauging construction of Levin and Gu [126]. This naturally brings together the

classification of SPT phases via fixed point models, gauging and anomalous boundary symmetries into a single unified approach that focuses only on MPOs which are properties of the ground states alone.

To achieve these goals we have developed tools to deal with orientation dependent MPO tensors. These tools allow us to calculate the symmetry action on monodromy defected and symmetry twisted states and also modular transformations, pre- and post- gauging, in a local way that is governed by a single tensor.

We first outline the general formalism for characterizing gapped phases in PEPS using matrix product operators (MPOs) in Section 2.2. Section 2.3 presents a set of local conditions that lead to a large class of PEPS with global symmetries which fit within the general formalism. Next, in Section 2.4, we identify a class of short-range entangled PEPS and discuss how SPT order manifests itself in these models via their anomalous edge physics. Section 2.5 explains how gauging a SPT PEPS with a discrete symmetry group yields a long-range entangled PEPS with topological order. In Section 2.6 we study symmetry twists and monodromy defects of SPT PEPS. These concepts are then illustrated with a family of examples that fall within the framework of SPT PEPS in Section 2.7. We show explicitly that gauging these states yields ground states of the twisted quantum double models [127, 128], which are the Hamiltonian formulations of Dijkgraaf-Witten discrete gauge theories [129, 130].

The appendices are organized into sections that review relevant background and others that provide technical details of novel results which are used throughout the paper. We first review the relevant properties of MPO-injective PEPS in Appendix 2.A, provide a novel argument that a MPO-injective PEPS with a single block projection MPO is the unique ground state of its parent Hamiltonian in Appendix 2.B and review the definition of the third cohomology of a single block MPO group representation in Appendix 2.C. In Appendix 2.D we present new results concerning possible orientation dependencies of MPO group representations. In Appendix 2.E we discuss different crossing tensors, their composition and the effect of modular transformations. Appendix 2.F contains a brief review of the quantum state gauging formalism and a novel proof that a gauged SPT PEPS is MPO-injective [109]. In Appendix 2.G we present an extension of the quantum state gauging procedure of Ref.[51] to arbitrary flat G-connections and use it to prove that the gauging procedure is gap preserving for arbitrary topologies and to furthermore construct the full topological ground space of a gauged SPT model. In Appendix 2.H we develop a novel description of symmetry twisted states, topological ground states and monodromy defected states in terms of MPOs and calculate their transformation under the residual symmetry group. Finally in Appendix 2.I we demonstrate that the quantum state gauging procedure for finite groups is equivalent to the standard minimal coupling scheme for gauging Hamiltonians.

2.2 Characterizing topological phases with matrix product operators

In this section we present a general framework for the classification of gapped phases with PEPS in terms of universal and discrete labels that arise directly from tensor network states. These discrete labels emerge from the set of MPO symmetries of the PEPS tensors and should remain invariant under continuous deformation of the MPOs.

A 2D PEPS can be defined on any directed graph Λ (most commonly a regular lattice) embedded in an oriented 2D manifold \mathcal{M} given a tensor

$$A_v := \sum_{i_v=1}^d \sum_{\{i_e\}_{e \in E_v}}^D (A_v)_{\{i_e\}}^{i_v} |i_v\rangle \bigotimes_{e \in E_v} (i_e|$$

for every vertex $v \in \Lambda$, where E_v is the set of edges with v as an endpoint, see Fig.2.1. Here i_v is the physical index running over a basis for the Hilbert space of a single site \mathbb{C}^d and each i_e is a virtual index of dimension D along an edge e adjacent to v in the graph Λ .

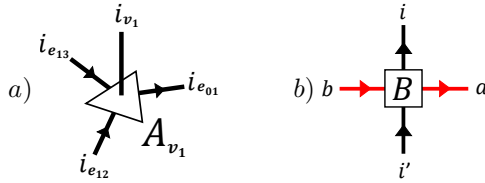


Figure 2.1: a) A PEPS tensor on a trivalent vertex. b) A right handed MPO tensor.

For any simply connected region $\mathcal{R} \subset \mathcal{M}$ whose boundary $\partial\mathcal{R}$ forms a contractible closed path in the dual graph Λ^* we define the PEPS map

$$A_{\mathcal{R}} : (\mathbb{C}^D)^{\otimes |\partial\mathcal{R}|_e} \rightarrow (\mathbb{C}^d)^{\otimes |\mathcal{R}|_v},$$

from $|\partial\mathcal{R}|_e$ virtual indices on the edges that cross $\partial\mathcal{R}$ to $|\mathcal{R}|_v$ physical indices on the vertices in \mathcal{R} , by taking the set of tensors $\{A_v | v \in \mathcal{R}\}$ and contracting each pair of indices that are assigned to an edge within \mathcal{R} , to yield

$$A_{\mathcal{R}} := \sum_{\{i_v\}_{v \in \mathcal{R}}} \sum_{\{i_e\}_{e \in \overline{\mathcal{R}}}} \bigotimes_{v \in \mathcal{R}} (A_v)_{\{i_e\}_{e \in E_v}}^{i_v} \bigotimes_{v \in \mathcal{R}} |i_v\rangle \bigotimes_{e \in \partial\mathcal{R}} (i_e|$$

where $\overline{\mathcal{R}} := \mathcal{R} \cup \partial\mathcal{R}$, see Fig.2.2.

Universal properties of the phase of matter containing the PEPS wave function are manifest in the local symmetries of $A_{\mathcal{R}}$. The specific symmetries we consider are of the form $U^{\otimes |\mathcal{R}|_v} A_{\mathcal{R}} = A_{\mathcal{R}} O^{\partial\mathcal{R}}$, where U is an on-site

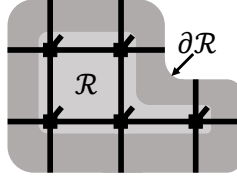


Figure 2.2: The PEPS map $A_{\mathcal{R}}$ from virtual indices on edges in $\partial\mathcal{R}$ to physical indices on vertices in \mathcal{R} .

unitary corresponding to a physical symmetry that is respected in our classification of phases. Since physical symmetries necessarily form a group under multiplication, we henceforth use the notation $U(g)$, $g \in \mathbb{G}$ (we do not consider non on-site symmetries such as lattice symmetries [131]). $O^{\partial\mathcal{R}}$ is a MPO acting on the virtual space associated to the edges crossing $\partial\mathcal{R}$. In general,

$$O^{\partial\mathcal{R}} = \sum_{\{i_n\}, \{i'_n\}=1}^D \text{tr} B_{\sigma_1}^{i_1, i'_1} \dots B_{\sigma_N}^{i_N, i'_N} |i_1 \dots i_N\rangle \langle i'_1 \dots i'_N|$$

where the edges crossing $\partial\mathcal{R}$ are ordered 1 to $N := |\partial\mathcal{R}|_e$, by fixing an arbitrary base point and following the orientation of $\partial\mathcal{R}$ (specifically the orientation induced by \mathcal{M}). Each $(B_{\sigma_n}^{i, i'})_{a, b}$ is a $\chi \times \chi$ matrix, see Fig.2.1, which can depend on the handedness $\sigma_n = \pm$ of the crossing of $\partial\mathcal{R}$ and edge n (+ for right, - for left).

Any truly topological symmetries should persist under arbitrary deformations of the region \mathcal{R} , hence the relevant task is to find a complete set \mathcal{S}_g of linearly independent single block [36] MPOs $O_{\alpha}^{\partial\mathcal{R}}(g)$ for every symmetry transformation $U(g)$ such that for every region \mathcal{R} (satisfying the conditions outlined above) we have

$$U(g)^{\otimes |\mathcal{R}|_v} A_{\mathcal{R}} = A_{\mathcal{R}} O_{\alpha}^{\partial\mathcal{R}}(g) \tag{2.1}$$

see Fig.2.3. There is an important subtlety in finding inequivalent MPOs that

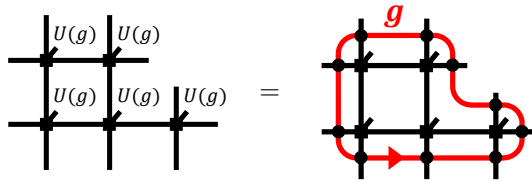


Figure 2.3: The symmetry of the PEPS map $A_{\mathcal{R}}$ on a region \mathcal{R} containing five sites.

satisfy Eq.(2.1) since two linearly independent solutions $O_1^{\partial\mathcal{R}}(g)$, $O_2^{\partial\mathcal{R}}(g)$

may coincide on the support of $A_{\mathcal{R}}$. This occurs precisely when they differ by an operator supported on the kernel of $A_{\mathcal{R}}$. To remove this redundancy one must first find the set of all single block MPO symmetries \mathcal{S}_1 for $U(1) = \mathbb{1}$. Assuming these MPOs are complete in the following sense $\sum_{\alpha} O_{\alpha}^{\partial\mathcal{R}}(1) = A_{\mathcal{R}}^{+} A_{\mathcal{R}}$, where $A_{\mathcal{R}}^{+}$ is a distinguished generalized inverse of $A_{\mathcal{R}}$, any MPO $\hat{O}^{\partial\mathcal{R}}$ can be projected onto the support of $A_{\mathcal{R}}$ to yield another MPO $A_{\mathcal{R}}^{+} A_{\mathcal{R}} \hat{O}^{\partial\mathcal{R}}$ with a (multiplicative) constant increase in the bond dimension. Hence the set of inequivalent single blocked MPO symmetries $\mathcal{S}_g := \{O_{\alpha}^{\partial\mathcal{R}}(g)\}_{\alpha}$ can be found by taking all linearly independent MPOs satisfying Eq.(2.1), projecting them onto the support subspace $A_{\mathcal{R}}^{+} A_{\mathcal{R}}$ and collecting the linearly independent single block MPOs that result.

Eq.(2.1) implies that $\mathcal{S} := \bigcup_g \mathcal{S}_g$ has a G-graded algebra structure. This algebra structure and the number of elements in \mathcal{S} must be independent of \mathcal{R} . Note the MPO matrices $B_{\sigma_e, \alpha}^{ij}(g)$ also do not depend on \mathcal{R} hence for every region the MPO $O_{\alpha}^{\partial\mathcal{R}}(g)$ is constructed from the same local tensors. The symmetry relations of Eq.(2.1), the graded algebra structure of \mathcal{S} and any discrete labels of the MPO representation of this graded algebra provide universal labels of a quantum phase, independent of the details of the local tensors A_v . We conjecture that the discrete labels of the MPO representation can be calculated in a purely local fashion [132, 133] and that they remain invariant under continuous physical perturbations.

Intrinsic topological order is defined without reference to any symmetry and thus corresponds to the $G = \{1\}$ case, in which PEPS are classified by \mathcal{S}_1 . Injective PEPS [103] always possess trivial topological order and have $\mathcal{S}_1 = \{\mathbb{1}^{\otimes |\partial\mathcal{R}|}\}$ whereas all known topological ordered PEPS [106–110] satisfy Eq.(2.1) with a nontrivial \mathcal{S}_1 . This was formalized in the framework of MPO-injectivity in Ref.[109], which was shown to capture all Levin-Wen string-net models (the Hamiltonian version of Turaev-Viro state sum invariants [134]). In Ref.[109] the independence of the MPO tensors from the region \mathcal{R} was guaranteed by the intuitive *pulling through* property and the more technical *generalized* and *extended inverse* properties, all of which were purely local conditions.

By taking a global symmetry G into account, a finer classification is achieved that contains symmetry-protected phases for $|\mathcal{S}_1| = 1$ and symmetry-enriched topological phases for $|\mathcal{S}_1| > 1$. In the next section we demonstrate how solutions of Eq.(2.1) can be obtained for nontrivial elements $g \in G$ in a similar fashion to [109].

2.3 Global symmetry in PEPS

In this section we present a set of local conditions that lead to a general class of solutions to Eq.(2.1).

Consider a PEPS on a trivalent directed graph Λ embedded in an oriented manifold \mathcal{M} , built from four index tensors A which we interpret as

linear maps from the virtual to physical indices $A : (\mathbb{C}^D)^{\otimes 3} \rightarrow \mathbb{C}^d$. Firstly, we require that the tensors A satisfy the axioms of MPO-injectivity [109], a framework describing general gapped phases without symmetry. Thus (potentially after some blocking of lattice sites, which we assume has already been carried out) the projection $P := A^+ A$ onto the subspace within which the tensor A is injective can be written as a matrix product operator

(2.2)

here the MPO tensors are denoted as black squares and satisfy the axioms listed in [109], see Appendix 2.A for a brief review. These axioms ensure that the same MPO is obtained for any larger region, independent of the order in which the generalized inverses are applied, and furthermore that this closed MPO is a projector independent of its length.

We now describe purely local sufficient conditions for a PEPS to be invariant under the on-site action $U(g)$ of a global symmetry group G . Hereto, we introduce another set of closed MPOs $\{V^{\partial\mathcal{R}}(g) \mid g \in G\}$ which inherit an orientation from $\partial\mathcal{R}$. These MPOs are composed of four index tensors that depend on a group element g . The tensors are depicted by filled circles in the following diagrams and are defined by conditions (2.3) and (2.4)

(2.3)

where $U(g)$ is a unitary representation of G , and

(2.4)

Note Eq.(2.4) with the directions reversed is implied by the above conditions. The orientation of the MPO tensors is significant as pulling the MPO through a PEPS tensor in a right handed fashion, as in Eq.(2.3), induces an action $U(g)$ on the physical index while pulling through in a left handed fashion results in a physical action $U^\dagger(g)$, this follows directly from Eq.(2.3) since U is a unitary representation.

With these two properties, it is clear that the ground space of a MPO-injective PEPS constructed from the tensor A on any closed system of arbitrary size is invariant under the global symmetry action $U(g)^{\otimes N}$. Hence

such MPO-injective PEPS that are unique ground states must be eigenvectors of the global symmetry. For the special case of injective PEPS [103] the MPO P is simply the identity $P = \mathbb{1}$ (i.e. a MPO with bond dimension 1), the symmetry MPOs $V(g)$ can always be factorized into a tensor product of local gauge transformations [135] and the ground state is unique.

From Eqs.(2.3) and (2.4) it immediately follows that the PEPS tensors are intertwiners, i.e. $U(g)A = AV(g)$, where $V(g)$ denotes a closed MPO acting on the three virtual indices. Without loss of generality, and in accordance with the general framework of Section 2.2, we impose that the MPOs $V(g)$ act within the support space of A such that $PV(g) = V(g)$, i.e.

$$\text{Diagram (2.5): } U(g)A = AV(g)$$

and in particular $V(1) = P$, for 1 the identity group element. Hence the MPOs $V(g)$ form a representation of G since we have $AV(g_1g_2) = U(g_1g_2)A = U(g_1)U(g_2)A = AV(g_1)V(g_2)$, and thus $PV(g_1g_2) = PV(g_1)V(g_2)$ where $P := A^+A$, see Eq.(2.2) (note $PV(g)P = A^+U(g)AP = PV(g)$). A similar argument shows that the symmetry MPO $V_{\text{rev}}(g)$ along the path with reversed orientation (inducing reversed arrows) equals $V(g^{-1})$ since $AV_{\text{rev}}(g) = U^\dagger(g)A = U(g^{-1})A = AV(g^{-1})$ which implies $PV_{\text{rev}}(g) = PV(g^{-1})$. The above two arguments extend to arbitrary contractible regions \mathcal{R} and boundary MPOs $P_{\partial\mathcal{R}}, V^{\partial\mathcal{R}}(g)$.

If we do not project the boundary symmetries onto the support subspace of A there are many equivalent choices for the symmetry action on the boundary. In particular, there might be choices for which the action is factorizable into a tensor product (see e.g. Ref.[111]), even if the support projector is not. However, the resulting boundary actions will generically not form a representation of the relevant symmetry group G . The procedure we have outlined of projecting these actions onto the injectivity subspace provides an unambiguous recipe to identify the relevant set of boundary operators that form a MPO representation of the physical symmetry group G . For the particular case of renormalization group fixed point models, our recipe matches the results of Ref.[111], as illustrated in Section 2.7.

With these properties it is clear that the class of symmetric PEPS satisfying Eqs.(2.3) and (2.4) constitute a special case of the general framework described in Section 2.2. Let $V^{\partial\mathcal{R}}(g)$ denote the MPO corresponding to group element g acting on the boundary of region \mathcal{R} then we have

$$U(g)^{\otimes |\mathcal{R}|_v} A_{\mathcal{R}} = A_{\mathcal{R}} V^{\partial\mathcal{R}}(g). \tag{2.6}$$

Note in the general case we may need to decompose $V^{\partial\mathcal{R}}(g)$ into a sum of single block MPOs to be consistent with Section 2.2.

This general class of solutions show that the formalism of Section 2.2 accommodates the description of both symmetries and topological order, and furthermore nontrivial actions of symmetries on states with topological order. Hence the formalism is well suited to describe symmetry-enriched topological phases within the PEPS framework. We plan to pursue this direction explicitly in future work[125].

2.4 Symmetry-protected topological PEPS

Having discussed the general framework for gapped phases and global symmetries in PEPS, we now focus on the subclass corresponding to states with symmetry-protected topological order. In the first subsection we identify the characteristic properties of short-range entangled SPT PEPS. We proceed in the second subsection with an analysis of the edge properties of non-trivial SPT PEPS.

2.4.1 Identifying SPT PEPS

First we must identify the relevant set of PEPS that accurately capture the short-range entanglement property characteristic of SPT phases. As shown in Ref.[109] and argued in the previous sections, MPO-injective PEPS can describe topological phases with long-range entanglement. To single out the short-range entangled PEPS that are candidates to describe SPT states we require that the projection MPO P has a single block when brought into its canonical form. Let B_P^{ij} denote the MPO matrix with external indices i and j , the single block property is equivalent to the transfer matrix $\mathbb{E}_P := \sum_{ij} B_P^{ij} \otimes \bar{B}_P^{ij}$ having a unique eigenvalue of largest magnitude with a corresponding unique eigenvector of full rank. For RG fixed-point PEPS, which are injective on the support subspace of P , we argue that the single block property implies the topological entanglement entropy [40, 136] is zero.

Proposition 1. *For a RG fixed point (zero correlation length) MPO-injective PEPS with a single blocked projector MPO P , the topological entanglement entropy of the PEPS is zero*

Note the rank of the reduced density matrix $\rho_{\mathcal{R}}$ on a finite homotopically trivial region \mathcal{R} of a MPO-injective PEPS on a sphere equals the rank of the projection MPO surrounding that region, i.e. $\text{rank}(\rho_{\mathcal{R}}) = \text{rank}(P_{\partial\mathcal{R}})$ [109]. Since the MPO P is a projection, we have $\text{rank}(P_{\partial\mathcal{R}}) = \text{tr}(P_{\partial\mathcal{R}}) = \text{tr}(P_{\partial\mathcal{R}}^2) = \text{tr}(\mathbb{E}_P^L)$, where $L = |\partial\mathcal{R}|_e$ is the number of virtual bonds crossing the boundary of the region \mathcal{R} under consideration. We then use the uniqueness of the largest eigenvalue λ_{\max} of \mathbb{E}_P to conclude that, for large regions, the rank of the reduced density matrix scales as λ_{\max}^L . This implies that the zero Rényi entropy has no topological correction and for RG fixed points this

furthermore implies that the topological entanglement entropy is zero [137]. We expect this property to hold throughout the gapped phase containing the fixed point.

A further crucial property of a SPT phase without symmetry breaking is the existence of a unique ground state on any closed manifold. For a PEPS to be a unique ground state its transfer matrix must have a unique fixed point. This excludes both symmetry-breaking and topological degeneracy [107, 138]. By taking a PEPS sufficiently close to its isometric form [106, 108, 109] we avoid the symmetry-breaking case (and assure the gap condition [104]). Furthermore, in Appendix 2.B we present an argument showing that MPO-injective PEPS with single block projection MPOs do not lead to topological degeneracy.

We have argued above that SPT PEPS should be MPO-injective on the support subspace of a single blocked projection MPO. In the language of Section 2.2 this implies $|\mathcal{S}_1| = 1$ for SPT PEPS. We now show that in this case the symmetry MPOs are also single blocked.

Proposition 2. *For any MPO-injective PEPS with a single blocked projection MPO, all symmetry MPOs of that PEPS can be chosen to be single blocked.*

Assume $V(g)$ contains multiple blocks when brought into canonical form $V(g) = \sum_i V_i(g)$, then we have $PV(g) = \sum_i V_{\pi(i)}(g)$ in canonical form (for some permutation π) since $V(g) = PV(g)$ for all lengths. This follows from the fact that a pair of MPOs which are equal for all lengths exhibit the same blocks when brought into canonical form [132]. Furthermore $\pi = 1$ since $V_i(g) = PV_{\pi^{-1}(i)}(g) = P^2V_{\pi^{-1}(i)}(g) = V_{\pi(i)}(g)$.

We have

$$P = V(g^{-1})V(g) = \sum_i V(g^{-1})V_i(g)$$

and since this equality holds for all lengths and P has a single block, there can be only one block on the right hand side after bringing it into canonical form [132]. Hence one term in the sum gives rise to a P block along with zero blocks in the canonical form and the others give rise only to zero blocks. Writing this out we have

$$P = V(g^{-1})V_i(g)$$

multiplying by $V(g)$ from the left and making use of the invariance under P implies

$$V(g) = V_i(g)$$

which has a single block (after throwing away the trivial zero blocks).

The arguments in this subsection show that the subclass of symmetric, MPO-injective PEPS satisfying Eqs.(2.3) and (2.4) which accurately describe SPT phases are precisely those with a single blocked projection MPO, provided they are taken sufficiently close to an isometric form to discount the possibility of a phase transition.

Hence the framework of Section 2.2 yields a classification of SPT phases in terms of the discrete labels of the (necessarily single blocked) MPO group representation $V(g)$ of the physical symmetry group G which include the group structure and the third cohomology class $[\alpha] \in H^3(G, U(1))$ [111] (see Appendix 2.C for a review).

2.4.2 Edge properties

We now focus on how the MPO symmetries affect the edge physics of a SPT PEPS and discuss how this can be used to diagnose nontrivial SPT order.

A short-range entangled PEPS with MPO symmetries $V(g)$ that satisfy Eqs.(2.3) and (2.4) has non-trivial SPT order if the third cohomology class $[\alpha]$ of the MPO representation is non-trivial. The existence of this non-trivial SPT order can be inferred by analyzing the edge physics when such a PEPS is defined on a finite lattice \mathcal{R} with a physical edge (boundary) $\partial\mathcal{R}$. In this case the PEPS has open (uncontracted) virtual indices along the physical boundary and all virtual boundary conditions give rise to exact ground states of the canonical PEPS (bulk) parent Hamiltonian H_{PEPS} (note boundary conditions orthogonal to the support of $P_{\partial\mathcal{R}}$ yield zero). Hence the ground space degeneracy scales exponentially with the length of the boundary, which is a generic property of any PEPS (bulk) parent Hamiltonian. The physically relevant question is whether the Hamiltonian can be perturbed by additional local terms $H_{\text{pert}} = \sum_v H_v$, which are invariant under G , to gap out these edge modes and give rise to a unique symmetric ground state.

In Ref.[138] an isometry \mathcal{W} was derived that maps any operator O acting on the physical indices of the PEPS to an effective operator acting on the virtual indices of the boundary $O \mapsto \mathcal{W}_{\mathcal{R}}^A[O]$. Let $A_{\mathcal{R}} = WH$ be a polar decomposition of $A_{\mathcal{R}}$, where W is an isometry from the virtual to physical level $(\mathbb{C}^D)^{\otimes |\partial\mathcal{R}|_e} \rightarrow (\mathbb{C}^d)^{\otimes |\mathcal{R}|_v}$. This induces the following isometry $\mathcal{W}_{\mathcal{R}}^A[O] := W^\dagger O W$ that maps bulk operators to the boundary in an orthogonality preserving way. Note there is some freedom in choosing W precisely when $P_{\partial\mathcal{R}}$ is nontrivial, in this case we make the choice that best preserves locality. Regardless of our choice of W we always have $P_{\partial\mathcal{R}} \mathcal{W}_{\mathcal{R}}^A[O] P_{\partial\mathcal{R}} = H^+ A_{\mathcal{R}}^\dagger O A_{\mathcal{R}} H^+$, see Fig.2.4. Away from an RG fixed point, however, it has not been proven that this isometry preserves locality. To this point we venture the following conjecture, which was numerically illustrated for a particular non-topological PEPS in Ref.[139],

Conjecture 1. *The boundary isometry of any PEPS with exponentially decaying correlations maps a local operator O_v acting on the physical indices near the boundary to a (quasi-) local operator $\tilde{O}_e^v := \mathcal{W}_{\mathcal{R}}^A[O_v]$ acting on the virtual degrees of freedom along the boundary.*

From properties (2.3) and (2.4) it is clear that acting with $U(g)$ on every physical site is equivalent to acting with the MPO $V^{\partial\mathcal{R}}(g)$ on the virtual boundary indices of the PEPS, hence a G -symmetric local perturbation H_v to

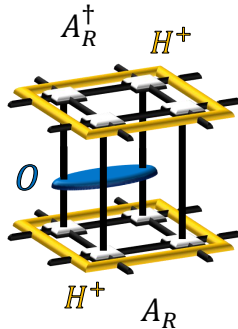


Figure 2.4: The bulk to boundary isometry, for a region \mathcal{R} containing four sites, projected onto the injectivity subspace $P_{\partial\mathcal{R}}\mathcal{W}_{\mathcal{R}}^A[O]P_{\partial\mathcal{R}} = H^+A_R^\dagger O A_R H^+$.

the Hamiltonian at the physical level H_{PEPS} is mapped to an effective (quasi-) local Hamiltonian term on the virtual boundary \tilde{H}_e^v that is invariant under $V^{\partial\mathcal{R}}(g)$. The full symmetric edge Hamiltonian is given by

$$\begin{aligned} \tilde{H}_{\text{edge}} &= P_{\partial\mathcal{R}} \mathcal{W}_{\mathcal{R}}^A[H_{\text{pert}}] P_{\partial\mathcal{R}} \\ &= V^{\partial\mathcal{R}}(1) \left(\sum_{e \in \partial\mathcal{R}} \sum_{v \mapsto e} \tilde{H}_e^v \right) V^{\partial\mathcal{R}}(1) \end{aligned} \quad (2.7)$$

where $v \mapsto e$ denotes that the bulk perturbation centered on site v becomes a (quasi-) local boundary term centered on virtual bond e .

Ground states of the perturbed physical Hamiltonian $H_{\text{bulk}} = H_{\text{PEPS}} + H_{\text{pert}}$ are given by contracting the virtual boundary indices of the ground state PEPS network with ground states of the effective edge Hamiltonian, i.e. $|\Psi_0^{\text{bulk}}\rangle = A_{\mathcal{R}}|\psi_0^{\text{edge}}\rangle$. If the edge Hamiltonian \tilde{H}_{edge} is gapped and does not exhibit spontaneous symmetry breaking then its ground state $|\psi_0^{\text{edge}}\rangle$ is well approximated by an injective MPS that is invariant under $V^{\partial\mathcal{R}}(g)$. However it was shown by Chen et al. that this results in a contradiction, since an injective MPS cannot be invariant under the action of a single blocked MPO group representation $V(g)$ with non-trivial third cohomology [111].

Consequently, the effective edge Hamiltonian \tilde{H}_{edge} either exhibits spontaneous symmetry breaking, in which case the MPS is not injective, or must be gapless, in which case its ground state cannot be well approximated by a MPS. In the former case, the physical state $A_{\mathcal{R}}|\psi_{0,i}^{\text{edge}}\rangle$ obtained by contracting the virtual boundary indices of the PEPS network with $|\psi_{0,i}^{\text{edge}}\rangle$, one of the symmetry breaking ground states of \tilde{H}_{edge} , also exhibits symmetry breaking and hence does not qualify as a symmetric state. The latter case, on the other hand, implies that a local symmetric perturbation to the physical

Hamiltonian is unable to gap out the gapless edge modes, which is one of the hallmarks of non-trivial SPT order.

Here we have again relied on a form of Conjecture 1, specifically that a PEPS with exponentially decaying correlations has a gapped transfer matrix, which implies that the gapless modes on the virtual boundary of the PEPS network are approximately identified, via the PEPS map $\mathcal{A}_{\mathcal{R}}$, with physical degrees of freedom that are an order of the correlation length from the boundary. Note this explicit identification of the gapless edge mode degrees of freedom is a major strength of the PEPS framework [139]. Our conjecture is consistent with the intuition that as a SPT PEPS is tuned to criticality the gap of the transfer matrix shrinks and the edge modes extend further into the bulk, and is also supported by the results of Ref.[140] concerning phase transitions between symmetry-protected and trivial phases.

In this section we have identified a subclass of symmetric PEPS with short-range entanglement that are MPO-injective with respect to a single blocked projection MPO. This led to a classification of SPT phases within the framework of Section 2.2 in terms of the third cohomology class of the MPO symmetry representation. Finally we described the influence of the possibly anomalous MPO symmetry action on the boundary physics of the PEPS. In the next section we explore an alternative approach to classifying SPT phases with PEPS via gauging.

2.5 Gauging SPT PEPS

In this section we discuss how gauging a SPT PEPS yields a long range entangled PEPS whose topological order is determined by the symmetry MPOs. We then proceed to show that the gauging procedure preserves the energy gap of a symmetric Hamiltonian. Our approach explicitly identifies how the symmetry MPOs that determine the boundary theory of a SPT model are mapped to topological MPOs that describe the anyons of a topological theory [133].

2.5.1 Gauging SPT PEPS to topologically ordered PEPS

We first outline the application of the gauging procedure from Ref.[51] to SPT PEPS and the effect this has upon the MPO symmetries.

Conditions (2.3) and (2.4) ensure that the SPT PEPS described in Section 2.4 are invariant under the global action $U(g)^{\otimes |\mathcal{M}|_v}$ of a symmetry group G , hence the quantum state gauging procedure of Ref.[51] is applicable. It was shown in Ref.[51] that the virtual boundary action of the physical symmetry in an injective PEPS becomes a purely virtual topological symmetry of the gauged tensors, with a trivial physical action. More precisely, it was shown that the gauging procedure transforms an injective PEPS, with virtual bonds in \mathbb{C}^D and a virtual symmetry representation that factorizes

as $V^{\partial\mathcal{R}}(g) = v(g)^{\otimes L}$ (with $v(g) : \mathbb{C}^D \rightarrow \mathbb{C}^D$), into a G -injective PEPS, with virtual bonds in $\mathbb{C}^D \otimes \mathbb{C}[G]$, that is injective on the support subspace of the projector $\sum_{g \in G} [v(g) \otimes R(g)]^{\otimes L}$. Here, $L := |\partial\mathcal{R}|_e$ is the number of virtual bonds crossing the boundary of the region \mathcal{R} under consideration and $R(g) |h\rangle := |hg^{-1}\rangle$ denotes the right regular representation of G on the new component $\mathbb{C}[G]$ of the virtual bonds. Let us recast this in the framework of Section 2.2. The ungauged symmetric injective PEPS map satisfies

$$A_{\mathcal{R}} V^{\partial\mathcal{R}}(g) = U(g)^{\otimes |\mathcal{R}|_v} A_{\mathcal{R}} \quad (2.8)$$

for any region $\mathcal{R} \subset \mathcal{M}$ and $g \in G$. Now let $O^{\partial\mathcal{R}}(g) := [v(g) \otimes R(g)]^{\otimes L}$, then the gauged PEPS map $A_{\mathcal{R}}^g$ for any region \mathcal{R} satisfies

$$A_{\mathcal{R}}^g O^{\partial\mathcal{R}}(g) = A_{\mathcal{R}}^g \quad (2.9)$$

for all $g \in G$, which implies that the gauged PEPS A^g is in the same phase as a quantum double model constructed from G , provided it is sufficiently close to a fixed point to ensure there is no symmetry breaking [106, 141].

The result of Ref.[51] can be extended to the general case outlined in Section 2.4 and Appendix 2.B where the PEPS map $A_{\mathcal{R}}$ in region \mathcal{R} has a non-factorizable MPO representation of the symmetry on the virtual level, given by $V^{\partial\mathcal{R}}(g) : (\mathbb{C}^D)^{\otimes L} \rightarrow (\mathbb{C}^D)^{\otimes L}$, and is only injective on the support subspace of the projection MPO $P_{\partial\mathcal{R}} = V^{\partial\mathcal{R}}(1)$ which is required to be single blocked. Hence we have

$$A_{\mathcal{R}} P_{\partial\mathcal{R}} = A_{\mathcal{R}} \quad (2.10)$$

$$A_{\mathcal{R}} V^{\partial\mathcal{R}}(g) = U(g)^{\otimes |\mathcal{R}|_v} A_{\mathcal{R}} \quad (2.11)$$

for all $g \in G$; note we have explicitly separated the $g = 1$ case for emphasis. In the language of Section 2.2 we have $\mathcal{S}_g = \{V^{\partial\mathcal{R}}(g)\}$, $\forall g \in G$.

The gauged PEPS A^g obtained by applying the procedure of Ref.[51] to A has virtual bonds in $\mathbb{C}^D \otimes \mathbb{C}[G]$ and satisfies the axioms of MPO-injectivity [109], but is now injective on the support subspace of the projection MPO $P_{\partial\mathcal{R}}^g := \frac{1}{|G|} \sum_{g \in G} O^{\partial\mathcal{R}}(g)$, where $O^{\partial\mathcal{R}}(g) := V^{\partial\mathcal{R}}(g) \otimes R(g)^{\otimes L}$, see Appendix 2.F for a detailed proof. Writing these conditions out, we have

$$A_{\mathcal{R}}^g O^{\partial\mathcal{R}}(g) = A_{\mathcal{R}}^g \quad (2.12)$$

for all $g \in G$, which implies $A_{\mathcal{R}}^g P_{\partial\mathcal{R}}^g = A_{\mathcal{R}}^g$. Note every MPO $O^{\partial\mathcal{R}}(g)$ is one of the original MPO symmetries $V^{\partial\mathcal{R}}(g)$ tensored with a tensor product representation on the new component $\mathbb{C}[G]$ of the virtual space that was introduced by gauging. The MPO representation of $P_{\partial\mathcal{R}}^g$ thus has a canonical form with multiple blocks labeled by $g \in G$ that correspond to the single block MPOs $O^{\partial\mathcal{R}}(g)$. Hence for the gauged PEPS $\mathcal{S}_1 = \{O^{\partial\mathcal{R}}(g) | g \in G\}$. Importantly, tensoring with a local action $R(g)$ on the additional virtual space $\mathbb{C}[G]$ does not change the bond dimension nor the third cohomology class of the MPO representation.

The topological order of the gauged SPT PEPS is a twisted Dijkgraaf-Witten model (provided it is sufficiently close to a fixed point to ensure there is no symmetry breaking) which is shown explicitly in Section 2.7.2. We emphasize that up to the trivial operators $R(g)^{\otimes L}$ the same MPOs determine both the gapless edge modes of the SPT phase and, as argued in [108, 109], the topological order of the gauged model. This realizes the gauging map from SPT models with a finite symmetry group to models with intrinsic topological order, explored at the level of Hamiltonians by Levin and Gu [126], explicitly on the level of states. In Appendix 2.I we apply the gauging procedure of Ref.[51] to families of SPT Hamiltonians with an arbitrary finite symmetry group, which yields an unambiguous gauging map to families of topologically ordered Hamiltonians.

We note that the PEPS gauging procedure can equally well be applied to gauge any normal subgroup $N \trianglelefteq G$ of the physical symmetry group G . This gives rise to states with symmetry-enriched topological order, where the topological component corresponds to a gauge theory with gauge group N and the global symmetry is given by the quotient group G/N ; we plan to investigate this direction further in future work [125].

2.5.2 Gauging preserves the gap

We now show that the gauging procedure of Ref.[51] preserves the energy gap of a symmetric Hamiltonian, which implies by contrapositive that two SPT PEPS are in different phases when the corresponding gauged PEPS lie in distinct topological phases.

Let H_m denote a local gapped symmetric ‘matter’ Hamiltonian, which captures the particular case of parent Hamiltonians for SPT PEPS. The Hamiltonian is a sum of local terms $H_m := \sum_v h_v$, where each h_v acts on a finite region within a constant distance of vertex v . Without loss of generality we take the Hamiltonian to satisfy $[h_v, U(g)^{\otimes |\mathcal{M}|_v}] = 0, \forall g \in G$ and shift the lowest eigenvalue of H_m to 0. The gap to the first excited energy level is denoted by $\Delta_m > 0$. We now apply the gauging procedure of Ref.[51] to obtain the gauged matter Hamiltonian defined by $H_m^G := \sum_v \mathcal{G}_{\Gamma_v}[h_v]$, for \mathcal{G}_{Γ_v} given in Eq.(2.112). This Hamiltonian is also local since each \mathcal{G}_{Γ_v} is locality preserving.

The gauging procedure introduces gauge fields on the links of the PEPS network and the full Hamiltonian of the gauged system contains local flux constraint terms $H_B := \sum_p (\mathbb{1} - \mathcal{B}_p)$ acting on these gauge fields by adding an energy penalty when the flux through a plaquette p is not the identity group element. Each local term \mathcal{B}_p is a Hermitian projector acting on the edges around plaquette p which has eigenvalue 1 on any gauge field configuration (G -connection) that satisfies the flux constraint and 0 otherwise, see Eq.(2.135). Furthermore \mathcal{B}_p is diagonal in the group basis on the edges, hence $[\mathcal{B}_p, \mathcal{B}_{p'}] = 0$.

The full Hamiltonian may also contain a sum of local commuting projections onto the gauge invariant subspace $H_P := \sum_v (\mathbb{1} - P_v)$, see Eq.(2.109), this corresponds to a model with an effective low energy gauge theory rather than a strict gauge theory. Hence the full Hamiltonian on the gauge and matter system is given by the following sum

$$H_{\text{full}} = H_m^{\mathcal{G}} + \Delta_B H_B + \Delta_P H_P$$

where $\Delta_B, \Delta_P \geq 0$. Note a strictly gauge invariant theory is recovered in the limit $\Delta_P \rightarrow \infty$. It is easy to verify that the components of the full Hamiltonian commute, i.e. $[H_m^{\mathcal{G}}, H_B] = [H_m^{\mathcal{G}}, H_P] = [H_B, H_P] = 0$, and hence are simultaneously diagonalizable. Furthermore, H_B and H_P each have lowest eigenvalue 0 and gap 1.

Assuming Δ_P is sufficiently large, the low energy subspace of H_{full} lies within the ground space of H_P and hence is spanned by states of the form $P[|\lambda\rangle_{\Lambda_v} \otimes |\phi\rangle_{\Lambda_e}]$, with $P = \prod_{v \in \Lambda} P_v$, for a basis $|\lambda\rangle$ of the matter (vertex) degrees of freedom (we will consider the eigenbasis of H_m) and a basis $|\phi\rangle$ of the gauge (edge) degrees of freedom (we will consider the group element basis).

Similarly, assuming Δ_B is sufficiently large, the low energy subspace of H_{full} lies within the ground space of H_B which is spanned by states whose gauge fields form a flat G-connection on the edge degrees of freedom. Since we additionally have $[B_p, P] = 0$ the common ground space of H_B and H_P is spanned by states of the form $P[|\lambda\rangle_{\Lambda_v} \otimes |\phi_{\text{flat}}\rangle_{\Lambda_e}]$, for a basis $|\phi_{\text{flat}}\rangle$ of the flat G-connections on the edge degrees of freedom (note these are product states).

G-connections form equivalence classes under the local gauge operations $a_v^g := \bigotimes_{e \in E_v^+} R_e(g) \bigotimes_{e \in E_v^-} L_e(g)$ (see appendix 2.F for a more detailed definition of a_v^g). On a 1-homotopy trivial manifold (no noncontractible loops) there is only 1 such equivalence class given by all connections of the form $|\phi_{\text{flat}}\rangle = \prod_i a_{v_i}^{g_i} |1\rangle_{\Lambda_e}$, where $|1\rangle_{\Lambda_e} := |1\rangle^{\otimes |\Lambda|_e}$.

Proposition 3. *For a 1-homotopy trivial manifold, the states $G|\lambda\rangle$ (for a basis $|\lambda\rangle$) span the common ground space of both H_B and H_P , where G is the quantum state gauging map defined in Eq.(2.111).*

Since $P_v = \int dg U_v(g) \otimes a_v^g$ one can easily see $P_v a_v^g = P_v U_v^\dagger(g)$ and hence for any state in the intersection of the ground spaces of H_B and H_P we have

$$\begin{aligned} P[|\psi\rangle_{\Lambda_v} \otimes |\phi_{\text{flat}}\rangle_{\Lambda_e}] &= P[|\psi\rangle_{\Lambda_v} \otimes \prod_i a_{v_i}^{g_i} |1\rangle_{\Lambda_e}] \\ &= P[[\prod_i U_{v_i}(g_i)]^\dagger |\psi\rangle_{\Lambda_v} \otimes |1\rangle_{\Lambda_e}] \\ &= G[\prod_i U_{v_i}(g_i)]^\dagger |\psi\rangle_{\Lambda_v} \end{aligned} \tag{2.13}$$

where we have started from our above characterization of the common ground space.

We now proceed to show that any eigenstate of H_m is mapped to an eigenstate of $H_m^{\mathcal{G}}$ by the quantum state gauging map G . See appendix 2.F for the details about the operator and state gauging maps \mathcal{G} and G as constructed in [51].

Proposition 4 ([51]). *The identity $\mathcal{G}_\Gamma[O]G = GO$ holds for any symmetric operator O .*

Suppose O acts on the sites $v \in \Gamma \subset \Lambda$ where Γ is a subgraph of the full lattice which contains all the edges between its vertices, then we have

$$\begin{aligned}
 \mathcal{G}_\Gamma[O]G &= \int \prod_{v \in \Gamma} dh_v \bigotimes_{v \in \Gamma} U_v(h_v) O \bigotimes_{v \in \Gamma} U_v^\dagger(h_v) \\
 &\bigotimes_{e \in \Gamma} |h_{v_e^-} h_{v_e^+}^{-1}\rangle \langle h_{v_e^-} h_{v_e^+}^{-1}| \int \prod_{v \in \Lambda} dg_v \bigotimes_{v \in \Lambda} U_v(g_v) \bigotimes_{e \in \Lambda} |g_{v_e^-} g_{v_e^+}^{-1}\rangle \\
 &= \int \prod_{v \in \Lambda} dg_v \prod_{v \in \Gamma} dh_v \bigotimes_{v \in \Lambda} U_v(g_v) \bigotimes_{v \in \Gamma} U_v(g_v^{-1} h_v) \\
 &O \bigotimes_{v \in \Gamma} U_v^\dagger(g_v^{-1} h_v) \prod_{e \in \Gamma} \delta_{(g_{v_e^-}^{-1} h_{v_e^-}), (g_{v_e^+}^{-1} h_{v_e^+})} \bigotimes_{e \in \Lambda} |g_{v_e^-} g_{v_e^+}^{-1}\rangle \\
 &= GO
 \end{aligned} \tag{2.14}$$

where edge e runs from vertex v_e^+ to v_e^- . The last equality follows since the δ condition forces $(g_v^{-1} h_v)$ to be equal for all $v \in \Gamma$ (assuming Γ is connected) and the operator O is symmetric under the group action $[O, \bigotimes_{v \in \Gamma} U_v(g)] = 0$.

This implies that any eigenstate $|\psi_\lambda\rangle$ of H_m with eigenvalue λ gives rise to an eigenstate $G|\psi_\lambda\rangle$ of $H_m^{\mathcal{G}}$ with the same eigenvalue. Note we have assumed that $G|\psi_\lambda\rangle \neq 0$, which is the case when the representation under which $|\psi_\lambda\rangle$ transforms contains the trivial representation. This always holds for a unique ground state (possibly after redefining the matrices of the group representation by multiplicative phases $U(g) \mapsto e^{i\theta(g)}U(g)$).

If H_m has a unique ground state $|\lambda_0\rangle$ the ground state of the full Hamiltonian is given by $G|\lambda_0\rangle$ (since $H_m^{\mathcal{G}} \geq 0$ for $H_m \geq 0$) and its gap satisfies $\Delta_{\text{full}} \geq \min(\Delta_m, \Delta_B, \Delta_P)$.

Hence if two local SPT Hamiltonians are connected by a gapped, continuous and symmetric path of local Hamiltonians then the gauged models are also connected by a gapped and continuous path of local Hamiltonians.

In Appendix 2.G we extend this proof to SPT Hamiltonians on topologically nontrivial manifolds where the gauging procedure leads to a topological degeneracy of the ground space. Orthogonal topological ground states are obtained by gauging distinct symmetry twisted SPT states, which are the subject of the next section.

2.6 Symmetry twists and monodromy defects

In this section we argue that symmetry twists and monodromy defects have a natural description in the tensor network formalism in terms of symmetry MPOs that correspond to anyons in the gauged model. We harness this description to calculate the effect that modular transformations have upon symmetry twisted and topological ground states via their effect on a four index *crossing tensor*. Similarly we calculate the projective transformation of a monodromy defect by composing two *crossing tensors*. Our approach explicitly identifies how the symmetry MPOs that describe defects of a SPT model become topological MPOs that describe the anyons of a topological model [133].

2.6.1 Symmetry twists in SPT PEPS

We first describe the construction of a symmetry twisted SPT PEPS in terms of the original SPT PEPS, symmetry MPOs and a crossing tensor. We then calculate the transformation of this state under the residual symmetry group.

For a flat gauge field configuration there is a well defined procedure for applying a corresponding symmetry twist to a local symmetric Hamiltonian, given by conjugating each local term by a certain product of on-site symmetries (see Appendix 2.G). On a trivial topology such a symmetry twist can be applied directly to a symmetric state by acting with a certain product of on-site symmetries. For example a symmetry twist on an infinite plane, specified by a pair of commuting group elements $(x, y) \in G \times G$ and oriented horizontal and vertical paths p_x, p_y in the dual lattice, acts on a state $|\psi\rangle$ in the following way

$$|\psi\rangle^{(x,y)} := \bigotimes_{v \in \mathcal{U}} U_v(x) \bigotimes_{v \in \mathcal{R}} U_v(y) |\psi\rangle$$

where \mathcal{R} is the half plane to the right of p_y , \mathcal{U} the half plane above p_x , see Fig.2.5. Note x and y must commute for the relevant gauge field configuration to be flat. One can also understand why they must commute by first applying the x -twist which reduces the symmetry group to $C(x)$ (the centralizer of x) and hence it only makes sense to implement a second twist for $y \in C(x)$. With this definition applying a symmetry twist to an eigenstate of a symmetric Hamiltonian (on a trivial topology) yields an eigenstate of the symmetry twisted Hamiltonian with the same eigenvalue.

The framework of SPT PEPS provides a natural prescription for the application of a symmetry twist directly to a PEPS on any topology, given by acting with symmetry MPOs on the virtual level of the PEPS. In the above example, assuming $|\psi\rangle$ is a SPT PEPS with local tensor A and symmetry MPOs $V(g)$, Eq.(2.3) implies that the symmetry twisted state $|\psi\rangle^{(x,y)}$ is given by acting on the virtual level of the PEPS $|\psi\rangle$ with the MPOs $V^{p_x}(x)$, $V^{p_y}(y)$

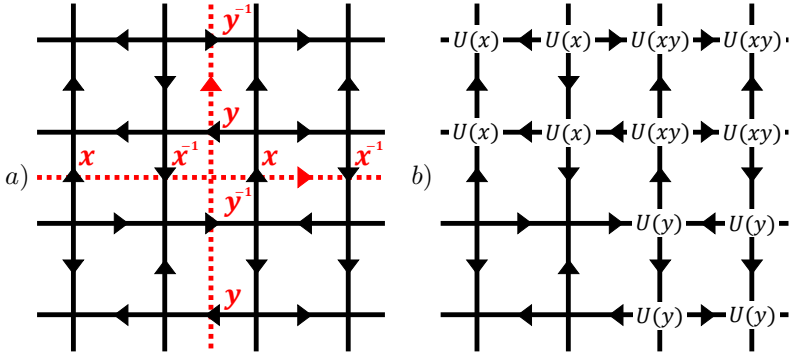


Figure 2.5: a) A symmetry twist (x, y) on an infinite plane. b) Physical action of the aforementioned symmetry twist.

(with inner indices contracted with the four index crossing tensor $Q_{x,y}$ (2.15) where p_x, p_y intersect) see Fig.2.6.

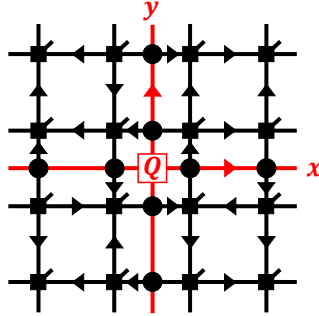
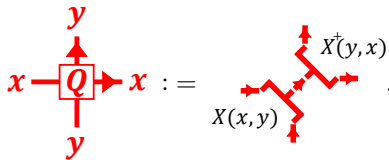


Figure 2.6: (x, y) symmetry twisted PEPS, for infinite or periodic boundary conditions.

The crossing tensor $Q_{x,y}$ is defined in terms of the local reduction tensor of the MPO representation $X(x, y)$ (see Eqs.(2.58,2.87))

$$\begin{aligned}
 Q_{x,y} &:= X(x, y)X^+(y, x) \\
 &= W_R^x(y)
 \end{aligned}
 \tag{2.15}$$



Eq.(2.3) and the zipper condition (2.72) for $X(x, y)$ imply that the $Q_{x,y}$

tensor contracted with MPOs $V^{p_x}(x), V^{p_y}(y)$ can be moved through the PEPS on the virtual level by applying appropriate on-site symmetries to the physical level.

This prescription extends straightforwardly to an arbitrary topology (see Appendix 2.G) as we now demonstrate with the example of a symmetry twist on a torus for a pair of commuting group elements (x, y) along distinct non-contractible cycles p_x, p_y . The symmetry twisted SPT PEPS $|\psi\rangle^{(x,y)}$ is again given by applying the MPOs $V^{p_x}(x), V^{p_y}(y)$ (with inner indices contracted with the crossing tensor $Q_{x,y}$) to the virtual level of the untwisted PEPS $|\psi\rangle$. Importantly this prescription fulfills the condition that applying a symmetry twist to a PEPS groundstate of a symmetric frustration free Hamiltonian yields a groundstate of the symmetry twisted Hamiltonian due to Eq.(2.3). We note that similar tensor network techniques allow a construction of symmetry twists for time reversal symmetry [142].

A symmetry twisted state with conjugated group elements (x^g, y^g) is related, up to a phase, to the symmetry twisted state with group elements (x, y) via a global symmetry action as follows $\theta_g^{x,y} |\psi\rangle^{(x^g, y^g)} = U(g)^{\otimes |\mathcal{M}|_v} |\psi\rangle^{(x,y)}$. Similarly a symmetry twisted state for a local deformation of the paths $(p_x, p_y) \mapsto (\tilde{p}_x, \tilde{p}_y)$ is related to the symmetry twisted state for (p_x, p_y) by a product of on-site symmetries corresponding to the deformation via Eq.(2.3). Hence the number of distinct classes of symmetry twisted states on a torus, under local operations, is given by the number of conjugacy classes of commuting pairs of group elements, which equals the number of irreducible representation of the quantum double $D(G)$ [106].

It is apparent that a symmetry twisted state $|\psi\rangle^{(x,y)}$ forms a 1D representation under the physical action of the residual symmetry group $C(x, y)$. Assuming that the untwisted ground state $|\psi\rangle$ is symmetric under G (which can always be achieved after rephasing the physical representation) the symmetry twisted states may still form nontrivial 1D representations of their respective residual symmetry groups, this fact becomes important when counting the ground space dimension of the gauged model. Calculating these 1D representations explicitly within the PEPS framework yields the result $\theta_g^{x,y} = \alpha^{(x,y)}(g)$ the second slant product of the 3-cocycle α that arose from the MPO group representation (see Appendix 2.E). Hence an (x, y) symmetry twisted state is symmetric under $C(x, y)$ iff $\alpha^{(x,y)} \equiv 1$, in which case y is called $\alpha^{(x)}$ -regular. If this property is satisfied by a given $y \in C(x)$ it is also holds for all conjugates of y . Furthermore the number of $\alpha^{(x)}$ -regular conjugacy classes is known to be equal to the number of irreducible projective representations with 2-cocycle $\alpha^{(x)}$ [129].

2.6.2 Gauging the symmetry twisted SPT PEPS

We now outline how the application of an appropriate gauging procedure to a symmetry twisted SPT PEPS yields a topological ground state.

There is a twisted version of the gauging procedure of Ref.[51] for each flat gauge field configuration which maps a symmetric Hamiltonian with the corresponding symmetry twist to a gauged Hamiltonian, the same one as obtained by applying the untwisted gauging procedure to the untwisted symmetric Hamiltonian (see Appendix 2.G for more detail). For a fixed representative (x, y) the twisted gauging operator $G_{x,y}$ is given by contracting the tensor product operators $R(x)^{\otimes |p_x|}, R(y)^{\otimes |p_y|}$ with the virtual level of the original gauging operator G . The twisted versions of the state gauging map are orthogonal for distinct symmetry twists in general and furthermore the fixed representatives satisfy $G_{x',y'}^\dagger G_{x,y} = \delta_{[x',y'],[x,y]} \int dg U(g)^{\otimes |\mathcal{M}|_v} \delta_{g \in \mathcal{C}(x,y)}$ (see Appendix 2.G.3). Hence each conjugacy class of symmetry twisted states that are symmetric under the residual symmetry group is mapped to an orthogonal ground state, while those that form a nontrivial 1D representation are mapped to 0. Consequently the dimension of the ground space for the gauged model is given by the number of irreducible representations of the twisted quantum double $D^\alpha(G)$ which can not be larger than the ground space dimension of a gauged trivial SPT model with the same symmetry group.

Given a SPT PEPS ground state $|\psi\rangle$, the orthogonal ground states of the gauged model can be constructed by applying the gauging tensor network operator and acting with the SPT symmetry MPO and a product of on-site symmetry actions $[V(g) \otimes R(g)^{\otimes L}]$ along noncontractible cycles on the virtual level of the gauged tensor network $G|\psi\rangle$. For a fixed representative (x, y) of a symmetric class of symmetry twists the corresponding gauged ground state is given by contracting the MPOs $[V^{p_x}(x) \otimes R(x)^{\otimes |p_x|}], [V^{p_y}(y) \otimes R(y)^{\otimes |p_y|}]$ (with the crossing tensor $Q_{x,y}$ at the intersection point $p_x \cap p_y$ [109]) with the virtual level of the gauged PEPS $G|\psi\rangle$.

2.6.3 Modular transformations

We calculate the effect of modular transformation on symmetry twisted and topological ground states via their effect on a set of four index crossing tensors.

Symmetry twisted ground states have been used to identify non trivial SPT order via the matrix elements of modular transformations taken with respect to them [143, 144]. We have calculated the SPT \tilde{S} & \tilde{T} matrices, corresponding to a $\frac{\pi}{2}$ rotation and a Dehn twist respectively, using our framework to find (see Eq.(2.107))

$$\langle x', y' | \tilde{S} | x, y \rangle = \alpha^{(y)}(x^{-1}, x)^{-1} \langle x', y' | y, x^{-1} \rangle \quad (2.16)$$

$$\langle x', y' | \tilde{T} | x, y \rangle = \alpha(x, y, x) \langle x', y' | x, xy \rangle \quad (2.17)$$

where we have used the abbreviation $|x, y\rangle := |\psi\rangle^{(x,y)}$ and note $y \in \mathcal{C}(x)$. The gauging procedure elucidates the precise correspondence between these matrix elements and the S & T -matrix of the gauged theory [44, 109,

145] which we have also calculated within the ground space (again see Eq.(2.107))

$$S = \sum_{xy=yx} \alpha^{(y)}(x^{-1}, x)^{-1} |[y, x^{-1}] \rangle \langle [x, y]| \quad (2.18)$$

$$T = \sum_{xy=yx} \alpha(x, y, x) |[x, xy] \rangle \langle [x, y]| \quad (2.19)$$

where $|[x, y] \rangle := G_{x,y} |\psi\rangle^{(x,y)}$ denotes a ground state of the gauged model. Note in our framework we consider a fixed but arbitrary choice of representative for each conjugacy class, rather than group averaging over them.

We have explicitly verified that S & T generate a linear representation of the modular group in agreement with known results for lattice gauge theories (See Subsection 2.E.4).

2.6.4 Projective symmetry transformation of monodromy defects

Here we describe an explicit construction of the projective representation that acts upon a monodromy defect. We calculate the 2-cocycle of this projective representation by considering the composition of pairs of crossing tensors.

Monodromy defects can be understood as symmetry twists along paths with open end points and have proven useful for the identification of SPT phases [87, 146]. The prescription for applying symmetry twists to SPT PEPS extends naturally to a construction of a pair of monodromy defects at the ends of a path p_g , for $g \in G$. This is given by applying a symmetry MPO $V^{p_g}(g)$ to the virtual level of the PEPS with an open inner index at either end of the path, which may be contracted with defect tensors replacing the PEPS tensors at each of the defects, see Fig.2.7. Applying the twisted gauging procedure for the corresponding gauge field configuration (which is flat except near the defect points) explicitly maps the symmetry twisted PEPS to a PEPS that describes a pair of flux anyon excitations in the gauged theory, see Appendix 2.H and Refs.[106, 133].

We now study a pair of monodromy defects on a twice punctured sphere topology, with a defect in each puncture, see Fig.2.7. This captures the case of a symmetry twist g applied to a path p_g along a cylinder, from one boundary to the other, and also the case of a pair of monodromy defects on a sphere, where each puncture is formed by removing a PEPS tensor and replacing it with a tensor that describes the defect.

Treating a symmetry twisted SPT PEPS on a cylinder (of fixed radius) as a one dimensional system, it is clear that the bulk is invariant under the residual symmetry group $C(g)$ since the symmetry twisted SPT PEPS on a torus formed by closing the cylinder (such that p_g becomes a noncontractible cycle) is symmetric. In this case the PEPS can be interpreted as a MPS and

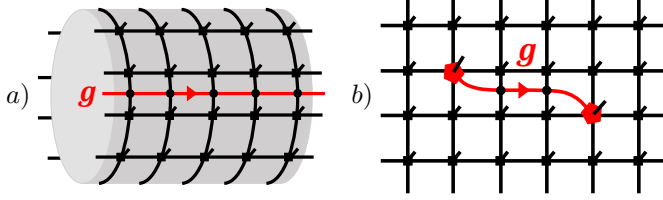


Figure 2.7: a) A symmetry twist along a cylinder PEPS. b) A pair of monodromy defects in a PEPS.

standard results in this setting imply that the global symmetry $U(h)^{\otimes |\mathcal{M}|_v}$ is intertwined by the PEPS to a tensor product of projective symmetry representations on the left and right virtual boundaries $\mathcal{V}_L^g(h) \otimes \mathcal{V}_R^g(h)$.

The projective boundary action $\mathcal{V}_R^g(h)$ of the symmetry can be explicitly constructed within the SPT PEPS framework. We find that it is given by a symmetry MPO acting on the PEPS virtual bonds entering the puncture, with its inner indices at the intersection of p_g and the boundary of the puncture contracted with the tensor $Y_R^g(h)$ (see Eq.(2.89)) that acts on the inner index of the symmetry twist MPO $V^{p_g}(g)$ entering the puncture.

$$\mathcal{V}_R^g(h) = \text{Diagram} \quad (2.20)$$

The diagram for equation (2.20) shows a red oval representing a boundary. Inside the oval, there are four horizontal black lines with dots at their ends. A red arrow labeled 'g' points to the right between the second and third lines. A red arrow labeled 'h' points to the right between the top and second lines. A red arrow labeled 'g' points to the right between the third and fourth lines. A red arrow labeled 'g' points to the right between the bottom and third lines.

The multiplication of physical symmetries induces a composition rule for the $Y_R^g(\cdot)$ tensors, see Appendix 2.H for details. Explicit calculation of these products yields the 2-cocycle factor set ω^g of the projective boundary representation $\mathcal{V}_R^g(k)\mathcal{V}_R^g(h) = \omega^g(k, h)\mathcal{V}_R^g(kh)$ in terms of the 3-cocycle α of the MPO symmetry representation $\omega^g(k, h) \sim \frac{\alpha(g, k, h)\alpha(k, h, g)}{\alpha(k, g, h)}$. This is consistent with the results of Ref.[87]. Note that altering α by a 3-coboundary induces a 2-coboundary change to the 2-cocycle ω^g , which hence forms a robust label of the SPT phase. The projective symmetry action is closely related to the braiding of anyons in the gauged theory.

2.7 Example: fixed-point SPT states

Inspired by the illuminating examples in Refs.[24] and [111] we now present a family of SPT PEPS with symmetry group G and 3-cocycle α satisfying

Eqs.(2.3) and (2.4), and explicitly demonstrate that gauging these states [51] yields MPO-injective PEPS that are the ground states of twisted quantum double Hamiltonians [128, 129].

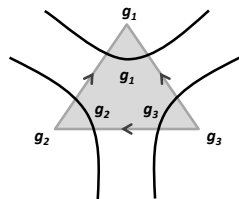
2.7.1 Fixed-point SPT PEPS

We describe our construction of fixed point SPT PEPS and calculate the MPOs induced by the symmetry action on a site. We explicitly give the fusion tensors for these MPOs and verify that they satisfy the *zipper* condition before determining the 3-cocycle of the MPO representation.

Our short-range entangled PEPS are defined on any trivalent lattice embedded in an oriented 2-manifold (dual to a triangular graph). They realize states equivalent to a standard SPT fixed point construction on the triangular graph [24, 147]. To this end we specify an ordering on the vertices of the triangular graph which induces an orientation of each edge, pointing from larger to smaller vertex. With this information we assign the following PEPS tensor $A_\Delta : \mathbb{C}(G)^{\otimes 6} \rightarrow \mathbb{C}(G)^{\otimes 3}$ to each vertex of the trivalent lattice

$$A_\Delta := \int \prod_{v \in \Delta} dg_v \tilde{\alpha}_\Delta \bigotimes_{v \in \Delta} |g_v\rangle_{\Delta,v} \bigotimes_{e \in \Delta} (g_{v_e^-} |_{\Delta,e,v_e^-} \langle g_{v_e^+} |_{\Delta,e,v_e^+} \tag{2.21}$$

where edge e is oriented from v_e^+ to v_e^- (hence $v_e^- < v_e^+$) in the triangular graph. The phase $\tilde{\alpha}_\Delta$ is defined on a vertex of the trivalent PEPS lattice dual to plaquette Δ of the triangular lattice, whose vertices appear in the order v, v', v'' following the orientation of the 2-manifold (note the choice of starting vertex is irrelevant), by a 3-cocycle α as follows $\tilde{\alpha}_\Delta := \alpha^{\sigma_\pi}(g_1 g_2^{-1}, g_2 g_3^{-1}, g_3)$. Where $(g_1, g_2, g_3) := \pi(g_v, g_{v'}, g_{v''})$ with π the permutation that sorts the group elements into ascending vertex order and $\sigma_\pi = \pm 1$ is the parity of the permutation (equivalently the orientation of Δ relative to the 2-manifold). In the following example the tensor A_Δ , possessing six virtual and three physical indices, has non zero entries given by



$$= \alpha(g_1 g_2^{-1}, g_2 g_3^{-1}, g_3). \tag{2.22}$$

Note the tensor diagrams in this section use the convention that physical vertex indices are written within the body of the tensor. Moreover we only depict the virtual and physical index combinations that give rise to non-zero values of the tensor.

The global symmetry of the PEPS on a closed manifold is ensured by the following transformation property of each local tensor

$$R(h)^{\otimes 3} A_{\Delta} = A_{\Delta} \bigotimes_{e \in \Delta} [Z_e^{\sigma_{\Delta,e}}(h) R(h)^{\otimes 2}], \quad (2.23)$$

where $Z_e(h) := \int dg_{v_e^-} dg_{v_e^+} \alpha(g_{v_e^-} g_{v_e^+}^{-1}, g_{v_e^+}, h) |g_{v_e^-}, g_{v_e^+}\rangle \langle g_{v_e^-}, g_{v_e^+}|$, and $\sigma_{\Delta,e} = \pm 1$ is $+1$ if e is directed along the clockwise orientation of $\partial\Delta$, and -1 otherwise. With this definition one can check that Eq.(2.23) is equivalent to the cocycle condition (2.61). Note the boundary actions on the shared edge of two neighboring tensors $A_{\Delta}, A_{\Delta'}$, induced by group multiplication on the physical sites Δ, Δ' , cancel out since $\sigma_{\Delta,e} = -\sigma_{\Delta',e}$ from which it follows that the full PEPS (on a closed manifold) is invariant under the group action applied to all physical indices. In our example the symmetry property is¹

$$= \quad (2.24)$$

Note that a tensor product of the virtual symmetry matrices $[Z_e^{\sigma_{\Delta,e}}(h) R(h)^{\otimes 2}]$ in general do not constitute a representation of G . A representation of G on the virtual level, $V(g)$, is obtained by projecting these matrices onto the subspace on which the PEPS tensor is injective. By doing so we construct MPOs that cannot be factorized as a tensor product. For the current fixed-point example we project $[Z_e^{\sigma_{\Delta,e}}(h) R(h)^{\otimes 2}]$ onto the subspace of virtual boundary indices corresponding to non-zero values of A_{Δ} , Eq.(2.21). This yields a MPO $V(h)$ constructed from the following tensors

$$h = \alpha(g_1 g_2^{-1}, g_2, h) \quad (2.25)$$

note that for fixed h these MPOs possess a single block. We introduce the

¹ Note the following subtlety, our tensor diagrams depict the coefficients of the map A_{Δ} and hence the group action $R(h)$ on the physical kets is equivalent to $R(h^{-1})$ on the coefficients, i.e. $R(h) \int dg f(g) |g\rangle = \int dg f(gh) |g\rangle$.

isometry $X(h_1, h_2)$

$$h_1 \rightarrow \quad \begin{array}{c} \text{---} g \\ \text{---} h_1 h_2 = \alpha(g, h_1, h_2) \\ \text{---} gh_1 \\ \text{---} h_2 \\ \text{---} gh_1 h_2 \end{array} \quad (2.26)$$

to describe the multiplication of two MPO tensors. With this isometry we have the following relation

$$\text{Diagram 1} = \text{Diagram 2} \quad (2.27)$$

where the left most tensor of Eq.(2.27) is $X^\dagger(h_1, h_2)$ and we have made use of the 3-cocycle condition (2.61). This implies that the MPOs $V(h)$ with fixed inner indices indeed form a representation of G . Note the stronger zipper condition

$$\text{Diagram 1} = \text{Diagram 2} \quad (2.28)$$

also holds for this MPO representation.

From Eq.(2.23) it is clear that the PEPS tensors A_Δ , Eq.(2.21), together with the MPOs $V(h)$, defined by Eq.(2.25), have SPT order described by the framework of Section 2.4. We now calculate the third cohomology class of the MPOs to determine which SPT phase the model belongs to. For this we see that X obeys the following associativity condition

$$X(h_1 h_2, h_3)[X(h_1, h_2) \otimes \mathbb{1}_{h_3}] = \alpha^{-1}(h_1, h_2, h_3) X(h_1, h_2 h_3)[\mathbb{1}_{h_1} \otimes X(h_2, h_3)], \quad (2.29)$$

which is again the 3-cocycle condition Eq.(2.61). From Eq.(2.29) we thus conclude that the short-range entangled states described by the tensors of Eq.(2.21) lie in a symmetry-protected topological phase labeled by the cohomology class $[\alpha^{-1}] \in H^3(G, U(1))$, see Appendix 2.A.

One may be surprised to notice that one layer of strictly local unitaries (equivalent to the local unitary circuit D_α (2.143)) acting on the vertices of the PEPS built from the tensors in Eq.(2.21) can remove the 3-cocycles, thus mapping it to a trivial product state. Superficially this seems to contradict the fact that SPT states cannot be connected to the trivial product state by low-depth local unitary circuits that preserve the symmetry. However, this is not the case as this definition requires every individual gate of the circuit to preserve the symmetry [148], which is not true for the circuit just described.

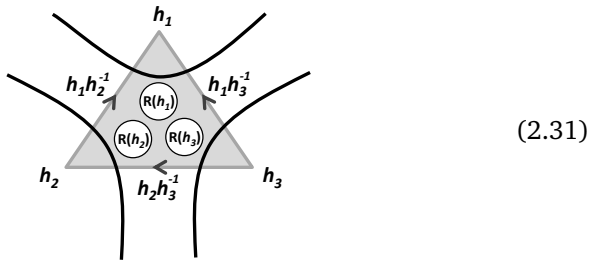
2.7.2 Gauging the fixed-point SPT PEPS

We now apply the quantum state gauging procedure of Ref.[51] to gauge the global symmetry of the fixed-point SPT PEPS defined in the previous subsection. For this we construct a gauging tensor network operator (matching that of Ref.[51] on the dual triangular graph) that couples gauge degrees of freedom to a given matter state. We proceed by applying a local unitary circuit to disentangle the gauge constraints and explicitly demonstrate that the resulting tensor describes the ground state of a twisted Dijkgraaf-Witten gauging theory.

The gauging map is defined by the following local tensors $G^\Delta : \mathbb{C}(\mathbb{G})^{\otimes 6} \otimes \mathbb{C}(\mathbb{G})^{\otimes 3} \rightarrow \mathbb{C}(\mathbb{G})^{\otimes 6}$

$$G^\Delta := \int \prod_{v \in \Delta} dh_v \bigotimes_{v \in \Delta} R_{\Delta,v}(h_v) \bigotimes_{e \in \Delta} [|h_{v_e^-} h_{v_e^+}^{-1} \rangle_{\Delta,e} \otimes (h_{v_e^+} |_{\Delta,e,v_e^+} (h_{v_e^-} |_{\Delta,e,v_e^-})] , \quad (2.30)$$

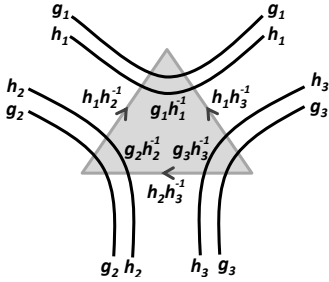
note G^Δ introduces gauge degrees of freedom on the edges. For our example the gauging tensor is



We can apply the gauging tensors locally to the SPT PEPS to form tensors for a gauge and matter PEPS

$$\bar{A}_\Delta := \int \prod_{v \in \Delta} dh_v dg_v \tilde{\alpha}_\Delta \bigotimes_{v \in \Delta} |g_v h_v^{-1} \rangle_{\Delta,v} \bigotimes_{e \in \Delta} |h_{v_e^-} h_{v_e^+}^{-1} \rangle_{\Delta,e} (g_{v_e^+}, h_{v_e^+} |_{\Delta,e,v_e^+} (g_{v_e^-}, h_{v_e^-} |_{\Delta,e,v_e^-}) \quad (2.32)$$

in our example these are



$$= \alpha(g_1 g_2^{-1}, g_2 g_3^{-1}, g_3). \quad (2.33)$$

The gauged PEPS $|\psi_g\rangle$, built from the tensors \bar{A}_Δ , satisfies local gauge constraints $\tilde{P}_v |\psi_g\rangle = |\psi_g\rangle$ for every vertex v , where

$$\tilde{P}_v := \int dg_v \bigotimes_{\Delta \ni v} [R_{\Delta,v}(h) \bigotimes_{e \in E_v^+} R_{\Delta,e}(g_v) \bigotimes_{e \in E_v^-} L_{\Delta,e}(g_v)]$$

The gauge and matter tensor \bar{A}_Δ is MPO-injective with respect to a purely virtual symmetry inherited from the symmetry transformation of the SPT tensor A_Δ and it also intertwines a physical symmetry to a virtual symmetry due to the transformation of the gauging tensors

$$\bar{A}_\Delta \bigotimes_{e \in \Delta} [Z_e^{\sigma_{\Delta,e}}(h) R(h)^{\otimes 2}] \otimes R(h)^{\otimes 2} = \bar{A}_\Delta \quad (2.34)$$

$$\begin{aligned} & \bigotimes_{v \in \Delta} R_{\Delta,v}(h) \bigotimes_{e \in \Delta} R_{\Delta,e}(h) L_{\Delta,e}(h) \bar{A}_\Delta \\ &= \bar{A}_\Delta \bigotimes_{e \in \Delta} \mathbb{1}^{\otimes 2} \otimes L(h)^{\otimes 2} \end{aligned} \quad (2.35)$$

the latter symmetry reflects the invariance of the full PEPS under the gauge constraints \tilde{P}_v .

We next apply a local unitary circuit \tilde{C}_Λ to explicitly map the gauge and matter model to a twisted quantum double ground state on the gauge degrees of freedom alone. This circuit is given by the tensor product of the following local unitary on each site

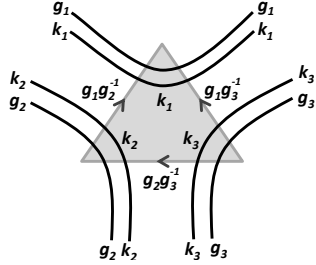
$$\tilde{C}_\Delta := \int \prod_{v \in \Delta} dg_v \bigotimes_{v \in \Delta} |g_v\rangle \langle g_v|_v \bigotimes_{e \in \Delta} L_e(g_{v_e^-}) R_e(g_{v_e^+}),$$

which maps the gauge constraints to local rank one projectors on the matter degrees of freedom at each vertex $\tilde{C}_\Lambda \tilde{P}_v \tilde{C}_\Lambda = \int dg_v \bigotimes_{\Delta \ni v} R_{\Delta,v}(h)$, fixing the state of the matter to be $\int dg_v \bigotimes_{\Delta \ni v} |g_v\rangle_{\Delta,v}$. From this we infer that the circuit \tilde{C}_Λ disentangles the gauge from the matter degrees of freedom. To see this explicitly we apply the circuit locally to each PEPS tensor, along

with a unitary change of basis on the virtual level (leaving the physical state invariant) to form the tensor $\bar{\bar{A}}_\Delta$ which is defined as follows

$$\begin{aligned} \bar{\bar{A}}_\Delta &:= \tilde{C}_\Delta \bar{A}_\Delta \bigotimes_{e \in \Delta} U_{\Delta, e, v_e^+} \otimes U_{\Delta, e, v_e^-} \\ &= \int \prod_{v \in \Delta} dk_v dg_v \tilde{\alpha}_\Delta \bigotimes_{v \in \Delta} |k_v\rangle_{\Delta, v} \bigotimes_{e \in \Delta} [|g_{v_e^-} g_{v_e^+}^{-1}\rangle_{\Delta, e} \\ &\quad \otimes (g_{v_e^+}, k_{v_e^+} |_{\Delta, e, v_e^+} (g_{v_e^-}, k_{v_e^-} |_{\Delta, e, v_e^-}] \end{aligned} \quad (2.36)$$

where $U := \int dg |g\rangle \langle g| \otimes SL^\dagger(g)$, with $S|g\rangle := |g^{-1}\rangle$, satisfies $(g, h|U = (g, gh^{-1}|$. For our example this tensor is given by



$$= \alpha(g_1 g_2^{-1}, g_2 g_3^{-1}, g_3) \quad (2.37)$$

This disentangled PEPS tensor $\bar{\bar{A}}_\Delta$ is now MPO-injective on the support subspace of the projection MPO given by a normalized sum of the symmetry MPOs from the SPT PEPS. Moreover the intertwining condition maps the physical vertex symmetry to a trivial action on the virtual space

$$\bar{\bar{A}}_\Delta \bigotimes_{e \in \Delta} [Z_e^{\sigma \Delta, e}(h) R(h)^{\otimes 2}] \otimes \mathbb{1}^{\otimes 2} = \bar{\bar{A}}_\Delta \quad (2.38)$$

$$\bigotimes_{v \in \Delta} R_{\Delta, v}(h) \bar{\bar{A}}_\Delta = \bar{\bar{A}}_\Delta \bigotimes_{e \in \Delta} \mathbb{1}^{\otimes 2} \otimes R(h)^{\otimes 2}. \quad (2.39)$$

From this we see that $\bar{\bar{A}}_\Delta$ separates into a trivial local component on the matter degrees of freedom yielding the state $\bigotimes_{v \in \Delta} \int dg_v \bigotimes_{\Delta \ni v} |g_v\rangle_{\Delta, v}$, and the following tensors on the gauge degrees of freedom

$$\int \prod_{v \in \Delta} dg_v \tilde{\alpha}_\Delta \bigotimes_{e \in \Delta} |g_{v_e^-} g_{v_e^+}^{-1}\rangle_{\Delta, e} (g_{v_e^+} |_{\Delta, e, v_e^+} (g_{v_e^-} |_{\Delta, e, v_e^-}. \quad (2.40)$$

These tensors define a PEPS on the gauge degrees of freedom that is a ground state of a 2D twisted quantum double with 3-cocycle α . Note this PEPS matches the standard representation of the ground state on the subspace obtained by mapping $\bigotimes_{\Delta \ni v} |g\rangle_{\Delta, v} \mapsto |g\rangle_v$ and $\bigotimes_{\Delta \ni e} |g\rangle_{\Delta, e} \mapsto |g\rangle_e$. For our

example this tensor is

$$= \alpha(g_1 g_2^{-1}, g_2 g_3^{-1}, g_3) \quad (2.41)$$

note in the Abelian case the tensors in Eq.(2.41) reduce to the string-net tensors [149, 150] after a suitable mapping between 3-cocycles and F -symbols [151] (in the non-Abelian case one has to change to the basis of irreducible representations to make the identification).

2.8 Conclusions

We have presented a unified picture for the characterization of all gapped phases, possibly with respect to certain physical symmetries, within the framework of PEPS in terms of virtual MPO symmetries. To achieve this we developed a characterization of global symmetry in the framework of MPO-injective PEPS [108, 109]. In contrast to the injective case [135], where the symmetry representation on the virtual indices factorizes into a tensor product, a MPO-injective PEPS tensors can have a virtual symmetry representation given by unfactorizable MPOs. We subsequently identified the short-range entangled PEPS to be those having a single block in the projection MPO onto the injectivity subspace. If the accompanying single block MPO virtual symmetry representation has a non-trivial third cohomology class it gives rise to unconventional edge properties and thus to symmetry-protected topological PEPS. Our identification of the virtual entanglement structure of PEPS with SPT order opens new routes to study transitions between SPT phases by utilizing methods that have been developed to study anyon condensation transitions of topological phases [52, 152].

We demonstrated that applying the quantum state gauging procedure [51] to a SPT PEPS transforms its MPO representation of G into a purely virtual symmetry of the gauged tensors. This implies that the resulting gauge-invariant PEPS also satisfies the axioms of MPO-injectivity, but with a projection MPO onto the injectivity subspace with a block structure labeled by the group elements $g \in G$. This block structure of the projection MPO, together with the third cohomology class label, characterize the phases of the twisted quantum double models which are known to have intrinsic topological order. It was shown in Ref.[109] that the projection MPO determines all the topological properties of the gauged PEPS. This relation explains the mechanism behind the braiding statistics approach to SPT phases [126] at the level of the corresponding quantum states. It furthermore reveals that both the gauging

and boundary theory approaches to classifying SPT phases are recast in the PEPS framework as the classification of a common set of MPOs. We have illustrated these concepts for a family of RG fixed-point states, containing a representative for all two-dimensional bosonic SPT phases with a finite on-site symmetry group.

To prove these results we developed new tools to deal with orientation dependent MPO tensors and used them to calculate the symmetry action on monodromy defected and symmetry twisted states and also modular transformations, before and after gauging, in terms of a single tensor.

The general formalism presented in this paper describes both local physical symmetries and topological order of PEPS with virtual MPO symmetries. Furthermore, it captures the general action of a symmetry on a PEPS with topological order and hence yields a natural framework for the study of symmetry-enriched topological phases. The quantum state gauging procedure can be adapted to gauge only a normal subgroup of the global symmetry group of a SPT PEPS, which allows one to explicitly construct families of SET PEPS. An open question is how the corresponding MPOs encode the discrete, universal labels of the SET phase and how to extract them. We further expect that a better understanding of excitations in MPO-injective PEPS [133] will yield insights into the physical properties of SET phases such as symmetry fractionalization. We plan to study these matters in future work [125].

Another question which presents itself is how to generalize the constructions presented in this paper to fermionic systems. It would be interesting to see if applying the same principles to the formalism of fermionic PEPS [68] naturally gives rise to the (partial) classification of fermionic SPT phases based on supercohomology theory [25]. The quantum state gauging procedure works equally well for fermionic systems, but the gauge degrees of freedom are always bosonic. It would thus be interesting to see how fermionic SPT order can be probed in this way.

Our identification of SPT PEPS in 2D as being injective with respect to an injective MPO hints at a hierarchical definition of SPT PEPS in arbitrary dimension with an injective tensor network object associated to each codimension. This appears to recover the cohomological classification of bosonic SPT states in arbitrary dimensions by a generalization of the argument from [111]. We plan to explore this further in future work.

2.A Axioms for MPO-injectivity

This section reviews the axioms of MPO-injectivity as presented in Ref.[109].

We interpret the tensors A of a MPO-injective PEPS as linear maps from the virtual to the physical space and apply a distinguished generalized inverse

A^+ , which gives rise to a projector that can be written as a MPO:

$$\text{Diagram (2.42)} \quad (2.42)$$

We further require this MPO to satisfy the *pulling through* property shown in Eq.(2.43).

$$\text{Diagram (2.43)} \quad (2.43)$$

The same property should also hold where the MPO gets pulled from three virtual indices to one or vice versa. This makes the presence of this MPO locally undetectable in the PEPS. Using the pulling through property, it is easy to check that the requirement for the MPO to be a projector is equivalent to the property shown in Eq.(2.44)

$$\text{Diagram (2.44)} \quad (2.44)$$

We also need a technical requirement such that the properties of the PEPS grow in a controlled way with the number of sites. For example, we want two concatenated tensors to be injective on the support subspace of the projection MPO surrounding these two tensors. For this we need that there exists a tensor X , depicted in (2.45),

$$X := \text{Diagram (2.45)} \quad (2.45)$$

such that we have the *extended inverse* property (2.46).

$$\text{Diagram (2.46)} \quad (2.46)$$

The extended inverse property allows one to prove many useful things like the intersection property or an explicit expression for the ground state manifold on a torus [109]. It turns out that under very reasonable assumptions about the projection MPO the extended inverse condition is automatically satisfied [133].

2.B Uniqueness of SPT PEPS ground state

In this appendix we demonstrate that the parent Hamiltonian of a MPO-injective PEPS with a single block projection MPO has a unique ground state on the torus (i.e. no topological degeneracy). A similar argument holds for higher genus surfaces.

For a Hermitian projection MPO there is no need to keep track of a direction on the internal leg of the MPO, we also ignore the explicit directions on the edges of the PEPS as they are irrelevant to our arguments. We require the following condition (stronger than Eq.(2.58))

We assume the projection MPO has been brought into a form satisfying the *zipper* condition, i.e. there are no off diagonal blocks in the product of two MPO tensors after it has been brought into canonical form, equivalently

$$(2.47)$$

where X is the reduction tensor for multiplication of copies of the MPO which forms a single block representation of the trivial group. This is true of the MPOs arising from fixed point models. For this representation we have the following version of Eq.(2.59)

$$(2.48)$$

we now rewrite this equality in a more suggestive fashion

$$(2.49)$$

in the above, and throughout the remainder of this appendix, we ignore explicit direction dependence as it does not affect the arguments made.

In the framework of MPO-injectivity different ground states of the PEPS parent Hamiltonian on the torus are spanned by tensor networks closed with different Q tensor solutions (see Ref.[109]) connected to MPOs on the virtual level along the inequivalent noncontractible loops of the torus

$$(2.50)$$

From the physical level one only has access to the Q tensor projected onto the support subspace of a MPO loop along the closure of the system.


(2.51)

Note this closure gives rise to the same ground state as the closed loop is a symmetry of the closed MPO-injective tensor network. Using condition (2.47) repeatedly (within the closed tensor network) leads to the following crossing tensor


(2.52)

which again gives rise to the same ground state. Following several more applications of Eqs.(2.47) & (2.49) we arrive at

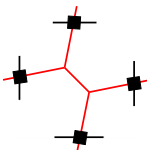

(2.53)

Note the overall phase of the ground state is irrelevant. Since the Q tensor can be placed anywhere in the tensor network we have that the following matrix



$$M_Q :=$$
(2.54)

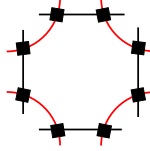
commutes through the virtual level of the single block (injective) projection MPO and hence must be proportional to the identity $M_Q = 1$. Plugging this in we have the following crossing tensor


(2.55)

which, by Eq.(2.47), yields the same state as the following


(2.56)

and with several applications of Eqs.(2.47) & (2.49) one can verify that this is equivalent to



(2.57)

which is easily seen to be a symmetry of a closed MPO-injective tensor network which hence yields the trivial ground state. To summarize we have seen that any Q tensor solution gives rise to the unique ground state obtained by closing the tensor network without any MPOs on the virtual level.

2.C Third cohomology class of a single block MPO group representation

In this appendix we recount the definition of the third cohomology class of an injective MPO representation of a finite group G , as first introduced in Ref.[111]. For details about group cohomology theory in the context of SPT order we refer the reader to Ref.[24].

In a MPO representation of G , multiplying a pair of MPOs labeled by the group elements g_0 and g_1 is equal to the MPO labeled by g_0g_1 for every length. Since the MPOs are injective we again know there exists a gauge transformation on the virtual indices of the MPO that brings both representations into the same canonical form [36]. This implies that there exists an operator (the reduction tensor) $X(g_0, g_1) : (\mathbb{C}^\times)^{\otimes 2} \rightarrow \mathbb{C}^\times$ such that Eq.(2.58) holds.

(2.58)

note $X(g_0, g_1)$ is only defined up to multiplication by a complex phase $\beta(g_0, g_1)$. If we now multiply three MPOs labeled by g_0, g_1 and g_2 there are two ways to reduce the multiplied MPOs to the MPO labeled by $g_0g_1g_2$. When only acting on the right virtual indices these two reductions are equivalent up to a nonzero complex number labeled by g_0, g_1 and g_2 . This is shown in

Eq.(2.59).

$$\begin{array}{c}
 \begin{array}{c}
 \bullet \\ \uparrow g_0 \\ \bullet \\ \uparrow g_1 \\ \bullet \\ \uparrow g_2 \\ \bullet \\ \uparrow g_3
 \end{array}
 \begin{array}{c}
 \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow
 \end{array}
 \begin{array}{c}
 X(g_0, g_1) \\ X(g_0, g_1, g_2)
 \end{array}
 \end{array}
 = \alpha(g_0, g_1, g_2)
 \begin{array}{c}
 \begin{array}{c}
 \bullet \\ \uparrow g_0 \\ \bullet \\ \uparrow g_1 \\ \bullet \\ \uparrow g_2 \\ \bullet \\ \uparrow g_3
 \end{array}
 \begin{array}{c}
 \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow
 \end{array}
 \begin{array}{c}
 X(g_0, g_1, g_2) \\ X(g_1, g_2)
 \end{array}
 \end{array}
 \quad (2.59)$$

By multiplying four MPOs one sees that α has to satisfy certain consistency conditions as the two different paths achieving the same reduction, shown in Eq.(2.60), should give rise to the same complex number.

$$\begin{array}{c}
 \begin{array}{c}
 \bullet \\ \uparrow g_0 \\ \bullet \\ \uparrow g_1 \\ \bullet \\ \uparrow g_2 \\ \bullet \\ \uparrow g_3
 \end{array}
 \begin{array}{c}
 \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow
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 \end{array}
 \rightarrow
 \begin{array}{c}
 \begin{array}{c}
 \bullet \\ \uparrow g_0 \\ \bullet \\ \uparrow g_1 \\ \bullet \\ \uparrow g_2 \\ \bullet \\ \uparrow g_3
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 \begin{array}{c}
 \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow
 \end{array}
 \begin{array}{c}
 \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow
 \end{array}
 \end{array}
 \rightarrow
 \begin{array}{c}
 \begin{array}{c}
 \bullet \\ \uparrow g_0 \\ \bullet \\ \uparrow g_1 \\ \bullet \\ \uparrow g_2 \\ \bullet \\ \uparrow g_3
 \end{array}
 \begin{array}{c}
 \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow
 \end{array}
 \begin{array}{c}
 \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow
 \end{array}
 \end{array}
 \downarrow
 \begin{array}{c}
 \begin{array}{c}
 \bullet \\ \uparrow g_0 \\ \bullet \\ \uparrow g_1 \\ \bullet \\ \uparrow g_2 \\ \bullet \\ \uparrow g_3
 \end{array}
 \begin{array}{c}
 \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow
 \end{array}
 \begin{array}{c}
 \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow
 \end{array}
 \end{array}
 \rightarrow
 \begin{array}{c}
 \begin{array}{c}
 \bullet \\ \uparrow g_0 \\ \bullet \\ \uparrow g_1 \\ \bullet \\ \uparrow g_2 \\ \bullet \\ \uparrow g_3
 \end{array}
 \begin{array}{c}
 \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow
 \end{array}
 \begin{array}{c}
 \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow
 \end{array}
 \end{array}
 \quad (2.60)$$

Using Eq.(2.59) one can easily verify that the consistency conditions are

$$\frac{\alpha(g_0, g_1, g_2)\alpha(g_0, g_1g_2, g_3)\alpha(g_1, g_2, g_3)}{\alpha(g_0g_1, g_2, g_3)\alpha(g_0, g_1, g_2g_3)} = 1 \quad (2.61)$$

which are exactly the 3-cocycle conditions and hence α is a 3-cocycle. As mentioned above $X(g_0, g_1)$ is only defined up to a complex number $\beta(g_0, g_1)$. This freedom can change the 3-cocycle defined in Eq.(2.59) by

$$\alpha'(g_0, g_1, g_2) = \alpha(g_0, g_1, g_2) \frac{\beta(g_1, g_2)\beta(g_0, g_1g_2)}{\beta(g_0, g_1)\beta(g_0g_1, g_2)} \quad (2.62)$$

thus we see that α is only defined up to a 3-coboundary. For this reason the single block MPO group representation is endowed with the label $[\alpha]$ from the

third cohomology group $H^3(G, \mathbb{C})$. Using the fact that $H^d(G, \mathbb{R}) = \mathbb{Z}_1$ [24] (and that \mathbb{R} as an additive group is isomorphic to \mathbb{R}^+ as a multiplicative group), we thus obtain that the third cohomology class of the MPO representation $[\alpha]$ is an element of $H^3(G, U(1))$.

2.D Orientation dependencies of MPO group representations

In this appendix we go beyond previous treatments of MPO group representations to consider subtleties that arise due to possible orientation dependencies of the tensors. We find a gauge transformation that reverses the orientation of MPO tensors, and use it to define the Frobenius-Schur indicator. We then find several *pivotal* phases and relate them to the 3-cocycle of the MPO group representation.

2.D.1 Orientation reversing gauge transformation

To describe the most general bosonic SPT phases one must use lattices with oriented edges, the internal index of the MPO also carries an orientation which leads to the definition of a pair of possibly distinct MPO tensors which depend on the handedness of the crossing upon which they sit

$$B_+(g) = \begin{array}{c} \uparrow \\ \text{---} g \text{---} \bullet \text{---} \\ \downarrow \end{array}, \quad B_-(g) = \begin{array}{c} \downarrow \\ \text{---} g \text{---} \bullet \text{---} \\ \uparrow \end{array}, \quad (2.63)$$

As shown in Section 2.3 reversing the orientation of the internal MPO index corresponds to inverting the group element which the MPO represents, i.e. $V_{\text{rev}}(g) = V(g^{-1})$. Since this holds for any injective group MPO of arbitrary length standard results from the theory of MPS imply that the local tensors are related by an invertible gauge transformation which we denote Z_g

$$\begin{array}{c} \uparrow \\ \text{---} g \text{---} \bullet \text{---} \\ \downarrow \end{array} = \begin{array}{c} \uparrow \\ \text{---} g \text{---} \triangleleft \text{---} \bullet \text{---} \triangleright \text{---} \\ \downarrow \end{array} \quad (2.64)$$

$$\begin{array}{c} \downarrow \\ \text{---} g \text{---} \bullet \text{---} \\ \uparrow \end{array} = \begin{array}{c} \downarrow \\ \text{---} g \text{---} \triangleleft \text{---} \bullet \text{---} \triangleright \text{---} \\ \uparrow \end{array} \quad (2.65)$$

where we use the following graphical notation for Z_g and related matrices

$$Z_g = \begin{array}{c} \text{---} g \text{---} \triangleleft \text{---} g^{-1} \end{array}, \quad Z_g^T = \begin{array}{c} \text{---} g^{-1} \text{---} \triangleright \text{---} g \end{array} \quad (2.66)$$

$$Z_g^{-1} = \begin{array}{c} \text{---} g^{-1} \text{---} \triangleright \text{---} g \end{array}, \quad (Z_g^{-1})^T = \begin{array}{c} \text{---} g \text{---} \triangleleft \text{---} g^{-1} \end{array} \quad (2.67)$$

which satisfy the relations

$$\begin{array}{c}
 \begin{array}{c} g \\ \leftarrow \blacktriangleleft \end{array} \begin{array}{c} g^{-1} \\ \rightarrow \blacktriangleright \end{array} \begin{array}{c} g \\ \leftarrow \end{array} = \begin{array}{c} g^{-1} \\ \rightarrow \end{array} \\
 \end{array} \tag{2.68}$$

$$\begin{array}{c}
 \begin{array}{c} g^{-1} \\ \leftarrow \end{array} \begin{array}{c} g \\ \rightarrow \blacktriangleleft \end{array} \begin{array}{c} g^{-1} \\ \rightarrow \blacktriangleright \end{array} = \begin{array}{c} g \\ \leftarrow \end{array} \\
 \end{array} \tag{2.69}$$

note while it seems apriori that the gauge transformations in Eq.(2.65) could be independent, the fact that the equation $V_{\text{rev}}(g) = V(g^{-1})$ holds for arbitrary orientations of the PEPS bonds implies that they can be chosen to be the same.

Applying the gauge transformation twice we arrive at the equality

$$\begin{array}{c} \uparrow \\ \bullet \\ \downarrow \end{array} \begin{array}{c} g \\ \leftarrow \end{array} = \begin{array}{c} g \\ \leftarrow \end{array} \begin{array}{c} g^{-1} \\ \rightarrow \blacktriangleleft \end{array} \begin{array}{c} g \\ \leftarrow \end{array} \begin{array}{c} \uparrow \\ \bullet \\ \downarrow \end{array} \begin{array}{c} g \\ \rightarrow \blacktriangleright \end{array} \begin{array}{c} g \\ \rightarrow \blacktriangleright \end{array} \begin{array}{c} g \\ \rightarrow \blacktriangleright \end{array} \tag{2.70}$$

which implies $Z_g(Z_{g^{-1}})^T = \chi_g \mathbb{1}$ for some $\chi_g \in U(1)$ since the MPO is injective. Hence $Z_g = \chi_g Z_{g^{-1}}^T$ i.e.

$$\begin{array}{c} g \\ \leftarrow \end{array} \begin{array}{c} g^{-1} \\ \rightarrow \blacktriangleleft \end{array} = \chi_g \begin{array}{c} g \\ \leftarrow \end{array} \begin{array}{c} g^{-1} \\ \rightarrow \blacktriangleright \end{array} \tag{2.71}$$

where χ_g is analogous to the Frobenius–Schur indicator and can be seen to satisfy $\chi_g = \chi_{g^{-1}}^{-1}$. Note χ_g can be absorbed by redefinition of Z_g whenever $g \neq g^{-1}$, but we will not do so at this point.

2.D.2 Pivotal phases

Since the multiplication of the injective MPOs forms a representation of G we have a local reduction as in Eq.(2.58). Again since this holds for arbitrary orientations of the PEPS bonds the reduction matrix $X(g_0, g_1)$ is the same for left and right handed MPOs. From here on we will work with a stronger restriction on the form of the MPOs such that the following *zipper* condition holds

$$\begin{array}{c} X(g, h) \\ \leftarrow \end{array} \begin{array}{c} gh \\ \uparrow \\ \bullet \\ \downarrow \end{array} \begin{array}{c} X(g, h) \\ \rightarrow \end{array} = \begin{array}{c} g \\ \uparrow \\ \bullet \\ \downarrow \end{array} \begin{array}{c} h \\ \uparrow \\ \bullet \\ \downarrow \end{array} \tag{2.72}$$

this is equivalent to there being no off diagonal blocks in the product of two MPO tensors after it has been brought into canonical form, and is true for MPOs that arise from fixed point models.

Let us now derive a relation between $\mathbb{1}_g \otimes (Z_h^{-1})^T X^{-1}(g, h)$ and $X(gh, h^{-1})$ in terms of a *one-line pivotal phase* which we then proceed to calculate in

terms of the three cocycle α of the MPO group representation. Consider

Diagrammatic equation (2.73) showing the decomposition of a product of two MPOs into a single MPO with a loop. The left side shows two MPOs stacked vertically, with the top one labeled g and the bottom one h . The input and output lines are labeled $X^\dagger(gh, h^{-1})$ and $X(gh, h^{-1})$. This is equal to a single MPO labeled g . This is further equal to a stack of three MPOs labeled g , h , and h with a red loop connecting the two h MPOs. This is equal to a stack of three MPOs labeled g , h , and h^{-1} with blue triangles on the h^{-1} MPO and red loops connecting the h and h^{-1} MPOs. Finally, this is equal to a stack of two MPOs labeled gh and h^{-1} with blue triangles on the h^{-1} MPO and red loops connecting the gh and h^{-1} MPOs. The right side of the equation is labeled (2.73).

which yields the desired equality

Diagrammatic equation (2.74) showing the definition of the phase γ . The left side shows a red line with a blue triangle labeled h^{-1} and a red loop above it, with input and output lines labeled $X^\dagger(g, h)$. This is equal to $\gamma(gh, h^{-1})$ times a red line with a blue triangle labeled h^{-1} and a red loop above it, with input and output lines labeled $X(gh, h^{-1})$. The right side of the equation is labeled (2.74).

where $\gamma(gh, h^{-1})$ is some yet to be determined one-line pivotal phase. We now separate $\gamma(gh, h^{-1})$ into a product of a phase specified by the cocycle α and another phase $b(g, h)$ which we show to be trivial. Multiplying Eq.(2.74) by $X^{-1}(g_0 g_1, g_1^{-1})$ yields

Diagrammatic equation showing the multiplication of γ by an inverse MPO. The left side shows a red line labeled $\gamma(gh, h^{-1})$ with a blue triangle labeled g above it. This is equal to a red line with a blue triangle labeled g above it, which then splits into two red lines. The top line is labeled $X^\dagger(gh, h^{-1})$ and the bottom line is labeled $X^\dagger(g, h)$. The bottom line then loops back to the top line with a blue triangle labeled h^{-1} above it. The right side of the equation is labeled (2.74).

$$\begin{aligned}
 &= \alpha^{-1}(g, h, h^{-1}) \rightarrow \begin{array}{c} X^{\dagger}(g, 1) \\ | \\ X^{\dagger}(h, h^{-1}) \\ | \\ \text{triangle} \\ | \\ g \end{array} \\
 &= \alpha^{-1}(g, h, h^{-1}) b(g, h) \rightarrow \text{---} g \text{---}
 \end{aligned} \tag{2.75}$$

Now considering

$$\begin{array}{c} X^{\dagger}(x, g) \quad x \quad X(x, g) \\ \left. \begin{array}{l} \text{---} X^{\dagger}(g, 1) \text{---} \\ \text{---} X^{\dagger}(h, h^{-1}) \text{---} \\ \text{---} \text{triangle} \text{---} \end{array} \right\} = b(g, h) \rightarrow xg
 \end{array} \tag{2.76}$$

after an application of Eq.(2.59) to the left most reductions tensors we see that $b(g, h) = b(xg, h)$, $\forall x$ and hence b has no dependence on the first input and can be absorbed into the definition of Z_h . Similar reasoning yields another useful equality

$$\begin{array}{c} g^{-1} \\ \left. \begin{array}{l} \text{---} X^{\dagger}(g, h) \text{---} \\ \text{---} \text{triangle} \text{---} \end{array} \right\} = \alpha(g^{-1}, g, h) \rightarrow \begin{array}{c} X(g^{-1}, gh) \\ | \\ \text{---} \end{array}
 \end{array} \tag{2.77}$$

In summary we have have calculated the one-line pivotal phases

$$\begin{aligned}
 \gamma(gh, h^{-1}) &= \alpha^{-1}(g, h, h^{-1}) \\
 \gamma'(gh, h^{-1}) &= \alpha(g^{-1}, g, h)
 \end{aligned} \tag{2.78}$$

We now proceed to define a *pivotal* phase relating the following different reductions of the same left handed MPO tensors

$$\begin{aligned}
 &\begin{array}{c} g \\ \bullet \\ \leftarrow \quad \rightarrow \\ h \\ \bullet \\ \leftarrow \quad \rightarrow \end{array} = \begin{array}{c} X^{\dagger}(h, g) \quad hg \quad X(h, g) \\ \left. \begin{array}{l} \text{---} \text{triangle} \text{---} \\ \text{---} \text{triangle} \text{---} \end{array} \right\} \\ \bullet \\ \leftarrow \quad \rightarrow \end{array} \\
 &= \begin{array}{c} X(g^{-1}, h^{-1}) \quad hg \quad X^{\dagger}(g^{-1}, h^{-1}) \\ \left. \begin{array}{l} \text{---} \text{triangle} \text{---} \\ \text{---} \text{triangle} \text{---} \end{array} \right\} \\ \bullet \\ \leftarrow \quad \rightarrow \end{array}
 \end{aligned} \tag{2.79}$$

Hence

$$\text{Diagram with } X(g^{-1}, h^{-1}) \text{ and } X(h, g) \text{ tensors connected to } \beta(g, h) \quad (2.80)$$

for some pivotal phase $\beta(g, h) \in U(1)$. By making use of Eqs.(2.74,2.77,2.78) we calculate β directly to find

$$\beta(g, h) = \varepsilon(g)\varepsilon(h)\tilde{\beta}(g, h) \quad (2.81)$$

where

$$\varepsilon(g) := \chi_g \alpha(g, g^{-1}, g)$$

$$\tilde{\beta}(g, h) := \frac{\alpha(h, g, g^{-1})}{\alpha(hg, g^{-1}, h^{-1})}$$

we proceed to show that $\varepsilon \cong 1$ and hence $\beta \cong \tilde{\beta}$.

Evaluating β in two different ways as follows

$$\beta(g, h) \text{ (diagram)} = \text{Diagram with } X(h, g) \text{ and } X(g^{-1}, h^{-1}) \text{ tensors} \quad (2.82)$$

$$= \chi_g \chi_h \text{ (diagram with } X(h, g) \text{ and } X(g^{-1}, h^{-1}) \text{ tensors)}$$

$$= \frac{\chi_g \chi_h \beta(h^{-1}, g^{-1})}{\chi_{gh}} \text{ (diagram with } hg \text{ and } (hg)^{-1} \text{ tensors)}$$

leads to the relation on ε

$$\varepsilon(k)\varepsilon(h)\varepsilon(hk) = 1 \quad (2.83)$$

after several applications of the 3-cocycle condition for α .

Using Eq.(2.59) we find

$$\text{Diagram with } g, h, k \text{ and } g^{-1}, h^{-1}, k^{-1} \text{ tensors} = \frac{\alpha(g^{-1}, h^{-1}, h^{-1})}{\alpha(k, h, g)}$$

(2.84)

applying Eq.(2.80) twice to both sides yields the further constraint on β

$$d\beta(a, b, c) := \frac{\beta(a, b)\beta(ab, c)}{\beta(b, c)\beta(a, bc)} = \frac{\alpha(a, b, c)}{\alpha(c^{-1}, b^{-1}, a^{-1})} \quad (2.85)$$

hence α forms a potential obstruction to β being a 2-cocycle. Note that $\tilde{\beta}$ also satisfies Eq.(2.85) as a consequence of the 3-cocycle condition for α and hence the function $\theta(a, b) := \varepsilon(a)\varepsilon(b)$ satisfies the 2-cocycle condition $d\theta(a, b, c) = 1$. This 2-cocycle condition, together with Eq.(2.83), implies that $\varepsilon(a) = \varepsilon(c)$, $\forall a, c \in G$ and since $\varepsilon(1) = 1$ consequently $\varepsilon \equiv 1$ is the constant function. This of course implies $\beta \equiv \tilde{\beta}$ which is the desired result

$$\beta(g, h) = \frac{\alpha(h, g, g^{-1})}{\alpha(hg, g^{-1}, h^{-1})}. \quad (2.86)$$

2.E Crossing tensors

In this Appendix we define four crossing tensors and demonstrate that they are related by phases involving only the 3-cocycle of the MPO representation. We proceed to define a composition operation on the crossing tensors and calculate the resulting crossing tensor. Building upon this result we determine the transformation of a crossing tensor under the global symmetry. Finally we calculate the effect of modular transformations on the crossing tensors.

2.E.1 Definitions

We now introduce several different forms for the crossing tensor (see Eq.(2.15)) that are related by phases which play an important role in our calculations

$$W_R^g(h) := X(g, h)X^+(h, g) = \text{Diagram} \quad (2.87)$$

$$W_L^g(h) := X(h, g)X^+(g, h) = \text{Diagram} \quad (2.88)$$

$$Y_R^g(h) := X^+(gh, h^{-1})[X^+(h, g) \otimes Z_h^{-1}]$$

$$= \begin{array}{c} \begin{array}{c} \xrightarrow{g} \xrightarrow{h} \xrightarrow{g} \\ \downarrow h \\ \xrightarrow{h} \end{array} \end{array} \quad (2.89)$$

$$Y_L^g(h) := [X(h, g) \otimes Z_h]X(g, h^{-1})$$

$$= \begin{array}{c} \begin{array}{c} \xrightarrow{h} \xrightarrow{g} \\ \downarrow h \\ \xrightarrow{h} \end{array} \end{array} \sim \begin{array}{c} \begin{array}{c} \xrightarrow{h^{-1}} \xrightarrow{g} \\ \downarrow h^{-1} \\ \xrightarrow{h^{-1}} \end{array} \end{array} \quad (2.90)$$

note $h \in C(g)$ and each tensor above is treated as a representative of an equivalence class of all crossing tensors that give rise to equal PEPS. Using Eqs.(2.59,2.78) one finds $Y_L^g(h) = \alpha(g, h, h^{-1})W_L^g(h)$, $W_L^g(h) = \alpha^{(g)}(h, h^{-1})^{-1}W_R^g(h^{-1})$, and $W_R^g(h) = \alpha(g, h, h^{-1})Y_R^g(h)$, i.e.

$$\begin{array}{ccc} W_L^g(h) & \xrightarrow{\alpha^{(g)}(h, h^{-1})} & W_R^g(h^{-1}) \\ \alpha(g, h, h^{-1}) \downarrow & & \uparrow \alpha(g, h^{-1}, h) \\ Y_L^g(h) & \xrightarrow{\omega^g(h, h^{-1})} & Y_R^g(h^{-1}) \end{array} \quad (2.91)$$

where

$$\alpha^{(g)}(k, h) := \alpha(g, k, h)\alpha(k, h, g)\alpha^{-1}(k, g, h) \quad (2.92)$$

is the slant product of α (which is a 2-cocycle) and

$$\omega^g(k, h) := \alpha^{(g)}(k, h) \frac{\alpha(g, kh, (kh)^{-1})}{\alpha(g, k, k^{-1})\alpha(g, h, h^{-1})} \quad (2.93)$$

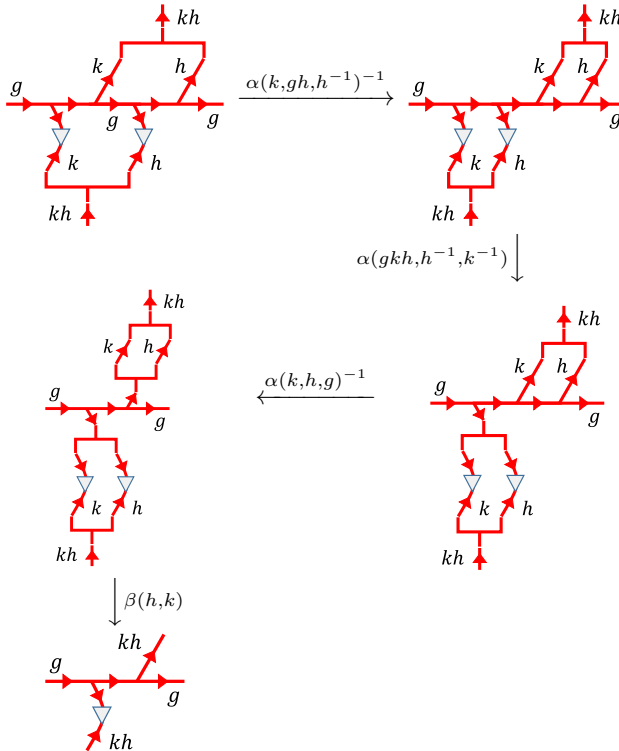
is an equivalent 2-cocycle, i.e. $[\omega^g] = [\alpha^{(g)}]$. One can easily verify that changing α by a 3-coboundary alters $\alpha^{(g)}$ by a 2-coboundary and hence the cohomology class $[\alpha]$ is mapped to $[\alpha^{(g)}]$ by the slant product.

2.E.2 Composition rule

There is a natural composition operation on the $Y_R^g(h)$ tensors induced by the action of a global symmetry $U(k)^{\otimes |\mathcal{M}|v}$, $k \in C(g, h)$, upon a symmetry twisted ground state as follows

$$Y_R^g(k) \times Y_R^g(h) := \begin{array}{c} \begin{array}{c} \xrightarrow{g} \xrightarrow{k} \xrightarrow{h} \\ \downarrow k \quad \downarrow h \\ \xrightarrow{k} \quad \xrightarrow{h} \end{array} \end{array} \quad (2.94)$$

note this product is associative but not commutative. The $Y_R^g(h)$ tensors in fact form a projective representation under this composition rule since



which yields

$$\begin{aligned}
 Y_R^g(k) \times Y_R^g(h) &= \frac{\alpha(k, gh, h^{-1})\alpha(k, h, g)}{\alpha(gkh, h^{-1}, k^{-1})\beta(h, k)} Y_R^g(kh) \\
 &= \alpha^{(g)}(k, h) \frac{\alpha(g, kh, h^{-1}k^{-1})}{\alpha(g, k, k^{-1})\alpha(g, h, h^{-1})} \\
 &\quad \frac{\alpha(k, h, h^{-1}k^{-1})}{\alpha(h, h^{-1}, k^{-1})\beta(h, k)} Y_R^g(kh) \\
 &= \omega^g(k, h) Y_R^g(kh)
 \end{aligned} \tag{2.95}$$

after several applications of the 3-cocycle condition for α , see Eq.(2.61).

2.E.3 Symmetry action

We are now in a position to calculate the effect of applying a global symmetry $k \in C(g, h)$ to an (x, y) symmetry twisted SPT PEPS on a torus as follows

$$g \sim g \quad (2.96)$$

$$\sim g \quad (2.97)$$

$$\sim g \quad (2.98)$$

$$= Y_R^g(k) \times W_R^g(h) \times Y_L^g(k) \quad (2.99)$$

$$= \frac{\alpha(g, h, h^{-1})}{\omega^g(k, k^{-1})} Y_R^g(k) \times Y_R^g(h) \times Y_R^g(k^{-1}) \quad (2.100)$$

$$= \frac{\alpha(g, h, h^{-1})\omega^g(k, h)}{\omega^g(k, k^{-1})} Y_R^g(kh) \times Y_R^g(k^{-1}) \quad (2.101)$$

$$= \frac{\omega^g(k, h)\omega^g(kh, k^{-1})\alpha(g, h, h^{-1})}{\omega^g(k, k^{-1})} Y_R^g(h) \quad (2.102)$$

$$= \frac{\omega^g(k, h)}{\omega^g(h, k)} W_R^g(h) \quad (2.103)$$

where we have made use of the 3-cocycle condition on α and the relations from Eq.(2.91). Hence we have found the group action $\pi_k[\cdot]$ induced on the crossing tensor by the physical symmetry to be

$$\begin{aligned} \pi_k[W_R^g(h)] &= (\omega^g)^{(h)}(k)^{-1} W_R^g(h) \\ &= \alpha^{(g,h)}(k)^{-1} W_R^g(h) \end{aligned} \quad (2.104)$$

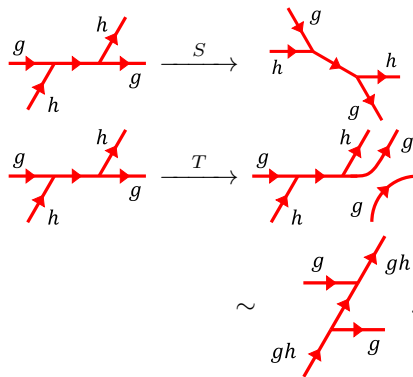
where $(\omega^g)^{(h)}$ is the slant product of ω^g (it is easy to see this equals the coefficient in Eq.(2.96)) and hence a 1D representation of $C(g, h)$ which equals the twice slant product of alpha $(\omega^g)^{(h)} = \alpha^{(g,h)}$ (since the slant product maps cohomology classes to cohomology classes). Now by the

orthogonality of characters we have that the projector $\Pi_{g,h}[\cdot] := \sum_{k \in C(g,h)} \pi_k[\cdot]$ maps a nonzero $W_R^g(h)$ to zero iff $\alpha^{(g,h)}$ is nontrivial i.e.

$$\Pi_{g,h}[W_R^g(h)] \neq 0 \iff \alpha^{(g,h)} \equiv 1. \tag{2.105}$$

2.E.4 Modular transformations

In this section we will calculate the effects of the S and T transformations ($\frac{\pi}{2}$ rotation and Dehn twist respectively) on the crossing tensor $W_R^g(h)$ which is relevant for both symmetry twisted and topological ground states. We use the following left handed convention



(2.106)

Using Eqs.(2.61,2.74,2.77,2.78,2.91) and the 3-cocycle condition on α we find

$$S[W_R^g(h)] = \alpha^{(h)}(g^{-1}, g)^{-1} W_R^h(g^{-1}) \tag{2.107}$$

$$T[W_R^g(h)] = \alpha(g, h, g) W_R^g(gh) \tag{2.108}$$

with these formulas we have explicitly verified that the action of S and T generate a linear representation of the modular group, i.e. they satisfy the relations

$$S^4 = \mathbb{1}, (ST)^3 = S^2.$$

It was sufficient to simply consider the multiplication of these generators since the gauge theories we deal with are doubled topological orders and consequently have zero modular central charge. We do not reproduce the tedious calculation here.

2.F Gauging SPT PEPS yields topological PEPS

In this appendix we recount the definition of the quantum state gauging procedure of Ref.[51] and generalize their proof to show that gauging a SPT PEPS results in a MPO-injective PEPS with a projection MPO that has multiple blocks in its canonical form, labeled by the group elements.

2.F.1 Quantum State Gauging Procedure

Let us first recount the definition of the global projector onto the gauge invariant subspace. This is defined on a directed graph Λ in which the vertices are enumerated and the edges are directed from larger to smaller vertex. To each vertex $v \in \Lambda$ we associate a Hilbert space \mathbb{H}_v together with a representation $U_v(g)$ of the group G and to each edge $e \in \Lambda$ we associate a Hilbert space isomorphic to the group algebra $\mathbb{H}_e \cong \mathbb{C}[G]$. We define the matter Hilbert space $\mathbb{H}_m := \bigotimes_{v \in \Lambda} \mathbb{H}_v$ and the gauge Hilbert space $\mathbb{H}_g := \bigotimes_{e \in \Lambda} \mathbb{H}_e$ which together form the full Hilbert space $\mathbb{H}_{g,m} := \mathbb{H}_g \otimes \mathbb{H}_m$. The states in $\mathbb{H}_{g,m}$ that are relevant for the gauge theory satisfy a local gauge invariance condition at each vertex. Specifically, they lie in the simultaneous $+1$ eigenspace of the following projection operators

$$P_v := \int dg_v U_v(g_v) \bigotimes_{e \in E_v^+} R_e(g_v) \bigotimes_{e \in E_v^-} L_e(g_v) \quad (2.109)$$

where E_v^+ (E_v^-) is the set of adjacent edges directed away from (towards) vertex v . $R(g), L(g)$ are the right and left regular representations, respectively. The projector onto the gauge invariant subspace is given by $P_\Lambda := \prod_v P_v$ and the analogous projector \mathcal{P}_Γ for any operator O supported on a subgraph $\Gamma \subset \Lambda$ (which contains the bounding vertices of all its edges) is defined to be

$$\begin{aligned} \mathcal{P}_\Gamma[O] := & \int \prod_{v \in \Gamma} dg_v \left[\bigotimes_{v \in \Gamma} U_v(g_v) \bigotimes_{e \in \Gamma} L_e(g_{v_e^-}) R_e(g_{v_e^+}) \right] \\ & \times O \left[\bigotimes_{v \in \Gamma} U_v(g_v) \bigotimes_{e \in \Gamma} L_e(g_{v_e^-}) R_e(g_{v_e^+}) \right]^\dagger \end{aligned} \quad (2.110)$$

where edge e points from v_e^+ to v_e^- .

We proceed to describe a gauging procedure for models defined purely on the matter degrees of freedom \mathbb{H}_m . To apply P_Λ and \mathcal{P}_Γ we first require a procedure to embed states and operators from \mathbb{H}_m into $\mathbb{H}_{g,m}$. For this we define the gauging map for matter states $|\psi\rangle \in \mathbb{H}_m$ by

$$G|\psi\rangle := P[|\psi\rangle \bigotimes_e |1\rangle_e], \quad (2.111)$$

and for matter operators $O \in \mathbb{L}(\mathbb{H}_m)$ acting on a subgraph $\Gamma \subseteq \Lambda$ (containing all edges between its vertices) by

$$\mathcal{G}_\Gamma[O] := \mathcal{P}_\Gamma[O \bigotimes_{e \in \Gamma} |1\rangle \langle 1|_e]. \quad (2.112)$$

2.F.2 Gauging SPT PEPS

In this section we show that a gauged SPT PEPS satisfies the axioms of MPO-injectivity.

Consider a region \mathcal{R} of a SPT PEPS $|\psi\rangle \in \mathbb{H}_m$ built from local tensor A . The PEPS map $A_{\mathcal{R}}$ on this region satisfies $A_{\mathcal{R}}^{\dagger} A_{\mathcal{R}} = P_{\partial\mathcal{R}}$ and hence is injective on the support subspace of a single block projection MPO $P_{\partial\mathcal{R}} = V^{\partial\mathcal{R}}(1)$ given by $\text{supp}(P_{\partial\mathcal{R}}) \subseteq (\mathbb{V}_e)^{\otimes L}$ where \mathbb{V}_e denotes the Hilbert space of a virtual index and $L := |\partial\mathcal{R}|_e$.

For the gauged PEPS $G|\psi\rangle \in \mathbb{H}_{g,m}$, the region \mathcal{R} is defined to include only those edges between vertices within \mathcal{R} , i.e. excluding the edges $e \in \partial\mathcal{R}$. Note our proof is easily adapted to the case where the edge degrees of freedom are ‘doubled’ and absorbed into the neighboring vertex degrees of freedom, as in Section 2.7.

The gauged PEPS map on region \mathcal{R} , $A_{\mathcal{R}}^g : (\mathbb{V}_e \otimes \mathbb{C}[G])^{\otimes L} \rightarrow \mathbb{H}_v^{\otimes |\mathcal{R}|_v} \otimes \mathbb{H}_e^{\otimes |\mathcal{R}|_e}$, naturally decomposes into the original PEPS map and a gauging tensor network operator multiplying the physical degrees of freedom $A_{\mathcal{R}}^g = G_{\mathcal{R}} A_{\mathcal{R}}$ where

$$G_{\mathcal{R}} := \int \prod_{v \in \mathcal{R}} dg_v \bigotimes_{v \in \mathcal{R}} U_v(g_v) \bigotimes_{e \in \mathcal{R}} |g_{v_e^-} g_{v_e^+}^{-1}\rangle_e \bigotimes_{e \in \partial\mathcal{R}} (g_{v_e^{\pm}}|_e \quad (2.113)$$

where $v_e^{\pm} \in \mathcal{R}$ denotes the unique vertex in \mathcal{R} adjacent to the edge $e \in \partial\mathcal{R}$.

Proposition 5. *A generalized inverse of the gauged PEPS is given by $(A_{\mathcal{R}}^g)^{\dagger} = A_{\mathcal{R}}^{\dagger} G_{\mathcal{R}}^{\dagger}$ which satisfies $(A_{\mathcal{R}}^g)^{\dagger} A_{\mathcal{R}}^g = \frac{1}{|G|} \sum_{g \in G} V^{\partial\mathcal{R}}(g) \otimes R(g)^{\otimes L}$. Furthermore,*

the gauged PEPS is MPO-injective with respect to the projection MPO $\frac{1}{|G|} \sum_{g \in G} V^{\partial\mathcal{R}}(g) \otimes R(g)^{\otimes L}$ which is a sum of single block injective MPOs labeled by $g \in G$.

Firstly we have

$$\begin{aligned} G_{\mathcal{R}}^{\dagger} G_{\mathcal{R}} &= \int \prod_{v \in \mathcal{R}} dh_v dg_v \bigotimes_{v \in \mathcal{R}} U_v(h_v^{-1} g_v) \\ &\quad \bigotimes_{e \in \mathcal{R}} \langle h_{v_e^-} h_{v_e^+}^{-1} | g_{v_e^-} g_{v_e^+}^{-1} \rangle \bigotimes_{e \in \partial\mathcal{R}} |h_{v_e^{\pm}}\rangle (g_{v_e^{\pm}}|_e \\ &= \int dg \bigotimes_{v \in \mathcal{R}} U_v(g) \bigotimes_{e \in \partial\mathcal{R}} R_e(g) \end{aligned} \quad (2.114)$$

since the delta conditions $\langle h_{v_e^-} h_{v_e^+}^{-1} | g_{v_e^-} g_{v_e^+}^{-1} \rangle$ force $h_{v_e^-}^{-1} g_{v_e^-} = h_{v_e^+}^{-1} g_{v_e^+}$ and hence $h_v^{-1} g_v =: g$ is constant across all $v \in \mathcal{R}$, assuming \mathcal{R} is connected. Hence

$$A_{\mathcal{R}}^{\dagger} G_{\mathcal{R}}^{\dagger} G_{\mathcal{R}} A_{\mathcal{R}} = P_{\partial\mathcal{R}} \int dg V^{\partial\mathcal{R}}(g) \bigotimes_{e \in \partial\mathcal{R}} R_e(g) \quad (2.115)$$

since $U(g)^{\otimes |\mathcal{R}|_v} A_{\mathcal{R}} = A_{\mathcal{R}} V^{\partial\mathcal{R}}(g)$ for a SPT PEPS (see Section 2.3) then the result follows as $P_{\partial\mathcal{R}} V^{\partial\mathcal{R}}(g) = V^{\partial\mathcal{R}}(g)$.

Let us now address the remaining conditions for MPO-injectivity. Most importantly the pulling through condition is easily seen to hold by Eq.(2.3) and since $P_v U_v^\dagger(g) = P_v \otimes_{e \in E_v^+} R_e(g) \otimes_{e \in E_v^-} L_e(g)$, see Appendix 2.G, Proposition 13 for more detail. The trivial loops condition for the MPO $V^{\partial\mathcal{R}}(g) \otimes R(g)^{\otimes L}$ follows directly from the trivial loops condition for $V^{\partial\mathcal{R}}(g)$ and the convention that $R(g)$ is inverted depending on the orientation of the crossing of the MPO loop with the virtual bond edge of the PEPS graph, see Eqs.(2.3),(2.4). Finally, as discussed at the end of Appendix 2.A the extended inverse condition is automatically satisfied when the projection MPO has a canonical form with injective blocks [133], which is the case for the MPO $V^{\partial\mathcal{R}}(g) \otimes R(g)^{\otimes L}$.

2.G Generalizing the gauging procedure to arbitrary flat G-connections

In this section we outline a generalization of the gauging procedure defined in Ref.[51] to arbitrary flat G-connections. For equivalent G-connections the gauging maps are related by local operations while for inequivalent G-connections, which are necessary to construct the full ground space of a gauged model on a nontrivial manifold, the gauging maps are topologically distinct. The gauging maps for nontrivial flat G-connections take inequivalent symmetry twisted states of the initial SPT models to orthogonal ground states of the topologically ordered gauged models.

2.G.1 Elementary definitions

Definition 1. A G-connection ϕ on a directed graph Λ , embedded in an oriented 2-manifold \mathcal{M} , is given by specifying a group element $\phi_e \in G$ for each edge $e \in \Lambda$.

$$\begin{aligned} \phi : \Lambda_e &\rightarrow G \\ e &\mapsto \phi_e \end{aligned}$$

ϕ can be thought of as a labeling $\{\phi_e\}$ of the edges in Λ by group elements $\phi_e \in G$. We view these connections as basis states $|\phi\rangle := \otimes_e |\phi_e\rangle_e \in \mathbb{C}[G]^{\otimes |\Lambda_e|}$.

Each G-connection ϕ defines a notion of transport along any oriented path (with origin and end point specified) $p \in \Lambda$ on the edges of the graph, the transport is specified by the group element

$$\phi_p := \prod_{i=|p|}^1 \phi_{e_i}^{\sigma_i} = \phi_{e_{|p|}}^{\sigma_{|p|}} \cdots \phi_{e_1}^{\sigma_1} \quad (2.116)$$

where the edges $e_i \in p$ are ordered as they occur following p along its orientation, and σ_i is 1 if the orientation of e_i matches that of p and -1 if it does not, see Fig.2.8. Note for paths p^1 , from v_0 to v_1 , and p^2 , from v_1 to v_2 , we have the following relation $\phi_{p^2} \phi_{p^1} = \phi_{p^{12}}$, where $p^{12} := p^1 \cup p^2$ is given by composing paths 1 and 2.

A pair of G-connections ϕ, φ are considered equivalent if they are related by a sequence of local gauge transformations from the set

$$\{a_v^g := \bigotimes_{e \in E_v^+} R_e(g) \bigotimes_{e \in E_v^-} L_e(g) \mid \forall g \in \mathbf{G}, v \in \Lambda\} \quad (2.117)$$

i.e. $\phi \sim \varphi \iff |\phi\rangle = \prod_i a_{v_i}^{g_i} |\varphi\rangle$.

One can easily verify that this constitutes an equivalence relation. Importantly, this equivalence relation preserves the conjugacy class of the G-holonomy ϕ_p of any closed path $p \in \Lambda$ with a fixed base point.

An important class of connections are the flat G-connections which are defined to have trivial holonomy along any contractible path.

Definition 2. A G-connection ϕ is flat iff $\phi_p = 1$ for any closed path $p \in \Lambda$ that is contractible in the underlying manifold \mathcal{M} .

This definition immediately implies that $\phi_p = \phi_{p'}$ for any pair of homotopic oriented paths p, p' with matching endpoints. It is easy to see that a G-connection is flat if and only if it satisfies the local condition $\phi_{\partial q} = 1$ for every plaquette q of the graph $\Lambda \subset \mathcal{M}$, where $\partial q \subset \Lambda$ is the boundary of q with the orientation inherited from \mathcal{M} . Moreover, one can easily verify that flatness is preserved under the equivalence relation (2.117) and hence the flat G-connections form equivalence classes under this relation. Note there can be multiple flat equivalence classes since it is possible for a flat G-connection to have a nontrivial holonomy $\phi_p \neq 1$ along a noncontractible loop $p \in \Lambda \subset \mathcal{M}$.

One can easily show that any contractible region $\Gamma \subseteq \Lambda \subset \mathcal{M}$ (formed by a set of vertices and the edges between them) of a flat G-connection $|\phi\rangle$ can be ‘cleaned’ by a sequence of operations $\prod_i a_{v_i}^{g_i}$, where each $v_i \in \Gamma$, such that the resulting equivalent connection $|\phi'\rangle := \prod_i a_{v_i}^{g_i} |\phi\rangle$ satisfies $\phi'_e = 1, \forall e \in \Gamma$.

Utilizing the cleaning procedure leads one to the following conclusion

Proposition 6. The equivalence class $[\phi]$ of a flat G-connection ϕ on an oriented 2-manifold (w.l.o.g. a genus- n torus or n -torus) \mathcal{M} is labeled uniquely by the conjugacy class of n pairs of group elements that commute with their neighbors, i.e. $\{(x_1, y_1), \dots, (x_n, y_n) \mid \exists x_i, y_i \in \mathbf{G}, x_i y_i = y_i x_i, y_i x_{i+1} = x_{i+1} y_i\}$, the set of such labels is henceforth referred to as $\mathcal{I}_{\mathcal{M}}$.

The argument proceeds as follows: any G-connection can be ‘cleaned’ onto the set of edges that cross any of the $2n$ closed paths $\{(p_x^i, p_y^i)\}$ in the

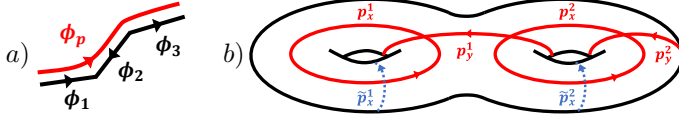


Figure 2.8: a) A simple example $\phi_p = \phi_3\phi_2^{-1}\phi_1$. b) Noncontractible cycles of the 2-torus.

dual graph Λ^* (where each (p_x^i, p_y^i) and (p_y^i, p_x^{i+1}) pair intersect once) that span the inequivalent noncontractible loops of the n -torus, see Fig.2.8. Now by the flatness condition the group elements along any loop must be the same (assuming w.l.o.g. the edges on that loop have the same orientation) and the group elements (x_i, y_i) and (y_i, x_{i+1}) of each pair of intersecting loops must commute. Furthermore, equivalence under the application of $\bigotimes_{v \in \Lambda} a_v^g, \forall g \in G$ implies that every set of labels in the same conjugacy class are equivalent.

Note there is a uniquely defined set of group elements

$$\begin{aligned} \{(x_1, y_1), \dots, (x_n, y_n) \mid x_i, y_i \in G, x_i y_i = y_i x_i, \\ y_i x_{i+1} = x_{i+1} y_i\} \end{aligned} \quad (2.118)$$

for each flat G -connection ϕ which are specified by the G -holonomies $x_i := \phi_{\tilde{p}_x^i}, y_i := \phi_{\tilde{p}_y^i}$ of pairs of paths $(\tilde{p}_y^i, \tilde{p}_x^i)$ in the graph Λ , where \tilde{p}_x^i is defined to be a path that intersects p_x^i once and all other paths $p_y^j, p_x^j, j \neq i$, zero times (\tilde{p}_y^i is defined similarly). Moreover, the conjugacy class $[(x_1, y_1), \dots, (x_n, y_n)] := \{(x_1^h, y_1^h), \dots, (x_n^h, y_n^h) \mid \forall h \in G\}$ labels the equivalence class $[\phi]$ of the G -connection ϕ , where $x^h := h x h^{-1}$.

For a fixed representative $\gamma = \{(x_i, y_i)\}$ of conjugacy class $[\gamma] \in \mathcal{I}_{\mathcal{M}}$ and choice of paths $\{(p_x^i, p_y^i)\}$ spanning the inequivalent noncontractible cycles of the n -torus, we construct a particularly simple representative flat G -connection as follows

Definition 3. *The simple representative flat G -connection ϕ^γ is defined by setting $\phi_e^\gamma := x_i^{\sigma_e^i}$ if p_x^i crosses e and $\phi_e^\gamma := y_i^{\sigma_e^i}$ if p_y^i crosses e , where σ_e^i is $+1$ if the crossing is right handed and -1 if it is left handed, and otherwise $\phi_e^\gamma := 1$ for edges that are not crossed by either p_x^i, p_y^i .*

Note an arbitrary flat connection $|\phi\rangle$ is related to some $|\phi^\gamma\rangle$ by a sequence of local operations $|\phi\rangle = \prod_i a_{v_i}^{g_i} |\phi^\gamma\rangle$. In particular, the representative connection $|\tilde{\phi}^\gamma\rangle$ corresponding to a deformation of the paths $(p_x^i, p_y^i) \mapsto (\tilde{p}_x^i, \tilde{p}_y^i)$ that does not introduce additional intersections (a planar isotopy) is related to $|\phi^\gamma\rangle$ by a sequence of local operations $\prod_i a_{v_i}^{g_i}$ that implements the deformation.

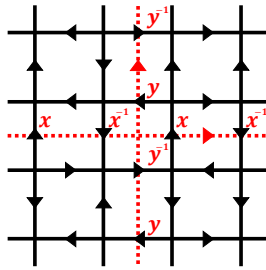


Figure 2.9: A representative flat G connection labeled by (x, y) .

2.G.2 Twisting and gauging operators and states

For any local operator O acting on the matter degrees of freedom in a contractible region $\Gamma \subseteq \Lambda$ there is a well defined notion of twisting O by a flat G -connection ϕ . Fixing a base vertex $v_0 \in \Gamma$ the twisted operator is given by

$$O^\phi := \int dg \bigotimes_{v \in \Gamma} U_v(\phi_{p_v} g) O \bigotimes_{v \in \Gamma} U_v^\dagger(\phi_{p_v} g) \quad (2.119)$$

where p_v is any path from v_0 to v within Γ (the choice does not matter since the connection is flat and Γ is contractible). The choice of distinguished base vertex v_0 is irrelevant since a change $v_0 \mapsto v'_0$ can be compensated by shifting $g \mapsto \phi_{p'}^{-1} g$, where p' is a path from v'_0 to v_0 , which has no effect since g is summed over. Note this definition of O^ϕ first projects O onto the space of symmetric operators, hence the sum over g is unnecessary if O is already symmetric. One can verify that O^ϕ commutes with the following twisted symmetry $\bigotimes_{v \in \Gamma} U_v(g^{\phi_{p_v}})$, $\forall g \in G$, where $g^h = h g h^{-1}$, independent of the choice of base point v_0 and paths $p_v \in \Gamma$ from v_0 to v .

The twisted state gauging map G_ϕ , for a flat G -connection ϕ , is defined by the following action

$$\begin{aligned} G_\phi |\psi\rangle &:= P[|\psi\rangle \otimes |\phi\rangle] \\ &= \int \prod_{v \in \Lambda} dg_v \left[\bigotimes_{v \in \Lambda} U_v(g_v) \right] |\psi\rangle \bigotimes_{e \in \Lambda} |g_{v_e} \phi_e g_{v_e}^{-1}\rangle_e \end{aligned} \quad (2.120)$$

where $|\psi\rangle \in \mathbb{H}_m$ is a state of the matter degrees of freedom. One can verify that $G_\phi^\dagger G_\phi = \int dg \bigotimes_{v \in \Lambda} U_v(g^{\phi_{p_v}}) \prod_i \delta_{g x_i, x_i g} \delta_{g y_i, y_i g}$ is the projection onto the symmetric subspace of the twisted symmetry, where (x_i, y_i) are the pairs of commuting group elements that label ϕ , see Eq.(2.118). The δ conditions arise since the state overlaps force the conjugation of g by the transport group elements $\phi_{p_v}, \phi_{p'_v}$ to agree for non homotopic paths p_v, p'_v from v_0 to v . These δ conditions also ensure the choice of fixed base point v_0 is irrelevant.

The twisted operator gauging map \mathcal{G}_Γ^ϕ is defined similarly

$$\begin{aligned} \mathcal{G}_\Gamma^\phi[O] := & \int \prod_{v \in \Gamma} dg_v \bigotimes_{v \in \Gamma} U_v(g_v) O \bigotimes_{v \in \Gamma} U_v^\dagger(g_v) \\ & \bigotimes_{e \in \Gamma} |g_{v_e^-} \phi_e g_{v_e^+}^{-1}\rangle \langle g_{v_e^-} \phi_e g_{v_e^+}^{-1}| \end{aligned} \quad (2.121)$$

where O is an operator that acts on the matter degrees of freedom on sites $v \in \Gamma \subseteq \Lambda$, and Γ is defined to include all the edges between its vertices. \mathcal{G}_Γ^ϕ is invertible on the space of ϕ -twisted symmetric local operators O^ϕ in the following sense

$$\begin{aligned} \text{Tr}_{e \in \Gamma} [\mathcal{G}_\Gamma^\phi[O^\phi] \bigotimes_{e \in \Gamma} |\phi_e\rangle \langle \phi_e|_e] &= \int \prod_{v \in \Gamma} dg_v \bigotimes_{v \in \Gamma} U_v(g_v) \\ & \quad \times O^\phi \bigotimes_{v \in \Gamma} U_v^\dagger(g_v) \prod_{e \in \Gamma} \delta_{g_{v_e^-} \phi_e g_{v_e^+}^{-1}, \phi_e} \\ &= \int dg_{v_0} \bigotimes_{v \in \Gamma} U_v(g_{v_0}^{\phi_{p_v}}) O^\phi \bigotimes_{v \in \Gamma} U_v^\dagger(g_{v_0}^{\phi_{p_v}}) \\ &= O^\phi \end{aligned} \quad (2.122)$$

where the final equality follows from the twisted symmetry of O^ϕ and the second equality follows since the δ conditions force $g_{v_e^-} = g_{v_e^+}^{\phi_e}$ which implies, after fixing a base point $v_0 \in \Lambda$, that $g_v = g_{v_0}^{\phi_{p_v}}$ for any path p_v from v_0 to v within Γ which is assumed to be contractible in the underlying manifold \mathcal{M} .

For the twisted gauging procedure we also have a version of Proposition 4, which states the useful equality $\mathcal{G}_\Gamma[O]G = GO$ for symmetric O . In the twisted case it must be modified in the following way

Proposition 7. *The identity $\mathcal{G}_\Gamma^\phi[O^\phi]G_\phi = G_\phi O^\phi$ holds for any symmetric operator O .*

We now proceed to show this

$$\begin{aligned} \mathcal{G}_\Gamma^\phi[O^\phi]G_\phi &= \int \prod_{v \in \Gamma} dh_v \bigotimes_{v \in \Gamma} U_v(h_v) O^\phi \bigotimes_{v \in \Gamma} U_v^\dagger(h_v) \\ & \quad \bigotimes_{e \in \Gamma} |h_{v_e^-} \phi_e h_{v_e^+}^{-1}\rangle \langle h_{v_e^-} \phi_e h_{v_e^+}^{-1}| \int \prod_{v \in \Lambda} dg_v \bigotimes_{v \in \Lambda} U_v(g_v) \\ & \quad \bigotimes_{e \in \Lambda} |g_{v_e^-} \phi_e g_{v_e^+}^{-1}\rangle \\ &= \int \prod_{v \in \Lambda} dg_v \prod_{v \in \Gamma} dh_v \bigotimes_{v \in \Lambda} U_v(g_v) \bigotimes_{v \in \Gamma} U_v(g_v^{-1} h_v) O^\phi \end{aligned}$$

$$\begin{aligned} & \bigotimes_{v \in \Gamma} U_v^\dagger(g_v^{-1} h_v) \prod_{e \in \Gamma} \delta_{(g_{v_e^-}^{-1} h_{v_e^-}), (g_{v_e^+}^{-1} h_{v_e^+})^{\phi_e}} \bigotimes_{e \in \Lambda} |g_{v_e^-} \phi_e g_{v_e^+}^{-1}\rangle \\ & = G_\phi O^\phi \end{aligned} \tag{2.123}$$

the last equality follows since the δ condition forces $g_v^{-1} h_v = (g_{v_0}^{-1} h_{v_0})^{\phi_{p_v}}$ (for a fixed choice of vertex v_0 and path $p_v \in \Gamma$ from v_0 to v which has no effect on the outcome) implying $\bigotimes_{v \in \Gamma} U_v(g_v^{-1} h_v) = \bigotimes_{v \in \Gamma} U_v((g_{v_0}^{-1} h_{v_0})^{\phi_{p_v}})$ which is precisely a twisted symmetry that commutes with O^ϕ to yield the desired result.

For a symmetric local Hamiltonian that has been twisted by a flat G-connection ϕ , $H_m^\phi = \sum_v h_v^\phi$, we define the twisted gauged Hamiltonian $(H_m^\phi)^{\mathcal{G}^\phi} := \sum_v \mathcal{G}_{\Gamma_v}^\phi[h_v^\phi]$ in a locality preserving way similar to the untwisted case. With this definition we pose the following proposition

Proposition 8. *For all flat G-connections ϕ we have $(H_m^\phi)^{\mathcal{G}^\phi} = H_m^{\mathcal{G}}$.*

To prove this it suffices to consider a generic local term h_v^ϕ acting on the subgraph Γ_v

$$\begin{aligned} \mathcal{G}_{\Gamma_v}^\phi[h_v^\phi] &= \int \prod_{v \in \Gamma} dg_v \bigotimes_{v \in \Gamma} U_v(g_v) U_v(\phi_{p_v}) h_v \bigotimes_{v \in \Gamma} U_v^\dagger(\phi_{p_v}) \\ & \quad U_v^\dagger(g_v) \bigotimes_{e \in \Gamma} |g_{v_e^-} \phi_e g_{v_e^+}^{-1}\rangle \langle g_{v_e^-} \phi_e g_{v_e^+}^{-1}| \\ &= \int \prod_{v \in \Gamma} dg_v \bigotimes_{v \in \Gamma} U_v(g_v \phi_{p_v}) h_v \bigotimes_{v \in \Gamma} U_v^\dagger(g_v \phi_{p_v}) \\ & \quad \bigotimes_{e \in \Gamma} |g_{v_e^-} \phi_{p_{v_e^-}} \phi_{p_{v_e^+}}^{-1} g_{v_e^+}^{-1}\rangle \langle g_{v_e^-} \phi_{p_{v_e^-}} \phi_{p_{v_e^+}}^{-1} g_{v_e^+}^{-1}| \\ &= \int \prod_{v \in \Gamma} d\tilde{g}_v \bigotimes_{v \in \Gamma} U_v(\tilde{g}_v) h_v \bigotimes_{v \in \Gamma} U_v^\dagger(\tilde{g}_v) \\ & \quad \bigotimes_{e \in \Gamma} |\tilde{g}_{v_e^-} \tilde{g}_{v_e^+}^{-1}\rangle \langle \tilde{g}_{v_e^-} \tilde{g}_{v_e^+}^{-1}| \\ &= \mathcal{G}_{\Gamma_v}[h_v] \end{aligned} \tag{2.124}$$

for the first equality we use the symmetry of h_v , for the second we use the fact $\phi_e = \phi_{p_{v_e^-}} \phi_{p_{v_e^+}}^{-1}$, note the choice of base point v_0 and paths p_v from v_0 to v in Γ have no effect since h_v is symmetric and Γ is contractible, for the third we use the invariance of the Haar measure under the change of group variables $g_v \mapsto \tilde{g}_v := g_v \phi_{p_v}$.

2.G.3 Gauging preserves the gap and leads to a topological degeneracy

We are now in a position to prove that gauging a SPT Hamiltonian defined on an arbitrary oriented 2-manifold \mathcal{M} preserves the energy gap, generalizing the proof presented in Section 2.5.2.

The full gauged Hamiltonian is given by $H_{\text{full}} := H_m^{\mathcal{G}} + \Delta_B H_B + \Delta_P H_P$, see Section 2.5.2 for a discussion of each term in the Hamiltonian. Note by Proposition 8 the same full Hamiltonian H_{full} is achieved by gauging any ϕ -twist of a given SPT Hamiltonian.

As argued in Section 2.5.2, for Δ_B, Δ_P sufficiently large, the low energy subspace of H_{full} lies within the common ground space of H_B and H_P . This subspace is spanned by the states $P[|\lambda\rangle_m \otimes |\phi\rangle_g] = G_\phi |\lambda\rangle$, where the matter states $|\lambda\rangle$ form a basis of \mathbb{H}_m , and the gauge states $|\phi\rangle$ span the flat G-connections. This leads to a generalization of Proposition 3 to arbitrary 2-manifolds

Proposition 9. *For an oriented 2-manifold \mathcal{M} the set of states $\{G_{\phi\gamma} |\lambda\rangle\}$, for $\{|\lambda\rangle\}$ a basis of \mathbb{H}_m and a fixed choice of representatives $\gamma \in [\gamma] \in \mathcal{I}_{\mathcal{M}}$, span the common ground space of H_B and H_P .*

Firstly, by Proposition 6, an arbitrary flat connection $|\phi\rangle$ is related to $|\phi^\gamma\rangle, \exists[\gamma] \in \mathcal{I}_{\mathcal{M}}$ by a sequence of local operations $|\phi\rangle = \prod_i a_{v_i}^{g_i} |\phi^\gamma\rangle$. Since $P_v = \int dg U_v(g) \otimes a_v^g$ one can easily see $P_v a_v^g = P_v U_v^\dagger(g)$ and hence we have

$$\begin{aligned} G_\phi |\psi\rangle_m &= P[|\psi\rangle_m \otimes \prod_i a_{v_i}^{g_i} |\phi^\gamma\rangle_g] \\ &= P[\left[\prod_i U_{v_i}(g_i)\right]^\dagger |\psi\rangle_m \otimes |\phi^\gamma\rangle_g] \\ &= G_{\phi^\gamma} \left[\prod_i U_{v_i}(g_i)\right]^\dagger |\psi\rangle_m. \end{aligned} \tag{2.125}$$

Therefore the common ground space of H_B and H_P is spanned by the states $\{G_{\phi^\gamma} |\lambda\rangle\}_{(\lambda,\gamma)}$ for a basis $\{|\lambda\rangle\}_\lambda$ of \mathbb{H}_m and a representative γ of each conjugacy class $[\gamma] \in \mathcal{I}_{\mathcal{M}}$.

We now bring together the definitions and propositions laid out thus far to show the following

Proposition 10. *Gauging a gapped SPT Hamiltonian on an arbitrary oriented 2-manifold \mathcal{M} yields a gapped local Hamiltonian with a topology dependent ground space degeneracy.*

Let $|\lambda^\gamma\rangle$ denote an eigenstate of the twisted SPT Hamiltonian $H_m^{\phi^\gamma}$ with eigenvalue λ . From Propositions 7 & 8 it follows that gauging an eigenstate of a ϕ -twisted SPT Hamiltonian yields an eigenstate of the gauged Hamiltonian, so we have $H_m^{\mathcal{G}} G_{\phi^\gamma} |\lambda^\gamma\rangle = \lambda G_{\phi^\gamma} |\lambda^\gamma\rangle$.

If H_m has a unique ground state $|\lambda_0\rangle$ Proposition 9 implies the ground space of the full Hamiltonian H_{full} is spanned by the states $\{G_{\phi^\gamma} |\lambda_0^\gamma\rangle\}_\gamma$ and its gap satisfies $\Delta_{\text{full}} \geq \min(\Delta_m, \Delta_B, \Delta_P)$

In the above we have assumed that $G_{\phi^\gamma} |\lambda_0^\gamma\rangle \neq 0$, for some γ . Note $G|\lambda_0\rangle \neq 0$ always holds for a unique ground state $|\lambda_0\rangle$ of a symmetric Hamiltonian (possibly after rephasing the matrices of the physical group representation which is assumed to have occurred).

We now proceed to show that the ground space degeneracy is equal to the number of distinct equivalence classes of symmetry twists which are invariant under the residual physical symmetry. This relies on the assumption that the distinct symmetry twisted SPT Hamiltonians $H_m^{\phi^\gamma}$ each have a nonzero unique ground state $|\lambda_0^\gamma\rangle$ with the same energy λ_0 . We show this to be the case, when the original frustration free SPT Hamiltonian H_m has a SPT PEPS ground state, by explicitly constructing tensor network representations of the twisted ground states, see Definition 4.

Proposition 11. *The overlap matrix of the gauged ground states $M_{[\gamma'],[\gamma]} := \langle \lambda_0^{\gamma'} | G_{\phi^{\gamma'}}^\dagger G_{\phi^\gamma} |\lambda_0^\gamma\rangle$ is diagonal, where γ, γ' are drawn from a fixed set of representatives for the conjugacy classes in \mathcal{I}_M . Furthermore, $M_{[\gamma'],[\gamma]}$ is invariant under a change of representatives and $M_{[\gamma],[\gamma]} = 0$ iff $|\lambda_0^\gamma\rangle$ transforms as a nontrivial representation of the physical symmetry action of $C(\gamma)$.*

The operators $G_\varphi^\dagger G_\phi$ that appear in the overlaps of the gauged twisted ground states imply that they are orthogonal. To see this consider the following

$$\begin{aligned} G_\varphi^\dagger G_\phi &= \int \prod_{v \in \Lambda} dk_v dg_v \bigotimes_{v \in \Lambda} U_v(k_v^{-1} g_v) \\ &\quad \prod_{e \in \Lambda} \langle k_{v_e^-} \varphi_e k_{v_e^+}^{-1} | g_{v_e^-} \phi_e g_{v_e^+}^{-1} \rangle \\ &= \int dg_{v_0} \bigotimes_{v \in \Lambda} U_v(\varphi_{p_v} g_{v_0} \phi_{p_v}^{-1}) \prod_i \delta_{x'_i g_{v_0}, g_{v_0} x_i} \delta_{y'_i g_{v_0}, g_{v_0} y_i} \end{aligned} \quad (2.126)$$

where we have fixed an arbitrary base vertex v_0 , p_v is any path from v_0 to v , and $\{(x'_i, y'_i)\}_i, \{(x_i, y_i)\}_i$ label the connections φ, ϕ respectively. The delta conditions arise since the overlaps in Eq.(2.126) force the transported group element $\varphi_{p_v} g_{v_0} \phi_{p_v}^{-1}$ to agree for any choice of path p_v (which may be homotopically distinct). This implies that $G_\varphi^\dagger G_\phi = 0$ whenever the labels $\{(x'_i, y'_i)\}_i, \{(x_i, y_i)\}_i$ fall into distinct equivalence classes of \mathcal{I}_M . For the particular case of the simple representative G-connections ϕ^γ we have

$$G_{\phi^{\gamma'}}^\dagger G_{\phi^\gamma} = \delta_{[\gamma'],[\gamma]} \int dg \bigotimes_{v \in \Lambda} U_v(g) \prod_i \delta_{x'_i g, g x_i} \delta_{y'_i g, g y_i}$$

for equivalence classes $[\gamma'], [\gamma] \in \mathcal{I}_{\mathcal{M}}$. Furthermore, if $\gamma' \sim \gamma$ then there exists a group element $h \in G$ such that $(x'_i, y'_i) = (x_i^g, y_i^g), \forall i \iff g \in h C(\gamma)$, a left coset of the centralizer of $\gamma = \{x_i, y_i\}_i$. In this case

$$G_{\phi\gamma'}^\dagger G_{\phi\gamma} = \int dg \bigotimes_{v \in \Lambda} U_v(g) \delta_{g \in h C(\gamma)} \quad (2.127)$$

and $H_m^{\phi\gamma'} = U(g)^{\otimes |\Lambda|_v} H_m^{\phi\gamma} U^\dagger(g)^{\otimes |\Lambda|_v}$ for any $g \in h C(\gamma)$, which implies

$$\theta_g^\gamma |\lambda_0^{\gamma'}\rangle = U(g)^{\otimes |\Lambda|_v} |\lambda_0^\gamma\rangle \quad (2.128)$$

for some phase $\theta_g^\gamma \in U(1)$. Hence

$$\langle \lambda_0^\gamma | G_{\phi\gamma'}^\dagger G_{\phi\gamma} | \lambda_0^\gamma \rangle = \theta_h^\gamma \langle \lambda_0^\gamma | G_{\phi\gamma'}^\dagger G_{\phi\gamma} | \lambda_0^{\gamma'} \rangle \iff [\gamma] = [\gamma'].$$

Moreover since $|\lambda_0^\gamma\rangle$ is the unique groundstate of a $C(\gamma)$ -symmetric Hamiltonian $\theta_{(\cdot)}^\gamma$ is a 1D representation of $C(\gamma)$. By the orthogonality of characters we have $G_{\phi\gamma'}^\dagger G_{\phi\gamma} |\lambda_0^\gamma\rangle \neq 0 \iff \theta_{(\cdot)}^\gamma \equiv 1$. Note $\theta_{(\cdot)}^\gamma \equiv 1$ is in fact a property of a conjugacy class as it does not depend on the choice of representative γ .

Consequently the choice of representative symmetry twist $\gamma \in [\gamma] \in \mathcal{I}_{\mathcal{M}}$ does not matter as all lead to the same gauged state $|\lambda_0, [\gamma]\rangle := G_{\phi\gamma} |\lambda_0^\gamma\rangle$. Hence the overlap matrix of the gauged twisted SPT groundstates is given by

$$\begin{aligned} M_{[\gamma'], [\gamma]} &= \langle \lambda_0, [\gamma'] | \lambda_0, [\gamma] \rangle \\ &= \delta_{[\gamma'], [\gamma]} \delta_{\theta_{(\cdot)}^\gamma, 1} \frac{|C(\gamma)|}{|G|} \langle \lambda_0^\gamma | \lambda_0^\gamma \rangle \end{aligned} \quad (2.129)$$

and the set of states $\{|\lambda_0, [\gamma]\rangle \mid [\gamma] \in \mathcal{I}_{\mathcal{M}}, \theta_{(\cdot)}^\gamma \equiv 1\}$ form an orthogonal basis for the ground space of the full gauged Hamiltonian H_{full} .

2.H Symmetry twists & monodromy defects

In this appendix we describe a general and unambiguous procedure for applying symmetry twists to SPT PEPS using virtual symmetry MPOs. We furthermore demonstrate that the gauging procedure maps the symmetry MPOs to freely deformable topological MPOs on the virtual level and hence the gauged symmetry twisted PEPS are locally indistinguishable while remaining globally orthogonal, implying that they exhibit topological order. We move on to discuss how the same MPOs can be arranged along open paths to describe monodromy defects in SPT PEPS and anyons in the gauged PEPS. Moreover, we explicitly calculate the projective transformation of individual monodromy defects under the residual symmetry group using tensor network techniques.

2.H.1 Symmetry twisted states

In this section we discuss the ground states of symmetry twisted Hamiltonians in more detail and show that the PEPS framework naturally accommodates a simple construction of these states.

On a trivial topology a symmetry twist can be applied directly to a state by acting on some region of the lattice with the physical symmetry. For example on an infinite square lattice in the 2D plane a symmetry twist (x, y) along an oriented horizontal and vertical path p_x, p_y , in the dual lattice, acts on a state $|\psi\rangle$ via

$$\begin{aligned} |\psi\rangle^\phi &:= \int dg \bigotimes_{v \in \Gamma} U_v(\phi_{p_v} g) |\psi\rangle \\ &= \bigotimes_{v \in \mathcal{U}} U_v(x) \bigotimes_{v \in \mathcal{R}} U_v(y) \int dg \bigotimes_{v \in \Gamma} U_v(g) |\psi\rangle \end{aligned}$$

where ϕ is the simple representative connection with label (x, y) on paths p_x, p_y , see Definition 3, and \mathcal{R} is the half plane to the right of p_y , \mathcal{U} the half plane above p_x , see Fig.2.5. Note this definition implicitly projects $|\psi\rangle$ onto the trivial representation and we have $O^\phi |\psi\rangle^\phi = (O |\psi\rangle)^\phi$ for symmetric operators O . Hence twisting an eigenstate $|\lambda\rangle$ of a SPT Hamiltonian H_m yields an eigenstate $|\lambda\rangle^\phi$ of the twisted Hamiltonian H_m^ϕ with the same eigenvalue. Note x and y must commute for ϕ to be a flat connection, equivalently if one thinks of first applying the x twist to a symmetric Hamiltonian, then the resulting operator will only be symmetric under the centralizer subgroup of x , $C(x) \leq G$, and hence it only makes sense to apply a second twist for an element $y \in C(x)$.

The effect of such a symmetry twist on a SPT PEPS $|\psi\rangle$ is particularly simple, it can be achieved by adding the virtual symmetry MPOs $V^{p_x}(x)$ and $V^{p_y}(y)$ (with inner indices contracted with the four index crossing tensor $Q_{x,y} = W_R^x(y)$ (2.15,2.87) where p_x, p_y intersect, see Fig.2.6) to the virtual level of the PEPS. Let us denote the resulting tensor network state $|\psi^{(x,y)}\rangle$, then by Eq.(2.3) we have $|\psi^{(x,y)}\rangle = |\psi\rangle^\phi$.

For nontrivial topologies the symmetry twist on a state $|\psi\rangle^{\phi^\gamma}$ is not well defined in terms of a physical symmetry action since two homotopically inequivalent paths p_v, p'_v can give rise to distinct transport elements $\phi_{p_v} \neq \phi_{p'_v}$. Note this problem does not arise when symmetry twisting local operators, such as the terms in a local Hamiltonian, since each operator acts within a contractible region. The PEPS formalism yields a simple resolution to this problem since the process of applying a symmetry twist ϕ^γ on the virtual level of a PEPS $|\psi^\gamma\rangle$ remains well defined, see Definition 4 and Fig.2.10.

The general scenario is as follows; we have a local gapped frustration free SPT Hamiltonian H_m defined on an oriented 2-manifold \mathcal{M} with a SPT PEPS $|\lambda_0\rangle$ as its unique ground state (note SPT PEPS parent Hamiltonians

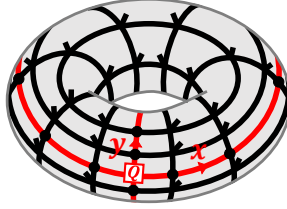


Figure 2.10: An (x, y) symmetry twisted PEPS on a torus.

satisfy these conditions) and we want to apply a symmetry twist along paths p_x^i, p_y^i in the dual graph labeled by $\gamma = \{(x_i, y_i)\}_i$.

Definition 4 (Symmetry Twisted SPT PEPS). *For a SPT PEPS $|\psi\rangle$ and a symmetry twist γ , specified by a set of pairwise intersecting paths in the dual graph $\{p_x^i, p_y^i\}_i$ and pairwise commuting group elements $\{(x_i, y_i)\}_i$ in \mathcal{G} , the symmetry twisted PEPS $|\psi^\gamma\rangle$ is constructed by taking the tensor network for $|\psi\rangle$ with open virtual indices on edges that cross $\{p_x^i, p_y^i\}_i$ and contracting these virtual indices with the MPOs $\{V^{p_x^i}(x_i), V^{p_y^i}(y_i)\}_i$. Moreover, at the intersection of the paths $p_x^i \cap p_y^i$ the internal indices of the MPOs $V^{p_x^i}(x_i), V^{p_y^i}(y_i)$ are contracted with four index crossing tensors $Q_{x_i, y_i} = W_R^{x_i}(y_i)$, defined in Eqs.(2.15,2.87) and similarly with $Q_{y_{i-1}, x_i} = W_R^{y_{i-1}}(x_i)$ at the intersections $p_y^{i-1} \cap p_x^i$. This is depicted in Fig. 2.10.*

It follows from Eq.(2.3) and the zipper condition (2.72) for $X(x_i, y_i)$ that the symmetry twisted ground state SPT PEPS $|\lambda_0^\gamma\rangle$ is the ground state of the twisted SPT Hamiltonian $H_m^{\phi^\gamma}$. More generally for any SPT PEPS $|\psi\rangle$ that is an eigenstate of each local term in H_m , Eq.(2.3) implies that $|\psi^\gamma\rangle$ is an eigenstate of $H_m^{\phi^\gamma}$ with the same eigenvalue (thereby justifying the notation). Note the twisted SPT PEPS $|\psi^\gamma\rangle$ for different choices of representative γ from the same conjugacy class $[\gamma] \in \mathcal{I}_{\mathcal{M}}$ are all related by the action of some global symmetry, which again follows from Eqs.(2.3),(2.72) and Proposition 6.

Proposition 12. *A γ -twisted SPT PEPS $|\psi^\gamma\rangle$ transforms as the following 1D representation*

$$\theta_{(\cdot)}^\gamma = \alpha^{(x_0, y_0)}(\cdot)^{-1} \prod_{i=1} [\alpha^{(y_{i-1}, x_i)}(\cdot) \alpha^{(x_i, y_i)}(\cdot)]^{-1} \quad (2.130)$$

under the physical action of the residual symmetry group $\mathcal{C}(\gamma)$.

The physical action of the symmetry $U(k)^{\otimes |\mathcal{M}|_v}$ induces a local action π_k on each crossing tensor $\{W_R^{x_i}(y_i), W_R^{y_{i-1}}(x_i)\}_i$ and by Eq.(2.104) we find the combined action to be $\alpha^{(x_0, y_0)}(\cdot)^{-1} \prod_{i=1} [\alpha^{(y_{i-1}, x_i)}(\cdot) \alpha^{(x_i, y_i)}(\cdot)]^{-1}$ as claimed.

2.H.2 Topological ground states

We now show that the twisted gauging procedure maps the virtual symmetry MPO to a freely deformable topological MPO on the virtual level.

Proposition 13. *Applying the twisted gauging map $G_{\phi\gamma}$ to a nonzero twisted SPT PEPS $|\psi^\gamma\rangle$ yields the MPO-injective PEPS $G|\psi\rangle$ with a set of freely deformable MPOs joined by crossing tensors, specified by $[\gamma]$, acting on the virtual level. The gauged state is zero iff $|\psi^\gamma\rangle$ transforms nontrivially under the residual symmetry group $C(\gamma)$, this property depends only on $[\gamma]$ and $[\alpha]$.*

We will first show that the tensor network $G_{\phi\gamma}|\psi^\gamma\rangle$ is given by contracting the MPOs $[V^{p_x^i}(x_i) \otimes_{e \in p_x^i} R_e(x_i)]$, $[V^{p_y^i}(y_i) \otimes_{e \in p_y^i} R_e(y_i)]$ (contracted with the crossing tensor $Q_{x_i, y_i} = W_R^{x_i}(y_i)$ at $p_x^i \cap p_y^i$) with the virtual indices of $G|\psi\rangle$ on edges that cross the paths $\{p_x^i, p_y^i\}$.

In general G_ϕ is a PEPO with vertex tensors $G_\phi^v = \int dg U_v(g) \otimes_{e \in E_v} (g| = G^v$ and edge tensors $G_\phi^e = \int dg_{v_e^+} dg_{v_e^-} L_e(g_{v_e^-}) R_e(g_{v_e^+}) |\phi_e\rangle \otimes (g_{v_e^+} | (g_{v_e^-} |$ [51]. Furthermore the edge tensors satisfy $G_\phi^e = G_1^e(R(\phi_e) \otimes \mathbb{1}) = G_1^e(\mathbb{1} \otimes R^\dagger(\phi_e))$. Hence the PEPO G_ϕ is given by the untwisted gauging map G with the tensor product operators $\{\otimes_{e \in p_x^i} R_e(x_i), \otimes_{e \in p_y^i} R_e(y_i)\}$ applied to the virtual indices that cross $\{p_x^i, p_y^i\}$.

Eqs.(2.3) and (2.72) together with $P_v a_v^g = P_v U_v^\dagger(g)$ imply $G_{\phi\gamma}|\psi^\gamma\rangle = G_{\phi\tilde{\gamma}}|\psi^{\tilde{\gamma}}\rangle$ for any deformation $\tilde{\gamma} = \{\tilde{p}_x^i, \tilde{p}_y^i\}$ of the paths $\gamma = \{p_x^i, p_y^i\}$ that does not introduce additional intersections (a planar isotopy). This furthermore implies that the MPOs $[V^p(g) \otimes_{e \in p} R_e(g)]$ satisfy the pulling through condition of Ref.[109] for any path p . Consequently, the MPO $\frac{1}{|G|} \sum_g [V^p(g) \otimes_{e \in p} R_e(g)]$, that was shown to be the projection onto the injectivity subspace of the gauged PEPS in Appendix 2.F, also satisfies the pulling through condition.

By Proposition 11 the gauged SPT PEPS $G_{\phi\gamma}|\psi^\gamma\rangle$ is zero iff $\theta_{(\cdot)}^\gamma$ is non-trivial, which is a property of the conjugacy class $[\gamma]$. Now by Proposition 12 and the fact that the slant product maps cohomology classes to cohomology classes we have the stated result.

Hence the nonzero gauged symmetry twisted PEPS ground states $|\lambda_0, [\gamma]\rangle := G_{\phi\gamma}|\lambda_0^\gamma\rangle$ are topologically ordered since the tensors Q_{x_i, y_i} that determine the ground state are locally undetectable, which follows from the pulling through condition satisfied by the topological MPOs and Eq.(2.72), while for $[\gamma] \neq [\gamma']$ the states are globally orthogonal $\langle \lambda_0, [\gamma] | \lambda_0, [\gamma'] \rangle = 0$, as shown above.

In fact there is a slight subtlety, as while the reduced density matrices for all $[\gamma], [\gamma'] \in \mathcal{I}_M$ are supported on the same subspace $\rho_{\mathcal{R}}^{\lambda_0, [\gamma]}, \rho_{\mathcal{R}}^{\lambda_0, [\gamma']} \in \text{Im}(A_{\mathcal{R}} \otimes A_{\mathcal{R}}^\dagger)$ for any contractible region \mathcal{R} , they are not necessarily equal [106] (or even exponentially close in the size of the region). One might also fret over the possibility that the state exhibits spontaneous symmetry breaking.

However neither of these complications can occur for the gauged symmetry twisted SPT PEPS, since an exact isometric fixed point SPT PEPS does not exhibit symmetry breaking and is gauged to a topologically ordered fixed point state which also does not exhibit symmetry breaking (see Section 2.7). Furthermore the gauging map is gap preserving, hence gauging any SPT PEPS in the same phase as an SPT fixed point maps it to a topological PEPS in the same phase as the gauged topological fixed point PEPS.

2.H.3 Monodromy defects in SPT PEPS

Monodromy defects can be created in a SPT theory by applying a symmetry twist along an open ended path in the dual graph p_g from plaquette q_0 to q_1 , specified by a G-connection ϕ^{p_g} , where $\phi_e^{p_g} = 1$, for $e \notin p_g$ and $\phi_e^{p_g} = g^{\sigma_e}$ for $e \in p_g$ (σ_e is +1 if p_g crosses e in a right handed fashion and -1 for left handed crossings) hence ϕ^{p_g} is flat on every plaquette except q_0, q_1 , the end points of p_g , see Fig.2.11. The defect states can be realized as ground states of some twisted Hamiltonians $H_m^{\phi^{p_g}} = \sum_{q \in \Lambda \setminus \partial p_g} h_q^{\phi^{p_g}} + h'_{q_0} + h'_{q_1}$ where the choice of the end terms h'_{q_0}, h'_{q_1} is somewhat arbitrary. These monodromy defects can be introduced into a SPT PEPS $|\psi\rangle$ following the framework set up for symmetry twists.

Definition 5 (Monodromy defected SPT PEPS). *A monodromy defect specified by p_g in a SPT PEPS $|\psi\rangle$ is described by a set of tensor network states parametrized by a pair of tensors B_0, B_1 where $B_0 : (\mathbb{C}^D)^{\otimes |E_{v_0}|} \otimes \mathbb{C}^\chi \rightarrow \mathbb{C}^d$ is a local tensor associated to a vertex $v_0 \in \partial q_0$ with a set of indices matching those of the tensor A_{v_0} , and an extra virtual index of the same bond dimension χ as the internal index of the MPO (B_1 is defined similarly).*

The monodromy defected tensor network states $|\psi^{p_g}, B_0, B_1\rangle$ are constructed from the SPT PEPS $|\psi\rangle$ by replacing the PEPS tensors A_{v_0}, A_{v_1} with B_0, B_1 and contracting the extra virtual indices thus introduced with the open end indices of the MPO $V^{p_g}(g)$ which acts on the virtual indices of the PEPS that cross p_g . This is depicted in Fig. 2.12 b).

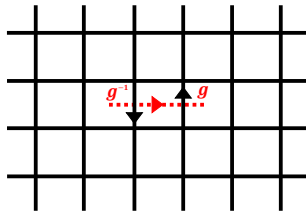


Figure 2.11: A symmetry twist g along an open path.

This provides an ansatz [133] for symmetry twists by choosing appropriate boundary tensors B_0, B_1 to close the free internal MPO indices at q_0, q_1 , the possibility of different boundary conditions corresponds to the ambiguity in the local Hamiltonian terms h'_{q_0}, h'_{q_1} , see Figs.2.11,2.12. Eq.(2.3) implies that the defect state ansatz $|\psi^{p_g}, B_0, B_1\rangle$ is in the ground space of the sum of Hamiltonian terms away from the end points of p_g , $\sum_{q \in \Lambda \setminus \partial p_g} h_q^{\phi^{p_g}}$, for any choice of tensors B_0, B_1 .

Since the connection ϕ^{p_g} is flat everywhere but q_0, q_1 , the gauging map can be applied, in the usual way, to operators that are supported away from these plaquettes. Hence the twisted gauged defect Hamiltonian is $(H_m^{\phi^{p_g}})^{S^{\phi^{p_g}}} := \sum_{q \in \Lambda \setminus \partial p_g} \mathfrak{G}_{\Gamma_q}^{\phi^{p_g}} [h_q^{\phi^{p_g}}] + h''_{q_0} + h''_{q_1}$ where again there is an ambiguity in the choice of end terms h''_{q_0}, h''_{q_1} . The SPT PEPS with monodromy defect p_g can be gauged via the standard gauging procedure for the G-connection ϕ^{p_g} to yield the tensor network $G_{\phi^{p_g}} |\psi^{p_g}, B_0, B_1\rangle$. Similar to the case of symmetry twists on closed paths, the gauged defect SPT PEPS $G_{\phi^{p_g}} |\psi^{p_g}, B_0, B_1\rangle$ is constructed from the untwisted gauged SPT PEPS $G |\psi\rangle$ by removing the tensors $G^{v_0} A_{v_0}, G^{v_1} A_{v_1}$ and replacing them with the pair of tensors $G^{v_0} B_0, G^{v_1} B_1$ connected by a virtual MPO $[V^{p_g}(g) \otimes_{e \in p_g} R_e(g)]$ acting on the virtual indices of the PEPS that cross p_g . Note the dimension of the inner indices of this MPO match the extra indices of $G^{v_0} B_0, G^{v_1} B_1$ since the newly introduced component of the MPO $\otimes_{e \in p_g} R_e(g)$ has trivial inner indices. To achieve a more general ansatz one may want to replace $G^{v_0} B_0, G^{v_1} B_1$ by arbitrary tensors $\tilde{B}_0, \tilde{B}_1 : (\mathbb{C}^D \otimes \mathbb{C}[G])^{\otimes |E_v|} \otimes \mathbb{C}^X \rightarrow \mathbb{C}^d$.

As shown above, the MPO $[V^{p_g}(g) \otimes_{e \in p_g} R_e(g)]$ satisfies the pulling through condition of Ref.[109] and hence $G_{\phi^{p_g}} |\psi^{p_g}, B_0, B_1\rangle = G_{\phi^{p'_g}} |\psi^{p'_g}, B_0, B_1\rangle$ for p'_g an arbitrary, end point preserving, deformation of p_g . By Eq.(2.124) we have $\mathfrak{G}_{\Gamma_q}^{\phi^{p_g}} [h_q^{\phi^{p_g}}] = \mathfrak{G}_{\Gamma_q} [h_q]$ and hence the gauged defect SPT PEPS $G_{\phi^{p_g}} |\psi^{p_g}, B_0, B_1\rangle$, for all B_0, B_1 , is in the ground space of the sum of gauged Hamiltonian terms away from the end points $\sum_{q \in \Lambda \setminus \partial p_g} \mathfrak{G}_{\Gamma_q} [h_q]$. Consequently $G_{\phi^{p_g}} |\psi^{p_g}, B_0, B_1\rangle$ must represent a superposition of anyon pairs, localized to the plaquettes q_0, q_1 , on top of the vacuum (ground state). Furthermore the freedom in choosing B_0, B_1 leads to a fully general anyon ansatz within the framework of MPO-injective PEPS [133].

2.H.4 Projective symmetry transformation of monodromy defects

We proceed to show that the internal degrees of freedom of a monodromy defect p_g transform under a projective representation of the residual global symmetry group $C(g)$ via a generalization of the mechanism for virtual symmetry actions in MPS [43, 104, 105].

We consider a SPT PEPS on an oriented manifold \mathcal{M} with a twice punctured sphere topology and a symmetry twist p_g running from one puncture

Π_0 to the other Π_1 . This captures both the case of a symmetry twisted SPT model defined on a cylinder (when the virtual bonds that enter the punctures are left open), and the case of a pair of monodromy defects on a sphere (when the punctures are formed by removing a pair of PEPS tensors A_{v_0}, A_{v_1} and contracting the virtual indices thus opened with B_0, B_1), see Fig. 2.12.

The bulk of the symmetry twisted state is invariant under the physical on-site representation $U(h)^{\otimes |\mathcal{M}|_v}$ of $C(g) \leq G$, but this may have some action on the virtual indices that enter the punctures. Treating the SPT PEPS on a cylinder of fixed radius as a one dimensional symmetric MPS implies, by well established arguments [104, 105], that the action of the symmetry on the virtual boundaries $\mathcal{V}_0^g(h) \otimes \mathcal{V}_1^g(h)$ forms a representation, while each individual boundary action $\mathcal{V}_0^g(h), \mathcal{V}_1^g(h)$ is free to form a projective representation.

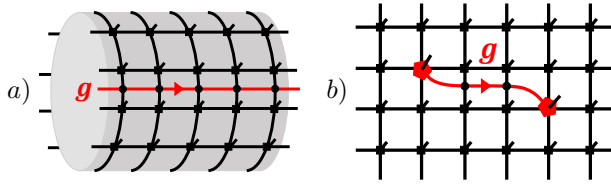


Figure 2.12: a) A symmetry twisted SPT PEPS on a cylinder. b) A pair of monodromy defects on a sphere.

Assuming the symmetry MPOs satisfy the *zipper* condition (2.72) one can directly calculate the effect that a physical symmetry action $U(h)^{\otimes |\mathcal{M}|_v}$, $h \in C(g)$ has on the virtual boundary, simultaneously demonstrating the symmetry invariance of the bulk.

$$\begin{array}{c}
 \text{Diagram 1} \\
 \text{Diagram 2} \\
 \text{Diagram 3}
 \end{array}
 = \begin{array}{c}
 \text{Diagram 4} \\
 \text{Diagram 5} \\
 \text{Diagram 6}
 \end{array}
 \quad (2.131)$$

$$\begin{array}{c}
 \text{Diagram 7} \\
 \text{Diagram 8} \\
 \text{Diagram 9}
 \end{array}
 = \begin{array}{c}
 \text{Diagram 10} \\
 \text{Diagram 11} \\
 \text{Diagram 12}
 \end{array}
 \quad (2.132)$$

Hence the symmetry action $\mathcal{V}_1^g(h)$ (see Eq.(2.20)) on the boundary of a single puncture Π_1 is given by the MPO $V^{\partial\Pi_1^-}(h)$, acting on the virtual indices along $\partial\Pi_1$, contracted with the crossing tensor $Y_R^g(h)$ (see Eq.(2.89)) acting on the inner MPO index of the symmetry twist $V^{P_g}(g)$ that enters the puncture. Similarly $\mathcal{V}_0^g(h)$, acting on the boundary of the other puncture Π_0 , is given by contracting the MPO $V^{\partial\Pi_0^-}(h)$ with the crossing tensor $Y_L^g(h)$.

There is a natural composition operation on the crossing tensors $Y_R^g(\cdot)$ that is induced by applying a product of global symmetries $U(k)^{\otimes |\mathcal{M}|_v} U(h)^{\otimes |\mathcal{M}|_v}$

and utilizing the reduction of Eq.(2.132) twice and then zipping the MPOs $V^{\partial\Pi_1^-}(k)V^{\partial\Pi_1^-}(h) = X(k, h)V^{\partial\Pi_1^-}(kh)X^+(k, h)$ by Eq.(2.72). This is nothing but the product $Y_R^g(k) \times Y_R^g(h)$ that was previously defined in Eq.(2.94).

Since the physical action $U(h)^{\otimes |\mathcal{M}|_v}$ forms a representation of the symmetry group $C(g)$ the simultaneous virtual action on both boundaries Π_0, Π_1 together $\mathcal{V}_0^g(h) \otimes \mathcal{V}_1^g(h)$ must also form a representation. However, there is a multiplicative freedom in the multiplication rule of the representation on a single boundary

$$\mathcal{V}_1^g(k)\mathcal{V}_1^g(h) = \omega_1^g(k, h)\mathcal{V}_1^g(kh)$$

(and similarly for $\mathcal{V}_0^g(h)$), under the constraint $\omega_0^g(k, h)\omega_1^g(k, h) = 1$, allowing the possibility of projective representations.

Using the result of Eq.(2.95), $Y_R^g(k) \times Y_R^g(h) = \omega^g(k, h)Y_R^g(kh)$, we can pin down the 2-cocycle ω_1^g explicitly in terms of the 3-cocycle α of the injective MPO representation $V^{\partial\Pi_0^-}(\cdot)$ as follows $\omega_1^g(k, h) = \omega^g(k, h)$ (see Eq.(2.93) for definition of ω^g). Hence the cohomology class of the projective representation $\mathcal{V}_1^g(\cdot)$ is given by

$$[\omega_1^g(k, h)] = [\alpha^{(g)}(k, h)].$$

It was shown above that a gauged SPT PEPS with a pair of defects $G_{\phi^{p_g}}|\psi^{p_g}, B_0, B_1\rangle$ describes a superposition of anyon pairs in the resulting topological theory. The projective transformation of the monodromy defects is intimately related to the braiding of the resulting anyons, which can be inferred from the following process, depicted in Fig. 2.13. First consider an isolated anyon formed by creating a pair of anyons and then moving the other arbitrarily far away. Next create a second pair and move them to encircle the isolated anyon, at this point one should fuse these anyons, but the full description of such fusion requires a systematic anyon ansatz which is beyond the scope of the current paper (see Ref.[133]). Instead we drag the pair arbitrarily far away as demonstrated in Fig. 2.13 and use the fact that this can be rewritten as some local action on the internal degrees of freedom of the isolated anyon, plus another locally undetectable action that can be moved arbitrarily far away.

2.I Gauging symmetric Hamiltonians and ground states

In this appendix we apply the gauging procedure developed in Ref.[51] to families of trivial and SPT Hamiltonians with symmetric perturbations and find that they are mapped to perturbed quantum double and twisted quantum double models respectively. We then go on to describe gauging the (unperturbed) fixed point ground states.

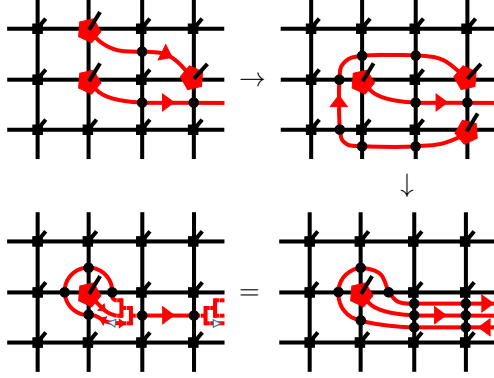


Figure 2.13: The process used to find the effect of braiding on the internal degrees of freedom of a single anyon.

2.I.1 Gauging the Hamiltonian

First we apply the gauging procedure to a symmetric Hamiltonian defined on the matter degrees of freedom, each with Hilbert space $\mathbb{H}_v \cong \mathbb{C}[G]$ and symmetry action $U_v(g) = R_v(g)$, associated to the vertices of a directed graph Λ embedded in a closed oriented 2-manifold \mathcal{M} . The Hamiltonian is given by

$$H_m = \alpha \sum_{v \in \Lambda} h_v^0 + \sum_{m \in G} \beta_m \sum_{e \in \Lambda} \mathcal{E}_e^m \quad (2.133)$$

the vertex terms are $h_v^0 := \int d\hat{g}_v dg_v |\hat{g}_v\rangle \langle g_v|$ while the edge interaction terms are $\mathcal{E}_e^m := \int dg_{v_e^-} dg_{v_e^+} \delta_{g_{v_e^-} g_{v_e^+}^{-1}, m} |g_{v_e^-}\rangle \langle g_{v_e^-}| \otimes |g_{v_e^+}\rangle \langle g_{v_e^+}|$. Each term in this

Hamiltonian is symmetric under the group action $\bigotimes_v R_v(g)$. For $\alpha, \beta_m < 0$ and $|\alpha| \gg |\beta_m|$ this Hamiltonian describes a symmetric phase with trivial SPT order, while for $|\beta_m| \gg |\alpha|$ the Hamiltonian describes different symmetry broken phases.

We construct the gauge and matter Hamiltonian $H_{\mathbf{g},m}$ by first gauging the local terms h_v^0 , which leaves them invariant $\mathcal{G}_v[h_v^0] = h_v^0$. Next we gauge the interaction terms \mathcal{E}_e^m with the gauging map on \bar{e} (the closure of edge e)

$$\begin{aligned} \mathcal{G}_{\bar{e}}[\mathcal{E}_e^m] &= \int dg_{v_e^-} dg_{v_e^+} dh_{v_e^-} dh_{v_e^+} \delta_{g_{v_e^-} g_{v_e^+}^{-1}, m} |g_{v_e^-} h_{v_e^-}^{-1}\rangle \\ &\langle g_{v_e^-} h_{v_e^-}^{-1}| \otimes |h_{v_e^-} h_{v_e^+}^{-1}\rangle \langle h_{v_e^-} h_{v_e^+}^{-1}|_e \otimes |g_{v_e^+} h_{v_e^+}^{-1}\rangle \langle g_{v_e^+} h_{v_e^+}^{-1}|. \end{aligned}$$

Finally we consider additional local gauge invariant Hamiltonian terms acting purely on the gauge degrees of freedom: symmetric local fields

$$\mathcal{F}_e^c := \int d\hat{g}_e dg_e \delta_{\hat{g}_e g_e^{-1} \in c} |\hat{g}_e\rangle \langle g_e| \quad (2.134)$$

where $c \in \mathcal{C}(G)$ are conjugacy classes of G , and plaquette flux-constraints

$$\mathcal{B}_p^m := \int \prod_{e \in \partial p} dg_e \delta_{g_{e_1}^{\sigma^{e_1}} \dots g_{e_{|\partial p|}}^{\sigma^{e_{|\partial p|}}}, m} \bigotimes_{e \in \partial p} |g_e\rangle \langle g_e|, \quad (2.135)$$

where each plaquette p has a fixed orientation induced by the 2-manifold \mathcal{M} , and the group elements $\{g_{e_1}, \dots, g_{e_{|\partial p|}}\}$ are ordered as the edges are visited starting from the smallest vertex label and moving against the orientation of ∂p , then $\sigma^{e_i} = \pm 1$ is $+1$ if the edge e_i points in the same direction as the orientation of p and -1 otherwise. Finally we require that the group elements lie in the center of the group $m \in C(G)$ which renders the choice of vertex from which we begin our traversal of ∂p irrelevant.

The full gauge and matter Hamiltonian is thus given by

$$\begin{aligned} H_{\mathbf{g},m} = & \alpha \sum_{v \in \Lambda} h_v^0 + \sum_{m \in G} \beta_m \sum_{e \in \Lambda} \mathcal{G}_e[\mathcal{E}_e^m] + \sum_{c \in \mathcal{C}(G)} \gamma_c \sum_{e \in \Lambda} \mathcal{F}_e^c \\ & + \sum_{m \in C(G)} \varepsilon_m \sum_{p \in \Lambda} \mathcal{B}_p^m. \end{aligned} \quad (2.136)$$

Note that each term commutes with all local gauge constraints $\{P_v\}$, see Eq.(2.109), and the physics takes place within this gauge invariant subspace.

2.1.2 Disentangling the constraints

To see more clearly that this gauge theory is equivalent to an unconstrained quantum double model we will apply a local disentangling circuit to reveal a clear tensor product structure, allowing us to ‘spend’ the gauge constraints to remove the matter degrees of freedom.

We define the disentangling circuit to be the product of local unitaries $C_\Lambda := \prod_v C_v$, where $C_v := \int dg_v |g_v\rangle \langle g_v|_v \prod_{e \in E_v^+} R_e(g) \prod_{e \in E_v^-} L_e(g)$. Note the order in the product is irrelevant since $[C_v, C_{v'}] = 0$. This circuit induces the following transformation on the gauge projectors: $C_\Lambda P_v C_\Lambda^\dagger = \int dg R_v(g)$, hence any state $|\psi\rangle$ in the gauge invariant subspace (simultaneous $+1$ eigenspace of all P_v) is disentangled into a tensor product of symmetric states on all matter degrees of freedom with an unconstrained state $|\psi'\rangle \in \mathbb{H}_{\mathbf{g}}$ on the gauge degrees of freedom $C_\Lambda |\psi\rangle = |\psi'\rangle \bigotimes_v \int dg_v |g_v\rangle$.

Now we apply the disentangling circuit to the Hamiltonian $H_{\mathbf{g},m}$. First note the pure gauge terms \mathcal{F}_e^c and \mathcal{B}_p^m are invariant under conjugation by C_v . The vertex terms are mapped to

$$C_v h_v^0 C_v^\dagger = \int dg_v R_v(g_v) \bigotimes_{e \in E_v^+} R_e(g_v) \bigotimes_{e \in E_v^-} L_e(g_v). \quad (2.137)$$

Since the disentangled vertex degrees of freedom are invariant under $R_v(g_v)$ we see that this Hamiltonian term acts as $\int dg_v \bigotimes_{e \in E_v^+} R_e(g_v) \bigotimes_{e \in E_v^-} L_e(g_v)$

on the relevant gauge degrees of freedom. We recognize this as the vertex term of a quantum double model. Finally we examine the transformation of the interaction terms $C_v \mathcal{G}_e[\mathcal{E}_e^m] C_v^\dagger = \frac{1}{|\mathbb{G}|} |m\rangle \langle m|_e$, which yield local fields on the gauge degrees of freedom that induce string tension. Hence we see that the gauge plus matter Hamiltonian after disentangling becomes a local Hamiltonian $H_g := C_v H_{g,m} C_v^\dagger$ acting purely on the gauge degrees of freedom

$$\begin{aligned}
 H_g = & \alpha \sum_v \int dg_v \bigotimes_{e \in E_v^+} R_e(g_v) \bigotimes_{e \in E_v^-} L_e(g_v) + \sum_{m \in \mathbb{G}} \frac{\beta_m}{|\mathbb{G}|} \\
 & \times \sum_{e \in \Lambda} |m\rangle \langle m|_e + \sum_{c \in \mathcal{C}(\mathbb{G})} \gamma_c \sum_{e \in \Lambda} \mathcal{F}_e^c + \sum_{m \in \mathcal{C}(\mathbb{G})} \varepsilon_m \sum_{p \in \Lambda} \mathcal{B}_p^m \quad (2.138)
 \end{aligned}$$

which describes a quantum double model with string tension and flux perturbations. Note that a spontaneous symmetry breaking phase transition in the ungauged model is mapped to a string tension induced anyon condensation transition by the gauging procedure.

2.1.3 Gauging nontrivial SPT Hamiltonians

The gauging procedure extends to nontrivial SPT Hamiltonians which are defined on triangular graphs embedded in closed oriented 2-manifolds \mathcal{M} . The only modification required is to replace the trivial vertex terms h_v^0 by nontrivial terms h_v^α which are defined by

$$\int d\hat{g}_v dg_v \prod_{v' \in L(v)} dg_{v'} \prod_{\Delta \in S(v)} \alpha_\Delta |\hat{g}_v\rangle \langle g_v| \bigotimes_{v' \in L(v)} |g_{v'}\rangle \langle g_{v'}| \quad (2.139)$$

where $S(v)$ is the star of v , $L(v)$ is the link of v and $\alpha_\Delta \in \text{U}(1)$ for plaquette Δ , whose vertices are given counterclockwise (relative to the orientation of the 2-manifold) by v, v', v'' , is defined by the 3-cocycle $\alpha_\Delta := \alpha^{\sigma_\pi} (g_1 g_2^{-1}, g_2 g_3^{-1}, g_3 g_4^{-1})$ where $(g_1, g_2, g_3, g_4) := \pi(\hat{g}_v, g_v, g_{v'}, g_{v''})$ for π the permutation that sorts the group elements into ascending vertex label order (with the convention that \hat{g}_v immediately precedes g_v) and $\sigma_\pi = \pm 1$ is the parity of the permutation. The terms h_v^α are clearly symmetric under global right group multiplication and are seen to be Hermitian since conjugation inverts the phase factor α_Δ and interchanges the role of \hat{g}_v and g_v which inverts the parity of π thereby compensating the conjugation of α_Δ .

We apply the gauging map on the region $\bar{S}(v)$ (the closure of the star of

v) to h_v^α

$$\begin{aligned} \mathcal{G}_{\bar{S}(v)}[h_v^\alpha] &= \int d\hat{g}_v dg_v dh_v \prod_{v' \in L(v)} dg_{v'} dh_{v'} \prod_{\Delta \in S(v)} \alpha_\Delta \\ &\quad |\hat{g}_v h_v^{-1}\rangle \langle g_v h_v^{-1}| \bigotimes_{v' \in L(v)} |g_{v'} h_{v'}^{-1}\rangle \langle g_{v'} h_{v'}^{-1}| \\ &\quad \bigotimes_{e \in \bar{S}(v)} |h_{v_e^-} h_{v_e^+}^{-1}\rangle \langle h_{v_e^-} h_{v_e^+}^{-1}|_e \end{aligned} \quad (2.140)$$

followed by the disentangling circuit $C_\Lambda \mathcal{G}_{\bar{S}(v)}[h_v^\alpha] C_\Lambda^\dagger$ which yields

$$\begin{aligned} &\int d\hat{g}_v dg_v dh_v \prod_{v' \in L(v)} dg_{v'} dh_{v'} \prod_{\Delta \in S(v)} \alpha_\Delta |\hat{g}_v h_v^{-1}\rangle \langle g_v h_v^{-1}| \\ &\quad \bigotimes_{v' \in L(v)} |g_{v'} h_{v'}^{-1}\rangle \langle g_{v'} h_{v'}^{-1}| \bigotimes_{e \in E_v^+} |g_{v_e^-} \hat{g}_v^{-1}\rangle \langle g_{v_e^-} g_v^{-1}| \\ &\quad \bigotimes_{e \in E_v^-} |\hat{g}_v g_{v_e^+}^{-1}\rangle \langle g_v g_{v_e^+}^{-1}| \bigotimes_{e \in L(v)} |g_{v_e^-} g_{v_e^+}^{-1}\rangle \langle g_{v_e^-} g_{v_e^+}^{-1}|. \end{aligned} \quad (2.141)$$

Note, importantly, the phase functions α_Δ now depend only on the gauge degrees of freedom. Finally in Eq.(2.142) we rewrite the pure gauge Hamiltonian terms without reference to the matter degrees of freedom, which become irrelevant as the matter degrees of freedom in any gauge invariant state are fixed to be in the symmetric state $\int dg_v |g_v\rangle_v$ by the disentangling circuit

$$\begin{aligned} &\int d\hat{g}_v dg_v \prod_{v' \in L(v)} dg_{v'} \prod_{\Delta \in S(v)} \alpha_\Delta \bigotimes_{e \in E_v^+} |g_{v_e^-} \hat{g}_v^{-1}\rangle \langle g_{v_e^-} g_v^{-1}| \\ &\quad \bigotimes_{e \in E_v^-} |\hat{g}_v g_{v_e^+}^{-1}\rangle \langle g_v g_{v_e^+}^{-1}| \bigotimes_{e \in L(v)} |g_{v_e^-} g_{v_e^+}^{-1}\rangle \langle g_{v_e^-} g_{v_e^+}^{-1}| \end{aligned} \quad (2.142)$$

This can be recognized as the vertex term of a 2D twisted quantum double model (the lattice hamiltonian version of a twisted Dijkgraaf Witten theory for the group G and cocycle α).

2.1.4 Gauging SPT groundstates

In this section we apply the gauging procedure directly to the ground states of the nontrivial SPT Hamiltonian that was defined in Eq.(2.139). These ground states are constructed using the following local circuit [147]

$$D_\alpha := \int \prod_{v \in \Lambda} dg_v \prod_{\Delta \in \Lambda} \tilde{\alpha}_\Delta \bigotimes_{v \in \Lambda} |g_v\rangle \langle g_v| \quad (2.143)$$

where $\tilde{\alpha}_\Delta \in U(1)$ is a function of the degrees of freedom on plaquette Δ , whose vertices are given counterclockwise, relative to the orientation of the 2-manifold \mathcal{M} , by v, v', v'' (note the choice of starting vertex is irrelevant) and is defined by a 3-cocycle as follows $\tilde{\alpha}_\Delta := \alpha^{\sigma_\pi}(g_1 g_2^{-1}, g_2 g_3^{-1}, g_3)$ where $(g_1, g_2, g_3) := \pi(g_v, g_{v'}, g_{v''})$ with π the permutation that sorts the group elements into ascending vertex label order and $\sigma_\pi = \pm 1$ is the parity of the permutation (equivalently the orientation of Δ embedded within the 2-manifold \mathcal{M}). Note D_α is easily expressed as a product of commuting 3-local gates.

To define SPT fixed point states we start with the trivial state $|\text{SPT}(0)\rangle := \bigotimes_v \int dg_v |g_v\rangle_v$, which is easily seen to be symmetric under global right group multiplication. One can also check that D_α is symmetric under conjugation by global right group multiplication by utilizing the 3-cocycle condition satisfied by each $\tilde{\alpha}_\Delta$. With this we define nontrivial SPT fixed point states $|\text{SPT}(\alpha)\rangle := D_\alpha |\text{SPT}(0)\rangle$, which are symmetric by construction. To see that $|\text{SPT}(\alpha)\rangle$ is the ground state of the SPT Hamiltonian $\sum_v h_v^\alpha$ we note $h_v^\alpha = D_\alpha h_v^0 D_\alpha^\dagger$ which again is proved using the 3-cocycle condition.

We will now gauge the SPT fixed point states by applying the state gauging map to D_α , since the input variables of the circuit carry the same information as the virtual indices of the fixed point SPT PEPS we hope this makes the correspondence between the two pictures more clear

$$GD_\alpha = \int \prod_{v \in \Lambda} dg_v dh_v \prod_{\Delta \in \Lambda} \tilde{\alpha}_\Delta \bigotimes_{e \in \Lambda} |h_{v_e^-} h_{v_e^+}^{-1}\rangle \bigotimes_{v \in \Lambda} |g_v h_v^{-1}\rangle \langle g_v|. \quad (2.144)$$

Under the local disentangling circuit this transforms to

$$C_\Lambda GD_\alpha = \int \prod_{v \in \Lambda} dg_v \prod_{\Delta \in \Lambda} \tilde{\alpha}_\Delta \bigotimes_{e \in \Lambda} |g_{v_e^-} g_{v_e^+}^{-1}\rangle \bigotimes_{v \in \Lambda} \langle g_v| \bigotimes_{v \in \Lambda} \int dk_v |k_v\rangle, \quad (2.145)$$

where it is clear that the matter degrees of freedom have been disentangled into symmetric states and the cocycles $\tilde{\alpha}_\Delta$ depend on both the group variables on the edges and the inputs on the vertices (which correspond to the PEPS virtual degrees of freedom).

The explicit connection to the fixed point SPT PEPS is made by replacing the basis at each vertex $|g_v\rangle_v$ by an analogous basis of the diagonal subspace of variables at each plaquette surrounding the vertex $\bigotimes_{\Delta \in \mathcal{S}(v)} |g_v\rangle_{\Delta, v}$. This construction lends itself directly to a PEPS description where a tensor is assigned to each plaquette of the original graph (i.e. the PEPS is constructed on the dual graph). This in turn is why we must apply a seemingly modified

version of the gauging operator of Ref.[51] to gauge the PEPS correctly and we note that on the subspace where redundant variables are identified the modified PEPS gauging operator becomes identical to the standard gauging operator.

Anyons and matrix product operator algebras

Synopsis

Quantum tensor network states and more particularly projected entangled-pair states provide a natural framework for representing ground states of gapped, topologically ordered systems. The defining feature of these representations is that topological order is a consequence of the symmetry of the underlying tensors in terms of matrix product operators. In this paper, we present a systematic study of those matrix product operators, and show how this relates entanglement properties of projected entangled-pair states to the formalism of fusion tensor categories. From the matrix product operators we construct a C^* -algebra and find that topological sectors can be identified with the central idempotents of this algebra. This allows us to construct projected entangled-pair states containing an arbitrary number of anyons. Properties such as topological spin, the S matrix, fusion and braiding relations can readily be extracted from the idempotents. As the matrix product operator symmetries are acting purely on the virtual level of the tensor network, the ensuing Wilson loops are not fattened when perturbing the system, and this opens up the possibility of simulating topological theories away from renormalization group fixed points. We illustrate the general formalism for the special cases of discrete gauge theories and string-net models.

Based on

‘Anyons and matrix product operator algebras’

N. Bultinck, M. Mariën, D. Williamson, M. Sahinoglu, J. Haegeman and F. Verstraete

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Contributions of the author: The author has contributed to all results

in this manuscript, except those regarding the numerical applications reported in section 3.6.2 and appendices 3.C, 3.D, 3.E and 3.F. The author has also written the largest part of the manuscript.

3.1 Introduction

Since the conception of quantum mechanics, the quantum many-body problem has been of central importance. Due to a lack of exact methods one has to study these systems using approximate techniques such as mean field theory or perturbative expansions in a small parameter, or using an effective description obtained from symmetry or renormalization arguments. Another approach that has proven to be very fruitful is the use of toy models and trial wave functions. Tensor network states constitute a class of such trial wave functions that has emerged in past decades from the interplay of quantum information theory and condensed matter theory [102]. The power of these states is two-sided. On the one hand, they can be used to study universal properties of quantum many-body systems, which makes them interesting objects from the theoretical perspective. On the other hand, they allow for novel methods to simulate the many-body problem, which makes them interesting from the point of view of computational physics. For example, in one dimension Matrix Product States not only underpin the highly successful Density Matrix Renormalization Group algorithm [35, 153], but have also been used to completely classify all gapped phases of matter in quantum spin chains [43, 104, 105].

In this work we focus on two-dimensional tensor network states, so-called Projected Entangled-Pair States (PEPS) [154]. Because of their local structure these trial states serve as a window through which we can observe the entanglement properties of ground states of complex quantum many-body systems. We use this to study ground states of local two-dimensional Hamiltonians that have topological order, a kind of quantum order characterized by locally indistinguishable ground states and exotic excitations which can behave differently from bosons and fermions [9, 100].

In recent years it became clear that topological order can be interpreted as a property of (a set of) states [155], the local Hamiltonian seems to be merely a tool to stabilize the relevant ground state subspace. It was realized that topological order manifests itself in entanglement properties such as the entanglement entropy [40, 41]. This has resulted in a definition of topological order via long-range entanglement [156]. More recent works have shown that the ground state subspace on a torus contains information about the topological excitations [157] and that for chiral phases the so-called entanglement spectrum reveals the nature of the edge physics [42]. In Ref. [158], it was even shown that for a restricted class of Hamiltonians a single ground state contains sufficient information to obtain the S matrix, an invariant for topological phases.

Utilizing the transparent entanglement structure of PEPS, we further examine this line of reasoning. We consider a class of PEPS with nonchiral topological order, which were introduced in [106, 108, 109, 159]. The intrinsic topological order in these states is characterized by a Matrix Product Operator (MPO) at the virtual level, which acts as a projector onto the virtual subspace on which the PEPS map is injective. This class of trial wave functions was shown to provide an exact description of certain renormalization group fixed-point models such as discrete gauge theories [160] and string-net models [109, 149, 150], but can also be perturbed away from the fixed point in order to study e.g. topological phase transitions [107, 152]. We show that the entanglement structure of these ‘MPO-injective’ PEPS enables a full characterization of the topological sectors of the corresponding quantum phase. In other words, the injectivity space of the tensors in a finite region of a single MPO-injective PEPS contains all information to fully determine the topological phase. More concretely, we show that the MPO that determines the entanglement structure of the PEPS allows one to construct a C^* -algebra whose central idempotents correspond to the topological sectors. A similar identification of topological sectors with central idempotents was made in [158, 161]. The advantage of the PEPS approach is that the idempotents can be used to explicitly write down generic wave functions containing anyonic excitations, which allows for a deeper understanding of how topological theories are realized in the ground states of local Hamiltonians. In addition, we obtain an intuitive picture of what happens in the wave function when these anyons are manipulated, and we can extract all topological information such as topological spins, the S matrix, fusion properties and braiding matrices. We would like to note that a very similar framework was recently discussed in the context of statistical mechanics [162], where universal information about the CFT describing the critical point was obtained.

Section 3.2 starts with an overview of the paper. In Section 3.3 we discuss general properties of projector MPOs and their connection to fusion categories. The construction of MPO-injective PEPS, as originally presented in [109], is worked out in detail in Section 3.4. Section 3.5 explains how to obtain the topological sectors and construct PEPS containing anyonic excitations. The corresponding anyon ansatz is illustrated for discrete gauge theories and string-nets in the examples of Section 3.6. Section 3.7 contains a discussion of the results and possible directions for future work. The appendices contain several technical calculations and detailed results for some specific examples.

3.2 Overview of the paper

In this section we convey the main ideas presented in this work, before obscuring them with technical details. We start by considering a large class of projector matrix product operators P that can be written as $P = \sum_a w_a O_a$,

where the w_a are complex numbers and O_a are injective (single block) matrix product operators with periodic boundary conditions:

$$O_a = \text{tr} \left(\begin{array}{c} \bullet \\ \circlearrowleft \\ \bullet \\ \bullet \\ \bullet \end{array} \right) \quad (3.1)$$

Because we want P to be a projector for every length it follows that $\{O_a\}$ forms the basis of a matrix algebra with positive integer structure coefficients: $O_a O_b = \sum_c N_{ab}^c O_c$, with $N_{ab}^c \in \mathbb{N}$. In section 3.3 we work out the details of this algebra and show that we can associate many concepts to it that are familiar from fusion categories.

In section 3.4 we turn to tensor network states on two-dimensional lattices, called Projected Entangled-Pair States (PEPS). We discuss how the MPO tensors can be used to construct a (family of) PEPS that satisfies the axioms of MPO-injectivity, i.e. the algebra $\{O_a\}$ constitutes the virtual ‘symmetry’ algebra of the local PEPS tensors and the virtual support of the PEPS on any topologically trivial region corresponds to the subspace determined by the MPO projector P along the boundary of that region. As shown in [109], the axioms of MPO-injectivity allow us to prove that such PEPS are unique ground states of their corresponding parent Hamiltonians on topologically trivial manifolds. We can also explicitly characterize the degenerate set of ground states on topologically non-trivial manifolds. The most important axiom of MPO-injectivity is the ‘pulling through’ property. To prove that it is satisfied by our construction, we need to impose that the MPO tensors satisfy the so-called *zipper* condition, i.e. there must exist a three-leg ‘fusion’ tensor X , which we depict as a grey box, such that the following identity holds:

$$\begin{array}{c} a \\ \bullet \\ \text{---} \\ \bullet \\ b \end{array} \begin{array}{c} \mu \\ \text{---} \\ \mu \end{array} \begin{array}{c} c \\ \text{---} \\ c \end{array} = \begin{array}{c} a \\ \text{---} \\ \mu \end{array} \begin{array}{c} \mu \\ \text{---} \\ \mu \end{array} \begin{array}{c} \bullet \\ \text{---} \\ c \end{array} \quad (3.2)$$

Remarkably, the same properties of the MPOs O_a that guarantee the pulling through property to hold also allow us to construct a *second type* of MPO algebra. The basis of this second algebra is bigger than that of the first one and its elements can be presented schematically as:

$$\text{tr} \left(\begin{array}{c} \bullet \\ \circlearrowleft \\ \bullet \\ \bullet \\ \bullet \end{array} \right) , \quad (3.3)$$

where the red square is a new type of tensor, defined in the main text, that is completely determined by the MPOs O_a . We show that this second algebra

is actually a C^* -algebra, hence it is isomorphic to a direct sum of full matrix algebras. We use this decomposition to identify the topological sectors with the different blocks, or equivalently, with the central idempotents that project onto these blocks. A large part of the paper is then devoted to show that, once one has identified these central idempotents (for which we give a constructive algorithm), one can construct MPO-injective PEPS containing anyonic excitations and study their topological properties. For example, the topological spin h_i of an anyon i can be obtained via the identity:

$$\text{Diagram with red lines and blue square } i = e^{i2\pi h_i} \text{Diagram with red lines and blue square } i, \quad (3.4)$$

where we used a blue square to denote a central idempotent (here the one corresponding to anyon i) as opposed to a red square, which denotes a basis element of the second algebra. In a similar manner one can extract the S -matrix, fusion relations and braiding matrices in a way that does not scale with the system size.

Let us now illustrate this general scheme for the simplest example, namely Kitaev’s Toric Code [163]. Note that the excitations in the Toric code are already completely understood in the framework of G -injective PEPS [106], which is a specific subset of the MPO-injective PEPS formalism with building blocks O_a that are tensor products of local operators, i.e. the MPOs have virtual bond dimension 1. However, as a pedagogical example we would like to study the anyons in the general language introduced above. In the standard PEPS construction of the Toric code [159] the virtual indices of the tensors are of dimension two and have a \mathbb{Z}_2 symmetry, i.e. they are invariant under $\sigma_z^{\otimes 4}$. So in this case the symmetry algebra is really a group and is given by the two MPOs $O_1 = \mathbb{1}^{\otimes 4}$ and $O_z = \sigma_z^{\otimes 4}$. Let us now introduce following tensor where all indices have dimension two:

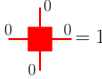
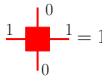
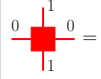
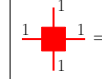
$$\text{Tensor with red 0 and black 0} = \mathbb{1} \quad \text{Tensor with red 1 and black 1} = \sigma_z. \quad (3.5)$$

All components that are not diagonal in the red indices are zero. One can clearly construct the Toric code symmetry MPOs O_1 and O_z using these tensors. By defining a fusion tensor where all indices have dimension two and with the following non-zero components:

$$\text{Fusion tensor with red indices } 0, 0, 1, 1 = 1, \quad (3.6)$$

one can verify that the zipper condition (3.2) is trivially satisfied.

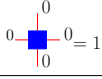
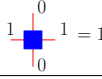
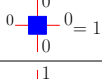
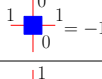
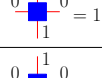
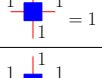

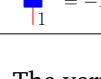
The second type of algebra is four-dimensional. The basis elements (3.3) can be obtained by using one of following tensors:

1	2	3	4
			

(3.7)

Each of these tensors has only one non-zero component, which is given in the table.

The central idempotents of this second algebra, labeled by the usual notation $\{1, e, m, em\}$, are now easily obtained by using following tensors:

1		
e		
m		
em		

(3.8)

Again, we only denote non-zero elements. The vertical indices in the tensors above with value one indicate that a string of σ_z is connected to these idempotents. This agrees with the G -injectivity construction of m and em anyons. From (3.4) one can now immediately see that the topological spins of these idempotents are $h_1 = h_e = h_m = 0$ and $h_{em} = 1/2$.

While our treatment of the Toric Code might seem overloaded, we will show in the remainder of the paper that it is in fact the correct language to describe anyons in general topological PEPS. We hope that this section can give some intuition and motivation to understand the more technical parts.

3.3 Projector Matrix Product Operators

3.3.1 Definition

We start the general theory with a discussion of Projector Matrix Product Operators (PMPO), the fundamental objects of MPO-injectivity, and their connection to known concepts of category theory. We consider PMPOs P_L that form translation invariant Hermitian projectors for every length L and

can be represented as

$$P_L = \sum_{\{i\},\{j\}=1}^D \text{tr}(\Delta B^{i_1 j_1} B^{i_2 j_2} \dots B^{i_L j_L}) |i_1 i_2 \dots i_L\rangle \langle j_1 j_2 \dots j_L|, \quad (3.9)$$

where B^{ij} are $\chi \times \chi$ matrices for fixed values of indices $i, j = 1, \dots, D$. We use this MPO to construct a PEPS in the next section, and D will then become the bond dimension of the resulting PEPS. Furthermore, Δ is a $\chi \times \chi$ matrix such that the specific position where it is inserted is irrelevant; every position of Δ will result in the same PMPO P_L . We also assume that the insertion of Δ still allows for a canonical form of the MPO such that the tensors have the following block diagonal structure [36]

$$B^{ij} = \bigoplus_{a=1}^{\mathcal{N}} B_a^{ij} \quad (3.10)$$

$$\Delta = \bigoplus_{a=1}^{\mathcal{N}} \Delta_a, \quad (3.11)$$

with B_a^{ij} and Δ_a $\chi_a \times \chi_a$ matrices such that $\sum_{a=1}^{\mathcal{N}} \chi_a = \chi$. P_L thus decomposes into a sum of MPOs

$$P_L = \sum_{a=1}^{\mathcal{N}} \sum_{\{i\},\{j\}=1}^D \text{tr}(\Delta_a B_a^{i_1 j_1} B_a^{i_2 j_2} \dots B_a^{i_L j_L}) |i_1 i_2 \dots i_L\rangle \langle j_1 j_2 \dots j_L| \quad (3.12)$$

The resulting MPOs labelled by a in this sum are injective, hence for each a the matrices $\{B_a^{ij}; i, j = 1, \dots, D\}$ and their products span the entire space of $\chi_a \times \chi_a$ matrices. Equivalently, the corresponding transfer matrices $\mathbb{E}_a = \sum_{i,j} B_a^{i,j} \otimes \bar{B}_a^{i,j}$ have a unique eigenvalue λ_a of largest magnitude that is positive and a corresponding (right) eigenvector equivalent to a full rank positive definite matrix ρ_a . The PMPO P_L can now only be translation invariant if the Δ_a commute with all the matrices B_a^{ij} . Injectivity of the tensors B_a then implies that $\Delta_a = w_a \mathbb{1}_{\chi_a}$, with w_a some complex numbers.

3.3.2 Fusion tensors

We thus arrive at the following form for P_L

$$\begin{aligned} P_L &= \sum_{a=1}^{\mathcal{N}} w_a O_a^L \\ &= \sum_{a=1}^{\mathcal{N}} w_a \sum_{\{i\},\{j\}=1}^D \text{tr}(B_a^{i_1 j_1} B_a^{i_2 j_2} \dots B_a^{i_L j_L}) |i_1 i_2 \dots i_L\rangle \langle j_1 j_2 \dots j_L| \end{aligned} \quad (3.13)$$

Since P_L is required to be a projector, we have that

$$P_L^2 = \sum_{a,b=1}^{\mathcal{N}} w_a w_b O_a^L O_b^L = \sum_{a=1}^{\mathcal{N}} w_a O_a^L = P_L, \quad (3.14)$$

which has to hold for all L . One can show that this implies that P_L and P_L^2 have the same blocks in their respective canonical forms¹ [164], leading to the following relations

$$O_a^L O_b^L = \sum_{c=1}^{\mathcal{N}} N_{ab}^c O_c^L, \quad (3.15)$$

$$\sum_{a,b=1}^{\mathcal{N}} N_{ab}^c w_a w_b = w_c, \quad (3.16)$$

where N_{ab}^c is a rank three tensor containing integer entrees. The theory of MPS representations [36] implies the existence of matrices $X_{ab,\mu}^c : \mathbb{C}^{\chi_a} \otimes \mathbb{C}^{\chi_b} \rightarrow \mathbb{C}^{\chi_c}$ for $\mu = 1, \dots, N_{ab}^c$ and left inverses $X_{ab,\mu}^{c+}$ satisfying $X_{ab,\nu}^{d+} X_{ab,\mu}^c = \delta_{de} \delta_{\mu\nu} \mathbb{1}_{\chi_c}$, such that we have following identities on the level of the individual matrices that build up the injective MPOs O_a^L ,

$$X_{ab,\mu}^{c+} \left(\sum_{j=1}^D B_a^{ij} \otimes B_b^{jk} \right) X_{ab,\mu}^c = B_c^{ik}. \quad (3.17)$$

We call the set of rank three tensors $X_{ab,\mu}^c$ the *fusion tensors*. These fusion tensors play an important role in constructing the anyon ansatz further on. From

$$\bigoplus_{\mu=1}^{N_{ab}^c} X_{ab,\mu}^{c+} \left(\sum_{j=1}^D B_a^{ij} \otimes B_b^{jk} \right) X_{ab,\mu}^c = \mathbb{1}_{N_{ab}^c} \otimes B_c^{ik}, \quad (3.18)$$

we see that the μ -label is arbitrary and the fusion tensors $X_{ab,\mu}^c$ are only defined up to a gauge transformation given by a set of invertible $N_{ab}^c \times N_{ab}^c$ matrices Y_{ab}^c ; every transformed set of fusion tensors $X'_{ab,\mu}{}^c = \sum_{\nu=1}^{N_{ab}^c} (Y_{ab}^c)_{\mu\nu} X_{ab,\nu}^c$ also satisfies (3.18). The MPO tensors and equation (3.17) are represented in figure 3.1 in a graphical language that is used extensively throughout this paper. Note in particular the difference between the square for the full MPO tensor B^{ij} with virtual indices (red lines) of dimension $\chi = \sum_a \chi_a$ and the disc for the injective MPO tensors B_a^{ij} with virtual indices (red line with symbol a) of dimension χ_a .

¹This essentially follows from the fact that $\lim_{L \rightarrow \infty} \text{tr}(O_a^L O_b^{L\dagger}) / \left(\sqrt{\text{tr}(O_a^L O_a^{L\dagger})} \sqrt{\text{tr}(O_b^L O_b^{L\dagger})} \right) = \delta_{a,b}$ for two injective MPOs O_a^L and O_b^L .

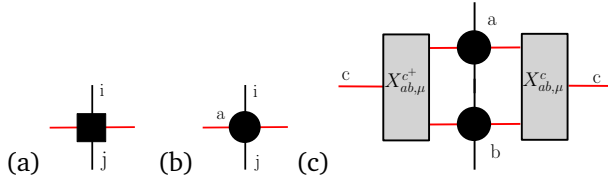


Figure 3.1: (a) MPO tensor B^{ij} . (b) Injective MPO tensor B_a^{ij} . (c) Left hand side of equation (3.17).

Two complications are worth mentioning. First, the canonical form of $O_a^L O_b^L$ can contain diagonal block matrices which are identically zero. Therefore, the fusion matrices $X_{ab,\mu}^c$ do not span the full space and $\sum_{c,\mu} \chi_c$ can be smaller than $\chi_a \times \chi_b$. Correspondingly, $\sum_{c,\mu} X_{ab,\mu}^c X_{ab,\mu}^{c+}$ is not necessarily the identity but only a projector on the support subspace of the internal MPO indices of $O_a^L O_b^L$.

Secondly, there can be nonzero blocks above the diagonal, i.e.

$$X_{ab,\mu}^{c+} \left(\sum_{j=1}^D B_a^{ij} \otimes B_b^{jk} \right) X_{ab,\nu}^d \neq 0 \quad (3.19)$$

for some $(c, \mu) < (d, \nu)$ (according to some ordering). These blocks do not contribute when the MPO is closed by the trace operation, but prevent us from writing

$$\sum_{c=1}^{\mathcal{N}} \sum_{\mu=1}^{N_{ab}^c} X_{ab,\mu}^c B_c^{ik} X_{ab,\mu}^{c+} = \sum_{j=1}^D B_a^{ij} \otimes B_b^{jk}. \quad (3.20)$$

We noticed above that a set of fusion tensors is only defined up to a gauge transformation Y . For PMPOs without nonzero blocks above the diagonal we now argue that the converse is also true, i.e. two collections of fusion tensors that satisfy equations (3.18) and (3.20) must be related by a gauge transformation Y . To see this, note that the absence of nonzero blocks above the diagonal is equivalent to the existence of an invertible matrix X_{ab} such that

$$X_{ab}^{-1} \left(\sum_{j=1}^D B_a^{ij} \otimes B_b^{jk} \right) X_{ab} = \bigoplus_c \left(\mathbb{1}_{N_{ab}^c} \otimes B_c^{ik} \right). \quad (3.21)$$

The fusion tensors that have the required properties are then simply the product of X_{ab} and the projector on the appropriate block: $X_{ab,\mu}^c = X_{ab} P_\mu^c$. It is clear that these fusion tensors are unique up to a matrix in the commutant of $\bigoplus_c \left(\mathbb{1}_{N_{ab}^c} \otimes B_c^{ik} \right)$. Since the B_c^{ik} are injective their commutant consists of multiples of the identity matrix. From this we can indeed conclude that the

only ambiguity in the definition of $X_{ab,\mu}^c$ is given by the gauge transformation Y .

Note that equation (3.20) is equivalent to

$$\left(\sum_{j=1}^D B_a^{ij} \otimes B_b^{jk} \right) X_{ab,\mu}^c = X_{ab,\mu}^c B_c^{ik}, \quad (3.22)$$

$$X_{ab,\mu}^{c+} \left(\sum_{j=1}^D B_a^{ij} \otimes B_b^{jk} \right) = B_c^{ik} X_{ab,\mu}^{c+}.$$

We refer to these last two equations as the *zipper condition*. While we continue somewhat longer in the general setting, we will need to assume that the zipper condition holds for most of the results in the remainder of the paper.

3.3.3 Hermiticity, duality and unital structure

If we also require P_L to be Hermitian for all L , then we find that for every block a there exists a unique block a^* such that

$$\bar{w}_a = w_{a^*} \quad (3.23)$$

$$O_a^{L\dagger} = O_{a^*}^L, \quad (3.24)$$

where the bar denotes complex conjugation. The tensor N then obviously satisfies

$$N_{ab}^c = N_{b^*a^*}^{c^*}. \quad (3.25)$$

Note that in general the tensors \bar{B}_a^{ji} and $B_{a^*}^{ij}$, which build up $O_a^{L\dagger}$ and $O_{a^*}^L$, are related by a gauge transformation: $\bar{B}_a^{ji} = Z_a^{-1} B_{a^*}^{ij} Z_a$ where Z_a is defined up to a multiplicative factor. By applying Hermitian conjugation twice we find

$$B_a^{ij} = \bar{Z}_a^{-1} \bar{B}_{a^*}^{ji} \bar{Z}_a \quad (3.26)$$

$$= \bar{Z}_a^{-1} Z_a^{-1} B_{a^*}^{ij} Z_a \bar{Z}_a. \quad (3.27)$$

Combining the above expression with the injectivity of B_a^{ij} we find $Z_a \bar{Z}_{a^*} = \gamma_a \mathbb{1} = \bar{Z}_{a^*} Z_a$, with $\gamma_a = \bar{\gamma}_{a^*}$ a complex number. If $a \neq a^*$, we can redefine one of the two Z matrices with an additional factor such that $\gamma_a = 1$. If, on the other hand, $a = a^*$ we find that γ_a must be real but we can at most absorb its absolute value in $Z_a \bar{Z}_a$ by redefining Z_a with an extra factor $|\gamma_a|^{-1/2}$. The sign $\varkappa_a = \text{sign}(\gamma_a)$ cannot be changed by redefining Z_a . It is a discrete invariant of the PMPO which is analogous to the Frobenius-Schur indicator in category theory.

To recapitulate, Hermitian conjugation associates to every block a a unique ‘dual’ block a^* in such a way that $(a^*)^* = a$. In fusion category

theory there is also a notion of duality, but it is defined in a different way. There, for every simple object a the unique dual simple object a^* is such that the tensor product of a and a^* contains the identity object 1 . The identity object is defined as the unique simple object that leaves all other objects invariant under taking the tensor product. Moreover, 1 appears only once in the decomposition of the tensor product of a and a^* . We now show that if a PMPO contains a trivial identity block then our definition of duality inferred from Hermitian conjugation coincides with the categorical definition. To do so, let us first revisit the transfer matrices

$$\begin{aligned}\mathbb{E}_a &= \sum_{i,j} B_a^{ij} \otimes \bar{B}_a^{ij} \\ &= (\mathbb{1} \otimes Z_a^{-1}) \sum_{i,j} B_a^{ij} \otimes B_{a^*}^{ji} (\mathbb{1} \otimes Z_a).\end{aligned}$$

We can thus use the tensors $(\mathbb{1} \otimes Z_a^{-1})X_{aa^*}^c$ (and their left inverses) to bring \mathbb{E}_a into a block form with nonzero blocks on and above the diagonal (upper block triangular). In particular, there are $N_{aa^*}^c$ diagonal blocks of size $\chi_c \times \chi_c$ that are given by $M_c = \sum_i B_c^{ii}$. They can be brought into upper triangular form by a Schur decomposition within the χ_c -dimensional space, such that we can identify the eigenvalue spectrum of \mathbb{E}_a with that of the different matrices M_c for c appearing in the fusion product of a and a^* . Since \mathbb{E}_a has a unique eigenvalue of largest magnitude λ_a , it must correspond to the unique largest eigenvalue of M_{c_a} for one particular block c_a , for which also $N_{aa^*}^{c_a} = 1$.

We now assume that there is a unique distinguished label c , which we choose to be $c = 1$, such that the spectral radius of M_1 is larger than the spectral radius of all other M_c for $c = 2, \dots, N$ (whose labeling is still arbitrary). We furthermore assume that $N_{aa^*}^1 \neq 0$ for all a , i.e. O_1^L appears in the product $O_a^L O_{a^*}^L$ for any a . This condition, as we now show, corresponds to imposing a unital structure and excludes cases where e.g. P_L is actually a sum of independent orthogonal projectors, corresponding to a partition A, B, \dots of the injective blocks that is completely decoupled (such that $N_{ab}^c = 0$ for any c if $a \in A$ and $b \in B$).

With this condition, we find that independent of a , $c_a = 1$ and all transfer matrices \mathbb{E}_a have $\lambda_a = \lambda$ as unique largest eigenvalue, with λ the largest magnitude eigenvalue of M_1 . This immediately gives rise to the following consequences. Firstly, $N_{aa^*}^1 = 1$ and not larger. Secondly, the largest eigenvalue of M_1 is positive and non-degenerate. Thirdly, any M_a for $a \neq 1$ has a spectral radius strictly smaller than λ . Fourthly, since the spectral radii of M_a and M_{a^*} are identical, it follows that $1^* = 1$. Furthermore, denoting the corresponding (right) eigenvector as \mathbf{v}_R and using $\bar{M}_1 = Z_1^{-1} M_1 Z_1$, we find $Z_1 \bar{\mathbf{v}}_R \sim \mathbf{v}_R$, where we can absorb the proportionality constant into Z_1 . Applying this relation twice reveals that $Z_1 \bar{Z}_1 \mathbf{v}_R = \mathbf{v}_R$, such that label 1 must have a trivial Frobenius-Schur indicator

$\approx_1 = 1$.

In addition, it is well known from the theory of MPS (but here applied to the MPOs by using the Hilbert-Schmidt inner product for the operators O_a^L) that for two injective MPO tensors B_a^{ij} and B_b^{ij} that are both normalized such that the spectral radius $\rho(\mathbb{E}_a) = \rho(\mathbb{E}_b) = \lambda$, the spectral radius of $\sum_{ij} B_a^{ij} \otimes \bar{B}_b^{ij} = (\mathbb{1} \otimes Z_b^{-1}) \sum_{i,j} B_a^{ij} \otimes B_b^{ji} (\mathbb{1} \otimes Z_b)$ is either λ (in which case O_a^L and O_b^L are identical and the tensors are related by a gauge transform) or the spectral radius is strictly smaller than λ . Since we can now use the fusion tensors $X_{ab;\mu}^c$ to bring $\sum_{i,j} B_a^{ij} \otimes B_b^{ji}$ into upper block triangular form with diagonal blocks M_c and thus to relate the spectra, this immediately shows that 1 cannot appear in the fusion product of a and b^* unless $b = a$, i.e. $N_{ab^*}^1 = \delta_{ab}$. We can continue along these lines to show some extra symmetry properties of the tensor N . If $N_{ab}^c \neq 0$, then $\sum_{ijk} B_a^{ij} \otimes B_b^{jk} \otimes \bar{B}_c^{ik}$ should have a largest magnitude eigenvalue λ with degeneracy N_{ab}^c . But using the Z matrices, and swapping the matrices in the tensor product, this also means that

$$N_{ab}^c = N_{bc^*}^{a^*} = N_{c^*a}^{b^*}, \quad (3.28)$$

which can further be combined with equation (3.25). In particular, this also shows that $N_{a1}^b = N_{1a}^b = \delta_{ab}$, such that the single block MPO O_1^L indeed corresponds to the neutral object of our algebra.

3.3.4 Associativity and the pentagon equation

Associativity of the product $(O_a^L O_b^L) O_c^L = O_a^L (O_b^L O_c^L)$ implies that

$$\sum_e N_{ab}^e N_{ec}^d = \sum_f N_{af}^d N_{bc}^f. \quad (3.29)$$

In addition, there are two compatible ways to obtain the block decomposition of $B_{abc}^{i,l} = \sum_{j,k} B_a^{i,j} \otimes B_b^{j,k} \otimes B_c^{k,l}$ into diagonal blocks of type $B_d^{i,l}$. Indeed, we have

$$\begin{aligned} X_{ec,\nu}^{d+} \left(X_{ab,\mu}^{e+} \otimes \mathbb{1}_{\chi_c} \right) B_{abc}^{i,l} \left(X_{ab,\mu}^e \otimes \mathbb{1}_{\chi_c} \right) X_{ec,\nu}^d &= B_d^{i,l} \\ X_{af,\sigma}^{d+} \left(\mathbb{1}_{\chi_a} \otimes X_{bc,\lambda}^{f+} \right) B_{abc}^{i,l} \left(\mathbb{1}_{\chi_a} \otimes X_{bc,\lambda}^f \right) X_{af,\sigma}^d &= B_d^{i,l}, \end{aligned}$$

as illustrated in figure 3.2. For PMPOs satisfying the zipper condition (3.22) similar reasoning as in section 3.3.2 shows that for every a, b, c, d there must exist a transformation

$$\left(X_{ab,\mu}^e \otimes \mathbb{1}_{\chi_c} \right) X_{ec,\nu}^d = \sum_{f=1}^{\mathcal{N}} \sum_{\lambda=1}^{N_{bc}^f} \sum_{\sigma=1}^{N_{af}^d} (F_d^{abc})_{e\mu\nu}^{f\lambda\sigma} \left(\mathbb{1}_{\chi_a} \otimes X_{bc,\lambda}^f \right) X_{af,\sigma}^d, \quad (3.30)$$

where F_d^{abc} are a set of invertible matrices. To see this, consider following identity, which follows from the zipper condition,

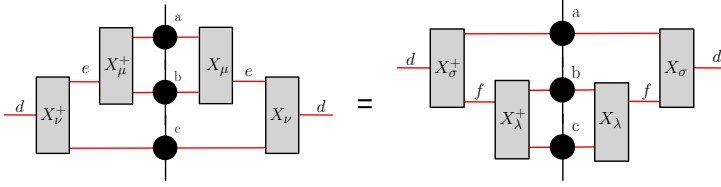


Figure 3.2: Property of MPO and fusion tensors that follows from associativity of the multiplication of O_a^L , O_b^L and O_c^L .

$$\sum_{d e \mu \nu} \begin{array}{c} a \\ b \\ c \end{array} \begin{array}{c} X_\mu^+ \\ X_\nu \end{array} \bullet \begin{array}{c} X_\nu^+ \\ X_\mu^+ \end{array} \begin{array}{c} a \\ b \\ c \end{array} = \sum_{d f \sigma \lambda} \begin{array}{c} a \\ b \\ c \end{array} \begin{array}{c} X_\lambda \\ X_\sigma \end{array} \bullet \begin{array}{c} X_\sigma^+ \\ X_\lambda^+ \end{array} \begin{array}{c} a \\ b \\ c \end{array} \quad (3.31)$$

Acting with fusion tensors on both sides of the equation gives

$$\begin{array}{c} a \\ b \\ c \end{array} \begin{array}{c} X_\mu^+ \\ X_\nu \end{array} \bullet d = \sum_{d' f \sigma \lambda} \begin{array}{c} a \\ b \\ c \end{array} \begin{array}{c} X_\lambda \\ X_\sigma \end{array} \bullet d' \begin{array}{c} X_\sigma^+ \\ X_\lambda^+ \end{array} \begin{array}{c} a \\ b \\ c \end{array} \begin{array}{c} X_\mu^+ \\ X_\nu \end{array} d \quad (3.32)$$

As a final step we use injectivity of the single block MPO tensors. This property implies that $(B_d^{ij})_{\alpha\beta}$, when interpreted as a matrix with rows labeled by ij and columns by $\alpha\beta$, has a left inverse B_d^+ such that $B_d^+ B_d = \delta_{dd'} \mathbb{1}_{\chi_d} \otimes \mathbb{1}_{\chi_d}$. Applying this inverse on both sides of (3.32) leads to the desired expression

$$\begin{array}{c} a \\ b \\ c \end{array} \begin{array}{c} X_\mu^+ \\ X_\nu \end{array} d \otimes d = \sum_{f \sigma \lambda} \begin{array}{c} a \\ b \\ c \end{array} \begin{array}{c} X_\lambda \\ X_\sigma \end{array} d \otimes \begin{array}{c} X_\sigma^+ \\ X_\lambda^+ \end{array} \begin{array}{c} a \\ b \\ c \end{array} \begin{array}{c} X_\mu^+ \\ X_\nu \end{array} d \quad (3.33)$$

The second tensor product factor on the right hand side is exactly $(F_d^{abc})_{e\mu\nu}^{f\lambda\sigma} \mathbb{1}_{\chi_d}$.

The F matrices have to satisfy a consistency condition called the pentagon equation, which is well-known in category theory. It results from deriving the matrix that relates $(X_{ab,\mu}^f \otimes \mathbb{1}_{\chi_c} \otimes \mathbb{1}_{\chi_d})(X_{fc,\nu}^g \otimes \mathbb{1}_{\chi_d})X_{gd,\rho}^e$ to $(\mathbb{1}_{\chi_a} \otimes \mathbb{1}_{\chi_d} \otimes X_{cd,\lambda}^h)(\mathbb{1}_{\chi_a} \otimes X_{bh,\kappa}^i)X_{ai,\sigma}^e$ in two different ways and equating the two resulting expressions. Written down explicitly, the pentagon equation reads

$$\sum_{h,\sigma\lambda\omega} (F_g^{abc})_{h\sigma\lambda}^{f\mu\nu} (F_e^{ahd})_{i\omega\kappa}^{g\lambda\rho} (F_i^{bcd})_{j\gamma\delta}^{h\sigma\omega} = \sum_{\sigma} (F_e^{fcd})_{j\gamma\sigma}^{g\nu\rho} (F_e^{abj})_{i\delta\kappa}^{f\mu\sigma}. \quad (3.34)$$

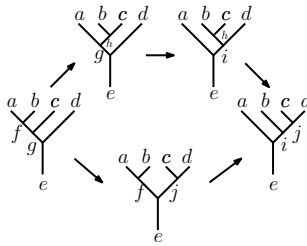


Figure 3.3: Two paths giving rise to the pentagon equation (3.34).

The two ways to obtain the same matrix leading to the pentagon equation are shown in figure 3.3. A standard result in category theory, called Mac Lane’s coherence theorem, states that the pentagon equation is the only consistency relation that needs to be checked; once it is satisfied all other possible consistency conditions are also automatically satisfied [32, 165].

The complete set of algebraic data we have associated to a Hermitian PMPO P_L that satisfies the zipper condition (3.22) is $(N_{ab}^c, F_d^{abc}, \varkappa_a)$. Note that (N_{ab}^c, F_d^{abc}) is (in many cases) known to be robust in the sense that every small deformation of the matrices F_d^{abc} that satisfies the pentagon equation can be absorbed in the fusion tensors via a suitable gauge transformation Y . This remarkable property is called Ocneanu rigidity [32, 166] and it shows that PMPOs satisfying the zipper condition naturally fall into discrete families.

$(N_{ab}^c, F_d^{abc}, \varkappa_a)$ is very similar to the algebraic data defining a fusion category. We argued in section 3.3.3 that when a PMPO has a unital structure then the definition of duality as derived from Hermitian conjugation is equivalent to the categorical definition. Similar kind of reasoning also shows that our definition of \varkappa_a coincides with that of the Frobenius-Schur indicator in fusion categories for a large class of PMPOs with unital structure that satisfy the zipper condition. We elaborate on this and other connections to fusion categories in Appendix 3.A. If the PMPO does not have a unital structure then the data $(N_{ab}^c, F_d^{abc}, \varkappa_a)$ defines a multi-fusion category, i.e. a kind of tensor category whose definition does not require the unit element to be simple.

3.4 MPO-injective PEPS

Using the PMPOs introduced in the previous section we can now define a class of states on two-dimensional lattices called MPO-injective PEPS, as introduced in [106, 108, 109]. The importance of this class of PEPS is that it can describe topologically ordered systems. For example, it was shown in [109] that all string-net ground states have an exact description in terms of MPO-injective PEPS. In section 3.4.1 we first impose some additional

properties on the PMPOs, which are required in order to construct PEPS satisfying all MPO-injectivity axioms in section 3.4.2. In section 3.4.3 we review some properties of the resulting class of MPO-injective PEPS.

3.4.1 Unitarity, zipper condition and pivotal structure

To be able to construct MPO-injective PEPS in section 3.4.2 we have to impose three properties on the PMPOs we consider.

Firstly, we require is that there exists a gauge on the internal MPO indices such that the fusion tensors $X_{ab,\mu}^c$ are isometries –such that $X_{ab,\mu}^{c+} = (X_{ab,\mu}^c)^\dagger$ – and the gauge matrices Z_a , introduced in section 3.3.3, are unitary. This brings PMPOs into the realm of unitary fusion categories, which will be required for various consistency conditions throughout. We now devise a new graphical language where the matrices Z_a are represented as

$$\begin{aligned}
 \begin{array}{c} a^* \\ \rightarrow \\ \blacktriangleleft \\ \leftarrow \\ a \end{array} &= Z_a & \begin{array}{c} a \\ \rightarrow \\ \blacktriangleright \\ \leftarrow \\ a^* \end{array} &= Z_a^T & (3.35) \\
 \begin{array}{c} a \\ \rightarrow \\ \blacktriangleright \\ \leftarrow \\ a^* \end{array} &= Z_a^{-1} & \begin{array}{c} a^* \\ \rightarrow \\ \blacktriangleleft \\ \leftarrow \\ a \end{array} &= (Z_a^{-1})^T
 \end{aligned}$$

Note that absolute orientation of the symbols used to represent the matrices has no meaning, as we will be using those in a two-dimensional setting where the tensors will be rotated. Rotating the first figure by 180° exchanges the row and column indices of the matrix and is thus equivalent to transposition, which is compatible with the graphic representation of Z_a^T . Because of unitarity, $(Z_a^{-1})^T = \bar{Z}_a$ and complex conjugation of the tensor simply amounts to reversing the arrows. The definition of the Frobenius-Schur indicator $Z_a \bar{Z}_{a^*} = \varkappa_a \mathbb{1}$ can now also be written as

$$\begin{array}{c} a^* \\ \rightarrow \\ \blacktriangleleft \\ \leftarrow \\ a \end{array} = \varkappa_a \begin{array}{c} a^* \\ \rightarrow \\ \blacktriangleright \\ \leftarrow \\ a \end{array} . \quad (3.36)$$

The second requirement is that the zipper condition (3.22) holds:

$$\begin{aligned}
 \begin{array}{c} a \\ \rightarrow \\ \bullet \\ \uparrow \\ b \\ \rightarrow \\ \bullet \\ \uparrow \\ \mu \end{array} &= \begin{array}{c} a \\ \rightarrow \\ \mu \\ \rightarrow \\ b \\ \rightarrow \\ \bullet \\ \uparrow \\ c \end{array} & (3.37) \\
 \begin{array}{c} c \\ \rightarrow \\ \mu \\ \rightarrow \\ a \\ \rightarrow \\ \bullet \\ \uparrow \\ b \\ \rightarrow \\ \bullet \\ \uparrow \\ \mu \end{array} &= \begin{array}{c} c \\ \rightarrow \\ \bullet \\ \uparrow \\ \mu \\ \rightarrow \\ a \\ \rightarrow \\ \bullet \\ \uparrow \\ b \\ \rightarrow \\ \mu \end{array}
 \end{aligned}$$

As already mentioned in section 3.3.2 this corresponds to the absence of blocks above the diagonal. In this new graphical notation, we no longer explicitly write X on the fusion tensors, but only the degeneracy label μ . A normal fusion tensor $X_{ab,\mu}^c$ has two incoming arrows and one outgoing, while its left inverse $X_{ab,\mu}^{c\dagger} = (X_{ab,\mu}^c)^\dagger$ has two outgoing arrows and one incoming. In order to determine the difference between e.g. X_{ab}^c and X_{ba}^c , any fusion tensor in a graphical diagram always has to be read by rotating it back to the above standard form; note that one should not flip (mirror) any symbol. Consistent use of the arrows is also indispensable in the graphical notation for MPO-injective PEPS in the next section.

The third and final requirement for the PMPO is that the fusion tensors satisfy a property which is closely related to the *pivotal structure* in fusion category theory:

$$\begin{array}{c} \text{a}^* \\ \text{b} \end{array} \rightarrow \begin{array}{|c|} \hline \mu \\ \hline \end{array} \begin{array}{c} \text{c} \\ \text{a} \end{array} = \sum_{\nu} (A_{ab}^c)_{\mu\nu} \begin{array}{|c|} \hline \nu \\ \hline \end{array} \begin{array}{c} \text{a} \\ \text{c} \end{array}, \quad (3.38)$$

where the square matrices A_{ab}^c satisfy $(A_{ab}^c)^\dagger A_{ab}^c = \frac{w_c}{w_b} \mathbb{1}$. A similar property holds if we bend the lower b index on the left hand side of (3.38), with a set of invertible matrices A'_{ab}^c satisfying $(A'_{ab}^c)^\dagger A'_{ab}^c = \frac{w_c}{w_a} \mathbb{1}$. Note that this is only possible when all the numbers w_a have the same phase. Using equation (3.23) this implies that all w_a are either positive or negative real numbers. From $\sum_{a,b=1}^N N_{ab}^c w_a w_b = w_c$ and the fact that N consists of nonnegative entries it then follows that all w_a must be positive. Furthermore, the pivotal property requires that the tensor N satisfies

$$N_{a^*b}^c = N_{ac}^b \quad (3.39)$$

which is indeed satisfied by combining the equalities (3.25) and (3.28) from Section 3.3.3. While we do believe that the pivotal property (3.38) follows from the zipper condition and the unitary/isometric property of the gauge matrices and the fusion tensors, the proof falls beyond the scope of this paper and we here impose it as an extra requirement.

By repeated application of the pivotal property, we obtain the following relation between the fusion tensors $X_{ab,\mu}^c$ and the gauge matrices Z_a :

$$\begin{array}{c} \text{a}^* \\ \text{b}^* \end{array} \rightarrow \begin{array}{|c|} \hline \mu \\ \hline \end{array} \begin{array}{c} \text{c} \\ \text{c}^* \end{array} = \sum_{\nu} (C_{ab}^c)_{\mu\nu} \begin{array}{|c|} \hline \nu \\ \hline \end{array} \begin{array}{c} \text{a}^* \\ \text{b}^* \end{array} \begin{array}{c} \text{c}^* \end{array}, \quad (3.40)$$

where $C_{ab}^c = A_{a^*b}^c \bar{A}_{a^*c^*}^b A_{b^*c^*}^{a^*}$ can be verified to be a unitary matrix. This relation also holds on more general grounds for any Hermitian PMPO satisfying the zipper condition, although with non-unitary C_{ab}^c in general.

Now that we have collected all the necessary properties for the relevant PMPOs we can turn to tensor network states on two-dimensional lattices in the next section. Note that the PMPOs that satisfy the properties discussed in this section could be thought of as classifying anomalous one-dimensional topological orders, i.e. the gapped topological orders that can be realized on the boundary of a two-dimensional bulk [167].

3.4.2 Entangled subspaces

The first step in our construction of a MPO-injective PEPS is to introduce two different types of MPO tensors. For the right handed type,

$$\begin{array}{c} j \\ | \\ \bullet \\ | \\ i \\ \leftarrow a \quad \rightarrow \beta \\ \alpha \end{array} = (B_{a,+}^{ij})_{\alpha\beta}, \quad (3.41)$$

we use the original tensors of the Hermitian PMPO we started from. The left handed type,

$$\begin{array}{c} j \\ | \\ \bullet \\ | \\ i \\ \leftarrow a \quad \rightarrow \beta \\ \alpha \end{array} = (B_{a,-}^{ij})_{\beta\alpha}, \quad (3.42)$$

is defined by complex conjugating $B_{a,+}$, which reverses the arrows, and then transposing i and j , i.e.

$$(B_{a,-}^{ij})_{\beta\alpha} = (\bar{B}_{a,+}^{ji})_{\alpha\beta}. \quad (3.43)$$

This is exactly the tensor that is obtained by applying Hermitian conjugation to the resulting MPO, as discussed in section 3.3.3. We can thus relate both tensors using the gauge matrices Z_a , which we now depict using the graphical notation as

$$\begin{array}{c} | \\ \bullet \\ | \\ a \\ \leftarrow a \quad \rightarrow \beta \\ \alpha \end{array} = \begin{array}{c} a \\ \leftarrow \triangleleft \bullet \triangleright \\ a^* \\ | \\ a \\ \leftarrow a \quad \rightarrow \beta \\ \alpha \end{array} \quad (3.44)$$

$$\begin{array}{c} | \\ \bullet \\ | \\ a \\ \leftarrow a \quad \rightarrow \beta \\ \alpha \end{array} = \begin{array}{c} a \\ \leftarrow \triangleleft \bullet \triangleright \\ a^* \\ | \\ a \\ \leftarrow a \quad \rightarrow \beta \\ \alpha \end{array}. \quad (3.45)$$

Here we also used that the matrices Z_a are unitary and the identity in Eq. (3.36).

With these tensors, MPO-injective PEPS can be constructed on arbitrary lattices. Firstly, assign an orientation to every edge of the lattice. Now define the MPO \tilde{F}_{C_v} at every vertex v , with C_v the coordination number of v , as follows: assign a counterclockwise orientation to v . At every edge

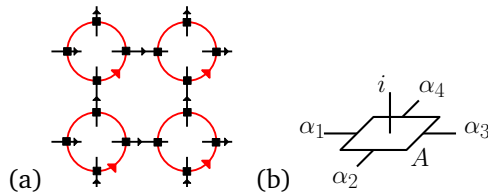


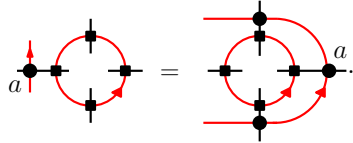
Figure 3.4: (a) A MPO-injective PEPS on a 2 by 2 square lattice with open boundaries. We assigned an orientation to every edge as indicated by the black arrows and an orientation to the internal MPO index represented by the red arrow. (b) A tensor A that can be used to complete the PEPS on the square lattice.

connected to v , place a right handed or left handed MPO tensor depending on the global orientation and the edge orientation. The MPO \tilde{P}_{C_v} is then obtained by contracting the C_v tensors along the internal MPO indices. With the unitary constraints on the gauge and fusion tensors, the original PMPO P_L that we started from allows for a unitary gauge freedom on the virtual indices of every MPO tensor B_a^{ij} . Note, however, that the choice of $B_{a,\pm}^{ij}$ and the transformation behavior of the gauge matrices Z_a is such that this is also a gauge freedom of the newly constructed \tilde{P}_{C_v} .

One can furthermore check that since the fusion tensors are isometries the resulting MPO \tilde{P}_L is a Hermitian projector just like P_L when the same weights w_a for the blocks are used. Note that reversing the internal orientation of a single block MPO in \tilde{P}_L amounts to taking the Hermitian conjugate and the weights satisfy $w_a = w_{a^*}$, so reversing the orientation of the internal index of \tilde{P}_{C_v} is equivalent to Hermitian conjugation, which leaves \tilde{P}_{C_v} invariant. So the counterclockwise global internal orientation on \tilde{P}_{C_v} is completely arbitrary.

Now that we have the Hermitian projectors \tilde{P}_{C_v} at every vertex we place a maximally entangled qudit pair $\sum_{i=1}^D |i\rangle \otimes |i\rangle$ on all edges of the lattice. We subsequently act at every vertex v with \tilde{P}_{C_v} on the qudits closest to v of the maximally entangled pairs on the neighboring edges. In this way we entangle the subspaces determined by \tilde{P}_{C_v} at each vertex. The resulting PEPS is shown in figure 3.4 for a 2 by 2 patch out of a square lattice. More general PEPS are obtained by placing an additional tensor $A[v] = \sum_{i=1}^d \sum_{\{\alpha\}=1}^D A[v]_{\alpha_1 \alpha_2 \dots \alpha_{C_v}}^i |i\rangle \langle \alpha_1 \alpha_2 \dots \alpha_{C_v}|$ at each vertex which maps the C_v indices on the inside of every MPO loop to a physical degree of freedom in \mathbb{C}^d . As long as $A[v]$ is injective as a linear map from $\mathbb{C}^{D^{C_v}}$ to \mathbb{C}^d (which requires $d \geq D^{C_v}$) the resulting PEPS satisfies the axioms of MPO injectivity as defined in [109], which we show below. For the particular case where each $A[v]$ is an isometry, the resulting network is an (MPO)-isometric PEPS. Throughout the remainder of this paper we ignore the tensors $A[v]$ as we will argue that the universal properties of the quantum phase of the PEPS are completely encoded in the entangled injectivity subspaces \tilde{P}_{C_v} .

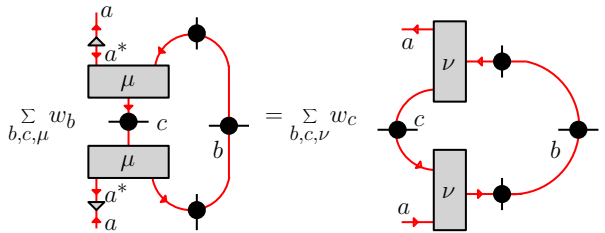
We can now prove the following central identity, which we henceforth refer to as the *pulling through equation*:



$$(3.46)$$

Note again the difference between squares that denote the superposition of the different injective MPOs $a = 1, \dots, N$ with suitable coefficients w_a and the discs that represent a single block MPO tensor of type a .

Using the zipper condition (3.37) we can write (3.46) as



$$(3.47)$$

From the pivotal property (3.38) and the fact that A_{ab}^c satisfy $(A_{ab}^c)^\dagger A_{ab}^c = \frac{w_c}{w_b} \mathbb{1}$ one can then indeed check the validity of (3.47).

Two additional notes are in order. Firstly, one could easily imagine different simple generalizations of the MPO-injectivity formalism. But as they are not necessary to understand the fundamental concepts we wish to illustrate, we keep the presentation simple and do not consider them here. However, in the string-net example later on we come across such a simple generalization and see how it leads to a slightly modified form of condition (3.38).

Secondly, rather than starting from a PMPO and using it to construct a PEPS tensor, we could have followed the reverse strategy and started from the set of injective MPOs that satisfy the pulling through equation for a given PEPS tensor. This set also forms an algebra (the product of two such MPOs is an MPO satisfying the pulling through equation and can therefore be decomposed into a linear combination of injective MPOs from the original set) and the PEPS tensor would naturally be supported on the virtual subspace corresponding to the central idempotent of that algebra, which corresponds to our PMPO \tilde{P}_{C_v} . Both approaches are of course completely equivalent.

3.4.3 Virtual support and parent Hamiltonians

The pulling through equation (3.46), which we have proven in the previous subsection, is the first property required for a PEPS to be MPO-injective according to the definition in Ref. [109]. The second property, or an alternative

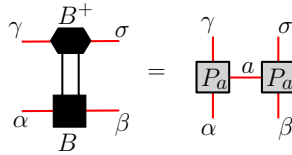


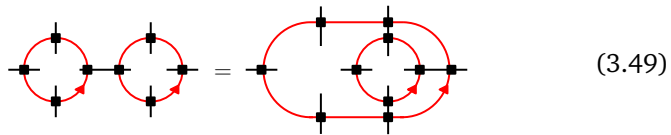
Figure 3.5: Acting with pseudo-inverse B^+ on the MPO tensor B gives a projector on block-diagonal matrices with \mathcal{N} blocks of dimension χ_a .

to it, is obtained automatically if we assume that the MPO has already been blocked such that the set of tensors $B^{ij}, \forall i, j = 1, \dots, D$ already span the full space $\oplus_{a=1, \dots, \mathcal{N}} \mathbb{C}^{\chi_a \times \chi_a}$ (corresponding to the injective blocks a in the canonical form) without having to consider any products. We then have the relation

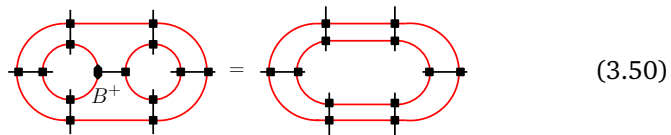
$$\sum_{i,j=1}^D B_{\gamma\sigma}^{+ij} B_{\alpha\beta}^{ij} = \sum_{a=1}^{\mathcal{N}} (P_a)_{\alpha\gamma} (P_a)_{\beta\sigma}, \tag{3.48}$$

where $B_{\gamma\sigma}^{+ij}$ is the pseudo-inverse of $B_{\alpha\beta}^{ij}$ interpreted as $D^2 \times \chi^2$ matrix. P_a are a set of \mathcal{N} projectors on the χ_a -dimensional subspaces labeled by a . The right hand side of (3.48) thus represents the projector on block diagonal matrices with \mathcal{N} blocks, labeled by a , of dimension χ_a . Equation (3.48) is also shown graphically in figure 3.5 and requires $D^2 > \sum_a \chi_a^2$. It essentially means that by acting with B^+ on a tensor B we can ‘open up’ the virtual indices of a closed projector MPO.

With these two properties, we can show that the virtual support of the PEPS map on every contractible region with boundary of length L is given by the PMPO \tilde{P}_L surrounding that region. Indeed, using the pulling through property we can grow the PMPO of a single tensor (note that we no longer explicitly indicate the orientation of every edge):



Then we can act with B^+ on the inner MPO loop to open up the indices and make it act on the entire boundary:



By repeating this trick we can indeed grow the PMPO to the boundary of any contractible region.

These arguments also imply that the rank of the reduced density matrix of the physical degrees of freedom in some finite region with a boundary of length L is equal to the rank of the PMPO \tilde{P}_L . Therefore, the zero Renyi entropy of a region with a boundary containing L virtual indices is

$$S_0 = \log(\text{Tr}(\tilde{P}_L)) = \log \text{tr} \left(\left(\sum_{i=1}^D B^{ii} \right)^L \right) = \log \left(\sum_{a=1}^{\mathcal{N}} w_a \text{tr} \left(M_a^L \right) \right), \quad (3.51)$$

where Tr denotes the trace over external MPO indices, tr denotes the trace over internal MPO indices and the matrices $M_a = \sum_i B_a^{ii}$ were defined in Section 3.3.3. Using the eigenvalue structure of the matrices M_a , we find that if the PMPO has a unital structure the zero Renyi entropy for large regions scales as

$$S_0 \approx \lambda_1 L - \log \left(\frac{1}{w_1} \right). \quad (3.52)$$

For fixed point models this constant correction will also appear in the von Neumann entropy, thus giving rise to the well-known topological entanglement entropy [40]. It was shown in [160] that if the PMPO has a unique block, i.e. if $\mathcal{N} = 1$, there is no topological entanglement entropy. In the next section, we show explicitly that using a single blocked PMPO in our PEPS construction does indeed not allow for the existence of different topological sectors.

The constructed MPO-injective PEPS corresponds to the exact ground state of a local, frustration free Hamiltonian. The so-called parent Hamiltonian construction is identical to that of standard injective PEPS [103] and takes the form

$$H = \sum_p h_p, \quad (3.53)$$

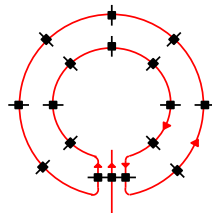
where the sum is over all plaquettes of the lattice and h_p is a positive semi-definite operator whose kernel corresponds to the image (physical support) of the PEPS map on that plaquette. For the square lattice, this is the image of the PEPS map shown in Fig. 3.4(a), interpreted as a matrix from the outer 8 to the inner 16 indices. Typically, h_p is defined as the projector onto the orthogonal complement of the physical support of the PEPS map. In [109] the pulling through property was shown to be sufficient to prove that all the ground states of the parent Hamiltonian (3.53) on a closed manifold are given by MPO-injective PEPS states whose virtual indices along the non-contractible cycles are closed using the same MPOs connected by a so-called ground state tensor Q . Because of the pulling through property these MPO loops can be moved freely on the virtual level of the PEPS, implying that all ground states are indistinguishable by local operators.

3.5 Anyon sectors in MPO-injective PEPS

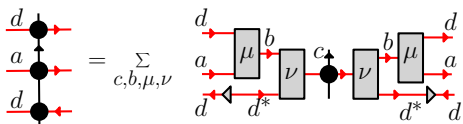
Having gathered all the concepts and technical tools of PMPOs and MPO-injective PEPS we can now turn to the question of how to construct topological sectors in these models. As argued in the previous section and shown in [109], MPO-injective PEPS give rise to degenerate ground states on nontrivial manifolds that are locally indistinguishable. Systems with this property that are defined on a large but finite open region are believed to have a low-energy eigenstate basis that can be divided into a finite number of topological superselection sectors, such that it is possible to measure in which sector a state is by acting only locally in the bulk of the region, but to go from a state in one sector to a state in another sector one necessarily has to act on both bulk and boundary. The elementary excitations in each sector are called *anyons* and can be seen as a generalization of bosons and fermions [7, 8]. In this section we show that the entanglement structure of the ground state PEPS as determined by the PMPO \tilde{P}_C contains all necessary information to find the anyonic sectors and their topological properties.

3.5.1 Topological charge

To find the topological sectors we start by looking at a patch of the ground state PEPS on an annulus. It was shown in [109] that the support of the ground state tensors in the annulus is equal to the support of the following tensor when we interpret it as a collection of matrices from the indices outside the annulus to the indices inside:


(3.54)

We now use following equality, which follows from the zipper condition (3.37) and (3.44),


(3.55)

to see that whatever tensor we put in the hole of the annulus, its relevant support space is given by the support of following tensors when interpreted

as matrices from the outer indices to the inner ones

$$A_{abcd,\mu\nu} = \text{Diagram} \tag{3.56}$$

A crucial observation is now that the matrices $A_{abcd,\mu\nu}$ form a C^* -algebra, i.e. we have that

$$A_{hegf,\lambda\sigma} A_{abcd,\mu\nu} = \delta_{ga} \sum_{ij,\rho\tau} \Omega_{(hegf,\lambda\sigma)(abcd,\mu\nu)}^{(hjc i,\rho\tau)} A_{hjc i,\rho\tau} \tag{3.57}$$

and

$$A_{abcd,\mu\nu}^\dagger = \sum_{e,\lambda\sigma} (\Theta_{abcd,\mu\nu})^{e\sigma\lambda} A_{cead^*,\sigma\lambda} \tag{3.58}$$

We show this explicitly in appendix 3.B. It is a well-known fact that every finite dimensional C^* -algebra is isomorphic to a direct sum of simple matrix algebras. We now claim that the topological sectors correspond to the different blocks in this direct sum decomposition of the algebra. This means we relate an anyon sector i to every minimal central idempotent \mathcal{P}_i satisfying $\mathcal{P}_i \mathcal{P}_j = \delta_{ij} \mathcal{P}_i$, $\mathcal{P}_i^\dagger = \mathcal{P}_i$ and $A_{abcd,\mu\nu} \mathcal{P}_i = \mathcal{P}_i A_{abcd,\mu\nu}$, where \mathcal{P}_i takes the form

$$\mathcal{P}_i = \sum_{abd,\mu\nu} c_{abd,\mu\nu}^i A_{abad,\mu\nu}. \tag{3.59}$$

Because we want to be able to measure the topological charge of an excitation it is a well-motivated definition to associate topological sectors to orthogonal subspaces. We note that in [161] a similar identification of anyons in string-net models with central idempotents was given. This idea dates back to the tube algebra construction of Ocneanu [168, 169]. In the remainder of this paper we represent the minimal central idempotents \mathcal{P}_i graphically as

$$\mathcal{P}_i = \text{Diagram} \tag{3.60}$$

One can easily see that the coefficients $c_{abd,\mu\nu}^i$ give the same central idempotent \mathcal{P}_i independent of the number of MPO tensors used to define $A_{abad,\mu\nu}$, i.e. the \mathcal{P}_i are projectors for every length. In appendix 3.C we give a numerical algorithm to explicitly construct the central idempotents \mathcal{P}_i .

3.5.2 Anyon ansatz

Having identified the topological sectors we would now like to construct MPO-injective PEPS containing anyonic excitations. To do so we first need to take a closer look at the C^* -algebra spanned by the elements $A_{abcd,\mu\nu}$.

A general central idempotent \mathcal{P}_i consists of a sum of idempotents $P_i^{a\alpha}$ that are not central:

$$\mathcal{P}_i = \sum_{a=1}^{D_i} \sum_{\alpha=1}^{d_{i,a}} P_i^{a\alpha}, \quad (3.61)$$

where the index a refers to the D_i MPO block labels that appear in \mathcal{P}_i , which we gave an arbitrary ordering. The $P_i^{a\alpha}$ satisfy $P_i^{a\alpha} P_j^{b\beta} = \delta_{i,j} \delta_{a,b} \delta_{\alpha,\beta} P_i^{a\alpha}$ and $P_i^{a\alpha\dagger} = P_i^{a\alpha}$. We also take the $P_i^{a\alpha}$ to be simple, i.e. they cannot be decomposed further as an orthogonal sum of idempotents. A central idempotent with $r_i \equiv \sum_{a=1}^{D_i} d_{i,a} > 1$ is called a higher dimensional central idempotent. From the algebra structure (3.57) and (3.58) we see that the simple idempotents have a diagonal block label, i.e. they can be expressed in terms of the basis elements as

$$P_i^{a\alpha} = \sum_{bd,\mu\nu} t_{bd,\mu\nu}^{a\alpha,i} A_{abcd,\mu\nu}. \quad (3.62)$$

The dimension of the algebra, i.e. the total number of basis elements $A_{abcd,\mu\nu}$, equals $\sum_i r_i^2$: for every \mathcal{P}_i the algebra also contains $r_i(r_i - 1)$ nilpotents $P_i^{a\alpha,b\beta}$. The nilpotents satisfy $(P_i^{a\alpha,b\beta})^\dagger = P_i^{b\beta,a\alpha}$ and $P_i^{a\alpha,b\beta} P_j^{c\gamma,d\delta} = \delta_{i,j} \delta_{b,c} \delta_{\beta,\gamma} P_i^{a\alpha,d\delta}$. Note that $P_i^{a\alpha,a\alpha} \equiv P_i^{a\alpha}$ is not a nilpotent but one of the non-central simple idempotents. Combining the simple idempotents and nilpotents we can define the projectors

$$\Pi_i^{[x]} = \sum_{a_\alpha, b_\beta=1}^{r_i} x_{a_\alpha b_\beta}^i P_i^{a_\alpha, b_\beta}, \quad (3.63)$$

where

$$\bar{x}_{a_\alpha b_\beta}^i = x_{b_\beta a_\alpha}^i \quad \text{and} \quad \sum_{b_\beta} x_{a_\alpha b_\beta}^i x_{b_\beta d_\delta}^i = x_{a_\alpha d_\delta}^i. \quad (3.64)$$

If $x_{a_\alpha b_\beta}^i = \bar{v}_{a_\alpha}^i v_{b_\beta}^i$ we call $\Pi_i^{[x]}$ a ‘rank one’ projector (note that $\Pi_i^{[x]}$ does not have to be a rank one matrix, but this terminology refers to the C^* -algebra structure.)

Let us now return to the MPO-injective PEPS. As explained above, every ground state tensor has virtual indices which are supported in the subspace \bar{P} . To introduce anyonic excitations in the tensor network we need a new type of PEPS tensor. If we want to place an anyon at vertex v with coordination number C_v this new type of tensor has C_v virtual indices of dimension D ,

one virtual index of dimension χ and one physical index of dimension d . On a square lattice for example, we depict this tensor as

$$I = \begin{array}{c} \diagup \\ \text{---} \square \text{---} \\ \diagdown \\ \uparrow \end{array} \quad i, \quad (3.65)$$

where the physical index points to the top left corner and the χ -dimensional index is on the bottom left corner. The label i and the name of the tensor I refer to the topological sector. A necessary condition for this tensor to describe an excitation with topological charge i is that its virtual indices are supported in the subspace determined by \mathcal{P}_i :

$$\begin{array}{c} \text{---} \square \text{---} \\ \diagup \quad \diagdown \\ \uparrow \end{array} \quad i = \delta_{i,j} \begin{array}{c} \text{---} \square \text{---} \\ \diagup \quad \diagdown \\ \uparrow \end{array} \quad i \equiv \delta_{i,j} I \quad (3.66)$$

This property provides a heuristic interpretation of topological sectors in terms of entanglement. For isometric PEPS the virtual indices along the boundary of a region label the Schmidt states of the physical indices and can therefore be interpreted as the ‘entanglement degrees of freedom’. Topological sectors are then characterized by entanglement degrees of freedom that live in orthogonal subspaces, so they are really the degrees of freedom that contain the topological information. When we go away from the fixed point the interpretation of virtual degrees of freedom as entanglement degrees of freedom starts to break down and one can understand how the construction fails beyond the phase transition.

Property (3.66) is not sufficient to obtain a good anyonic excitation tensor. To see what additional properties it should have we construct a MPO-injective PEPS containing an anyon pair (i, i^*) , where i^* will be defined in a moment. We can do this by starting from the ground state PEPS, replacing the tensors at two vertices by the excitation tensors corresponding to sectors i and i^* and then connecting the χ -dimensional indices of the excitation tensors with the appropriate MPO on the virtual level. See figure 3.6 for an example on the 3 by 3 square lattice. Note that the position of the virtual MPO is irrelevant since it can be moved by using the pulling through property.

If we interpret I as a matrix with the rows labeled by the physical index and the columns by the virtual indices then we can write (3.66) as $IP_j = \delta_{i,j}I$. To construct the PEPS containing the (i, i^*) anyon pair we do not use the full tensor I but project its virtual indices in the space corresponding to the simple idempotent $P_i^{a\alpha}$: $I^{a\alpha} \equiv IP_i^{a\alpha}$, where a is one of the MPO block labels appearing in (3.61). Let us assume that we have connected the

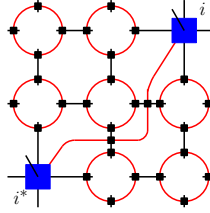


Figure 3.6: A MPO-injective PEPS on a 3 by 3 square lattice containing an anyon pair (i, i^*) located at the lower left and upper right corner.

tensors I^{a_α} and I^{*a_α} on the virtual level with a single block MPO a . We now want the total anyon pair to be in the vacuum sector. We can impose this by surrounding the tensors with the vacuum projector \tilde{P} . If we ignore the ground state PEPS environment we can represent the vacuum anyon pair graphically as

(3.67)

The anyon type i^* is defined as the unique topological sector such that (3.67) is non-zero for a fixed i (see section 3.5.5 for more details). Using (3.55) we can rewrite (3.67) as

$$\sum_{bcd, \mu\nu} w_d \dots$$
(3.68)

Here we again recognize the algebra basis elements $A_{abcd, \mu\nu}^\dagger$ and $A_{abcd, \mu\nu}$ (see Appendix 3.B.2 for more details on how to identify the Hermitian conjugate). We now make use of the fact that the basis elements can be written as

$$A_{abcd, \mu\nu} = \sum_{i, \alpha\gamma} u_{abcd, \mu\nu}^{i, a_\alpha c_\gamma} P_i^{a_\alpha, c_\gamma}, \tag{3.69}$$

$$A_{abcd, \mu\nu}^\dagger = \sum_{i, \alpha\gamma} \tilde{u}_{abcd, \mu\nu}^{i, c_\gamma a_\alpha} P_i^{a_\alpha, c_\gamma}. \tag{3.70}$$

Note that once we have found the idempotents we can easily obtain the coefficients $u_{abcd, \mu\nu}^{i, a_\alpha c_\gamma}$ by $P_i^{a_\alpha} A_{abcd, \mu\nu} P_i^{c_\gamma} = u_{abcd, \mu\nu}^{i, a_\alpha c_\gamma} P_i^{a_\alpha, c_\gamma}$. If we represent the simple idempotents and nilpotents as

$$P_i^{a_\alpha, b_\beta} = \text{Diagram}, \quad (3.71)$$

then we can write (3.68) as

$$\sum_{c, \gamma \lambda} \left(\sum_{bcd, \mu \nu} u_{abcd, \mu \nu}^{i, a_\alpha c_\gamma} \bar{u}_{abcd, \mu \nu}^{i^*, c_\lambda a_\sigma} w_d \right) \text{Diagram} \quad (3.72)$$

So we see that in order to be able to take the tensors I and I^* and connect them on the virtual level such that they are in the vacuum state it should hold that

$$I^{a_\alpha} P_i^{a_\alpha, c_\gamma} \propto I^{c_\gamma}. \quad (3.73)$$

Equation (3.73) tells us something about the injectivity property of I . Suppose that I would be injective on the subspace corresponding to \mathcal{P}_i when we interpret it as a matrix from the virtual to the physical indices, i.e. there is a left inverse I^+ such that $I^+ I = \mathcal{P}_i$. (Note that we know from non-topological tensor networks that excitation tensors are generically not injective [170, 171]. However, they could become injective by blocking them with multiple surrounding ground state tensors. Even if this would not be the case we want our formalism to hold irrespective of the specific Hamiltonian so we can focus on the extreme cases where the excitation tensors are injective.) Acting with I^+ on both sides of equation (3.73) would give $P_i^{a_\alpha, b_\beta} \propto P_i^{b_\beta}$, which is clearly an inconsistency. For this reason we consider the more general case

$$I^+ I = \Pi_i^{[x]}, \quad (3.74)$$

where we need to determine the coefficients $x_{a_\alpha b_\beta}^i$. Now we get from (3.73)

$$\sum_{c_\gamma} x_{c_\gamma a_\alpha}^i P_i^{c_\gamma, b_\beta} \propto \sum_{c_\gamma} x_{c_\gamma b_\beta}^i P^{c_\gamma, b_\beta} \quad \forall b_\beta. \quad (3.75)$$

This shows that all columns of the matrix $[x]$ are proportional, implying that $\Pi_i^{[x]}$ is rank one, i.e. $x_{a_\alpha b_\beta}^i = \bar{v}_{a_\alpha}^i v_{b_\beta}^i$ and $\sum_{a_\alpha} \bar{v}_{a_\alpha}^i v_{a_\alpha}^i = 1$. This is consistent with the fact that it should not be possible to differentiate between the (i, i^*) -pair before and after vacuum projection via the physical indices of only I or I^* . That (i, i^*) are together in the vacuum state is a global, topological property and this information should not be accessible by looking at only one anyon in the pair. Anyons also detect each other's presence via nonlocal,

topological interactions that can be thought of as a generalized Aharonov-Bohm effect [172]. In section 3.5.6 we elaborate on how the virtual MPO strings implement this topological interaction. The fact that the virtual MPO strings implement topological interactions is consistent with the rank one property of $\Pi_i^{[x]}$ because the physical indices of a single excitation tensor should not allow one to deduce which virtual MPO string is connected to the tensor on the virtual level.

With the rank one $[x]$ we get from (3.73)

$$I^{a_\alpha} P^{a_\alpha, c_\gamma} = \frac{v_{a_\alpha}^i}{v_{c_\gamma}^i} I^{c_\gamma}. \quad (3.76)$$

So we can always choose tensors I^{a_α} such that

$$I^{a_\alpha} P^{a_\alpha, c_\gamma} = I^{c_\gamma} \quad \text{and} \quad I^+ I = \left(\sum_{a_\alpha} P_i^{a_\alpha, x} \right) \left(\sum_{b_\beta} P_i^{x, b_\beta} \right). \quad (3.77)$$

Using this choice for I we can write the equality of equations (3.67) and (3.72) as

$$\begin{aligned} (I^{a_\alpha} \otimes_a I^{a_\sigma}) \tilde{P} &= \sum_{c, \gamma \lambda} \left(\sum_{bcd, \mu\nu} u_{abcd, \mu\nu}^{i, a_\alpha c_\gamma} \bar{u}_{abcd, \mu\nu}^{i^*, c_\lambda a_\sigma} w_d \right) I^{c_\gamma} \otimes_c I^{c_\lambda} \\ &\equiv \sum_{c, \gamma \lambda} M_{c\gamma\lambda, a\alpha\sigma} I^{c_\gamma} \otimes_c I^{c_\lambda}, \end{aligned} \quad (3.78)$$

$$(3.79)$$

where we used \otimes_a to denote the tensor product of two anyonic excitation tensors connected with the single block MPO a and introduced the matrix M . We get from (3.79)

$$\left(\sum_{a\alpha\sigma} y_{a\alpha\sigma} I^{a_\alpha} \otimes_a I^{a_\sigma} \right) \tilde{P} = \sum_{c\gamma\lambda} \left(\sum_{a\alpha\sigma} M_{c\gamma\lambda, a\alpha\sigma} y_{a\alpha\sigma} \right) I^{c_\gamma} \otimes_c I^{c_\lambda} \quad (3.80)$$

So in order for the (i, i^*) pair to be in the vacuum we should choose $y_{a\alpha\sigma}$ to be an eigenvector of M :

$$\sum_{a\alpha\sigma} M_{c\gamma\lambda, a\alpha\sigma} y_{a\alpha\sigma} = y_{c\gamma\lambda}. \quad (3.81)$$

Because \tilde{P} is a projector the matrix M is also a projector and therefore has eigenvalues one or zero. Note that in general the vector $y_{c\gamma\lambda}$ will be entangled in the indices γ and λ . However, this is purely ‘virtual’ entanglement that cannot be destroyed by measurements on only one anyon in the pair because of the rank-one injectivity structure of I .

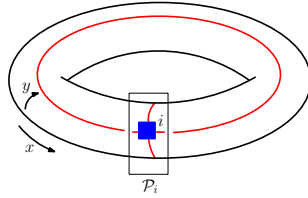


Figure 3.7: A schematic representation of the minimally entangled state $|\Xi_i^x\rangle$ with anyon flux i through the hole in the x -direction. It is obtained by placing the projector \mathcal{P}_i on the virtual level of the tensor network on the torus along the non-contractible loop in the y -direction and connecting the open indices with a MPO along the x -direction.

As a final remark we would like to stress that we only looked at the universal properties of the anyonic excitation tensors. These tensors of course also contain a lot of degrees of freedom that one needs to optimize over using a specific Hamiltonian in order to construct eigenstates of the system. This one can do using similar methods as for non-topological PEPS [170, 171].

3.5.3 Ground states on the torus and the S matrix

The projectors \mathcal{P}_i automatically allow one to construct the Minimally Entangled States (MES) on a torus [157]; one can simply put \mathcal{P}_i along the non-contractible loop in the y -direction and close the ‘inner’ and ‘outer’ indices of \mathcal{P}_i with an MPO along the non-contractible loop in the orthogonal x -direction. See figure 3.7 for a schematic representation. The resulting structure on the virtual level of the tensor network can be moved around freely because of the pulling through property and is therefore undetectable via local operators, implying we have constructed a ground state $|\Xi_i^x\rangle$ with an anyon flux of type i threaded through the hole in the x -direction. A similar construction also allows one to construct a MES $|\Xi_i^y\rangle$ with an anyon flux through the hole in the y -direction. Since for $|\Xi_i^x\rangle$ \mathcal{P}_i lowers the rank of the reduced density matrix of a segment of the torus obtained by cutting along two non-contractible loops in the y -direction it indeed implies (for fixed-point models) that we have minimized the entanglement entropy. In [157] the topological entanglement entropy for such a bipartition in a MES $|\Xi_i^x\rangle$ was found to be $\gamma_i = 2(\log D - \log d_i)$, where D is the so-called total quantum dimension and d_i is the quantum dimension of anyon type i . The PEPS construction then shows that the topological entanglement entropy for any bipartition in a low-energy excited state with a contractible boundary surrounding an anyon in sector i will be given by $\gamma'_i = \log D - \log d_i$.

This identification of the MES gives direct access to the S matrix, which is defined as the unitary matrix that implements the basis transformation from one minimally entangled basis $\{|\Xi_i^x\rangle\}$ to the other $\{|\Xi_i^y\rangle\}$. The advantage

of the MPO-injectivity formalism is that we can compute the S matrix in a way that does not scale with the system size. For this we take a single PMPO \tilde{P}_{C_4} with four tensors and use it to construct the smallest possible ‘torus’ by contracting the virtual indices along the x direction and the ones along the y direction. Defining T_i^x as the vector obtained by putting central idempotent \mathcal{P}_i along the y -direction on the virtual level of the minimal torus and T_i^y by putting \mathcal{P}_i along the x -direction we then have

$$T_i^y = \sum_{j=1} S_{ij} T_j^x. \quad (3.82)$$

We have numerically verified the validity of this expression for all examples below and found that it indeed holds.

Recall that the central idempotents can be written as a sum of simple idempotents

$$\mathcal{P}_i = \sum_{a=1}^{D_i} \sum_{\alpha=1}^{d_{i,\alpha}} P_i^{a\alpha}, \quad (3.83)$$

where each of the $P_i^{a\alpha}$ satisfies $P_i^{a\alpha} P_i^{b\beta} = \delta_{a,b} \delta_{\alpha,\beta} P_i^{a\alpha}$ and $P_i^{a\alpha\dagger} = P_i^{a\alpha}$. In principle one could use each of the $P_i^{a\alpha}$ to construct a ground state on the torus, in a similar way as explained above for \mathcal{P}_i . For the examples below we have numerically verified that each $P_i^{a\alpha}$ for fixed i gives the same ground state, implying that the ground state degeneracy on the torus is indeed given by the number of central idempotents.

3.5.4 Topological spin

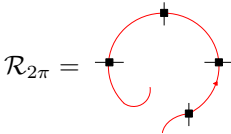
Even in the absence of rotational symmetry an adiabatic 2π rotation of the system should not be observable. Normally, we would conclude from this that the 2π rotation acts as the identity times a phase (called the Berry phase in continuous systems [173]) on the total Hilbert space: $R(2\pi) = e^{i\theta} \mathbf{1}$. However, the existence of topological superselection sectors changes this conclusion [174]. Because there are no local, i.e. physical, operators that couple states in different sectors the 2π rotation could produce a different phase $e^{i2\pi h_i}$ in each sector and still be unobservable. The number h_i in a particular sector is generally called the *topological spin* of the corresponding anyon.

To see this kind of behavior in MPO-injective PEPS it is important to realize that to define a 2π rotation one has to specify a specific (discrete) path of states, in the same way one has to define a continuous family of states in order to obtain a Berry phase. For example, in the case of a square lattice we can define the path using 4 successive rotations over $\pi/2$. When dealing with a non-regular lattice we have to use a family of different lattices along the path. We can now consider a region of MPO-injective PEPS in the sector defined by \mathcal{P}_i . This region has an open internal MPO-index along the

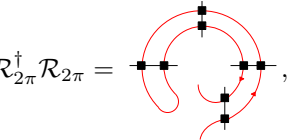
boundary that cannot be moved freely. We show that one can obtain the topological spin associated to sector \mathcal{P}_i by rotating the PEPS on a finite region while keeping the virtual boundary conditions fixed. After a 2π rotation \mathcal{P}_i surrounding the PEPS region is transformed to


(3.84)

Equation (3.84) can be interpreted as \mathcal{P}_i acting on the matrix $\mathcal{R}_{2\pi}$ defined by


(3.85)

By looking at the graphical expression for $\mathcal{R}_{2\pi}^\dagger \mathcal{R}_{2\pi}$


(3.86)

one can easily see by embedding it in a MPO-injective PEPS and using the pulling through property (3.46) that we can reduce it to a trivial action, implying $\mathcal{R}_{2\pi}$ is unitary on the relevant subspace. Using the zipper condition (3.37), the pivotal property (3.38) and again the pulling through property one can show via some graphical calculus that the following identity holds

$$\mathcal{R}_{2\pi}^\dagger A_{abcd,\mu\nu} \mathcal{R}_{2\pi} = A_{abcd,\mu\nu} \tag{3.87}$$

on the relevant subspace for all elements $A_{abcd,\mu\nu}$ in the algebra. Schur's lemma thus allows us to conclude that $\mathcal{R}_{2\pi} = \sum_i \theta_i \mathcal{P}_i$, with θ_i some phases because of the unitarity of $\mathcal{R}_{2\pi}$. We thus arrive at the desired result, i.e.

$$\mathcal{P}_i \mathcal{R}_{2\pi} = \theta_i \mathcal{P}_i, \tag{3.88}$$

where $\theta_i = e^{i2\pi h_i}$ gives the topological spin of the anyon in sector i .

3.5.5 Fusion

We can associate an algebra, called the fusion algebra, to the topological sectors. Consider a state which has the ground state energy everywhere except for two spatially separated regions. Using operators that surround one of those individual regions, we can measure the topological charge within both regions. Say these measurements reveal topological charges i and j . By considering the two different regions and a part of the ground state between them as one big region and using loop operators surrounding this bigger region, we can similarly measure the total topological charge. This measurement will typically have several outcomes, i.e. the total state is in a superposition of different topological sectors. The sectors appearing in this superposition for every i and j determine the integer rank three tensor \mathcal{N}_{ij}^k and we formally write the fusion algebra as $i \times j = \sum_k \mathcal{N}_{ij}^k k$. It is also clear that this algebra is by construction commutative, i.e. $\mathcal{N}_{ij}^k = \mathcal{N}_{ji}^k$. Assuming that all states in the same topological sector are connected via local operators we should be able to move an anyon i from one place to another using a string operator [11, 32, 33, 175]. Applying this string operator to a region that does not contain an excitation will create a pair (i, i^*) of anyons, where i^* is the unique dual/anti particle of anyon i . From this we see that $\mathcal{N}_{ij}^1 = \delta_{j, i^*}$.

This fusion algebra is very easily and explicitly realized in MPO-injective PEPS. In the simplest case, we just place two single-site idempotents \mathcal{P}_i and \mathcal{P}_j , next to each other on neighboring lattice sites. We can then fuse together the MPO strings emanating from \mathcal{P}_i and \mathcal{P}_j into one string. Looking at an annular ground state region surrounding the two anyons and using similar reasoning as in section 3.5.1 we find that the sum of all idempotents $\sum_k \mathcal{P}_k$ surrounding both anyons acts as a resolution of the identity on the relevant subspace. We can easily determine the subspaces \mathcal{P}_k on which the combination of both anyons are supported. These subspaces correspond to the possible fusion products of \mathcal{P}_i and \mathcal{P}_j . We illustrate this in figure 3.9, which uses a new, simplified diagrammatic notation that is defined in figure 3.8. From now on we shall denote the ground state by a tensor network consisting of black colored sites, omitting the physical indices. A site that contains an excitation is colored blue or red. Note that the procedure of figure 3.9 does not allow one to determine fusion multiplicities, i.e. it only tells whether \mathcal{N}_{ij}^k is non-zero. The multiplicities –the specific values of \mathcal{N}_{ij}^k – are in general harder to obtain directly since they arise from the number of linearly independent ways the MPO strings emanating from the idempotents can be connected on the virtual level. One could of course also just calculate the fusion multiplicities from the S matrix using the Verlinde formula [176].

Note that a projective measurement of the topological charge in some region via the physical PEPS indices greatly depends on the details of the tensors A and A' used to complete the tensor network. This is to be expected since the physical measurement is determined by the specific microscopic

realization of the quantum phase.

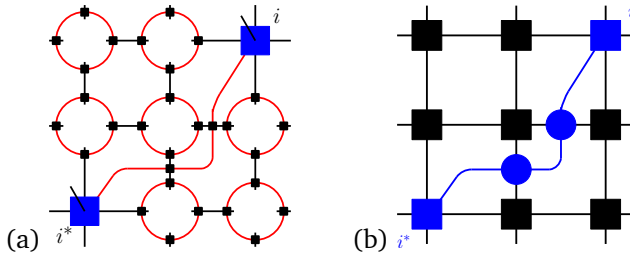


Figure 3.8: (a) The original tensor diagram for the ground state with an anyon pair (i, i^*) in the corners of the lattice. (b) Simplified tensor diagram for the state. In the remainder of the paper we will only use simplified diagrams. The ground state tensors are denoted by black squares and the physical indices are omitted. The blue squares describe an anyon of type i, i^* living on the respective sites. The blue tensors are supposed to be invariant under the virtual action of the idempotent corresponding to the label i or i^* . We use blue and red to denote sites containing an anyon, whereas other colors such as grey are reserved for fusion product of MPOs or anyons.

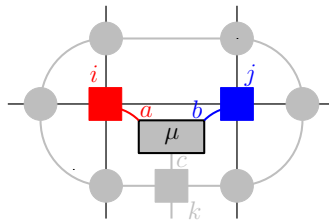


Figure 3.9: The procedure to determine the fusion product of two anyons in the new, simplified graphical notation (see also figure 3.8). The anyons are given by the red and blue idempotents $\mathcal{P}_i, \mathcal{P}_j$. We first fuse their outgoing strings a, b to all possible products c . We can now measure the fusion product of the anyons by projecting the result on the subspaces determined by the idempotents \mathcal{P}_k . The idempotents that give rise to a non zero projection correspond to the possible fusion products (k) of the red (i) and blue (j) anyons. Importantly, the sum over all grey idempotents \mathcal{P}_k acts as the identity on the virtual labels.

3.5.6 Braiding

When introducing the PEPS anyon ansatz in section 3.5.2 we mentioned that anyons detect each others presence in a non-local, topological way. We will now make this statement more precise. To every fixed configuration of anyons in the plane we can associate a collection of quantum many-body states. This set of states forms a representation of the colored braid group. This means that when we exchange anyons or braid them around

each other this induces a non-trivial unitary transformation in the subspace corresponding to the configuration. If there is only one state that we can associate to every anyon configuration then we only get one-dimensional representations. This situation is commonly referred to as Abelian statistics and the anyons are called Abelian anyons. With non-Abelian anyons we can associate multiple orthogonal states to one or more anyon configurations and these will form higher dimensional representations of the colored braid group.

One can obtain a basis for the subspace associated to a certain anyon configuration by assigning an arbitrary ordering to the anyons and projecting the first two anyons in a particular fusion state. One subsequently does the same for the fusion outcome of the first two anyons and the third anyon. This can be continued until a final projection on the vacuum sector is made. So the degeneracy of an anyon configuration is given by the number of different ways an ordered array of anyons can fuse to the vacuum.

Just as in relativistic field theories there is a spin-statistics relation for anyons, connecting topological spin and braiding. It is expressed by the so-called ‘pair of pants’ relation, which we show graphically using the same set-up as presented in figure 3.9:

$$\begin{aligned}
 & \begin{array}{ccc}
 \text{Diagram 1} & \xrightarrow{R} & \text{Diagram 2} \\
 \text{Diagram 3} & & \text{Diagram 4}
 \end{array} \\
 & = \begin{array}{ccc}
 \text{Diagram 5} & = e^{2\pi i(h_k - h_i - h_j)} & \text{Diagram 6}
 \end{array} \quad (3.89)
 \end{aligned}$$

The pair of pants relation shows that braiding acts diagonally on two anyons that are in a particular fusion state, which is realized in the figures by the grey idempotent k surrounding i and j . Because the topological spins can be shown to be rational numbers [177], the spin-statistics connection reveals that every anyon configuration provides a representation of the truncated colored braid group, i.e. there exists a natural number n such that $R^{2n} = \mathbb{1}$.

To describe the exchange and braiding of two anyons that are not in a particular fusion state we look for a generalization of the pulling through condition (3.49), (3.46). The goal is to obtain tensors $\mathcal{R}_{\mathcal{P}_i, b}$ that describe the pulling of a MPO string of type b through a site that contains an anyon

corresponding to \mathcal{P}_i according to the defining equation

$$(3.90)$$

If there is no anyon on the site we consider, i.e. the idempotent on this site is \mathcal{P}_1 corresponding to the trivial anyon, the operator $\mathcal{R}_{\mathcal{P}_i, b}$ is equal to the identity on the MPO indices as follows from the pulling through property (3.46).

While in practice one could solve the equation that determines \mathcal{R} numerically, we can in fact obtain the tensors $\mathcal{R}_{\mathcal{P}, b}$ analytically also for a nontrivial idempotent \mathcal{P}_i with $i \neq 1$. We thereto rewrite the left hand side of (3.90) by using relation (3.37) as follows (Note that we do not depict the required orientations on the indices and that we omit the corresponding gauge transformations Z_a to keep the presentation simple. These issues will also not have to be taken into account for the string-net examples further on.),

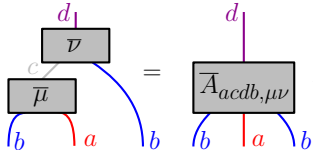
$$(3.91)$$

If by $\mathcal{P}_i A_{abcd}$ we denote the multiplication of \mathcal{P}_i and A_{abcd} in the anyon algebra defined in (3.57), we find that

$$(3.92)$$

With a slight abuse of notation, the grey rectangle containing $\bar{A}_{acdb, \mu\nu}$ denotes a similar tensor as the algebra object $A_{acdb, \mu\nu}$ in (3.56), but without

the MPO tensors,



The tensors $\mathcal{P}_i \cdot A_{acdb, \mu\nu} = P_i^a \cdot A_{acdb, \mu\nu}$ [see Eq. (3.61)] can easily be determined using the structure constants. Note that all tensors $\mathcal{P}_i \cdot A_{acdb}$ are supported on the subspace determined by \mathcal{P}_i , hence they all correspond to the same topological sector. Indeed, braiding an anyon around another one cannot change the topological charges. Remark that after the blue MPO is pulled through the site containing the anyon, the tensor on the site and the braid tensor linking the MPOs are in general entangled, due to the summation over a, c, d .

If \mathcal{P}_i is a one dimensional idempotent, the tensor $\mathcal{P}_i \cdot A_{acdb, \mu\nu}$ is only nonzero for a unique choice of $d = a$ and is in that case equal to \mathcal{P}_i , up to a constant. Hence, in that case there is no entanglement between the tensor on the site and the tensor that connects the MPOs.

Once we obtain these tensors $\mathcal{R}_{\mathcal{P}_i, b}$ we know how to resolve the exchange of anyons and we can compute the R matrix (braiding matrix). Suppose we have two anyons, described by idempotents $\mathcal{P}_i, \mathcal{P}_j$ and we want to compare the fusion of these anyons with and without exchanging them. Both situations correspond to figures 3.10(a) and 3.10(b) respectively.

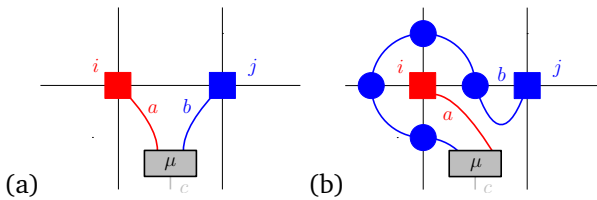


Figure 3.10: Two anyons, described by idempotents $\mathcal{P}_i, \mathcal{P}_j$, can be fused before exchanging them, as in Figure (a), or after exchanging, as in (b). To compare both diagrams we first use the tensor \mathcal{R} to redraw figure (b). The result is shown in equation (3.93).

All we need to resolve this situation is the tensor $\mathcal{R}_{\mathcal{P}_i, b}$ for all b for which \mathcal{P}_j is non zero. With this tensor we can redraw figure 3.10(b) in a way similar to the left hand side of (3.93). It is now clear that the $\mathcal{R}_{\mathcal{P}_i, b}$ tensors encode the R matrices of the topological phase, i.e. the braiding information of the anyonic excitations.

$$(3.93)$$

Analogously, we now show how the full braiding, or double exchange, of one anyon around another can be determined. As before, this information is completely contained within the \mathcal{R} tensors, as shown in figure 3.11. We study the situation where there are two anyon pairs present and we braid one anyon of the first pair completely around an anyon of the second pair. The procedure is shown in figure 3.11. If we compare figures 3.11 (a) and (d), we note that two different changes occurred in the transition between both diagrams. First, the use of relation (3.90) can induce a non-trivial action on the inner degrees of freedom of the idempotent. While it cannot change the support of the idempotent itself, as this determines the topological superselection sector, the degrees of freedom within a sector can change. This is important if the idempotent corresponding to the anyon is higher dimensional.

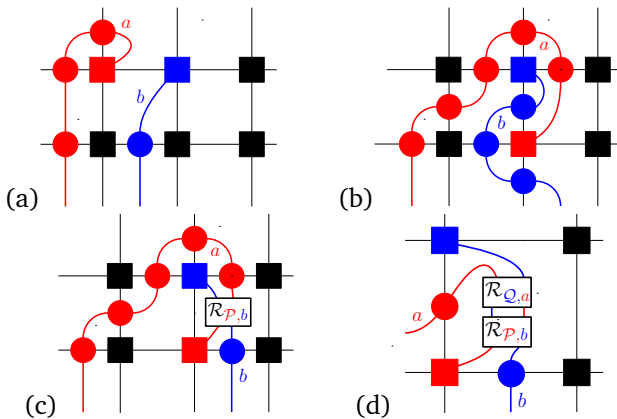


Figure 3.11: Figure (a): two anyons in a lattice, the lattice sites that contain the central idempotents \mathcal{P}, \mathcal{Q} are colored red and blue respectively. Figure (b): we can move the red anyon until the configuration is suited to apply equation (3.90). Figure (c): We pull the blue line through the red anyon, using the tensor $\mathcal{R}_{\mathcal{P},b}$ that depends on the red idempotent and the label of the blue line. Figure (d): a similar operation, now with $\mathcal{R}_{\mathcal{Q},a}$.

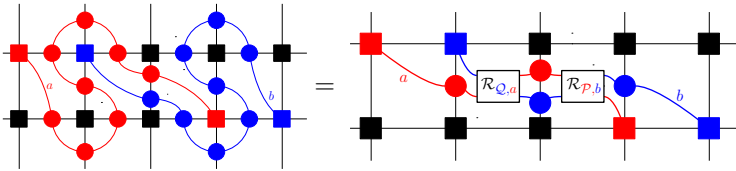


Figure 3.12: A more symmetric version of the braiding process described in figure 3.11. Completely braiding a red around a blue anyon is described by the contraction of the tensors $\mathcal{R}_{\mathcal{P},b}$ and $\mathcal{R}_{\mathcal{Q},a}$.

Secondly, the fusion channels of the red and blue anyon pair can change. Both pairs were originally in the vacuum sector, but can be in a superposition of sectors after braiding, as is illustrated in Figure 3.13.

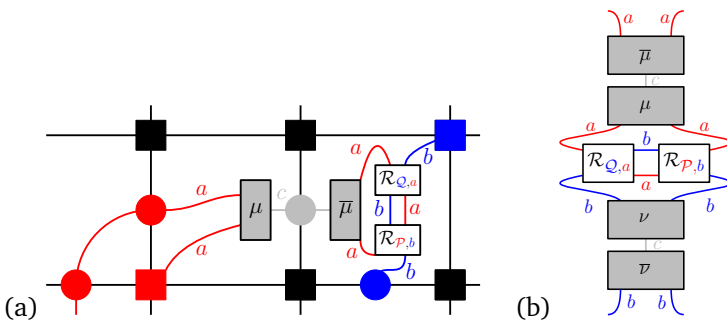


Figure 3.13: (a) The result of braiding the red anyon around the blue, as in figure 3.11(b). The gray label correspond to the possible fusion channels of the pair of red (or blue) anyons. Before braiding, the pair of red anyons was in the trivial topological sector. After braiding, several fusion results are possible. They can be measured at the gray line. A sum over the different possible fusion outcome values for these lines is implied. (b) A more symmetric (and rotated) version of (a). Due to the structure of the tensors \mathcal{R} , the gray lines c at the top and bottom are equal.

3.6 Examples

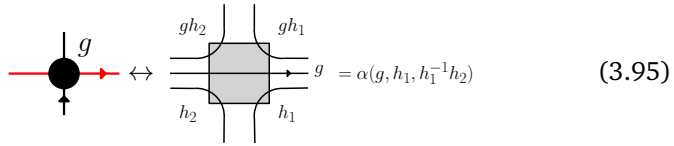
We will now illustrate the general formalism of anyons in MPO-injective PEPS with some examples and show that we indeed find all topological sectors. First, we focus on discrete twisted gauge theories [33, 128, 129, 178]. After that we turn to string-net models [175, 179].

3.6.1 Discrete gauge theories

The projector MPO for twisted quantum double models takes the form

$$P = \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} V(g), \tag{3.94}$$

where \mathbb{G} is an arbitrary finite group of order $|\mathbb{G}|$ and $V(g)$ are a set of injective MPOs that form a representation of \mathbb{G} , i.e. $V(g)V(h) = V(gh)$. $V(g)$ is constructed from the tensors



where the internal MPO indices are the horizontal ones. All indices are $|\mathbb{G}|$ -dimensional and are labeled by group elements. We use the convention that indices connected in the body of the tensors are enforced to be equal. In (3.95) we only drew the non-zero tensor components, i.e. for lower indices h_1 and h_2 there is only one non-zero tensor component, namely the one where the upper indices are related by a left group multiplication by g . The number $\alpha(g_1, g_2, g_3) \in \mathbb{U}(1)$ is a so-called 3-cocycle satisfying the 3-cocycle condition

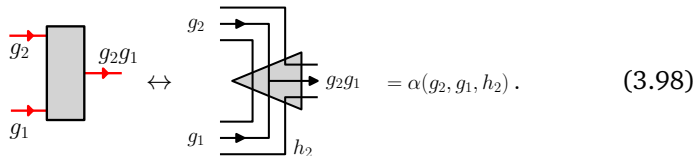
$$\alpha(g_1, g_2, g_3)\alpha(g_1, g_2g_3, g_4)\alpha(g_2, g_3, g_4) = \alpha(g_1g_2, g_3, g_4)\alpha(g_1, g_2, g_3g_4) \tag{3.96}$$

Without loss of generality one can take the 3-cocycles to satisfy

$$\alpha(e, g, h) = \alpha(g, e, h) = \alpha(g, h, e) = 1, \tag{3.97}$$

with e the identity group element, for all $g, h \in \mathbb{G}$. For this twisted quantum double MPO we have $g^* = g^{-1}$ and $Z_g = \sum_{h_1} \alpha(g, g^{-1}, h_1) |g^{-1}h_1, h_1\rangle \langle h_1, g^{-1}h_1|$. The specific form of this MPO also allows one to see immediately that the topological entanglement entropy of a contractible region in the corresponding MPO-injective PEPS is given by $\ln |\mathbb{G}|$.

The fusion tensors $X_{g_1g_2}$ for the twisted quantum double MPO take the form



Using (3.95), (3.98) and (3.96) one can check that the injective MPOs $V(g)$ indeed form a representation of \mathbb{G} . Using the same data one also sees that

the zipper condition (3.37) holds for the tensors of $V(g)$. Again using the cocycle condition the fusion tensors are seen to satisfy the equation

$$(X_{g_3 g_2} \otimes \mathbb{1}_{g_1}) X_{g_3 g_2, g_1} = \alpha(g_3, g_2, g_1) (\mathbb{1}_{g_3} \otimes X_{g_2, g_1}) X_{g_3, g_2 g_1} \quad (3.99)$$

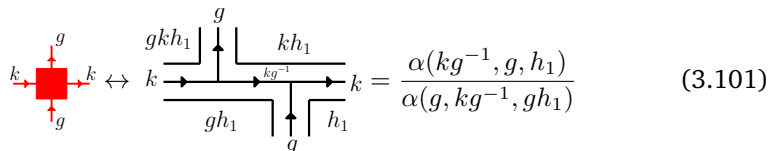
So the 3-cocycles α play the role of the F matrices in the general equation (3.30). This connection between MPO group representations and three cocycles was first established in [50]. For more details about the MPOs under consideration and the corresponding PEPS we refer to [160].

Topological charge

Using the MPO and fusion tensors defined above we can now construct the algebra elements A_{g_1, g_2, g_3, g_4} defined by Eq. 3.56; note that the indices μ, ν are always one dimensional in the group case so we can safely discard them. To construct the central idempotents we focus on the following algebra elements

$$A_{g, g^{-1} k^{-1}, g, k} = \delta_{[k, g], e} R_g(k^{-1}), \quad (3.100)$$

where $[k, g] = k g k^{-1} g^{-1}$ is the group commutator and e the trivial group element. For convenience, our choice for the basis of the algebra $R_g(k)$ deviates slightly from Eq. (3.56). It is constructed by closing a single block MPO (3.95) labeled by group element k , satisfying $[k, g] = e$, with a tensor that has as non-zero components



$$k \begin{array}{c} \uparrow g \\ \square \\ \downarrow g \\ \leftarrow k \end{array} \leftrightarrow k \begin{array}{c} \uparrow gh_1 \\ \leftarrow k \\ \rightarrow kg^{-1} \\ \downarrow g \\ \rightarrow kh_1 \\ \downarrow h_1 \end{array} = \frac{\alpha(kg^{-1}, g, h_1)}{\alpha(g, kg^{-1}, gh_1)} \quad (3.101)$$

Note that this tensor is chosen slightly different as the one in Eq. (3.56) and that the direction of k has been reversed.

By repeated use of the cocycle condition and the fact that $[g, k] = [g, m] = e$ one can now derive the multiplication rule of the algebra elements

$$R_g(m) R_g(k) = \bar{\omega}_g(m, k) \frac{\epsilon_g(mk)}{\epsilon_g(m) \epsilon_g(k)} R_g(mk) \quad (3.102)$$

where

$$\begin{aligned} \bar{\omega}_g(m, k) &= \frac{\alpha(m, g, k)}{\alpha(m, k, g) \alpha(g, m, k)} \\ \frac{\epsilon_g(mk)}{\epsilon_g(m) \epsilon_g(k)} &= \frac{\alpha(g, mk g^{-1}, g)}{\alpha(g, m g^{-1}, g) \alpha(g, k g^{-1}, g)} \end{aligned} \quad (3.103)$$

One can check that $\omega_g(m, k)$ is a 2-cocycle satisfying the 2-cocycle condition

$$\omega_g(m, k) \omega_g(mk, l) = \omega_g(m, kl) \omega_g(k, l), \quad (3.104)$$

when m , k and l commute with g . So the algebra elements $R_g(k)$ form a projective representation of the centralizer \mathcal{Z}_g of g . We now define the following projective irreducible representations of \mathcal{Z}_g labeled by μ

$$\Gamma_g^\mu(m)\Gamma_g^\mu(k) = \omega_g(m, k)\Gamma_g^\mu(mk), \quad (3.105)$$

and the corresponding projective characters $\chi_g^\mu(k) = \text{tr}(\Gamma_g^\mu(k))$. We denote the dimension of projective irrep μ by d_μ . Using the Schur orthogonality relations for projective irreps one can now check that

$$P_{(g,\mu)} = \frac{d_\mu}{|\mathcal{Z}_g|} \sum_{k \in \mathcal{Z}_g} \epsilon_g(k) \chi_g^\mu(k) R_g(k) \quad (3.106)$$

are Hermitian orthogonal projectors, i.e. $P_{(g,\mu)}^\dagger = P_{(g,\mu)}$ and $P_{(g,\mu)}P_{(h,\nu)} = \delta_{g,h}\delta_{\mu,\nu}P_{(g,\mu)}$. To obtain the central idempotents we have to sum over all elements in the conjugacy class \mathcal{C}_A of g , so the final anyon ansatz is

$$\mathcal{P}_{(\mathcal{C}_A,\mu)} = \sum_{g \in \mathcal{C}_A} P_{(g,\mu)}. \quad (3.107)$$

In this way we indeed recover the standard labeling of dyonic excitations in discrete twisted gauge theories: the flux is labeled by a conjugacy class \mathcal{C}_A and the charge is labeled by a projective irrep of the centralizer \mathcal{Z}_g of a representative element g in \mathcal{C}_A [180, 181].

Anyon ansatz

In this section we will illustrate some aspects of the anyon ansatz that were discussed in section 3.5.2. Firstly, in figure 3.14 we show the explicit PEPS ground state and excitation tensors for the non-twisted $(\alpha(g_1, g_2, g_3) \equiv 1)$ quantum double PEPS on the hexagonal lattice. This provides an explicit example of an anyonic excitation tensor that has a rank-one injectivity structure on each virtual subspace corresponding to a topological sector.

Secondly, we look at a pair of pure charges. Using similar reasoning as in the previous section we can construct the simple idempotents and nilpotents with diagonal group label as

$$P_{(\mathcal{C}_A,\mu)}^{(g,i),(g,j)} = \frac{d_\mu}{|\mathcal{Z}_g|} \sum_{k \in \mathcal{Z}_g} \epsilon_g(k) [\Gamma_g^\mu(k)]_{ij} R_g(k), \quad (3.108)$$

where i, j are matrix indices of the irrep $\Gamma_g^\mu(k)$. The simple idempotents and nilpotents with off-diagonal group label can be obtained via a straightforward generalization, but we will not need them here.

We consider a charge μ and its anti-charge μ^* . The relevant idempotents and nilpotents are $P_{\mu}^{i,j} \equiv P_{(e,\mu)}^{(e,i),(e,j)}$. To construct a topological PEPS

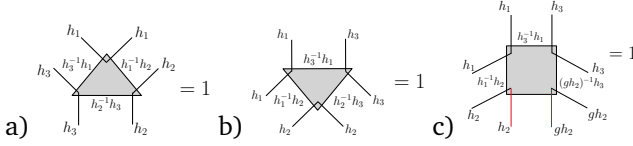


Figure 3.14: Tensors for the non-twisted ($\alpha(g_1, g_2, g_3) \equiv 1$) quantum double PEPS on a hexagonal lattice. a) Ground state tensors for the A -sublattice. b) Ground state tensors for the B -sublattice. All indices are $|\mathbb{G}|$ -dimensional and are labeled by group elements. There are two virtual indices for every link in the lattice. Indices that are connected in the tensors are enforced to be equal. There are three physical indices on each tensor, of which we write the index value between the virtual indices. All non-zero tensor components have index configurations as indicated in the figures and have value one. The resulting PEPS is MPO-injective with virtual support PMPO (3.94). c) An anyonic excitation tensor for the A -sublattice. The extra lower index, which we colored red for clarity, is to be connected to a MPO on the virtual level. Multiplying all the physical indices of an A -sublattice ground state tensor counter clockwise gives the identity group element. For the excitation tensor the multiplied value of the physical indices is $h_2^{-1}g^{-1}h_2$, which indicates the presence of a non-trivial flux. The physical indices can distinguish between virtual MPOs corresponding to group elements in different conjugacy classes. However, the rank-one injectivity structure of the anyonic tensor is reflected in the fact that elements in the same conjugacy class give equivalent configurations of the physical indices.

containing the charge pair we start with two tensors C_μ^i and $C_{\mu^*}^j$, which have as many virtual indices as the coordination number of the lattice and one physical index. Their virtual indices are supported on the subspaces determined by respectively $P_\mu^{i,i}$ and $P_{\mu^*}^{j,j}$. If we interpret the charge tensors as matrices with the physical index as row index and the virtual indices together as the column index then this implies $C_\mu^i P_\nu^{k,k} = \delta_{\mu,\nu} \delta_{i,k} C_\mu^i$ and $C_{\mu^*}^j P_{\nu^*}^{k,k} = \delta_{\mu^*,\nu^*} \delta_{j,k} C_{\mu^*}^j$. We now want to find the complete anyonic excitation tensors C_μ and C_{μ^*} such that $C_\mu P_\mu^{i,i} = C_\mu^i$ and $C_{\mu^*} P_{\mu^*}^{j,j} = C_{\mu^*}^j$. For this we proceed as before: we take both tensors and project them in the vacuum sector. We will ignore the PEPS environment and simply work with the tensor product of both charge tensors $C_\mu^i \otimes C_{\mu^*}^j$. The vacuum projector (3.94) on this tensor product can be written as

$$\tilde{P} = \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} V(g) \otimes V(g) = \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} R_e(g) \otimes R_e(g). \quad (3.109)$$

Using the orthogonality relations for irreps we rewrite the vacuum projector as

$$\tilde{P} = \sum_{\nu} \frac{1}{d_\nu} \sum_{p,q=1}^{d_\nu} P_\nu^{p,q} \otimes P_{\nu^*}^{p,q}, \quad (3.110)$$

where $[\Gamma^{\nu^*}(g)]_{pq} = [\bar{\Gamma}^\nu(g)]_{pq}$. We therefore get for the vacuum projected

charge pair

$$\left(C_\mu^i \otimes C_{\mu^*}^j \right) \left(\sum_\nu \frac{1}{d_\nu} \sum_{p,q=1}^{d_\nu} P_\nu^{p,q} \otimes P_{\nu^*}^{p,q} \right) = \delta_{i,j} \frac{1}{d_\mu} \sum_q C_\mu^i P_\mu^{i,q} \otimes C_{\mu^*}^i P_{\mu^*}^{i,q}. \quad (3.111)$$

By taking $C_\mu^q \equiv C_\mu^i P_\mu^{i,q}$ we obtain

$$\left(\sum_{i=1}^{d_\mu} C_\mu^i \otimes C_{\mu^*}^i \right) \tilde{P} = \left(\sum_{i=1}^{d_\mu} C_\mu^i \otimes C_{\mu^*}^i \right). \quad (3.112)$$

So we see that for the pair to be in the vacuum state both charges should form a maximally entangled state in the irrep matrix indices. However, as explained in the general discussion of section 3.5.2, this is purely virtual entanglement that cannot be destroyed by physical operators acting on only one charge in the pair.

Topological spin

To calculate the topological spin we first note following relation

$$\Gamma_g^\mu(k) \Gamma_g^\mu(g) = \Gamma_g^\mu(g) \Gamma_g^\mu(k) \frac{\omega_g(k, g)}{\omega_g(g, k)} = \Gamma_g^\mu(g) \Gamma_g^\mu(k), \quad (3.113)$$

which holds for all $k \in \mathcal{Z}_g$. Using Schur's lemma this implies that $\Gamma_g^\mu(g) = e^{i2\pi h_g^\mu} \mathbb{1}_{d_\mu}$. One can also easily check that

$$\Gamma_g^\mu(g^{-1}) = \omega_g(g, g^{-1}) \Gamma_g^\mu(g)^\dagger. \quad (3.114)$$

With these observations we now obtain

$$\begin{aligned} P_{(g,\mu)} R_g(g) &= \frac{d_\mu}{|\mathcal{Z}_g|} \sum_{k \in \mathcal{Z}_g} \chi_g^\mu(k) R_g(kg) \\ &= \frac{d_\mu}{|\mathcal{Z}_g|} \sum_{x \in \mathcal{Z}_g} \text{tr}(\Gamma_g^\mu(x) \Gamma_g^\mu(g^{-1}) \omega_g^*(x, g^{-1})) R_g(x) \\ &= e^{-i2\pi h_g^\mu} \frac{d_\mu}{|\mathcal{Z}_g|} \sum_{x \in \mathcal{Z}_g} \epsilon_g(x) \chi_g^\mu(x) R_g(x) \\ &= e^{-i2\pi h_g^\mu} P_{(g,\mu)} \end{aligned}$$

Since $e^{-i2\pi h_g^\mu}$ is the same for all elements in the conjugacy class \mathcal{C}_A of g we obtain the desired result

$$\mathcal{P}_{(\mathcal{C}_A, \mu)} \mathcal{R}_{2\pi} = \mathcal{P}_{(\mathcal{C}_A, \mu)} \sum_{g \in \mathbb{G}} R_g(g) = \theta_{(\mathcal{C}_A, \mu)} \mathcal{P}_{(\mathcal{C}_A, \mu)}, \quad (3.115)$$

where $\mathcal{R}_{2\pi}$ was introduced in section 3.5.4. The phase $\theta_{(\mathcal{C}_A, \mu)} = e^{-i2\pi h_g^\mu}$ gives the topological spin of the corresponding anyon.

Fusion

In the group case fusion is easy to calculate analytically because of the following identity for the basis elements of our algebra:

$$\text{Diagram} = \delta_{k,l} \text{Diagram} \tag{3.116}$$

This implies that to calculate fusion relations we can simply trace over the inner indices at the shared boundary of two central idempotents to create a bigger loop.

We subsequently act with the fusion tensor X_{gh} on the two red inner indices on the right hand side of (3.116), which acts as a unitary on the support of these indices. We also attach X_{gh}^\dagger to the outer indices in (3.116), which can obviously be obtained by decomposing the product of the two MPOs $V(g)$ and $V(h)$ that are connected to the central idempotents once we embed them in a MPO-injective PEPS. Using the 3-cocycle condition one can now check that we have

$$\text{Diagram} = \beta(k, g, h) \text{Diagram}, \tag{3.117}$$

where $\beta(k, g, h)$ is given by

$$\beta(k, g, h) = \omega_k(g, h) \frac{\epsilon_{gh}(k)}{\epsilon_g(k)\epsilon_h(k)}. \tag{3.118}$$

So we obtain

$$P_{(g,\mu)} \times P_{(h,\nu)} = \frac{d_\mu d_\nu}{|\mathcal{Z}_g||\mathcal{Z}_h|} \sum_{k \in \mathcal{Z}_{gh}} \epsilon_{gh}(k) \chi_g^\mu(k) \chi_h^\nu(k) \omega_k(g, h) R_{gh}(k). \tag{3.119}$$

We now define $\Gamma_{gh}^{\mu\nu}(k) = \Gamma_g^\mu(k) \otimes \Gamma_h^\nu(k) \omega_k(g, h)$ for all k such that $[k, g] = [k, h] = e$. Then repeated use of the 3-cocycle condition (3.96) shows that

$$\Gamma_{gh}^{\mu\nu}(k_1) \Gamma_{gh}^{\mu\nu}(k_2) = \omega_{gh}(k_1, k_2) \Gamma_{gh}^{\mu\nu}(k_1 k_2), \tag{3.120}$$

i.e. $\Gamma_{gh}^{\mu\nu}(k)$ is a projective representation of \mathcal{Z}_{gh} . This representation will in general be reducible

$$\Gamma_{gh}^{\mu\nu}(k) \simeq \bigoplus_{\lambda} \mathbb{1}_{W_{\mu\nu}^\lambda} \otimes \Gamma_{gh}^\lambda(k), \tag{3.121}$$

where the integer $W_{\mu\nu}^\lambda$ denotes the number of times a projective irrep λ appears in the decomposition of $\Gamma_{gh}^{\mu\nu}$. From this we get following relation between the projective characters

$$\chi_g^\mu(k)\chi_h^\nu(k)\omega_k(g, h) = \sum_{\lambda} W_{\mu\nu}^\lambda \chi_{gh}^\lambda(k). \quad (3.122)$$

So we find

$$P_{(g,\mu)} \times P_{(h,\nu)} = \sum_{\lambda} W_{\mu\nu}^\lambda P_{(gh,\lambda)}, \quad (3.123)$$

up to some normalization factors. In this way we obtain the final fusion rules

$$\mathcal{P}_{(\mathcal{C}_A,\mu)} \times \mathcal{P}_{(\mathcal{C}_B,\nu)} = \sum_{(\mathcal{C}_C,\lambda)} \mathcal{N}_{(\mathcal{C}_A,\mu),(\mathcal{C}_B,\nu)}^{(\mathcal{C}_C,\lambda)} \mathcal{P}_{(\mathcal{C}_C,\lambda)}, \quad (3.124)$$

where the fusion coefficients can be written down explicitly using the orthogonality relations for projective characters [129, 180]:

$$\mathcal{N}_{(\mathcal{C}_A,\mu),(\mathcal{C}_B,\nu)}^{(\mathcal{C}_C,\lambda)} = \frac{1}{|\mathbb{G}|} \sum_{g_1 \in \mathcal{C}_A} \sum_{g_2 \in \mathcal{C}_B} \sum_{g_3 \in \mathcal{C}_C} \sum_{h \in \mathcal{Z}_{g_1} \cap \mathcal{Z}_{g_2} \cap \mathcal{Z}_{g_3}} \delta_{g_1 g_2, g_3} \chi_{g_1}^\mu(h) \chi_{g_2}^\nu(h) \bar{\chi}_{g_3}^\lambda \omega_h(g_1, g_2) \quad (3.125)$$

3.6.2 String-nets

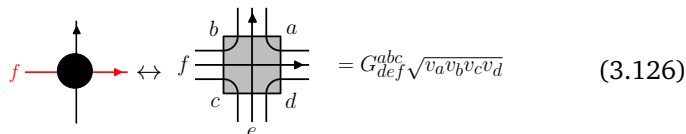
The next example we consider are the string-net models. For simplicity, we restrict ourselves to models without higher dimensional fusion spaces, i.e. all N_{ab}^c in equation (3.15) are either 0 or 1. Also, we only deal with models where each single block MPO is self-dual: $a = a^*$ and $N_{aa}^1 = 1$. Both restrictions can easily be lifted.

The description of string-nets in the framework presented here was introduced in [109]. The string-net models are a prime example of the MPO-injectivity formalism. The PMPO is constructed from the G -symbols and the quantum dimensions of a unitary fusion category. The single block MPOs correspond one-to-one with the simple objects of the input fusion category. The fusion matrices X_{ab}^c are also easily constructed from the G -symbols and the quantum dimensions. These tensors give rise to an MPO-injective PEPS and they satisfy the properties listed in section 3.4.1. The validity of the general requirements in our formalism follows mainly from the pentagon relation of the G -symbols. The properties of section 3.4.1 are rooted in the spherical property of unitary fusion categories.

To describe the string-nets as a tensor network, there is one extra technical subtlety we need to take into account. Every closed loop in the PEPS representation of a string-net wave function gives rise to a factor equal to the quantum dimension of the label of this loop. In [109], this was taken care of by incorporating such factors both in the tensors and by adding extra factors for every bend in an MPO. Because of this convention, the MPOs give

rise to projectors P_L for every length that are not Hermitian on a closed loop. Luckily, as all these operators are still similar to Hermitian operators via a local, positive similarity transformation, this has no implications for the general theory. For example, we still find that every single block MPO labeled by a has a unique corresponding single block MPO a^* that is obtained by Hermitian conjugation, where a^* is just the categorical dual of a . The tensors we describe next are used on a square lattice, similar tensors can be used on different lattices.

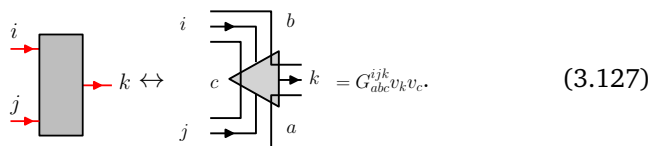
First we describe the PMPO. We have



$$= G_{def}^{abc} \sqrt{v_a v_b v_c v_d} \quad (3.126)$$

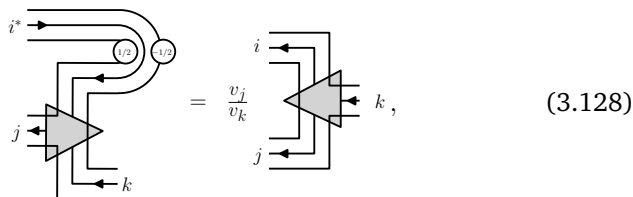
where the internal MPO indices are the horizontal ones and all indices are N dimensional. The single block MPOs are determined by fixing the label f . The corresponding weights w_f used to construct a PMPO are given by the quantum dimensions d_f divided by $\mathcal{D}^2 = \sum_a d_a^2$, the total quantum dimension of the fusion category squared. The factors v_a in the definition of the MPO are included to take care of the closed loop factors. They are given by the square roots of the quantum dimensions: $v_a = d_a^{1/2}$. The single block MPOs obtained by fixing f satisfy the algebraic structure of the fusion algebra of the category we used to construct the MPOs.

For the string-net MPOs we consider here the gauge transformations Z_a are all trivial; they amount to simply swapping the double line structure which is present in the virtual indices of the MPO tensor. The fusion tensors X_{ab}^c are given by



$$= G_{abc}^{ijk} v_k v_c \quad (3.127)$$

The factor v_c is only present for the closed loop condition (and could be taken care of differently). The pivotal property for these fusion tensors is



$$= \frac{v_j}{v_k} \quad (3.128)$$

which is equivalent to (3.38) up to the diagonal matrices labeled by $1/2$ and $-1/2$, which denote the power of the quantum dimensions that are added

to satisfy the closed loop condition. More specifically, these matrices are $\sum_a d_a^{\pm 1/2} |a\rangle \langle a|$.

With this information, the MPO and fusion tensors can now be used in our framework in order to obtain an ansatz for anyons in string-nets. Unlike in the case of discrete gauge theories, we now need the ansatz (3.56) in full generality. We recall the form of the algebra elements

$$A_{abcd, \mu\nu} = \text{Diagram}$$

The structure constants that define the multiplication of these objects can be computed analytically with formula (3.144) or numerically. The algebra that describes the anyons is similar to a construction proposed in [161], although obtained from a very different motivation. To obtain the central idempotents of this algebra we use a simple algorithm described in Appendix 3.C, see also [182]. As expected, we obtain both one and higher dimensional central idempotents.

In Appendix 3.D we list the central idempotents and their properties for the Fibonacci, Ising and $\text{Rep}(S_3)$ string-nets. For each of those, we also compute the topological spin using the standard procedure described in subsection 3.5.4. For string-nets, these spins can in principle be computed analytically from the central idempotents. Furthermore, we compute the fusion table describing the fusion of two anyons. Thereto, we have numerically performed the procedure explained in subsection 3.5.5. We indeed recover the known fusion rules for the anyonic excitations of these theories. Note that there are no fusion multiplicities larger than one in the models we consider. Finally, we explicitly work out the braid tensor \mathcal{R} using the procedure of 3.5.6 for two anyons in the Fibonacci string-net model in Appendix 3.F.

3.7 Discussion and outlook

For all the examples considered here the PEPS anyon construction is equivalent to calculating the Drinfeld center [183] of the input theory, i.e. the algebraic structure determined by the single block MPOs O_a , which was either a finite group (which can be generalized to a Hopf algebra) or a unitary fusion category. This center construction leads to a modular tensor category, which describes a consistent anyon theory [184]. When the input theory is already a modular tensor category by itself, the center construction

gives a new modular tensor category, which is isomorphic to two copies of the original anyon theory, one of which is time-reversed [184]. It is then clear that the new anyon theory cannot correspond to a chiral phase. This is actually true in general, i.e. the set of modular tensor categories obtained via the center construction cannot describe chiral phases. In [185] the set of center modular tensor categories was identified with the set of modular tensor categories containing a so-called Lagrangian subalgebra. A physical connection between the existence of a Lagrangian subgroup and the non-chirality of the quantum phase was given in [186] for the case of Abelian statistics.

We have found that PMPOs of the form (3.9) that can be used to build MPO-injective PEPS give rise to many concepts familiar from the theory of unitary fusion categories: a finite number of simple objects and associated fusion relations, the pentagon equation, a generalized notion of duality and the Frobenius-Schur indicator \varkappa_a , pivotal structure and unitarity. However, there is one important property of unitary fusion categories that does not seem to immediately come out of MPO-injectivity, namely the existence of a unique, simple unit element. In other words, we have not found a property of MPO-injectivity that requires the projector MPO to contain a single block MPO O_1 , satisfying $O_1 O_i = O_i O_1 = O_i$ for all i . However, if such identity block is not present then we can associate a multi-fusion category to the PMPO. It is known that multi-fusion categories can also be used to construct string-net models [187].

So at this point it seems that the only possibilities to have MPO-injective PEPS that describe physics beyond discrete gauge theories and string-nets without having to extend the MPO-injectivity formalism of [109] are given by:

- (1) using PMPOs that have no canonical form;
- (2) defining different left handed MPO tensors to construct \tilde{P}_{C_v} ;
- (3) not imposing the zipper condition (3.37).

Trying option (2) will most likely lead to a violation of unitarity, in which case the algebra $A_{abcd,\mu\nu}$ can no longer be proven to be a C^* -algebra. This will lead to non-Hermitian central idempotents, which to some extent obscures their interpretation as topological sectors. Options (1) and (3) are at the moment much less clear to us, so we will not try to speculate on their implications. It would be very interesting to better understand the implications of options (1) - (3) and see if there is any relation between MPO-injective PEPS and the recently constructed tensor network states for chiral phases [112, 113].

To conclude, we have not only established a connection between MPO-injective PEPS and unitary fusion categories as mentioned above but also a formalism to obtain the topological sectors of the corresponding quantum

phase. Similar to previous results [158, 161] we can relate topological sectors to the central idempotents of an algebra, which in our case is a C^* -algebra constructed from the MPO that determines the injectivity subspace of the ground space tensors. The formalism is constructive and gives the correct anyon types for all the examples we worked out. It furthermore allows us to write down explicit PEPS wave functions that contain an arbitrary number of anyons. This gives an interpretation of topological sectors in terms of entanglement. From the PEPS wave functions containing anyons we can extract universal properties such as fusion relations and topological spins in a very natural way. For certain string-net models we also studied the effect of braiding on the PEPS.

Several open questions concerning topological order in tensor networks remain. As mentioned above, it is not clear if chiral topological phases fit into the MPO-injectivity formalism, or what –if any– is the correct formalism to describe gapped chiral theories with tensor networks. For non-chiral topological phases the construction presented here defines an equivalence relation for PMPOs, i.e. two PMPOs are said to be equivalent if the resulting central idempotents have the same topological properties. At this point the (Morita) equivalence relation between PMPOs is very poorly understood. It is also known that there is a substantial interplay between the topological order and global symmetries of a quantum system. Some first progress in capturing universal properties of these so-called symmetry-enriched topological phases with tensor networks was made in [188]. A direction for future research which enforces itself upon us at the end of this paper is of course the extension of the presented formalism to fermionic PEPS [68]. We expect that the concept of MPO algebras should also be connected to topological sectors in fermionic tensor networks. It is conceivable that the concepts introduced here might also be relevant for other types of tensor networks, e.g. the Multi-scale Entanglement Renormalization Ansatz (MERA) descriptions of topological phases [189, 190]. Besides these theoretical questions there are also a lot of new applications of MPO-injectivity that come within reach, especially the study of topological phase transitions in non-Abelian anyon theories. We hope to make progress on these matters in future work.

3.A Hermitian PMPOs with unital structure and fusion categories

In this appendix we will further consider the connection between (unitary) fusion categories and PMPOs that satisfy the zipper condition (3.37) and have a unital structure. As explained in section 3.3.3 a PMPO is said to have a unital structure if there exists a unique single block MPO labeled by 1 such

that

$$\rho(M_1) \geq \rho(M_b) \quad \forall b \quad (3.129)$$

$$N_{bb^*}^1 \geq 1 \quad \forall b, \quad (3.130)$$

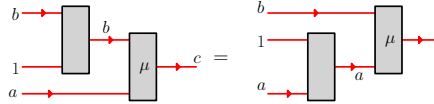
where $M_a = \sum_{i=1}^D B_a^{ii}$ and $\rho(M_a)$ denotes the spectral radius of M_a . It was shown in the main text that this definition implies that $\rho(M_1) > \rho(M_b), \forall b \neq 1$ and $N_{bb^*}^1 = 1, \forall b$, with in addition $1^* = 1$ and $\varkappa_1 = 1$. From the symmetry of the tensor N

$$N_{ab}^c = N_{bc^*}^{a^*} = N_{c^*a}^{b^*} \quad (3.131)$$

and properties of injective MPS it then follows that

$$N_{ab^*}^1 = N_{a1}^b = N_{1a}^b = \delta_{ab}, \quad (3.132)$$

such that 1 is indeed the trivial element of the algebra of single block MPOs. We now also require that fusing with the unit element 1 is trivial as expressed by the triangle equation [32]:



$$(3.133)$$

Because the PMPO satisfies the zipper condition we can define the F matrices as in section 3.3.4. The triangle equation can then equivalently be stated as

$$[F_c^{b1a}]_{b1\mu}^{a1\mu} = \delta_{\mu\nu}. \quad (3.134)$$

Note that the triangle equation fixes the relative norm and phase of X_{1a}^a and X_{b1}^b . Combining the triangle equation (3.133) with the pentagon equation (3.34) gives rise to additional triangle equations:

$$[F_c^{1ab}]_{a1\mu}^{c\nu 1} = \delta_{\mu\nu} \quad (3.135)$$

$$[F_c^{ab1}]_{c\mu 1}^{b1\nu} = \delta_{\mu\nu}. \quad (3.136)$$

With these assumptions one can use results from the theory of injective MPS to show that there exists a choice of fusion tensors such that:

$$[F_a^{aa^*a}]_1^1 = \frac{\varkappa_a}{d_a} \quad (3.137)$$

$$[F_a^{a^*aa^*}]_1^1 = [(F_a^{aa^*a})^{-1}]_1^1 = \frac{\varkappa_{a^*}}{d_{a^*}} \quad (3.138)$$

$$\frac{1}{d_a} = \frac{1}{d_{a^*}} > 0, \quad (3.139)$$

where $\varkappa_a = \pm 1$ is defined as in section 3.3.3 via $Z_a \bar{Z}_{a^*} = \varkappa_a \mathbb{1}$. If we now also assume the unitarity condition of section 3.4.1, then we can relate the numbers d_a obtained from the F -symbol to the Perron-Frobenius vector of the N coefficients, i.e.:

$$d_a d_b = \sum_c N_{ab}^c d_c \tag{3.140}$$

Identities (3.137) to (3.140) are very tedious to prove. Since they are not the main focus of this paper, the proofs will be given elsewhere.

The positive numbers d_a are called the *quantum dimensions* of the simple objects in the unitary fusion category. Given the quantum dimensions and the F matrices, equations (3.137) and (3.138) are then used to define the Frobenius-Schur indicator \varkappa_a in category theory [32]. So we see that our definition of \varkappa_a via the gauge matrices Z_a coincides with that of the Frobenius-Schur indicator in fusion categories for this special class of PMPOs.

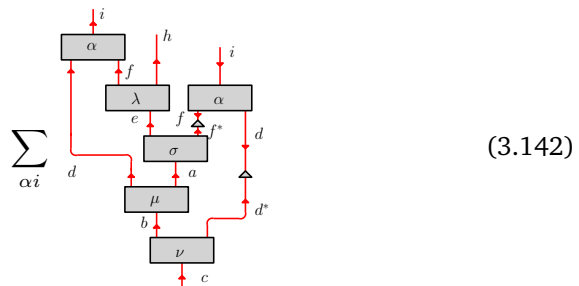
3.B C^* -Algebra structure of $A_{abcd,\mu\nu}$

3.B.1 Closedness under multiplication

We consider the objects $A_{abcd,\mu\nu}$ defined in (3.56) and show they form an algebra under matrix multiplication, i.e. we show that

$$A_{hegf,\lambda\sigma} A_{abcd,\mu\nu} = \delta_{ga} \sum_{ij,\rho\tau} \Omega_{(hegf,\lambda\sigma)(abcd,\mu\nu)}^{(hjc i,\rho\tau)} A_{hjc i,\rho\tau}. \tag{3.141}$$

Using the zipper condition (3.37) we see that we can neglect the MPO tensors and that the object we have to decompose is given by



As a first step we use (3.40) and a ‘ F -move’ (3.30) to obtain

$$= \sum_{\alpha\beta\gamma\delta ij} \left(C_{f^*d^*}^{i^*-1} \right)_{\alpha\beta} \left(F_b^{def^*} \right)_{(j\gamma\delta)}^{(a\sigma\mu)} \quad (3.143)$$

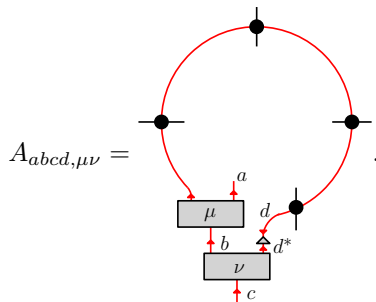
A final two F -moves then lead to

$$= \sum_{\alpha\gamma\delta j\rho i\kappa\tau} \left(C_{f^*d^*}^{i^*-1} \right)_{\rho\kappa} \left(F_b^{def^*} \right)_{(j\gamma\delta)}^{(a\sigma\mu)} \left(F_j^{dfh} \right)_{(i\alpha\rho)}^{(e\lambda\gamma)} \left(F_c^{j f^* d^* -1} \right)_{(i^*\beta\tau)}^{(b\nu\delta)} \quad (3.144)$$

So we indeed obtain a decomposition of the composite object in terms of the original ones, giving the desired algebra structure.

3.B.2 Closedness under Hermitian conjugation

We now show that the algebra formed by the elements $A_{abcd,\mu\nu}$ is closed under Hermitian conjugation, i.e. $A_{abcd,\mu\nu}^\dagger = \sum_{e,\kappa\lambda} (\Theta_{abcd,\mu\nu})^{e\kappa\lambda} A_{cead^*,\kappa\lambda}$. Starting from the basis element



we can implement Hermitian conjugation in the following way:

- Complex conjugation and exchanging the inner and outer indices of the MPO tensors amounts simply to reversing the arrow on the red line, due to the relation between left- and right-handed MPO tensors in Eq. (3.43).
- Complex conjugation of the gauge matrix Z_d , which also simply amounts to reversing the red arrows as discussed in section 3.4.1.
- Exchanging the inner and outer indices connected to (the left inverses of) the fusion tensors.
- Complex conjugation of the fusion tensors, which reverses the red arrows and reconnects them to the other side of the box: the complex conjugate of the fusion tensor is the transpose of the inverse (=hermitian conjugated) fusion tensor.

This gives rise to the following diagram for $A_{abcd,\mu\nu}^\dagger$:

$$A_{abcd,\mu\nu}^\dagger = \quad (3.145)$$

Restoring the orientation of the original loop results in

$$A_{abcd,\mu\nu}^\dagger = \quad (3.146)$$

We can now use an A and A' move [see Eq. (3.38)] to obtain

$$A_{abcd,\mu\nu}^\dagger = \sum_{\rho\sigma} (A_{d^*a}^b)_{\mu\rho} (A_{bd}^{c'})_{\nu\sigma} \quad (3.147)$$

Using a final F move and Eq. (3.36) we obtain the required relation

$$A_{abcd,\mu\nu}^\dagger = \sum_{\rho\sigma\epsilon\kappa\lambda} (A_{d^*a}^b)_{\mu\rho} (A_{bd}^{c'})_{\nu\sigma} \mathcal{Z}_d (F_a^{d^*cd})_{\epsilon\kappa\lambda}^{b\sigma\rho} A_{ced^*,\kappa\lambda}. \quad (3.148)$$

3.C Finding central idempotents

In this appendix we present a simple and constructive algorithm to calculate the decomposition of an algebra \mathcal{A} over \mathbb{C} in primitive central idempotents. The constructive approach to the Artin-Wedderburn theorem is well known in the literature [182] and can be generalized to algebras over different base fields. We assume that the Jacobson radical of \mathcal{A} is trivial, one can check this for instance by computing the kernel of a proper matrix, see [182] for more details.

The input of the algorithm are the structure constants d_{ij}^k of the algebra \mathcal{A} with respect to a vector space basis $\{b_1, \dots, b_r\}$. We have $b_i b_j = \sum_{k=1}^r d_{ij}^k b_k$. The output of the algorithm are the coefficients in this basis of the minimal central idempotents. These are the elements $p \in \mathcal{A}$ such that $p \neq 0, p^2 = p$, p commutes with every element in \mathcal{A} and p cannot be written as $p = p_1 + p_2$ where p_1, p_2 also satisfy the previous requirements. Finding the minimal central idempotents is equivalent to determining the block decomposition of a matrix algebra.

We denote the column vector of coefficients of an element x with respect to this basis as $c(x)$. We first calculate the center $Z(\mathcal{A})$ of \mathcal{A} . Let $x = \sum_{j=1}^r x_j b_j$. It holds that $x \in Z(\mathcal{A})$ iff $b_i x = x b_i$ for all i . It is easy to see that this is equivalent to $\sum_{j=1}^r (d_{ij}^k - d_{ji}^k) x_j = 0$ for all k, i . We conclude that $x \in Z(\mathcal{A})$ iff $c(x) \in \text{Kern}(Z)$ with $Z_{(i-1)r+k,j} = d_{ij}^k - d_{ji}^k$.

Let $\{z_1, \dots, z_c\}$ be a basis of $\text{Kern}(Z)$. We can easily obtain the structure constants f_{ij}^k with respect to this basis by solving the linear system

$$\sum_k f_{ij}^k c(z_k) = c(z_i z_j)$$

for all i, j .

We now forget the algebra \mathcal{A} and only work in the commutative algebra $\mathcal{C} := Z(\mathcal{A})$. From now on, we denote by $c(z)$ the column vector of coefficients of an element $z \in \mathcal{C}$ with respect to the basis $\{z_1, \dots, z_c\}$.

Given an element z , recall that the ideal generated by z is defined by $\langle z \rangle = \text{span}\{xz \mid x \in \mathcal{C}\}$. If we take a random element $z \in \mathcal{C}$, we expect that $\langle z \rangle = \mathcal{C}$. Let us now show how to decompose an ideal as $\langle z \rangle = \langle z_1 \rangle \oplus \langle z_2 \rangle$.

First, we find a basis of the space $\langle z \rangle$. This is easily done by computing a basis of the column space of the matrix $[c(z z_1) \dots c(z z_c)]$. Let $\{y_1, \dots, y_d\}$ be a basis of $\langle z \rangle$. Second, we compute the identity I_z of the ideal, this is the unique element with $I_z y_i = y_i$ for all i . After a straightforward calculation we obtain that the coefficients C_j of the identity I_z with respect to the basis $\{y_1, \dots, y_d\}$ are given by the solution of the linear system

$$\sum_{j=1}^d \left(\sum_{l=1}^c \sum_{m=1}^c c(y_j)_l c(y_k)_m f_{lm}^p \right) C_j = c(y_k)_p$$

for all p .

We can now decompose the ideal $\langle z \rangle$. The minimal polynomial P with $P(z) = 0$ can be calculated as follows. Find the smallest q such that the matrix $[c(z^q) \dots c(z) c(I_z)]$ is rank deficient. The zero vector of this matrix gives the coefficients of P . Let n_1, \dots, n_q be the complex roots of P , hence $P(x) = \prod_{i=1}^q (x - n_i)$. If $q = 1$, the ideal $\langle z \rangle$ is one dimensional. This implies that $z^2 = \lambda z$, hence z/λ is an idempotent. If $q > 1$ we decompose $P(x) = P_1(x)P_2(x)$ such that P_1, P_2 have no common roots.

We claim that $\langle P_1(z) \rangle \oplus \langle P_2(z) \rangle := R(z)$ is the sought after decomposition of $\langle z \rangle$. First, we show that the equality holds in $\langle z \rangle = R(z)$. Clearly the inclusion \supseteq holds. We now show the reverse inclusion. Since P_1 and P_2 are polynomials over \mathbb{C} and have no common roots, they are coprime. Bézout's identity ensures the existence of two polynomials Q_1, Q_2 such that $1 = Q_1P_1 + Q_2P_2$. Evaluating both sides in z gives that $I_z \in R(z)$. Since $R(z)$ is an ideal, $xI_z \in R(z)$ for all x , by which we can conclude that $\langle z \rangle \subseteq R(z)$. It is worth noting that $Q_1(z)P_1(z)$ is the identity of $\langle P_1(z) \rangle$, hence the calculation of the identity only needs to be performed once at the start of the algorithm.

Second, we show that $\langle P_1(z) \rangle$ and $\langle P_2(z) \rangle$ are orthogonal spaces. Take $w_1P_1(z) \in \langle P_1(z) \rangle$ and $w_2P_2(z) \in \langle P_2(z) \rangle$, then the equality $w_1P_1(z)w_2P_2(z) = 0$ holds since \mathcal{C} is commutative and $P(z) = P_1(z)P_2(z) = 0$. This implies that the sum is direct and that $\langle z \rangle = \langle P_1(z) \rangle \oplus \langle P_2(z) \rangle$. Since \mathcal{C} is finite, we can apply this decomposition recursively and after a finite number of steps we find the primitive idempotents of \mathcal{C} , from which we can easily obtain those of \mathcal{A} .

3.D Results for string-nets

3.D.1 Fibonacci string-net

The first example we discuss is the simplest non-Abelian string-net model. As input we use the modular tensor category of Fibonacci anyons. We expect to find central idempotents corresponding to the topological sectors of the doubled Fibonacci theory.

MPO-tensors

The categorical data of the Fibonacci theory is well known. The theory has two labels 1 and τ that satisfy the non-Abelian fusion rules

$$N_{11}^1 = N_{\tau 1}^\tau = N_{1\tau}^\tau = N_{\tau\tau}^1 = N_{\tau\tau}^\tau = 1,$$

other multiplicities are zero. The quantum dimensions are given by $d_1 = 1$ and $d_\tau = \frac{1+\sqrt{5}}{2} := \phi$. The remaining crucial information are the F -symbols

of this theory. They are given by

$$[F_d^{abc}]_e^f = F_{def}^{abc} = \delta_{abe}\delta_{cde}\delta_{adf}\delta_{bcf}F_{def}^{abc}, \tag{3.149}$$

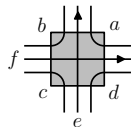
where $\delta_{ijk} = 1$ if i, j, k can fuse to 1, i.e. $N_{ij}^k > 0$, and $\delta_{ijk} = 0$ zero otherwise. The non-trivial elements of F are given by

$$F_{\tau 11}^{\tau \tau \tau} = \frac{1}{\phi}, \quad F_{\tau \tau 1}^{\tau \tau \tau} = \frac{1}{\sqrt{\phi}}, \quad F_{\tau 1 \tau}^{\tau \tau \tau} = \frac{1}{\sqrt{\phi}}, \quad F_{\tau \tau \tau}^{\tau \tau \tau} = -\frac{1}{\phi}.$$

All other non-zero components of F are one. The construction of the tensors is most easily described using the scalars $v_i = \sqrt{d_i}$ and the G symbols,

$$G_{def}^{abc} = \frac{1}{v_e v_f} F_{def}^{abc}. \tag{3.150}$$

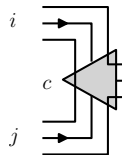
As shown in [109], the Fibonacci string-net state can now be described by a projector MPO constructed from the tensors



$$= G_{def}^{abc} \sqrt{v_a v_b v_c v_d} \tag{3.151}$$

After removing the zero rows and columns, this MPO has bond dimension 5 and consists of two blocks B_1 and B_τ of dimension 2 and 3 respectively. The blocks B_1, B_τ satisfy the Fibonacci fusion rules. The diagonal matrix Δ from equation (3.9) is given by the quantum dimensions of the block labels divided by the square of the total quantum dimension: $w_1 = \frac{1}{1+\phi^2}$ and $w_\tau = \frac{\phi}{1+\phi^2}$.

For these MPOs we also know the explicit form of the fusion tensors X :



$$= G_{abc}^{ijk} v_k v_c. \tag{3.152}$$

Central idempotents

Here we give the central idempotents and their topological spins for the Fibonacci string-net. Recall that the algebra we decompose is generated by the following basis elements

$$A_{11111}, A_{\tau \tau \tau 1}, A_{1 \tau 1 \tau}, A_{1 \tau \tau \tau}, A_{\tau 1 \tau \tau}, A_{\tau \tau 1 \tau}, A_{\tau \tau \tau \tau}.$$

All other possible elements are zero due to the fusion rules. We find 4 different idempotents, of which $\mathcal{P}_1, \mathcal{P}_2, \mathcal{P}_3$ are one-dimensional and \mathcal{P}_4 has

dimension two:

$$\begin{aligned}\mathcal{P}_1 &= \frac{1}{\sqrt{5}} \left(\frac{1}{\phi} A_{1111} + \sqrt{\phi} A_{1\tau 1\tau} \right) \\ \mathcal{P}_2 &= \frac{1}{\sqrt{5}} \left(\frac{1}{\phi} A_{\tau\tau\tau 1} + \frac{1}{\sqrt{\phi}} e^{-\frac{4\pi i}{5}} A_{\tau 1\tau\tau} + e^{\frac{3\pi i}{5}} A_{\tau\tau\tau\tau} \right) \\ \mathcal{P}_3 &= \frac{1}{\sqrt{5}} \left(\frac{1}{\phi} A_{\tau\tau\tau 1} + \frac{1}{\sqrt{\phi}} e^{\frac{4\pi i}{5}} A_{\tau 1\tau\tau} + e^{-\frac{3\pi i}{5}} A_{\tau\tau\tau\tau} \right) \\ \mathcal{P}_4 &= \frac{1}{\sqrt{5}} \left(\phi A_{1111} + A_{\tau\tau\tau 1} - \sqrt{\phi} A_{1\tau 1\tau} + \sqrt{\phi} A_{\tau 1\tau\tau} + \frac{1}{\phi} A_{\tau\tau\tau\tau} \right).\end{aligned}$$

We recognize \mathcal{P}_1 as the vacuum particle. Indeed, when we write out this tensor, we find a diagonal tensor with weights depending on the inner MPO label. These weights correspond exactly to the weights that determine the ground state tensors in the MPO framework [109], denoted by Δ in equation (3.9). More generally, we see in all other examples that we always recover the vacuum particle corresponding to the ground state.

There are some other general remarks we can already see in this example. The vectors $A_{1\tau\tau\tau}$ and $A_{\tau\tau 1\tau}$ are not present in any of the idempotents. These are exactly the vectors A_{abcd} with a different incoming a and outgoing c label. We do not expect them to be present in the decomposition of a central idempotent, as they correspond exactly to off diagonal nilpotent matrices that are not in the center of the algebra. The decomposition of the higher dimensional central idempotent \mathcal{P}_4 in irreducible, but not central, one-dimensional idempotents is very simple. The element \mathcal{P}_4 contains both terms with $a, c = 1$ and $a, c = \tau$. The decomposition of \mathcal{P}_4 in two one-dimensional idempotents is obtained by grouping all terms with $a, c = 1$ as one idempotent and all terms with $a, c = \tau$ as the second idempotent. This procedure also holds for more general models. All other, one-dimensional, idempotents only contain terms with $a, c = 1$ or $a, c = \tau$. Note that a d -dimensional idempotent projects onto a d^2 dimensional subspace, such that we indeed recover the algebra dimension as $7 = 1^2 + 1^2 + 1^2 + 2^2$. This is required for our set of central idempotents to be complete.

The topological spins we obtain are given by

$$h_1 = 0, h_2 = -\frac{4}{5}, h_3 = \frac{4}{5}, h_4 = 0.$$

Clearly, we can now make the identification with the well-known anyons from the doubled Fibonacci theory:

$$\mathcal{P}_1 = (1, 1), \mathcal{P}_2 = (1, \bar{\tau}), \mathcal{P}_3 = (\tau, 1), \mathcal{P}_4 = (\tau, \bar{\tau}).$$

We can compare this result with the idempotents obtained in [161] and see that both solutions have a similar structure. With a slightly different convention of the basis elements A_{abcd} , corresponding to a normalization that depends on a, b, c, d , we obtain exactly the same multiplication table and idempotents.

3.D.2 Ising string-net

As a second example we look at the string-net obtained from the Ising fusion category.

MPO-tensors

As we saw in the analysis of the Fibonacci model in the previous subsection, we only need the fusion rules, quantum dimensions and F -symbols to construct the relevant tensors. The Ising category has three labels $1, \sigma, \psi$ with fusion rules

$$N_{11}^1 = 1, N_{1\sigma}^\sigma = 1, N_{1\psi}^\psi = 1, N_{\sigma\sigma}^1 = 1,$$

up to the usual allowed permutations of the labels. The only non-trivial fusion rule is $\sigma \times \sigma = 1 + \psi$. The quantum dimension are given by $d_1 = 1, d_\sigma = \sqrt{2}, d_\psi = 1$.

The F -symbols are again given by $F_{def}^{abc} \neq 0$ iff all appearing fusion processes are allowed, see equation (3.149). The non-trivial elements are given by

$$F_{\sigma 11}^{\sigma\sigma\sigma} = \frac{1}{\sqrt{2}}, F_{\sigma\psi 1}^{\sigma\sigma\sigma} = \frac{1}{\sqrt{2}}, F_{\sigma 1\psi}^{\sigma\sigma\sigma} = \frac{1}{\sqrt{2}}, F_{\sigma\psi\psi}^{\sigma\sigma\sigma} = -\frac{1}{\sqrt{2}}, F_{\sigma\sigma\sigma}^{\psi\sigma\psi} = -1, F_{\psi\sigma\sigma}^{\psi\sigma\psi} = -1,$$

other allowed non-zero components are one. Similarly as for the Fibonacci model, we can now construct the G -symbols and from these all necessary tensors, see equations (3.150), (3.151), (3.152) in the previous subsection.

Central idempotents

We now have all the tensors required to calculate the central idempotents of the Ising string-net. From the fusion rules we find that there are 12 non-zero basis elements A_{abcd} . The algebra generated by these elements has 9 central idempotents, given by

$$\begin{aligned} \mathcal{P}_1 &= \frac{1}{4} \left(A_{1111} + 2^{3/4} A_{1\sigma 1\sigma} + A_{1\psi 1\psi} \right) \\ \mathcal{P}_2 &= \frac{1}{4} \left(A_{\sigma\sigma\sigma 1} + 2^{1/4} e^{\frac{\pi i}{8}} A_{\sigma 1\sigma\sigma} + 2^{1/4} e^{-\frac{3\pi i}{8}} A_{\sigma\psi\sigma\sigma} + e^{\frac{\pi i}{2}} A_{\sigma\sigma\sigma\psi} \right) \\ \mathcal{P}_3 &= \frac{1}{4} \left(A_{\sigma\sigma\sigma 1} + 2^{1/4} e^{-\frac{\pi i}{8}} A_{\sigma 1\sigma\sigma} + 2^{1/4} e^{\frac{3\pi i}{8}} A_{\sigma\psi\sigma\sigma} + e^{-\frac{\pi i}{2}} A_{\sigma\sigma\sigma\psi} \right) \\ \mathcal{P}_4 &= \frac{1}{4} \left(A_{\psi\psi\psi 1} + 2^{3/4} e^{\frac{\pi i}{2}} A_{\psi\sigma\psi\sigma} - A_{\psi 1\psi\psi} \right) \\ \mathcal{P}_5 &= \frac{1}{4} \left(A_{\psi\psi\psi 1} + 2^{3/4} e^{-\frac{\pi i}{2}} A_{\psi\sigma\psi\sigma} - A_{\psi 1\psi\psi} \right) \\ \mathcal{P}_6 &= \frac{1}{4} \left(A_{\sigma\sigma\sigma 1} + 2^{1/4} e^{-\frac{7\pi i}{8}} A_{\sigma 1\sigma\sigma} + 2^{1/4} e^{\frac{5\pi i}{8}} A_{\sigma\psi\sigma\sigma} + e^{\frac{\pi i}{2}} A_{\sigma\sigma\sigma\psi} \right) \\ \mathcal{P}_7 &= \frac{1}{4} \left(A_{\sigma\sigma\sigma 1} + 2^{1/4} e^{\frac{7\pi i}{8}} A_{\sigma 1\sigma\sigma} + 2^{1/4} e^{-\frac{5\pi i}{8}} A_{\sigma\psi\sigma\sigma} + e^{-\frac{\pi i}{2}} A_{\sigma\sigma\sigma\psi} \right) \end{aligned}$$

$$\mathcal{P}_8 = \frac{1}{4} \left(A_{1111} - 2^{3/4} A_{1\sigma 1\sigma} + A_{1\psi 1\psi} \right)$$

$$\mathcal{P}_9 = \frac{1}{2} \left(A_{1111} + A_{\psi\psi\psi\psi} - A_{1\psi 1\psi} + A_{\psi 1\psi\psi} \right)$$

The corresponding topological spins are found to be

$$h_1 = 0, h_2 = \frac{1}{16}, h_3 = -\frac{1}{16}, h_4 = \frac{1}{2}, h_5 = -\frac{1}{2}$$

$$h_6 = -\frac{7}{16}, h_7 = \frac{7}{16}, h_8 = 0, h_9 = 0.$$

All central idempotents are one dimensional, except for \mathcal{P}_9 which is two-dimensional, such that we indeed obtain $12 = 8 \cdot 1^2 + 2^2$. We can now identify these central idempotents with the anyons in the double Ising model as follows,

$$\mathcal{P}_1 = (1, 1), \mathcal{P}_2 = (\sigma, 1), \mathcal{P}_3 = (1, \bar{\sigma}),$$

$$\mathcal{P}_4 = (\psi, 1), \mathcal{P}_5 = (1, \psi), \mathcal{P}_6 = (\sigma, \bar{\psi}),$$

$$\mathcal{P}_7 = (\psi, \bar{\sigma}), \mathcal{P}_8 = (\psi, \bar{\psi}), \mathcal{P}_9 = (\sigma, \bar{\sigma}).$$

3.D.3 Rep(S_3) string-net

As a final example we consider the string-net with input fusion category the representation theory of S_3 . As this last category is not modular, the anyons of the string-net are not just doubled versions of the labels of the input data.

MPO-tensors

Again, we need to specify the categorical data of the input category and can construct the tensors of the Rep(S_3) string-net from these. The Rep(S_3) fusion category has three labels 1, 2, 3 with following fusion rules,

$$N_{11}^1 = 1, N_{12}^2 = 1, N_{13}^3 = 1, N_{33}^2 = 1, N_{33}^3 = 1.$$

up to the allowed permutations of the labels. The non-trivial fusion rule is $3 \times 3 = 1 + 2 + 3$. The quantum dimensions of the labels are $d_1 = 1, d_2 = 1, d_3 = 2$.

As always, the F -symbols are given by $F_{def}^{abc} \neq 0$ if all appearing fusion processes are allowed as in equation (3.149). The non-trivial elements are given by

$$F_{333}^{323} = -1, \quad F_{333}^{332} = -1, \quad F_{333}^{233} = -1, \quad F_{233}^{333} = -1,$$

$$F_{311}^{333} = \frac{1}{2}, \quad F_{312}^{333} = \frac{1}{2}, \quad F_{313}^{333} = \frac{1}{\sqrt{2}}, \quad F_{321}^{333} = \frac{1}{2}, \quad F_{322}^{333} = \frac{1}{2},$$

$$F_{323}^{333} = -\frac{1}{\sqrt{2}}, \quad F_{331}^{333} = \frac{1}{\sqrt{2}}, \quad F_{332}^{333} = -\frac{1}{\sqrt{2}}, \quad F_{333}^{333} = 0,$$

other allowed coefficients are 1. Similarly as for the Fibonacci model, we can now construct the G -symbols and from these all necessary tensors, see equations (3.150), (3.151) and (3.152).

Central idempotents

The algebra for the given fusion rules is 17-dimensional. We find 8 different central idempotents,

$$\begin{aligned} \mathcal{P}_1 &= \frac{1}{6}A_{3331} - \frac{1}{6}A_{3332} + \frac{1}{3\sqrt{2}}e^{-2\pi i/3}A_{3133} + \frac{1}{3\sqrt{2}}e^{\pi i/3}A_{3233} + \frac{1}{3}e^{2\pi i/3}A_{3333} \\ \mathcal{P}_2 &= \frac{1}{6}A_{2221} + \frac{1}{6}A_{2122} - \frac{\sqrt{2}}{3}A_{2323} \\ \mathcal{P}_3 &= \frac{1}{2}A_{2221} + \frac{1}{4}A_{3331} - \frac{1}{2}A_{2122} + \frac{1}{4}A_{3332} - \frac{1}{2\sqrt{2}}A_{3133} - \frac{1}{2\sqrt{2}}A_{3233} \\ \mathcal{P}_4 &= \frac{1}{6}A_{3331} - \frac{1}{6}A_{3332} + \frac{1}{3\sqrt{2}}e^{2\pi i/3}A_{3133} + \frac{1}{3\sqrt{2}}e^{-\pi i/3}A_{3233} + \frac{1}{3}e^{-2\pi i/3}A_{3333} \\ \mathcal{P}_5 &= \frac{1}{6}A_{3331} - \frac{1}{6}A_{3332} + \frac{1}{3\sqrt{2}}A_{3133} - \frac{1}{3\sqrt{2}}A_{3233} + \frac{1}{3}A_{3333} \\ \mathcal{P}_6 &= \frac{1}{3}A_{1111} + \frac{1}{3}A_{2221} + \frac{1}{3}A_{1212} + \frac{1}{3}A_{2122} - \frac{\sqrt{2}}{3}A_{1313} + \frac{\sqrt{2}}{3}A_{2323} \\ \mathcal{P}_7 &= \frac{1}{2}A_{1111} + \frac{1}{4}A_{3331} - \frac{1}{2}A_{1212} + \frac{1}{4}A_{3332} + \frac{1}{2\sqrt{2}}A_{3133} + \frac{1}{2\sqrt{2}}A_{3233} \\ \mathcal{P}_8 &= \frac{1}{6}A_{1111} + \frac{1}{6}A_{1212} + \frac{\sqrt{2}}{3}A_{1313}. \end{aligned}$$

The idempotents $\mathcal{P}_3, \mathcal{P}_6, \mathcal{P}_7$ are two-dimensional; all other central idempotents have dimension one. We again check the consistency condition $17 = 1 + 1 + 1 + 1 + 1 + 2^2 + 2^2 + 2^2$, which ensures our set of central idempotents is complete.

The only non-zero topological spins are given by

$$h_1 = -\frac{1}{3}, h_3 = \frac{1}{2}, h_4 = \frac{1}{3}.$$

The S -matrix can be calculated as explained in subsection 3.5.3. We find that

$$S = \frac{1}{6} \begin{pmatrix} 1 & 3 & 2 & 1 & 2 & 3 & 2 & 2 \\ 3 & 3 & 0 & -3 & 0 & -3 & 0 & 0 \\ 2 & 0 & 4 & 2 & -2 & 0 & -2 & -2 \\ 1 & -3 & 2 & 1 & 2 & -3 & 2 & 2 \\ 2 & 0 & -2 & 2 & -2 & 0 & -2 & 4 \\ 3 & -3 & 0 & -3 & 0 & 3 & 0 & 0 \\ 2 & 0 & -2 & 2 & -2 & 0 & 4 & -2 \\ 2 & 0 & -2 & 2 & 4 & 0 & -2 & -2 \end{pmatrix}.$$

These results agree with the theoretical findings in the literature, see for instance [191].

3.E Vacuum $(\tau, \bar{\tau})$ -pair

Suppose we have a $\mathcal{P}_{\tau\bar{\tau}}$ anyon pair. We can write the tensors that live on the sites containing an anyon as a sum of a tensor with a 1 MPO attached to it and a tensor with a τ MPO attached to it,

Diagrammatic equation (3.153): A tensor with a purple square (labeled I) and a purple circle (labeled I) is equal to the sum of two tensors. The first tensor has a blue square (labeled I^1) and a blue circle (labeled 1). The second tensor has a red square (labeled I^τ) and a red circle (labeled τ). All tensors are connected to a central black square tensor.

$$I \text{ (square)} \text{ --- } I \text{ (circle)} = I^1 \text{ (square)} \text{ --- } 1 \text{ (circle)} + I^\tau \text{ (square)} \text{ --- } \tau \text{ (circle)}. \quad (3.153)$$

As we created this pair from the ground state, it is itself in the trivial topological sector, hence invariant under the idempotent of the trivial sector, which is the MPO projector. Hence the tensor network containing this pair is equivalent to the network containing the pair projected on the MPO subspace,

Diagrammatic equation showing the projection of the anyon pair onto the MPO subspace. The left side shows a tensor network with a purple anyon pair. The right side shows the sum of two tensor networks: one with a blue anyon pair (labeled I^1 and 1) and one with a red anyon pair (labeled I^τ and τ). The coefficients are $\frac{1}{\mathcal{D}^2}$ and $\frac{\phi}{\mathcal{D}^2}$.

$$\text{Tensor Network with } I \text{ (square)} \text{ --- } I \text{ (circle)} = \frac{1}{\mathcal{D}^2} \text{Tensor Network with } I^1 \text{ (square)} \text{ --- } 1 \text{ (circle)} + \frac{\phi}{\mathcal{D}^2} \text{Tensor Network with } I^\tau \text{ (square)} \text{ --- } \tau \text{ (circle)} + \frac{1}{\mathcal{D}^2} \text{Tensor Network with } I^\tau \text{ (square)} \text{ --- } \tau \text{ (circle)} + \frac{\phi}{\mathcal{D}^2} \text{Tensor Network with } I^1 \text{ (square)} \text{ --- } 1 \text{ (circle)}.$$

Here, $\mathcal{D}^2 = 1 + \phi^2$ is the square of the total quantum dimension of the Fibonacci model. We can now apply the same procedure as in the calculation

of $\mathcal{R}_{\mathcal{P}_{\tau,\tau}}$, which yields,

$$\begin{aligned}
 &= \frac{1}{\mathcal{D}^2} \begin{array}{c} I^1.A_{1111} \\ \text{Diagram 1} \end{array} + \frac{\phi}{\mathcal{D}^2} \begin{array}{c} I^1.A_{1\tau 1\tau} \\ \text{Diagram 2} \end{array} \\
 &+ \frac{\phi}{\mathcal{D}^2} \begin{array}{c} I^1.A_{1\tau\tau\tau} \\ \text{Diagram 3} \end{array} + \frac{1}{\mathcal{D}^2} \begin{array}{c} I^\tau.A_{\tau\tau\tau 1} \\ \text{Diagram 4} \end{array} \\
 &+ \frac{\phi}{\mathcal{D}^2} \begin{array}{c} I^\tau.A_{\tau 1\tau\tau} \\ \text{Diagram 5} \end{array} + \frac{\phi}{\mathcal{D}^2} \begin{array}{c} I^\tau.A_{\tau\tau\tau\tau} \\ \text{Diagram 6} \end{array} \\
 &+ \frac{\phi}{\mathcal{D}^2} \begin{array}{c} I^\tau.A_{\tau\tau 1\tau} \\ \text{Diagram 7} \end{array}.
 \end{aligned}
 \tag{3.154}$$

The products $\mathcal{P}_{\tau\bar{\tau}}.A_{abcd}$ are easily calculated. We find that

$$\begin{aligned}
 &= \frac{1}{\mathcal{D}^2} \begin{array}{c} I^1 \\ \text{Diagram 1} \end{array} + \frac{1}{\mathcal{D}^2\phi^2} \begin{array}{c} I^1 \\ \text{Diagram 2} \end{array} \\
 &+ \frac{\phi}{\mathcal{D}^2} \begin{array}{c} I^1.A_{1\tau\tau\tau} \\ \text{Diagram 3} \end{array} + \frac{1}{\mathcal{D}^2} \begin{array}{c} I^\tau \\ \text{Diagram 4} \end{array} \\
 &+ \frac{1}{\mathcal{D}^2} \begin{array}{c} I^\tau \\ \text{Diagram 5} \end{array} + \frac{1}{\mathcal{D}^2\phi^3} \begin{array}{c} I^\tau \\ \text{Diagram 6} \end{array} \\
 &+ \frac{\phi}{\mathcal{D}^2} \begin{array}{c} I^\tau.A_{\tau\tau 1\tau} \\ \text{Diagram 7} \end{array}.
 \end{aligned}
 \tag{3.155}$$

As the pair of anyons is in the vacuum sector we can equate the right hand side of equation (3.153) to the right hand side of equation (3.155). Now, the difference between a 1 or τ string can be decided in the presence of other anyons. Hence for this equality to hold it needs to hold for the diagrams with a 1 and τ string separately. This gives the following two

relations,

$$\begin{aligned}
 I^1 \text{---} \square \text{---} \square \text{---} \square &= \frac{1 + \frac{1}{\phi^2}}{\mathcal{D}^2} I^1 \text{---} \square \text{---} \square \text{---} \square + \frac{\phi}{\mathcal{D}^2} I^\tau \cdot A_{\tau\tau 1\tau} \\
 I^\tau \text{---} \square \text{---} \square \text{---} \square &= \frac{2 + \frac{1}{\phi^3}}{\mathcal{D}^2} I^\tau \text{---} \square \text{---} \square \text{---} \square + \frac{\phi}{\mathcal{D}^2} I^1 \cdot A_{1\tau\tau\tau}
 \end{aligned}
 \tag{3.156}$$

Let us denote by B_1, B_τ the local tensors supported on $P_{\tau, \bar{\tau}}^1, P_{\tau, \bar{\tau}}^\tau$ respectively. In the figures, B_1 is denoted by a blue square and B_τ by a red square.

Clearly the pair of tensors $B_\tau \cdot A_{\tau\tau 1\tau}$ give rise to the same tensor network as the pair B_1 . Similar, the pair $B_1 \cdot A_{1\tau\tau\tau}$ and B_τ give rise to the same network. Hence we can choose

$$B_1 = \left(\frac{\sqrt{5}}{\phi} \right)^{-1/2} B_\tau \cdot A_{\tau\tau 1\tau}, \quad B_\tau = \left(\frac{\sqrt{5}}{\phi^2} \right)^{-1/2} B_1 \cdot A_{1\tau\tau\tau}. \tag{3.157}$$

Both requirements are consistent as $A_{\tau\tau 1\tau} \cdot A_{1\tau\tau\tau} = \frac{\sqrt{5}}{\phi\sqrt{\phi}} P_{\tau, \bar{\tau}}^1$ and $A_{1\tau\tau\tau} \cdot A_{\tau\tau 1\tau} = \frac{\sqrt{5}}{\phi\sqrt{\phi}} P_{\tau, \bar{\tau}}^\tau$. We see that, as expected, the requirement that a pair of $\mathcal{P}_{\tau, \bar{\tau}}$ anyons is in the topologically trivial sectors, restricts the choice of different B_1, B_τ tensors by enforcing a strict relation between them.

Let us now take such a pair of $\mathcal{P}_{\tau, \bar{\tau}}$ anyons and compute the braiding tensor $\mathcal{R}_{\mathcal{P}_{\tau, \bar{\tau}}, \tau}$. The calculation is the same as we already did for the general pair B_1, B_τ , we only need the results for the τ string in this calculation. Due to the relation (3.157) there is no additional entanglement between the degrees of freedom on the site containing the anyon and the \mathcal{R} tensor. We find that

$$\mathcal{R}_{\mathcal{P}_{\tau, \bar{\tau}}, \tau} = -\frac{1}{\phi^{3/2}} \bar{A}_{1212} + \frac{5^{1/4}}{\sqrt{\phi}} \bar{A}_{1222} + \frac{1}{\sqrt{\phi}} \bar{A}_{2122} + \frac{1}{\phi^2} \bar{A}_{2222} + \frac{5^{1/4}}{\phi} \bar{A}_{2212}.$$

On the virtual level, this is a 8×8 orthogonal matrix.

3.F Braiding in the Fibonacci string-net

To illustrate the general braiding formalism developed in section 3.5.6 of the main text we now work out some details for the Fibonacci string-net. As explained above, the crucial information to write down the relevant tensors are the F -symbols and the quantum dimensions of this theory. We can use the anyon ansatz to numerically determine the four central idempotents; we listed the outcome of this calculation in Appendix 3.D.

First we focus on the idempotent that describes a $(\tau, 1)$ anyon in the PEPS. We denote this idempotent by \mathcal{P}_τ . If we recall the definition of the tensors A_{abcd} , we can express this idempotent as

$$\mathcal{P}_\tau = \frac{1}{\sqrt{5}} \left(\frac{1}{\phi} A_{\tau\tau\tau 1} + \frac{1}{\sqrt{\phi}} e^{\frac{4\pi i}{5}} A_{\tau 1\tau\tau} + e^{-\frac{3\pi i}{5}} A_{\tau\tau\tau\tau} \right).$$

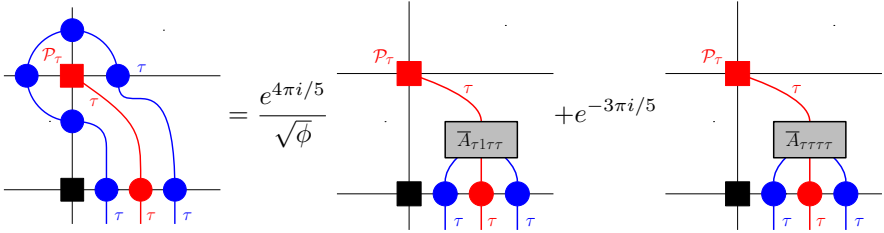
Suppose we have two such anyons, then we can determine their possible fusion outcomes. For this we use the fusion procedure explained in Figure 3.9 in section 3.5.5. Clearly, the outgoing τ strings of the two anyons can be fused to a 1 or τ string. The 1 string can give rise to a fusion product supported in the subspace corresponding to \mathcal{P}_1 or $\mathcal{P}_{\tau\bar{\tau}}$, while the τ string can give rise to a support in all idempotents except \mathcal{P}_1 . Although it is not easy to determine this analytically, one can readily determine the sectors where the two \mathcal{P}_τ anyons are supported numerically. These sectors are the \mathcal{P}_1 and \mathcal{P}_τ sector, as we expect from the fusion rules of Fibonacci anyons.

Let us now concentrate on the exchange of two such τ anyons and determine the tensor $\mathcal{R}_{\mathcal{P}_\tau, \tau}$. We first show how one can analytically determine these tensors. This gives insight in the close relation between the idempotents and the \mathcal{R} tensors. The calculation we use to determine the tensor \mathcal{R} resembles the well-known teleportation protocol from quantum information theory. We follow the derivation of section 3.5.6 in the main text. This gives

(3.158)

Since \mathcal{P}_τ is a one dimensional idempotent, $\mathcal{P}_\tau A_{abcd} = \lambda_{abcd} \mathcal{P}_\tau$ for complex numbers λ_{abcd} that can easily be calculated from the structure constants of the algebra. We find that $\lambda_{\tau 1\tau\tau} = \frac{1}{\sqrt{\phi}} e^{4\pi i/5}$, $\lambda_{\tau\tau 1\tau} = 0$ and $\lambda_{\tau\tau\tau\tau} = e^{-3\pi i/5}$,

such that Eq. (3.158) is simplified to



We conclude from this calculation that the tensor $\mathcal{R}_{\mathcal{P}_\tau, \tau}$ is given by

$$\mathcal{R}_{\mathcal{P}_\tau, \tau} = \frac{1}{\sqrt{\phi}} e^{4\pi i/5} \bar{A}_{\tau 1 \tau \tau} + e^{-3\pi i/5} \bar{A}_{\tau \tau \tau \tau}.$$

We can now also look at the contraction of two of these tensors as in figure 3.13, which describes the full braiding of two anyons. This tensor then describes the monodromy matrix of two Fibonacci anyons. It is known that the elements are given by $e^{2\pi i(h_c - h_\tau - h_\tau)}$ where c is the fusion product of the two anyons, $c = 1, \tau$. As the spins of the anyons are $h_1 = 0$ and $h_\tau = 2/5$ we expect the tensor in Figure 3.13 to contain the phases $e^{-4\pi i/5}$ and $e^{\pi i/5}$ in the respective topological sectors. One can readily check that this is indeed the case.

We can also look at the higher dimensional idempotent $\mathcal{P}_{\tau\bar{\tau}}$. In general, the situation gets more complicated due to entanglement between the degrees of freedom on the site where the anyon lives and the tensors \mathcal{R} in the virtual network. However, if we obtain the anyons by acting on the ground state, such that we have an anyon pair in the trivial sector, we can simplify the expression for $\mathcal{R}_{\mathcal{P}_{\tau\bar{\tau}}, \tau}$. The reason this is possible is that by acting locally on the topologically trivial vacuum, we can only create very specific excitation pairs in the $\mathcal{P}_{\tau\bar{\tau}}$ sector. Indeed, the crucial fact that the entire pair is in the trivial sector, determines the relation between the anyon tensors in the different minimal, but non-central, idempotent sectors of a higher dimensional idempotent. For the same reason, one can only create a fluxon pair with zero topological charge in the quantum doubles [106, 163, 192]. Such a pair exactly corresponds to the equal superposition of all string types in a given conjugacy class. We now illustrate that this reasoning is still valid in our more general formalism by looking at a $\mathcal{P}_{\tau\bar{\tau}}$ created on top of the trivial sector.

Fermionic projected entangled-pair states and topological phases

Synopsis

We study fermionic matrix product operator algebras and identify the associated algebraic data. Using this algebraic data we construct fermionic tensor network states in two dimensions that have non-trivial symmetry-protected or intrinsic topological order. The tensor network states allow us to relate physical properties of the topological phases to the underlying algebraic data. We illustrate this by calculating defect properties and modular matrices of supercohomology phases. Our formalism also captures Majorana defects as we show explicitly for a class of \mathbb{Z}_2 symmetry-protected and intrinsic topological phases. The tensor networks states presented here are well-suited for numerical applications and hence open up new possibilities for studying interacting fermionic topological phases.

Based on

‘Fermionic projected entangled-pair states and topological phases’
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Contributions of the author: The author has contributed to all results and has written the manuscript, except for appendix 4A.

4.1 Introduction

In recent years there has been substantial progress in the understanding of topological phases in spin systems and their representations via tensor network states. Tensor networks are ideally suited for describing topolog-

ical phases of matter because, nonlocal, topological features of a system are captured by the symmetries of local tensors. In one-dimensional spin systems Matrix Product States (MPS) were used to classify all Symmetry-Protected Topological (SPT) phases [46–49]. A complete understanding of two-dimensional SPT phases in terms of Projected Entangled-Pair States (PEPS) was developed in [59, 160, 193]. A first systematic study of intrinsic topological order in PEPS was done in Ref. [56], where the concept of G -injectivity was introduced. The concept of G -injectivity was soon after generalized to twisted G -injectivity [57] and to matrix product operator (MPO)-injectivity [194], the latter describing the same class of topological phases as those captured by string-net models [179, 195]. A detailed understanding of the anyonic excitations in MPO-injective PEPS and how to construct them was developed in [109].

For topological fermionic systems, the understanding is much less developed. Building on the work of Ref. [66] a complete description of interacting fermionic SPT phases in one dimension using fermionic MPS (fMPS) was given in Refs. [196, 197]. In [61–63], it was shown that free fermions systems with nonzero thermal Hall conductance can be represented as Gaussian PEPS. The first steps in generalizing MPO-injectivity to fermionic PEPS were reported in Refs. [94, 95], but those formulations did not develop the theory of Majorana defects.

In this work we will focus on topological phases with zero thermal Hall conductance in two dimensions and develop a general formalism for understanding the universal properties of fermionic tensor network states representing these phases of matter. We do this by first studying fermionic Matrix Product Operator (fMPO) algebras. The structural data associated to such algebras, which can be seen as a fermionic version of the fusion categories underlying bosonic topological tensor networks, will allow us to construct the relevant topological PEPS. Similarly to the bosonic case, the crucial property giving rise to the non-trivial topological order is the *pulling through* equation. The advantage of the tensor network language is that many interesting universal physical properties of the topological phases can be calculated in a straightforward way. We illustrate this by calculating the symmetry properties of defects and the modular matrices of symmetry-twisted states on a torus for Gu-Wen or supercohomology phases [25]. We also show that the formalism presented here goes beyond supercohomology and fermionic string-net phases [53, 54] and captures systems with Majorana defects [92, 93], and our construction is hence related to the state sum constructions of spin topological field theories reported in Ref. [91].

Many equivalent formulations of fermionic tensor networks based on fermionic mode operators, Grassmann variables or swap gates exist in the literature [67, 68, 88, 198, 199]. In this work we use the graded vector space approach presented in Ref. [196], as it turns out to be the natural framework for generalizing the MPO symmetries of the bosonic case.

4.2 Fermionic tensor networks

In this section we review the fermionic tensor network formalism as introduced in [196]. To define fermionic tensors we will make use of super vector spaces. A super vector space V has a natural direct sum structure

$$V = V^0 \oplus V^1, \quad (4.1)$$

where vectors in V^0 or in V^1 are called homogeneous vectors. A vector in V^0 (V^1) is said to have even (odd) parity. We denote the parity of homogeneous basis vectors $|i\rangle$ as

$$|i| = \begin{cases} 0 & \text{if } |i\rangle \in V^0 \\ 1 & \text{if } |i\rangle \in V^1. \end{cases} \quad (4.2)$$

The tensor product of two homogeneous vectors $|i\rangle$ and $|j\rangle$ is again a homogeneous vector and has parity $|i| + |j| \bmod 2$. This implies that V and the associated operation of taking tensor products is \mathbb{Z}_2 graded. We denote the graded tensor product as

$$|i\rangle \otimes_{\mathfrak{g}} |j\rangle \in V \otimes_{\mathfrak{g}} V. \quad (4.3)$$

For super vector spaces we will always use the following canonical tensor product isomorphism:

$$\mathcal{F} : V \otimes_{\mathfrak{g}} W \rightarrow W \otimes_{\mathfrak{g}} V : |i\rangle \otimes_{\mathfrak{g}} |j\rangle \rightarrow (-1)^{|i||j|} |j\rangle \otimes_{\mathfrak{g}} |i\rangle. \quad (4.4)$$

This isomorphism of course connects the mathematical concept of super vector spaces to physical systems of fermions. The dual vector space V^* inherits the \mathbb{Z}_2 grading from V and \mathcal{F} can be extended in the following way:

$$\mathcal{F} : V^* \otimes_{\mathfrak{g}} W \rightarrow W \otimes_{\mathfrak{g}} V^* : \langle i| \otimes_{\mathfrak{g}} |j\rangle \rightarrow (-1)^{|i||j|} |j\rangle \otimes_{\mathfrak{g}} \langle i|, \quad (4.5)$$

and similarly for the action on $V^* \otimes_{\mathfrak{g}} W^*$.

Fermionic tensors are defined in the graded tensor product of super vector spaces. We will always restrict to homogeneous tensors, i.e. those tensors that have a well-defined parity. Let us now introduce the contraction map \mathcal{C} :

$$\mathcal{C} : V^* \otimes_{\mathfrak{g}} V : \langle i| \otimes_{\mathfrak{g}} |j\rangle \rightarrow \langle i|j\rangle = \delta_{i,j}. \quad (4.6)$$

The contraction map \mathcal{C} can be generalized to arbitrary tensor contractions in the following way: first we take the graded tensor product of the tensors one wishes to contract, secondly, use \mathcal{F} to bring the bra and ket to be contracted next to each other and last, apply \mathcal{C} as defined in (4.6). For tensor contraction to be well defined it is crucial that the tensors have a definite

parity, as we explain in more detail at the end of this section. Note that following the fermionic contraction rules, we get

$$\mathcal{C}(|i\rangle \otimes_{\mathfrak{g}} |j\rangle) = (-1)^{|i||j|} \mathcal{C}(|j\rangle \otimes_{\mathfrak{g}} |i\rangle) = (-1)^{|i|} \delta_{i,j}, \quad (4.7)$$

which results in the fermionic super trace. Vice versa, if we want to write the ordinary trace of an operator as a tensor contraction, we need to insert an additional parity tensor on the contracted index. As an illustration of more general fermionic tensor contraction, let us define the following fermionic tensors (we will not always explicitly denote the graded tensor product symbol $\otimes_{\mathfrak{g}}$)

$$C = \sum_{\alpha\beta\gamma} C_{\alpha\beta\gamma} |\alpha\rangle |\beta\rangle \langle \gamma|$$

$$D = \sum_{\lambda\kappa} D_{\lambda\kappa} |\lambda\rangle \langle \kappa|,$$

where we wish to contract the β index of C with the κ index of D . As a first step we take the graded tensor product of C and D :

$$C \otimes_{\mathfrak{g}} D = \sum_{\alpha\beta\gamma\lambda\kappa} C_{\alpha\beta\gamma} D_{\lambda\kappa} |\alpha\rangle |\beta\rangle \langle \gamma| \otimes_{\mathfrak{g}} |\lambda\rangle \langle \kappa|.$$

Next, we bring the κ bra next to the β ket using fermionic reordering:

$$\mathcal{F}(C \otimes_{\mathfrak{g}} D) = \sum_{\alpha\beta\gamma\lambda\kappa} C_{\alpha\beta\gamma} D_{\lambda\kappa} (-1)^{|\kappa|(|\lambda|+|\gamma|+|\beta|)} |\alpha\rangle \langle \kappa| |\beta\rangle \langle \gamma| |\lambda\rangle.$$

If the tensors C and D are even, this is equivalent to

$$\mathcal{F}(C \otimes_{\mathfrak{g}} D) = \sum_{\alpha\beta\gamma\lambda\kappa} C_{\alpha\beta\gamma} D_{\lambda\kappa} (-1)^{|\kappa|+|\kappa||\alpha|} |\alpha\rangle \langle \kappa| |\beta\rangle \langle \gamma| |\lambda\rangle.$$

Now we apply the contraction to obtain the final tensor:

$$F \equiv \sum_{\alpha\gamma\lambda} \left(\sum_{\beta} C_{\alpha\beta\gamma} D_{\lambda\beta} (-1)^{|\beta|+|\beta||\alpha|} \right) |\alpha\rangle \langle \gamma| |\lambda\rangle.$$

Note that in the definition of fermionic tensors we have to include an internal ordering of the basis vectors. It therefore only makes sense to compare tensors that have the same internal ordering, but we can easily switch to a different ordering by absorbing minus signs from the fermionic reordering in the tensor components. Tensor identities obtained in this way will of course continue to hold when suitably transformed to a different internal ordering.

With this definition of tensor contraction the diagrammatic notation familiar from bosonic tensor networks still applies to the fermionic case.

However, note that the diagrammatic notation does not unambiguously specify the order in which the tensors are put in the tensor product before contracting. This choice is irrelevant as long as all tensors have total even parity, or there is at most one tensor with odd parity, since we can then always swap the order of the tensors before performing contractions. In later sections, we will also need to consider diagrams with two odd tensors, and will be more careful in that case. Another important point is that the order in which the contractions are performed is also irrelevant, on which we further elaborate. Let us thereto highlight some special cases that relate to matrix multiplication and are noteworthy for the following sections. Two-index tensors of the form $\sum_{\alpha,\beta} C_{\alpha,\beta} |\alpha\rangle \langle\beta|$, $\sum_{\gamma,\delta} D_{\gamma,\delta} |\gamma\rangle \langle\delta|$ will give rise to ordinary matrix multiplication of the components when contracting index β with γ , resulting in $\sum_{\alpha,\delta} (CD)_{\alpha,\delta} |\alpha\rangle \langle\delta|$. As expected, we can introduce an identity tensor $\sum_{\beta',\gamma'} \delta_{\beta',\gamma'} |\beta'\rangle \langle\gamma'|$ in between this contraction (now contracting β with β' and γ' with γ) without changing the result. If we want to contract index β and γ of $\sum_{\alpha,\beta} C_{\alpha,\beta} \langle\alpha| |\beta\rangle$ and $\sum_{\gamma,\delta} D_{\gamma,\delta} \langle\gamma| |\delta\rangle$, we obtain $\sum_{\alpha,\beta,\delta} C_{\alpha,\beta} D_{\beta,\delta} (-1)^{|\beta|} \langle\alpha| |\delta\rangle = \sum_{\alpha,\delta} (CPD)_{\alpha,\delta} \langle\alpha| |\delta\rangle$, with P the parity matrix. The identity tensor for this contraction is $\sum_{\beta',\gamma'} P_{\beta',\gamma'} \langle\beta'| |\gamma'\rangle = \sum_{\beta',\gamma'} (-1)^{|\beta'|} \delta_{\beta',\gamma'} \langle\beta'| |\gamma'\rangle \xrightarrow{\mathcal{F}} \sum_{\beta',\gamma'} \delta_{\gamma',\beta'} |\gamma'\rangle \langle\beta'|$. The identity tensor in this case is thus equivalent to the former identity tensor, but just expressed with a different internal ordering. For the diagrammatic tensor notation to be well-defined, the identity tensor should indeed not depend on the type of contraction, i.e. whether bra is contracted with ket or vice versa depends on which tensor is taken first and which second, and this is not specified by the diagrammatic notation. From the above observations it follows that once every individual tensor is specified (with internal ordering) every diagram with contracted indices can be unambiguously translated in a fermionic tensor contraction. We will use the diagrammatic notation extensively in the remainder of this manuscript.

As a final point about fermionic tensor contraction, we consider multi-index tensors which can be interpreted as matrices with compound indices. Contracting index β with γ , as well as β' with γ' , in the two tensors $\sum_{\alpha,\alpha',\beta,\beta'} C_{(\alpha,\alpha'),(\beta,\beta')} |\alpha\rangle |\alpha'\rangle \langle\beta| \langle\beta'|$ and $\sum_{\gamma,\gamma',\delta,\delta'} D_{(\gamma,\gamma'),(\delta,\delta')} |\gamma\rangle |\gamma'\rangle \langle\delta| \langle\delta'|$ gives rise to $\sum_{\alpha,\alpha',\delta,\delta'} (CD)_{(\alpha,\alpha'),(\delta,\delta')} |\alpha\rangle |\alpha'\rangle \langle\delta| \langle\delta'|$. Note that in order to obtain simple matrix multiplication, the order of the indices in the tensor components and the order of the indices in the fermionic basis vectors are chosen differently.

4.3 fMPO algebras

Similar to the bosonic case [109], we start with a finite number of irreducible fMPOs which arise as the virtual symmetries of the topologically ordered PEPS and which constitute a C^* algebra. Specifically, we consider

N irreducible fMPOs of length L $\{O_a^L | a = 1 \dots N\}$ that are closed under multiplication and Hermitian conjugation for every L :

$$O_a^L O_b^L = \sum_{c=1}^N N_{ab}^c O_c^L \quad (4.8)$$

$$(O_a^L)^\dagger \equiv O_{a^*}^L, \quad (4.9)$$

with $N_{ab}^c \in \mathbb{N}$ and $O_a^L \in \{O_a^L | a = 1 \dots N\}$. The reason for these requirements is that we want to be able to construct a Hermitian projector $P^L = \sum_{a=1}^N w_a O_a^L$ from the irreducible fMPOs, which then determines the virtual support space of a PEPS tensor.

The fMPOs are constructed from even fermionic tensors

$$B[a] = \sum_{i,j,\alpha,\beta} \left(B_a^{ij} \right)_{\alpha,\beta} | \alpha \rangle | i \rangle \langle j | \langle \beta | \quad \text{with } |i| + |j| + |\alpha| + |\beta| = 0 \pmod{2} \quad (4.10)$$

and the parity tensor $P = \sum_{\alpha} (-1)^{|\alpha|} | \alpha \rangle \langle \alpha |$ as:

$$\begin{aligned} O_a^L &\equiv \mathcal{C}(P \otimes_{\mathfrak{g}} B[a] \otimes_{\mathfrak{g}} B[a] \otimes_{\mathfrak{g}} \dots \otimes_{\mathfrak{g}} B[a]) \\ &= \sum_{\{i\}\{j\}} \text{tr} \left(B_a^{i_1 j_1} B_a^{i_2 j_2} \dots B_a^{i_L j_L} \right) | i_1 \rangle \langle j_1 | \otimes_{\mathfrak{g}} | i_2 \rangle \langle j_2 | \otimes_{\mathfrak{g}} \dots \otimes_{\mathfrak{g}} | i_L \rangle \langle j_L | \end{aligned}$$

The reason for inserting the extra parity matrix arises from the PEPS construction explained in the following section, which indeed ensures that such a parity tensor is inserted in every closed virtual loop. Physically, this parity tensor encodes anti-periodic boundary conditions. Note that the parity matrix gets canceled by the super trace generated by the fermionic contraction rules, such that the final expression in terms of the tensor components is identical to that of the bosonic MPO algebras with periodic boundary conditions, and enables us to recycle many of the results. However, unlike in the bosonic case, there are two types of irreducible fMPOs. In Ref. [196], it was shown that irreducibility for a fMPO implies that the matrices B^{ij} span a simple \mathbb{Z}_2 graded matrix algebra over \mathbb{C} , which come in two different types: the even and odd type [76]. An even simple \mathbb{Z}_2 graded algebra is simple as an ungraded algebra implying that its center consists of multiples of the identity. An odd simple \mathbb{Z}_2 graded algebra is not simple as an ungraded algebra and its graded center consists of multiples of the identity and multiples of Y , where Y is an odd matrix satisfying $Y^2 \propto \mathbb{1}$. Without loss of generality we adopt the convention that $Y^2 = -\mathbb{1}$. The type of irreducible fMPO will be denoted by $\epsilon_a \in \{0, 1\}$, where $\epsilon_a = 0$ implies that O_a^L is of even type while $\epsilon_a = 1$ implies O_a^L is of odd type, which we will also refer to as Majorana type. For simplicity, we take ϵ_a to be a \mathbb{Z}_2 grading of the fMPO algebra. Another consequence of the anti-periodic boundary conditions is that both

types of irreducible fMPOs have a total fermion parity that is even, whereas fMPOs with periodic boundary conditions have a total fermion parity that matches the value ϵ of the underlying algebra.

4.3.1 Fusion tensors

Multiplying two fMPOs O_a^L and O_b^L gives rise to a new fMPO with a tensor that can be written as

$$\sum_{\alpha, \alpha', i, k, \beta, \beta'} (B_{ab}^{ik})_{(\alpha, \alpha'), (\beta, \beta')} |\alpha\rangle |\alpha'\rangle |i\rangle \langle k| \langle \beta'| \langle \beta|$$

where the ordering was chosen such that the fMPO coefficients reduce to a matrix product of the matrices B_{ab}^{ik} , which are given by

$$(B_{ab}^{ik})_{(\alpha, \alpha'), (\beta, \beta')} = (-1)^{|\alpha'|(|\alpha|+|\beta|)} \sum_j (B_a^{ij})_{\alpha, \beta} (B_b^{jk})_{\alpha', \beta'}$$

Similar to the bosonic case, the fact that $O_a^L O_b^L = \sum_{c=1}^N N_{ab}^c O_c^L$ for every L implies the existence of a gauge transformation X_{ab} that simultaneously brings the matrices B_{ab}^{ik} into a canonical form (block upper triangular), where the diagonal blocks correspond to B_c^{ik} appearing N_{ab}^c times [75].

From the columns of the the gauge transform X_{ab} and the rows of its inverse X_{ab}^{-1} , we can build fermionic splitting and fusion tensors $X_{ab, \mu}^c$ and $X_{ab, \mu}^{c+}$ ($\mu = 1, \dots, N_{ab}^c$), such that

$$\mathcal{C}(X_{ab, \mu}^{c+} \otimes_{\mathfrak{g}} \mathbb{B}[a] \otimes_{\mathfrak{g}} \mathbb{B}[b] \otimes_{\mathfrak{g}} X_{ab, \mu}^c) = \mathbb{B}[c]. \quad (4.12)$$

We introduce the following graphical notation for the tensors $\mathbb{B}[a]$, $X_{ab, \mu}^c$ and $X_{ab, \mu}^{c+}$

$$\begin{array}{c} a \\ | \\ \circ \\ | \\ b \end{array} = \mathbb{B}[a] \quad \begin{array}{c} a \\ | \\ \boxed{\mu} \\ | \\ b \end{array} \begin{array}{c} c \\ | \\ \text{---} \end{array} = X_{ab, \mu}^c \quad \begin{array}{c} a \\ | \\ \boxed{\mu^+} \\ | \\ b \end{array} \begin{array}{c} c \\ | \\ \text{---} \end{array} = X_{ab, \mu}^{c+}, \quad (4.13)$$

where the red (horizontal) indices represent the internal fMPO indices and the black (vertical) indices represent the external fMPO indices. We can then denote the contraction in equation (4.12) graphically as

$$\begin{array}{c} a \\ | \\ \circ \\ | \\ b \end{array} \begin{array}{c} a \\ | \\ \boxed{\mu^+} \\ | \\ b \end{array} \begin{array}{c} c \\ | \\ \text{---} \end{array} = \begin{array}{c} c \\ | \\ \circ \\ | \\ c \end{array} \quad (4.14)$$

Note that although the fMPO tensors $\mathbb{B}[a]$ have even parity, the fusion tensors have a well defined parity that can be either even or odd. This parity depends on the degeneracy label μ and adds a \mathbb{Z}_2 grading denoted as $|\mu|$ to the degeneracy space.

The fusion tensors satisfy following properties:

$$\begin{aligned}
 & \text{Diagram: } \begin{array}{c} a \\ \text{---} \\ \mu^+ \\ \text{---} \\ b \end{array} \text{---} \begin{array}{c} a \\ \text{---} \\ \mu \\ \text{---} \\ c \end{array} = \delta_{\mu,\nu} \delta_{c,d} \text{---} c \\
 & \sum_{c,\mu} \begin{array}{c} a \\ \text{---} \\ \mu \\ \text{---} \\ b \end{array} \text{---} \begin{array}{c} a \\ \text{---} \\ \mu^+ \\ \text{---} \\ b \end{array} = \begin{array}{c} a \\ \text{---} \\ P_{ab} \\ \text{---} \\ b \end{array} , \tag{4.15}
 \end{aligned}$$

where P_{ab} is the projector onto the support of the internal indices of the fMPO tensor $\mathcal{C}(B[a] \otimes_{\mathfrak{g}} B[b])$. For our purposes we are interested in fMPOs that satisfy a slightly stronger condition than equation (4.14). Namely, we assume that the following *zipper condition* holds:

$$\begin{array}{c} a \\ \circ \\ \text{---} \\ b \\ \circ \end{array} = \sum_{c,\mu} \begin{array}{c} a \\ \text{---} \\ \mu \\ \text{---} \\ b \end{array} \begin{array}{c} c \\ | \\ \circ \\ | \\ c \end{array} \begin{array}{c} a \\ \text{---} \\ \mu^+ \\ \text{---} \\ b \end{array} . \tag{4.16}$$

Up to this point, the properties of fMPO super algebras are very similar to those of bosonic MPO algebras. We will now discuss the implications of the presence of $\epsilon_a = 1$ irreducible fMPOs. Because the graded center of the matrices $B[a]^{ij}$ for $\epsilon_a = 1$ contains the odd matrix Y , it is clear that we can contract Y onto any index of a fusion tensor corresponding to an irreducible fMPO with $\epsilon = 1$ to get another fusion tensor that also satisfies the defining equations (4.14) and (4.16). Because Y is odd this changes the parity of the fusion tensor $X_{ab,\mu}^c$. Let us start with the situation $\epsilon_a = \epsilon_b = 1$ and consider the matrix

$$\begin{array}{c} a \\ \circ \\ \text{---} \\ \mu^+ \\ \text{---} \\ b \end{array} \begin{array}{c} a \\ \text{---} \\ Y \\ \text{---} \\ c \end{array} \begin{array}{c} a \\ \text{---} \\ \mu \\ \text{---} \\ c \end{array} , \tag{4.17}$$

where without loss of generality we take $X_{ab,\mu}^c$ and $X_{ab,\mu}^{c+}$ to have even parity. Eq. (4.17) represents an odd matrix that commutes with the matrices $B[c]^{ij}$ because of Eq. (4.16). But $\epsilon_c = 0$ so the center of the matrix algebra $B[c]^{ij}$ consists only of multiples of the identity. For this reason, the matrix in Eq. (4.17) is zero when $\epsilon_a = \epsilon_b = 1$. Similar reasoning shows that also the odd matrix

$$\begin{array}{c} a \\ \text{---} \\ \mu^+ \\ \text{---} \\ b \end{array} \begin{array}{c} a \\ \text{---} \\ Y \\ \text{---} \\ c \end{array} \begin{array}{c} a \\ \text{---} \\ \mu \\ \text{---} \\ c \end{array} \tag{4.18}$$

is zero when $\epsilon_a = \epsilon_b = 1$. On the other hand, the matrix

$$\begin{array}{c} a \\ \circ \\ \text{---} \\ \mu^+ \\ \text{---} \\ b \end{array} \begin{array}{c} a \\ \text{---} \\ Y \\ \text{---} \\ c \end{array} \begin{array}{c} a \\ \text{---} \\ \mu \\ \text{---} \\ c \end{array} \tag{4.19}$$

is an even matrix commuting with all matrices $B[c]^{ij}$, which implies that it is a multiple of the identity. Since $(Y \otimes_{\mathfrak{g}} Y)^2 = -\mathbb{1} \otimes_{\mathfrak{g}} \mathbb{1}$ we thus find that the matrix in Eq. (4.19) equals $\pm i\mathbb{1}$. Combining all the properties just derived we can conclude that N_{ab}^c is a multiple of two when $\epsilon_a = \epsilon_b = 1$. The index μ labeling the fusion tensors $X_{ab,\mu}^c$ has a natural tensor product structure $\mu = (\hat{\mu}, |\mu|)$, where $\hat{\mu} \in \{1, \dots, N_{ab}^c/2\}$ and $|\mu|$ also denotes the parity of the fusion tensor $X_{ab,(\hat{\mu},|\mu|)}^c$. We will adopt following graphical notation for the fusion tensors and the property derived from matrix (4.19):

$$\begin{aligned}
 & \begin{array}{c} a \\ \text{---} \\ \text{---} \\ b \end{array} \left[\begin{array}{c} \mu \\ \text{---} \\ \text{---} \\ c \end{array} \right] = X_{ab,(\hat{\mu},0)}^c & \begin{array}{c} a \\ \text{---} \circledast Y \\ \text{---} \\ b \end{array} \left[\begin{array}{c} \hat{\mu} \\ \text{---} \\ \text{---} \\ c \end{array} \right] = X_{ab,(\hat{\mu},1)}^c \\
 & \begin{array}{c} a \\ \text{---} \circledast Y \\ \text{---} \\ b \\ \text{---} \circledast Y \end{array} \left[\begin{array}{c} \hat{\mu} \\ \text{---} \\ \text{---} \\ c \end{array} \right] = (-1)^{\eta_{ab,\hat{\mu}}^c} \begin{array}{c} a \\ \text{---} \\ \text{---} \\ b \end{array} \left[\begin{array}{c} \hat{\mu} \\ \text{---} \\ \text{---} \\ c \end{array} \right] , & (4.20)
 \end{aligned}$$

where $\eta_{ab,\hat{\mu}}^c \in \{0, 1\}$ are discrete quantities that are part of the algebraic structure defining the fMPO super algebra.

Let us revisit the matrix in Eq. (4.17) when $\epsilon_a = 1$ and $\epsilon_b = 0$. Now $\epsilon_c = 1$ so the fact that this odd matrix commutes with all $B[c]^{ij}$ implies that it is a multiple of Y . Since $(Y \otimes_{\mathfrak{g}} \mathbb{1})^2 = -\mathbb{1} \otimes_{\mathfrak{g}} \mathbb{1}$ this implies that

$$\begin{array}{c} a \\ \text{---} \\ \text{---} \\ b \end{array} \left[\begin{array}{c} \mu \\ \text{---} \\ \text{---} \\ c \end{array} \right] \circledast Y = (-1)^{\zeta_{ab,\mu}^c} \begin{array}{c} a \\ \text{---} \circledast Y \\ \text{---} \\ b \end{array} \left[\begin{array}{c} \mu \\ \text{---} \\ \text{---} \\ c \end{array} \right] . \quad (4.21)$$

Similar reasoning for the matrix in Eq. (4.18) when $\epsilon_a = 0$ and $\epsilon_b = 1$ shows that

$$\begin{array}{c} a \\ \text{---} \\ \text{---} \\ b \end{array} \left[\begin{array}{c} \mu \\ \text{---} \\ \text{---} \\ c \end{array} \right] \circledast Y = (-1)^{\chi_{ab,\mu}^c} \begin{array}{c} a \\ \text{---} \\ \text{---} \circledast Y \\ b \end{array} \left[\begin{array}{c} \mu \\ \text{---} \\ \text{---} \\ c \end{array} \right] . \quad (4.22)$$

So when $\epsilon_c = 1$ there is no further restriction on N_{ab}^c and the parity of the fusion tensor for each μ is completely arbitrary. We will keep the graphical notation introduced in Eq. (4.13) for the even parity fusion tensor $X_{ab,\mu}^c$ and use the left hand sides of Eq. (4.21) and (4.22) as a graphical notation for the odd fusion tensors $X_{ab,\mu}^c$. In Appendix 4.A we give a more detailed derivation of the fusion tensors and their properties.

4.3.2 F move and pentagon equation

Associativity of the product of three fMPOs $O_a^L O_b^L O_c^L$ clearly implies that $\sum_d N_{ab}^d N_{dc}^e = \sum_f N_{bc}^f N_{af}^e$. Associativity also allows one to derive an important property of the fusion tensors. The fMPO tensor of $O_a^L O_b^L O_c^L$, $\mathcal{C}(\mathbb{B}[a] \otimes_{\mathfrak{g}} \mathbb{B}[b] \otimes_{\mathfrak{g}} \mathbb{B}[c])$, can be written as a sum in two different ways by either

applying equation (4.16) first to $\mathcal{C}(\mathbb{B}[a] \otimes_{\mathfrak{g}} \mathbb{B}[b])$ or first to $\mathcal{C}(\mathbb{B}[b] \otimes_{\mathfrak{g}} \mathbb{B}[c])$. Let us first consider the case where $\epsilon \equiv 0$. Equality of the two sums in this case implies that the fusion tensors satisfy ¹

$$\begin{array}{c} a \\ \text{---} \\ \mu \\ \text{---} \\ b \\ \text{---} \\ \nu \\ \text{---} \\ c \end{array} \begin{array}{c} d \\ \text{---} \\ \nu \\ \text{---} \\ e \end{array} = \sum_{f,\lambda,\kappa} [F_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} \begin{array}{c} a \\ \text{---} \\ \kappa \\ \text{---} \\ b \\ \text{---} \\ f \\ \text{---} \\ c \end{array} \begin{array}{c} \lambda \\ \text{---} \\ e \end{array}, \quad (4.23)$$

where $[F_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu}$ is an invertible even matrix. We will often refer to this identity as an F -move and to the matrices $[F_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu}$ as the F -symbols.

As is familiar from bosonic fusion categories, the F -symbols have to satisfy a consistency equation called the (super) pentagon equation. This consistency condition arises from equating the two different paths one can follow to get from $\mathcal{C}((X_{ab,\mu}^f \otimes_{\mathfrak{g}} \mathbb{1} \otimes_{\mathfrak{g}} \mathbb{1}) \otimes_{\mathfrak{g}} (X_{fc,\nu}^g \otimes_{\mathfrak{g}} \mathbb{1}) \otimes_{\mathfrak{g}} X_{gd,\rho}^e)$ to $\mathcal{C}((\mathbb{1} \otimes_{\mathfrak{g}} \mathbb{1} \otimes_{\mathfrak{g}} X_{cd,\delta}^j) \otimes_{\mathfrak{g}} (\mathbb{1} \otimes_{\mathfrak{g}} X_{bj,\gamma}^i) \otimes_{\mathfrak{g}} X_{ai,\omega}^e)$ using F -moves. These different paths are shown in figure 4.1. Written down explicitly, the super pentagon equation is

$$\sum_{h,\sigma,\lambda,\kappa} [F_g^{abc}]_{h,\sigma\lambda}^{f,\mu\nu} [F_e^{ahd}]_{i,\omega\kappa}^{g,\sigma\rho} [F_i^{bcd}]_{j,\gamma\delta}^{h,\lambda\kappa} = \sum_{\sigma} [F_e^{fcd}]_{j,\sigma\delta}^{g,\nu\rho} [F_e^{abj}]_{i,\omega\gamma}^{f,\mu\sigma} (-1)^{|\mu||\delta|}, \quad (4.24)$$

where $|\mu|$ ($|\delta|$) denotes the parity of fusion tensor $X_{ab,\mu}^f$ ($X_{cd,\delta}^j$). We see that for $\epsilon \equiv 0$, the only difference between the fermionic pentagon equation and the standard, bosonic pentagon equation is the minus sign depending on $|\mu|$ and $|\delta|$. This sign arises from the reordering of two fusion tensors so that a subsequent F -move can be applied. This step is also shown in figure 4.1. For $\epsilon \equiv 0$ the super pentagon equation was previously derived in the construction of fermionic string-net models [53, 54].

Let us now also take fMPOs with $\epsilon = 1$ into account. As in equation (4.23), we want to relate $\mathcal{C}(X_{ab,\mu}^d \otimes_{\mathfrak{g}} X_{dc,\nu}^e)$ and $\mathcal{C}(X_{bc,\kappa}^f \otimes_{\mathfrak{g}} X_{af,\lambda}^e)$, which both reduce $\mathcal{C}(\mathbb{B}[a] \otimes_{\mathfrak{g}} \mathbb{B}[b] \otimes_{\mathfrak{g}} \mathbb{B}[c])$ to a direct sum of $\mathbb{B}[e]$. Since $\mathbb{B}[e]$ has a non-trivial center $\{\mathbb{1}_e, Y_e\}$ when $\epsilon_e = 1$ we find

$$\begin{aligned} & \mathcal{C}(X_{ab,\mu}^d \otimes_{\mathfrak{g}} X_{dc,\nu}^e) \\ &= \begin{cases} \sum_{f,\lambda,\kappa} \mathcal{C}(X_{bc,\kappa}^f \otimes_{\mathfrak{g}} X_{af,\lambda}^e \otimes_{\mathfrak{g}} ([F_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} \mathbb{1}_e)), & \epsilon_e = 0 \\ \sum_{f,\lambda,\kappa} \mathcal{C}(X_{bc,\kappa}^f \otimes_{\mathfrak{g}} X_{af,\lambda}^e \otimes_{\mathfrak{g}} ([F_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} \mathbb{1}_e + [G_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} Y_e)), & \epsilon_e = 1 \end{cases} \end{aligned}$$

From parity consideration, it follows for $\epsilon_e = 0$ that $[F_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} = 0$ if $|\mu| + |\nu| + |\kappa| + |\lambda| \pmod 2 \neq 0$. For $\epsilon_e = 1$, we have $[F_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} = 0$ if $|\mu| + |\nu| + |\kappa| + |\lambda| \pmod 2 = |\mu| + |\kappa| \pmod 2 \neq 0$ and $[G_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} = 0$ if $|\mu| + |\nu| + |\kappa| + |\lambda|$

¹The proof is similar to the bosonic case [109].

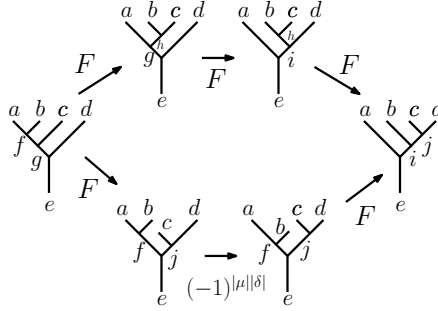


Figure 4.1: Schematic representation of the two paths giving rise to the super pentagon equation. The upper path consists of three F -moves and is similar to the bosonic case. In the lower path there are two F -moves and one fermionic reordering of the fusion tensors, leading to a potential minus sign depending on their parity.

$\text{mod } 2 = |\mu| + |\kappa| \pmod{2} \neq 1$. If the fusion tensors are isometric, such that $X_{ab,\mu}^{c+} = X_{ab,\mu}^{c\dagger}$, we find that

$$\begin{cases} \sum_{f,\lambda\kappa} [\bar{F}_e^{abc}]_{f,\lambda\kappa}^{d',\mu'\nu'} [F_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} = \delta_{d,d'} \delta_{\mu,\mu'} \delta_{\nu,\nu'}, & \epsilon_e = 0, \\ \sum_{f,\lambda\kappa} [\bar{F}_e^{abc}]_{f,\lambda\kappa}^{d',\mu'\nu'} [F_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} + [\bar{G}_e^{abc}]_{f,\lambda\kappa}^{d',\mu'\nu'} [G_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} = \delta_{d,d'} \delta_{\mu,\mu'} \delta_{\nu,\nu'}, & \epsilon_e = 1, \\ \sum_{f,\lambda\kappa} [\bar{F}_e^{abc}]_{f,\lambda\kappa}^{d',\mu'\nu'} [G_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} - [\bar{G}_e^{abc}]_{f,\lambda\kappa}^{d',\mu'\nu'} [F_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} = 0, & \epsilon_e = 1. \end{cases} \quad (4.25)$$

This means that, for $\epsilon_e = 0$, F_e^{abc} is itself a unitary matrix (note that it's square as $\sum_d N_{ab}^d N_{dc}^e = \sum_f N_{bc}^f N_{af}^e$), while for $\epsilon_e = 1$, the matrix $F_e^{abc} \otimes \mathbb{1} + G_e^{abc} \otimes y$ is unitary and symplectic.

Having the F -move interact with the virtual fMPO indices is inconvenient in order to derive the super pentagon equation and to construct an explicit fPEPS tensor satisfying the pulling through equation in the following section. Indeed, the latter requires that we have scalar coefficient $[F_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu}$ rather than a matrix. We can therefore switch to a different convention for the fusion tensors, where we redefine $\frac{1}{\sqrt{2}} X_{ab,\mu}^c \rightarrow \tilde{X}_{ab,(\hat{\mu},0)}^c$ and $\frac{1}{\sqrt{2}} \mathcal{C}(X_{ab,\mu}^c \otimes_{\mathfrak{g}} Y_c) \rightarrow \tilde{X}_{ab,(\hat{\mu},1)}^c$ when $\epsilon_c = 1$, while $\tilde{X}_{ab,(\hat{\mu},|\mu|)}^c = X_{ab,(\hat{\mu},|\mu|)}^c$ when $\epsilon_a = \epsilon_b = 1$ and $\tilde{X}_{ab,\mu}^c = X_{ab,\mu}^c$ when $\epsilon_a = \epsilon_b = 0$. In all cases, $|\mu|$ denotes the parity of the fusion tensor $\tilde{X}_{ab,\mu}^c$. The factors $\frac{1}{\sqrt{2}}$ are introduced such that

$$\sum_{c,\mu} \mathcal{C}(\tilde{X}_{ab,\mu}^c \otimes_{\mathfrak{g}} \tilde{X}_{ab,\mu}^{c+}) = \sum_c \sum_{\hat{\mu}=1}^{N_{ab}^c} \sum_{|\mu|=0,1} \mathcal{C}(\tilde{X}_{ab,(\hat{\mu},|\mu|)}^c \otimes_{\mathfrak{g}} \tilde{X}_{ab,(\hat{\mu},|\mu|)}^{c+}) \quad (4.26)$$

still defines a properly normalized projector onto the support subspace of the tensor B_{ab} , while

$$\mathcal{C}(\tilde{X}_{ab,\mu}^{c+} \otimes_{\mathfrak{g}} \tilde{X}_{ab,\nu}^d) = \delta_{c,d} \begin{cases} \delta_{\mu,\nu} \mathbb{1}_c, & \epsilon_c = 0 \\ \frac{1}{2}(\delta_{\mu,\nu} \mathbb{1}_c - Y_{\mu,\nu} Y_c), & \epsilon_c = 1 \end{cases} \quad (4.27)$$

with $Y_{\mu,\nu} = \delta_{\hat{\mu},\hat{\nu}} y_{|\mu|,|\nu|} = \delta_{\hat{\mu},\hat{\nu}} (|\nu| - |\mu|)$. The latter expression for the case ϵ_c is reminiscent of the pseudo-inverse of a Majorana fMPS.

The fusion tensors $\tilde{X}_{ab,\mu}^c$ have the degeneracy structure $\mu = (\hat{\mu}, |\mu|)$ as soon as either ϵ_a, ϵ_b or ϵ_c is nonzero. Contraction with Y_c switches between $(\hat{\mu}, 0)$ and $(\hat{\mu}, 1)$ if $\epsilon_c = 1$, i.e.

$$\mathcal{C}(\tilde{X}_{ab,\mu}^c \otimes_{\mathfrak{g}} Y_c) = \sum_{\nu} Y_{\nu,\mu} \tilde{X}_{ab,\nu}^c \quad \text{if } \epsilon_c = 1. \quad (4.28)$$

For the case with $\epsilon_a = \epsilon_b = 1$ we have:

$$\mathcal{C}(Y_a \otimes_{\mathfrak{g}} \tilde{X}_{ab,\mu}^c) = \sum_{\nu} (M_{ab}^c)_{\nu,\mu} \tilde{X}_{ab,\nu}^c \quad (4.29)$$

$$\mathcal{C}(Y_b \otimes_{\mathfrak{g}} \tilde{X}_{ab,\mu}^c) = \sum_{\nu} (L_{ab}^c)_{\nu,\mu} \tilde{X}_{ab,\nu}^c, \quad (4.30)$$

where M_{ab}^c and L_{ab}^c are odd (i.e. they are nonzero only for $|\mu| \neq |\nu|$). From the results of the previous section it follows that $(M_{ab}^c)_{\mu\nu} = \delta_{\hat{\mu},\hat{\nu}} y_{|\mu|,|\nu|}$ and $L_{ab}^c = (-1)^{\eta_{ab}+1} i \delta_{\hat{\mu},\hat{\nu}} x_{|\mu|,|\nu|}$, with $x_{|\mu|,|\nu|} = 1 - \delta_{|\mu|,|\nu|}$.

When $\epsilon_c = 0$ we have $\mu = 1, \dots, N_{ab}^c$ whereas if $\epsilon_c = 1$, we have $\hat{\mu} = 1, \dots, N_{ab}^c$ and thus $\mu = 1, \dots, 2N_{ab}^c$. But here, N_{ab}^c only represents the number of times O_c originates from multiplying O_a and O_b if these fMPOs are built from the fermionic tensors B_a, B_b and B_c without normalization factor. Since we take ϵ to act as a \mathbb{Z}_2 grading, we can define all Majorana fMPOs to have an additional global factor $1/\sqrt{2}$, so that in the case $\epsilon_a = \epsilon_b = 1$ we would also have $\mu = 1, \dots, 2N_{ab}^c$, i.e. $\hat{\mu} = 1, \dots, N_{ab}^c$, if we fix N_{ab}^c in the relation $O_a O_b = \sum_c N_{ab}^c O_c$.

The advantage of working with an overcomplete basis of fusion tensors is that we can now write the F -move as an even transformation acting purely on the degeneracy spaces and not on the virtual indices of fMPOs, exactly as in the bosonic case, i.e. we can write

$$\mathcal{C}(\tilde{X}_{ab,\mu}^d \otimes_{\mathfrak{g}} \tilde{X}_{dc,\nu}^e) = \sum_{f,\lambda,\kappa} [\tilde{F}_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} \mathcal{C}(\tilde{X}_{bc,\kappa}^f \otimes_{\mathfrak{g}} \tilde{X}_{af,\lambda}^e). \quad (4.31)$$

Let us explain this in more detail by providing an explicit recipe for going from the F -symbols to the \tilde{F} -symbols.

1. Step 1: We first write

$$\mathcal{C}(X_{ab,\mu}^d \otimes_{\mathfrak{g}} \tilde{X}_{dc,\nu}^e) = \sum_{f,\lambda,\kappa} [(f_1)_{e}^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} \mathcal{C}(X_{bc,\kappa}^f \otimes_{\mathfrak{g}} \tilde{X}_{af,\lambda}^e), \quad (4.32)$$

where $[(f_1)_{e}^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} = [F_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu}$ if $\epsilon_e = 0$, and

$$[(f_1)_{e}^{abc}]_{f,(\hat{\lambda},0)\kappa}^{d,\mu(\hat{\nu},0)} = [F_e^{abc}]_{f,\hat{\lambda}\kappa}^{d,\mu\hat{\nu}} \quad [(f_1)_{e}^{abc}]_{f,(\hat{\lambda},0)\kappa}^{d,\mu(\hat{\nu},1)} = [G_e^{abc}]_{f,\hat{\lambda}\kappa}^{d,\mu\hat{\nu}} \quad (4.33)$$

$$[(f_1)_{e}^{abc}]_{f,(\hat{\lambda},1)\kappa}^{d,\mu(\hat{\nu},0)} = -[G_e^{abc}]_{f,\hat{\lambda}\kappa}^{d,\mu\hat{\nu}} \quad [(f_1)_{e}^{abc}]_{f,(\hat{\lambda},1)\kappa}^{d,\mu(\hat{\nu},1)} = [F_e^{abc}]_{f,\hat{\lambda}\kappa}^{d,\mu\hat{\nu}} \quad (4.34)$$

if $\epsilon_e = 1$. From the properties of F and G , we can check that $(f_1)_e^{abc}$ is still a unitary matrix, and is even, i.e. its elements $[(f_1)_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu}$ vanish if $|\mu| + |\nu| + |\kappa| + |\lambda| \pmod 2 \neq 0$. Furthermore, in the isometric case, $(f_1)_e^{abc}$ is unitary, i.e.

$$\sum_{f,\lambda\kappa} [(\bar{f}_1)_e^{abc}]_{f,\lambda\kappa}^{d',\mu'\nu'} [(f_1)_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} = \delta_{d',d} \delta_{\mu',\mu} \delta_{\nu',\nu}, \quad (4.35)$$

from which also follows

$$\sum_{d,\mu,\nu} [(f_1)_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} [(\bar{f}_1)_e^{abc}]_{f',\lambda'\kappa'}^{d,\mu\nu} = \delta_{f,f'} \delta_{\kappa,\kappa'} \delta_{\lambda,\lambda'}. \quad (4.36)$$

2. Step 2:

$$\mathcal{C}(\tilde{X}_{ab,\mu}^d \otimes_{\mathfrak{g}} \tilde{X}_{dc,\nu}^e) = \sum_{f,\lambda,\kappa} [(f_2)_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} \mathcal{C}(X_{bc,\kappa}^f \otimes_{\mathfrak{g}} \tilde{X}_{af,\lambda}^e) \quad (4.37)$$

with $[(f_2)_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} = [(f_1)_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu}$ if $\epsilon_d = 0$. If $\epsilon_d = 1$, we obtain

$$[(f_2)_e^{abc}]_{f,\lambda\kappa}^{d,(\hat{\mu},0)\nu} = \frac{1}{\sqrt{2}} [(f_1)_e^{abc}]_{f,\lambda\kappa}^{d,\hat{\mu}\nu}, \quad (4.38)$$

$$[(f_2)_e^{abc}]_{f,\lambda\kappa}^{d,(\hat{\mu},1)\nu} = \frac{1}{\sqrt{2}} \sum_{\nu'} (M_{dc}^e)_{\nu',\nu} [(f_1)_e^{abc}]_{f,\lambda\kappa}^{d,\hat{\mu}\nu'}. \quad (4.39)$$

Note that $(f_2)_e^{abc}$ is still even, because M_{dc}^e is odd. Furthermore, in the isometric case, we obtain

$$\begin{aligned} & \sum_{f,\lambda\kappa} [(\bar{f}_2)_e^{abc}]_{f,\lambda\kappa}^{d',\mu'\nu'} [(f_2)_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} \\ &= \delta_{d',d} \begin{cases} \delta_{\mu',\mu} \delta_{\nu',\nu}, & \epsilon_d = 0 \\ [\delta_{\mu',\mu} \delta_{\nu',\nu} + Y_{\mu',\mu} (M_{dc}^e)_{\nu',\nu}] / 2, & \epsilon_d = 1 \end{cases} \end{aligned} \quad (4.40)$$

and

$$\sum_{d,\mu,\nu} [(f_2)_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} [(\bar{f}_2)_e^{abc}]_{f',\lambda'\kappa'}^{d,\mu\nu} = \delta_{f,f'} \delta_{\kappa,\kappa'} \delta_{\lambda,\lambda'}. \quad (4.41)$$

Note that if there is a d with $\epsilon_d = 1$ present, the matrix $(f_2)_e^{abc}$ has more columns than rows and can therefore no longer be unitary. However, the above expression shows that it is still isometric and defines a projector upon premultiplication with its hermitian conjugate.

3. Step 3:

$$\mathcal{C}(\tilde{X}_{ab,\mu}^d \otimes_{\mathfrak{g}} \tilde{X}_{dc,\nu}^e) = \sum_{f,\lambda,\kappa} [\tilde{F}_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} \mathcal{C}(\tilde{X}_{bc,\kappa}^f \otimes_{\mathfrak{g}} \tilde{X}_{af,\lambda}^e) \quad (4.42)$$

with $[\tilde{F}_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} = [(f_2)_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu}$ if $\epsilon_f = 0$. If $\epsilon_f = 1$, we obtain the required relation by the following substitution:

$$\begin{aligned} & \mathcal{C}(\mathbb{X}_{bc,\kappa}^f \otimes_{\mathfrak{g}} \tilde{\mathbb{X}}_{af,\lambda}^e) \\ &= \mathcal{C}\left(\mathbb{X}_{bc,\kappa}^f \otimes_{\mathfrak{g}} \frac{1}{2}(\mathbb{1}_f - \mathbb{Y}_f \otimes_{\mathfrak{g}} \mathbb{Y}_f) \otimes_{\mathfrak{g}} \tilde{\mathbb{X}}_{af,\lambda}^e\right) \\ &= \frac{1}{\sqrt{2}}\mathcal{C}\left(\tilde{\mathbb{X}}_{bc,(\hat{\kappa},0)}^f \otimes_{\mathfrak{g}} \tilde{\mathbb{X}}_{af,\lambda}^e\right) - \frac{1}{\sqrt{2}}\mathcal{C}\left(\tilde{\mathbb{X}}_{bc,(\kappa,1)}^f \otimes_{\mathfrak{g}} (\mathbb{Y}_f \otimes_{\mathfrak{g}} \tilde{\mathbb{X}}_{af,\lambda}^e)\right) \\ &= \frac{1}{\sqrt{2}}\mathcal{C}\left(\tilde{\mathbb{X}}_{bc,(\hat{\kappa},0)}^f \otimes_{\mathfrak{g}} \tilde{\mathbb{X}}_{af,\lambda}^e\right) - \frac{1}{\sqrt{2}}\sum_{\lambda'}(L_{af}^e)_{\lambda,\lambda'}\mathcal{C}\left(\tilde{\mathbb{X}}_{bc,(\kappa,1)}^f \otimes_{\mathfrak{g}} \tilde{\mathbb{X}}_{af,\lambda'}^e\right) \end{aligned}$$

So we get for the final \tilde{F} -symbols

$$[\tilde{F}_e^{abc}]_{f,\lambda(\hat{\kappa},0)}^{d,\mu\nu} = \frac{1}{\sqrt{2}}[(f_2)_e^{abc}]_{f,\lambda\hat{\kappa}}^{d,\mu\nu}, \quad (4.43)$$

$$[\tilde{F}_e^{abc}]_{f,\lambda(\kappa,1)}^{d,\mu\nu} = -\frac{1}{\sqrt{2}}\sum_{\lambda'}(L_{af}^e)_{\lambda,\lambda'}[(f_2)_e^{abc}]_{f,\lambda'\hat{\kappa}}^{d,\mu\nu}. \quad (4.44)$$

The resulting \tilde{F}_e^{abc} is even (because L_{af}^e is odd), not necessarily square and in the isometric case satisfies

$$\sum_{f,\lambda\kappa} [\tilde{F}_e^{abc}]_{f,\lambda\kappa}^{d',\mu'\nu'} [\tilde{F}_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} = \delta_{d',d} \begin{cases} \delta_{\mu',\mu} \delta_{\nu',\nu}, & \epsilon_d = 0, \\ [\delta_{\mu',\mu} \delta_{\nu',\nu} + Y_{\mu',\mu}(M_{dc}^e)_{\nu',\nu}] / 2, & \epsilon_d = 1, \end{cases} \quad (4.45)$$

and

$$\sum_{d,\mu,\nu} [\tilde{F}_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} [\tilde{F}_e^{abc}]_{f',\lambda'\kappa'}^{d,\mu\nu} = \delta_{f,f'} \begin{cases} \delta_{\kappa,\kappa'} \delta_{\lambda,\lambda'}, & \epsilon_f = 0, \\ [\delta_{\kappa,\kappa'} \delta_{\lambda,\lambda'} + Y_{\kappa,\kappa'}(L_{af}^e)_{\lambda,\lambda'}] / 2, & \epsilon_f = 1. \end{cases} \quad (4.46)$$

Fusing the product of four MPOs using these fusion tensors in two different ways gives rise to the super pentagon equation for \tilde{F} .

4.3.3 Frobenius-Schur indicator

As a final point on fMPO super algebras, we want to consider the irreducible fMPOs for which $a^* = a$, i.e. the irreducible fMPOs satisfying $(O_a^L)^\dagger = O_a^L$. It was shown in Ref. [109] that in the bosonic case one can associate an invariant $\varkappa_a \in \{-1, 1\}$ to such MPOs, which coincides with the Frobenius-Schur indicator from fusion categories. In the fermionic case, this invariant has a natural generalization. A crucial observation to obtain the correct generalization is that Hermitian conjugation involves a reordering of the basis vectors for operators that act on the graded tensor product of super

vector spaces. Hermitian conjugation is most naturally defined in the following basis, where contraction coincides with matrix multiplication of the components:

$$\left(\sum_{i_1, i_2, j_1, j_2} M_{i_1, i_2, j_1, j_2} |i_1\rangle |i_2\rangle \langle j_2| \langle j_1| \right)^\dagger = \sum_{i_1, i_2, j_1, j_2} \bar{M}_{i_1, i_2, j_1, j_2} |j_1\rangle |j_2\rangle \langle i_2| \langle i_1|. \quad (4.47)$$

However, the natural basis in which fMPOs are expressed is of the form $|i_1\rangle \langle j_1| \otimes_{\mathfrak{g}} |i_2\rangle \langle j_2|$, on which Hermitian conjugation then acts as

$$(|i_1\rangle \langle j_1| \otimes_{\mathfrak{g}} |i_2\rangle \langle j_2|)^\dagger = (-1)^{(|i_1|+|j_1|)(|i_2|+|j_2|)} |j_1\rangle \langle i_1| \otimes_{\mathfrak{g}} |j_2\rangle \langle i_2|. \quad (4.48)$$

So Hermitian conjugation does not only result in complex conjugation for the components but also produces additional signs. For this reason it might not be clear at first sight that $(O_a^L)^\dagger$ is actually also an fMPO. However, the minus sign produced by Hermitian conjugation is the same as the minus sign one gets from reordering of fermion modes under reflection symmetry, and we know this sign can be absorbed in the fMPO tensors by redefining them as $B^{i,j} \rightarrow P^{|i|+|j|} B^{i,j}$ (or equivalently as $B^{i,j} P^{|i|+|j|}$) [196], where P is the matrix containing the components of P as defined earlier. One can check this by explicitly evaluating the redefined fMPO components:

$$\begin{aligned} & \text{tr}(P^{|i_1|+|j_1|} B^{i_1, j_1} \dots P^{|i_{N-1}|+|j_{N-1}|} B^{i_{N-1}, j_{N-1}} P^{|i_N|+|j_N|} B^{i_N, j_N}) \\ &= (-1)^{(|i_N|+|j_N|)(|i_1|+\dots+|j_{N-1}|)} \\ & \quad \text{tr}(P^{|i_1|+|j_1|+|i_N|+|j_N|} B^{i_1, j_1} \dots P^{|i_{N_1}|+|j_{N-1}|} B^{i_{N-1}, j_{N-1}} B^{i_N, j_N}) \\ &= (-1)^{(|i_N|+|j_N|)(|i_1|+\dots+|j_{N-1}|)+(|i_{N-1}|+|j_{N-1}|)(|i_1|+\dots+|j_{N-2}|)} \\ & \quad \text{tr}(P^{|i_1|+|j_1|+|i_N|+|j_N|+|i_{N_1}|+|j_{N-1}|} B^{i_1, j_1} \dots B^{i_{N-1}, j_{N-1}} B^{i_N, j_N}) \\ &= \dots \\ &= (-1)^{(|i_N|+|j_N|)(|i_1|+\dots+|j_{N-1}|)+(|i_{N-1}|+|j_{N-1}|)(|i_1|+\dots+|j_{N-2}|)+\dots+(|i_2|+|j_2|)(|i_1|+|j_1|)} \\ & \quad \text{tr}(P^{\sum_{\alpha=1}^N (|i_\alpha|+|j_\alpha|)} B^{i_1, j_1} \dots B^{i_{N-1}, j_{N-1}} B^{i_N, j_N}). \end{aligned} \quad (4.49)$$

Since we work with anti-periodic boundary conditions all irreducible fMPOs are even so $\sum_{\alpha=1}^N (|i_\alpha| + |j_\alpha|) = 0 \pmod{2}$, which indeed shows that $P^{|i|+|j|} B^{i,j}$ produces the original fMPO with the desired minus sign.

The property $(O_a^L)^\dagger = O_a^\dagger$ now implies that the matrices of tensor components $B^{i,j}$ satisfy [75]

$$P^{|i|+|j|} \bar{B}_a^{j,i} = Z_a^{-1} B_a^{i,j} Z_a, \quad (4.50)$$

where Z_a is an invertible matrix with parity μ_a . Iterating this relation twice we find

$$(-1)^{\mu_a(|i|+|j|)} B_a^{i,j} = \left(\bar{Z}_a^{-1} Z_a^{-1} \right) B_a^{i,j} (Z_a \bar{Z}_a) . \quad (4.51)$$

If $\epsilon_a = 0$ the center of the algebra spanned by $B_a^{i,j}$ consists only of multiples of the identity. Therefore, if $\mu_a = 0$, we can conclude from (4.51) that $Z_a \bar{Z}_a = \alpha \mathbb{1}$ and thus $\bar{Z}_a Z_a = \bar{\alpha} \mathbb{1}$, where without loss of generality we can take α to be a phase by rescaling Z_a . Combining these two equations gives $\alpha^2 = 1$ and thus $Z_a \bar{Z}_a = (-1)^{\rho_a} \mathbb{1}$, where $\rho_a \in \{0, 1\}$. If $\mu_a = 1$, we similarly find that $Z_a \bar{Z}_a = (-1)^{\rho_a} iP$. For $\epsilon_a = 1$ the center of the algebra spanned by $B_a^{i,j}$ contains the odd matrix Y , so that both Z_a and $Y Z_a$ are valid gauge transformations satisfying (4.51). This implies that the parity of Z_a is ambiguous and we can take it to be even. In this case we find similarly to the situation with $\epsilon_a = 0$ that $Z_a \bar{Z}_a = (-1)^{\rho_a} \mathbb{1}$. By defining $Z_a^1 \equiv Y Z_a$ one can obtain another invariant by $Z_a^1 \bar{Z}_a^1 = (-1)^{\tilde{\rho}_a} iP$. One can check that these two invariants are independent. The invariant obtained from the odd gauge transformation $Z_a Y$, however, is not independent. So in total we have found eight different possibilities. For $\epsilon_a = 0$ we have four possibilities labeled by μ_a and ρ_a . When $\epsilon_a = 1$ we also find four possibilities, labeled by $\hat{\rho}_a$ and $\tilde{\rho}_a$. Using similar techniques as for fermionic matrix product states with time reversal symmetry or reflection symmetry one can show that these eight possibilities form a \mathbb{Z}_8 group where the group structure corresponds to taking the graded tensor product of fMPOs [196]. So if we take the invariant ϵ_a as part of the definition of the Frobenius-Schur indicator we see that it is isomorphic to \mathbb{Z}_8 in the fermionic case, while it is only isomorphic to \mathbb{Z}_2 in the bosonic case.

4.4 Fixed-point PEPS construction

In the previous section we extracted the structural data associated to a fMPO super algebra. In this section we will apply a bootstrap method to construct fermionic PEPS and associated fMPOs from this algebraic data. The fMPOs constructed in this way form explicit representations of the fMPO super algebras described in the previous section, and we can construct such a representation for each consistent set of structural data. Imposing two extra conditions on the \tilde{F} -symbols ensures that the PEPS and fMPOs satisfy the pulling through identities, which endow the PEPS with non-trivial topological properties. The topological phases described by the tensor networks constructed in this section coincide with the phases captured by fermionic string-nets [53, 54] when $\epsilon \equiv 0$.

4.4.1 PEPS tensors

For simplicity we will restrict our construction to the honeycomb lattice. To specify fermionic tensors one does not only have to specify the coefficients, but also in what ordering of the basis vectors these coefficients are defined. For the fermionic PEPS tensors on the A-sublattice we will choose the following internal ordering:

$$\begin{array}{c} \gamma \\ \swarrow \quad \nearrow \\ \nu \\ \uparrow \\ \lambda \end{array} \leftrightarrow |\nu\rangle|\lambda\rangle\langle\gamma| \quad (4.52)$$

where ν is the physical index and λ, γ, β are the virtual ones. Note that the arrows in the graphical notation denote which indices correspond to bra's, and which to kets. In the basis just specified, the tensor components are

$$\begin{array}{c} \nu \quad c' \quad d' \\ \swarrow \quad \nearrow \\ \kappa \\ \uparrow \\ \lambda \\ e' \quad f' \quad a \end{array} = \delta_{a,a'} \delta_{b,b'} \delta_{c,c'} \delta_{d,d'} \delta_{e,e'} \delta_{f,f'} [\tilde{F}_e^{abc}]_{f,\lambda\kappa}^{\mu\nu} \frac{(d_a d_c)^{1/6} (d_c d_b)^{1/4}}{d_d^{1/3} d_f^{1/4}} \quad (4.53)$$

This graphical notation requires some explanation. Each index is specified by four labels: three labels are denoted by Latin letters and one label is denoted by a Greek letter, which is also exactly the data that specified a fusion tensor $X_{ab,\mu}^c$ in the previous section. Each external line in the graphical notation carries a label denoted by a Latin letter. The tensor components are zero when lines that are connected in the body of the tensor carry a different label. This is taken into account by the delta tensors in equation (4.53). However, in the remainder of this paper these delta conditions will be implicit in our definition of fixed-point tensor components and should be clear from the graphical notation. The physical index is labeled by the three labels carried by the lines that end in the body of the tensor (in the figure these are labels b, c and f) and a corresponding Greek label (κ in the figure). The possibly non-zero tensor components are given by the \tilde{F} -symbols of the previous section, where each of the four tensor indices maps to a fusion tensor that defines the \tilde{F} -symbol. The parity of the index also equals the parity of the corresponding fusion tensor.

The tensors on the B-sublattice are defined with following internal ordering:

$$\begin{array}{c} \gamma \\ \uparrow \\ \nu \\ \swarrow \quad \searrow \\ \lambda \quad \beta \end{array} \leftrightarrow |\nu\rangle|\beta\rangle\langle\lambda| \quad (4.54)$$

And in this basis, the tensor coefficients are analogously represented as

$$\begin{array}{c} \lambda \\ \uparrow \\ e \quad \kappa \quad a \\ \swarrow \quad \downarrow \quad \searrow \\ c \quad d \quad \mu \\ \nu \end{array} = \left[\tilde{F}_e^{abc} \right]_{f,\lambda\kappa}^{d,\mu\nu} \frac{(d_a d_c)^{1/6} (d_b d_e)^{1/4}}{d_d^{1/3} d_f^{1/4}}, \tag{4.55}$$

where the bar denotes complex conjugation. All PEPS tensor components are given in terms of \tilde{F} symbols. When $\epsilon \equiv 0$ the \tilde{F} -symbols are equivalent to the standard F -symbols and the fermionic PEPS is very closely related to the bosonic string-net PEPS. However, when taking Majorana fMPOs into account, the \tilde{F} symbols are a particular choice of associators, and their explicit construction is given in section 4.3.2.

Let us also comment on the choice of arrows in our definition of the PEPS tensors. Reversing the arrows interchanges bra's with kets and for fermionic PEPS this has a non-trivial effect for the simple reason that $\mathcal{C}(|\alpha\rangle \otimes_{\mathfrak{g}} |\beta\rangle) = \delta_{\alpha,\beta}$ while $\mathcal{C}(|\beta\rangle \otimes_{\mathfrak{g}} |\alpha\rangle) = (-1)^{|\alpha|} \delta_{\alpha,\beta}$. From this we see that reversing the arrow on a link is equivalent to inserting a parity matrix $P = \mathbb{1}_0 \oplus -\mathbb{1}_1$ on the corresponding virtual index in the contracted network, where $\mathbb{1}_0$ ($\mathbb{1}_1$) is the identity on the parity even (odd) subspace. So if we would flip all the arrows surrounding a vertex, the three resulting parity matrices on the neighbouring virtual indices can be intertwined to a parity matrix on the physical index since the PEPS tensors are even. This shows that to every fermionic PEPS we can actually associate an entire family of PEPS, that are related to the original one by on-site parity actions, by flipping the arrows surrounding vertices. For this reason, the choice of arrows is very reminiscent of a lattice spin structure.

4.4.2 Fermionic pulling through

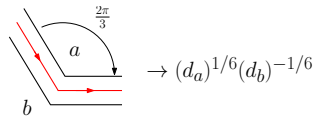
We will define two types of tensors to construct fMPOs on the virtual level of the fermionic PEPS. The first, right-handed type, defined with the internal ordering

$$\begin{array}{c} \gamma \\ \uparrow \\ \beta \quad \delta \\ \circ \\ \alpha \uparrow \end{array} \leftrightarrow |\alpha\rangle |\beta\rangle \langle \gamma| \langle \delta|, \tag{4.56}$$

has components which are again determined by the \tilde{F} -symbols in the following way:

$$\begin{array}{c} \nu \\ \uparrow \\ e \quad d \\ \left[\begin{array}{cc} \square & \square \\ \square & \square \end{array} \right] \mu \\ \lambda \quad \downarrow \\ f \quad \kappa \quad b \end{array} = \left[\tilde{F}_e^{abc} \right]_{f,\lambda\kappa}^{d,\mu\nu} \left(\frac{d_e d_b}{d_f d_a} \right)^{1/4}. \tag{4.57}$$

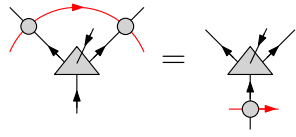
In appendix 4.B we show that the fMPOs constructed from tensors (4.56), (4.57) form an explicit representation of the fMPO algebra whose \tilde{F} -symbols we took to define the tensor components. To place the fMPO on the virtual level of the fermionic PEPS we will introduce an additional convention. The closed fMPO should be interpreted as a polygon, i.e. as a closed collection of straight lines and angles between them. On every angle we place a diagonal matrix that inserts some weights, depending on the labels carried by the outer lines. The rule to add the weights is the following: to each label a we associate a positive number d_a (the choice of d_a is not arbitrary as we will see further on) and the weights are then given by $d_a^{\frac{1}{2}(1-\frac{\alpha}{\pi})}$, where α is the inner (outer) angle in radians for the inner (outer) line. For example, when the fMPO contains an angle of $\frac{2\pi}{3}$ the weights are:



$$\rightarrow (d_a)^{1/6} (d_b)^{-1/6} \quad (4.58)$$

For notational simplicity this convention will always be implicit in our graphical notation from now on.

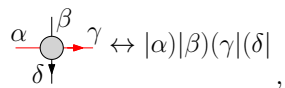
The reason to define the right-handed fMPO tensors as in (4.56,4.57) is that the pentagon equation now implies that the following pulling through identity holds:



$$\quad (4.59)$$

Note that equation (4.59) is only equivalent to the pentagon equation when we use the \tilde{F} -symbols in defining the tensor components. The underlying reason is as follows. Every index of the fixed point tensors corresponds to a fusion tensor, and the four fusion tensors from every index in a tensor together correspond to an F move whose \tilde{F} -symbol determines the tensor component. Since the indices are defined in a super vector space, an even and an odd vector are necessarily orthogonal. However, as explained in section 4.3, when $\epsilon_c = 1$, the even and odd version of the fusion tensor $X_{ab,\mu}^c$ correspond to the same fusion channel. Because of this, equation (4.59) would only be equal to the pentagon equation up to factors of two when the tensors are defined in terms of the F symbols.

Let us now define the second, left-handed, type of fMPO tensor with the internal ordering



$$\quad (4.60)$$

and components

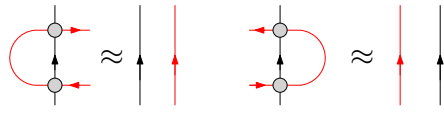
$$\begin{array}{c} \nu \\ \begin{array}{|c|c|} \hline d & e \\ \hline \mu & \lambda \\ \hline b & f \\ \hline \kappa & \end{array} \\ \end{array} \lambda = \left[\tilde{F}_e^{abc} \right]_{f,\lambda\kappa}^{d,\mu\nu} \left(\frac{d_e d_b}{d_f d_d} \right)^{1/4} \quad (4.61)$$

We will now restrict to \tilde{F} -symbols that are unitary or isometric matrices, i.e. \tilde{F} -symbols that satisfy equations (4.45) and (4.46), which we restate here for convenience:

$$\sum_{f,\lambda\kappa} [\tilde{F}_e^{abc}]_{f,\lambda\kappa}^{d',\mu'\nu'} [\tilde{F}_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} = \delta_{d',d} \begin{cases} \delta_{\mu',\mu} \delta_{\nu',\nu}, & \epsilon_d = 0, \\ [\delta_{\mu',\mu} \delta_{\nu',\nu} + Y_{\mu',\mu}(M_{dc}^e)_{\nu',\nu}] / 2, & \epsilon_d = 1, \end{cases} \quad (4.62)$$

$$\sum_{d,\mu,\nu} [\tilde{F}_e^{abc}]_{f,\lambda\kappa}^{d,\mu\nu} [\tilde{F}_e^{abc}]_{f',\lambda'\kappa'}^{d,\mu\nu} = \delta_{f,f'} \begin{cases} \delta_{\kappa,\kappa'} \delta_{\lambda,\lambda'}, & \epsilon_f = 0, \\ [\delta_{\kappa,\kappa'} \delta_{\lambda',\lambda'} + Y_{\kappa,\kappa'}(L_{af}^e)_{\lambda,\lambda'}] / 2, & \epsilon_f = 1. \end{cases} \quad (4.63)$$

In this case, one sees that with our definition of the left-handed fMPO tensors the following properties are satisfied

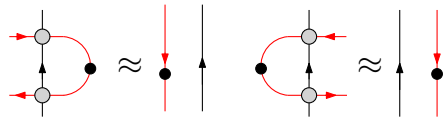


$$\quad (4.64)$$

where we used approximate equality to denote that these are not strict tensor identities, but are only satisfied on the relevant subspaces. In other words, these identities should only hold when the fMPO is embedded within the fermionic PEPS. One can check that this is indeed the case for the fMPOs and fermionic PEPS just defined. As a final step, we require that the \tilde{F} -symbols satisfy

$$\left[\tilde{F}_e^{abc} \right]_{f,\lambda\sigma}^{d,\mu\nu} \frac{\sqrt{d_e d_b}}{\sqrt{d_f d_d}} = \left[\tilde{F}_f^{adc} \right]_{e,\lambda\nu}^{b,\mu\sigma} \frac{\theta_b^{ac,\mu} \theta_e^{ac,\lambda}}{\theta_d^{ac,\mu} \theta_f^{ac,\lambda}} \frac{\theta_\sigma^{ac}}{\theta_\nu^{ac}} t_\mu^{ac} s_\lambda^{ac}, \quad (4.65)$$

where $\theta \in U(1)$ and $t, s \in \{1, -1\}$. It is this condition that fixes the positive numbers d_a . Eq. (4.65) is a generalization of the pivotal property for bosonic fusion categories, which together with the isometric property implies that the fMPOs also satisfy following properties:



$$\quad (4.66)$$

where the black dot is a graphical notation for the parity matrix $P = \sum_{\alpha} (-1)^{|\alpha|} |\alpha\rangle\langle\alpha|$. The reason for requiring unitarity and a generalization of the pivotal property is that from the pulling through identity (4.59) we can now derive the complete set of pulling through identities for the A-sublattice:

(4.67)

In a similar way one can derive the pulling through identities for the B-sublattice:

(4.68)

where the identity in the top left corner follows from the (complex conjugate of the) super pentagon equation, and all other identities can be derived from this one using properties (4.64) and (4.66). Note that the pulling through identities (4.67) and (4.68) imply that closed fMPOs on the virtual level of the PEPS contain parity matrices on their internal indices. They encode the rules of how these parity matrices move or change in their total number by a multiple of two when the fMPO moves through the PEPS tensors. One can check that these rules completely determine the position of the parity matrices on every closed fMPO and imply that their number is always odd

for every fMPO along a contractible cycle. This implies that our formalism survives an important consistency check. In Ref. [196] it was explained that an $\epsilon = 1$ fMPO evaluates to zero when it is closed with an even number of parity matrices P inserted on its internal indices; in particular we cannot close it without inserting any parity matrix. But we just argued that the pulling through identities imply that every fMPO along a contractible cycle contains an odd number of parity matrices, thus preventing the fermionic PEPS with Majorana symmetry fMPOs from contracting to the zero vector. fMPOs along non-contractible cycles require a more detailed analysis. We will come back to this point in section 4.6.1.

In this section we have constructed fermionic PEPS tensors on the honeycomb lattice and fMPO tensors, both right- and left-handed, such that the pulling through identities hold. The pulling through identities are a fingerprint of non-trivial topological order in PEPS, which can –for example– be seen by defining the fermionic PEPS on a torus. In this situation, one can place fMPOs on the virtual level along non-contractible cycles. This will lead to PEPS that are locally indistinguishable from each other, since the fMPOs can move freely on the virtual level. This results in a topological ground state degeneracy.

4.5 Gu-Wen symmetry-protected phases

Up to this point we have studied fMPO super algebras to construct fermionic tensor networks that have non-trivial topological order. But as explained in [59, 60] fMPO group representations $\{O_g^L \mid g \in G\}$ are also relevant for symmetry-protected topological (SPT) phases. In this section we will restrict to the case $\epsilon_g = 0, \forall g \in G$. We again work on the honeycomb lattice, and the SPT PEPS tensors on the A-sublattice are

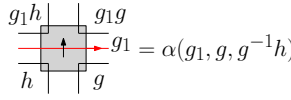
$$\begin{array}{c}
 \begin{array}{c}
 \nearrow h \\
 \triangle \\
 \searrow k \\
 \uparrow g
 \end{array}
 \end{array}
 = \left[F_k^{g, g^{-1}h, h^{-1}k} \right]_{g^{-1}k}^h \equiv \alpha(g, g^{-1}h, h^{-1}k)
 \tag{4.69}$$

Note that this is a modified version of the PEPS tensor (4.53) defined previously; the only difference is that we left out the middle label in the virtual indices since it is redundant in the group case and the virtual labels g, h and k now get copied to the physical index. The internal ordering is the same as defined in (4.52). To completely specify this tensor we also have to specify the grading, i.e. we have to specify the parity of the basis vectors. We do this by defining a function $Z : G \times G \rightarrow \{0, 1\}$. The parities of the virtual indices are then given by $Z(g, g^{-1}k)$, $Z(g, g^{-1}h)$, $Z(h, h^{-1}k)$ and the parity of the physical index is given by $Z(g^{-1}h, h^{-1}k)$. Requiring the PEPS tensor to be even implies that $Z(g, h)$ is a 2-cocycle. The tensors for the B-sublattice are obtained via a similar modification of the tensor defined in (4.54), (4.55).

For fMPO group representations with $\epsilon_g \equiv 0$, the super pentagon relation can be expressed in terms of the $\alpha(g_1, g_2, g_3)$ as

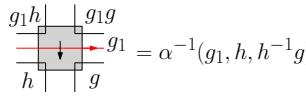
$$\frac{\alpha(g_1, g_2, g_3)\alpha(g_1, g_2g_3, g_4)\alpha(g_2, g_3, g_4)}{\alpha(g_1g_2, g_3, g_4)\alpha(g_1, g_2, g_3g_4)} = (-1)^{Z(g_1, g_2)Z(g_3, g_4)}, \quad (4.70)$$

which is the supercocycle relation as defined previously by Gu and Wen to construct fermionic SPT phases [25]. From the supercocycle relation it follows that a left-regular symmetry action on the physical indices gets intertwined to a virtual fMPO symmetry action on the virtual indices, where the fMPO is constructed from the tensors



$$g_1 = \alpha(g_1, g, g^{-1}h) \quad (4.71)$$

and

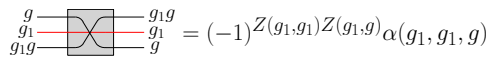


$$g_1 = \alpha^{-1}(g_1, h, h^{-1}g) \quad (4.72)$$

The parities of the indices of the right-handed fMPO tensor are $Z(g, g^{-1}h)$, $Z(g_1, g)$, $Z(g_1g, g^{-1}h)$ and $Z(g_1, h)$. The parities of the left-handed tensor are $Z(g_1h, h^{-1}g)$, $Z(g_1, h)$, $Z(h, h^{-1}g)$ and $Z(g_1, g)$. Evenness of both tensors again follows from the fact that $Z(g, h)$ is a 2-cocycle. The internal ordering of the fMPO tensors is the same as in (4.56) and (4.60)

The intertwining property of the PEPS tensors (4.69) implies that the resulting short-range entangled tensor network has a global symmetry G , which contains fermion parity in its center. For more details on PEPS with a global symmetry that is realized on the virtual level by MPOs we refer to Ref. [60]. It was shown in Ref. [60] that the topologically ordered PEPS discussed in the previous section can be obtained from the SPT PEPS by gauging this global symmetry [51]. We note that fermionic tensor networks using Grassmann variables for the gauged models were constructed in Ref.[95].

The fMPOs constructed from the tensors (4.71) and (4.72) have the property that $O_g^\dagger = O_{g^{-1}}$. So to group elements g_1 satisfying $g_1^2 = e$, where e is the identity group element, we can associate a Frobenius-Schur indicator as defined in the general theory of fMPO super algebras in section 4.3. Again using the supercocycle relation one finds that Z_{g_1} is given by



$$Z_{g_1} = (-1)^{Z(g_1, g_1)Z(g_1, g)}\alpha(g_1, g_1, g), \quad (4.73)$$

where without loss of generality we have taken representative cocycles

satisfying $\alpha(e, g, h) = 1$ and $Z(e, g) = 0$ ². The parity of Z_{g_1} is $Z(g_1, g_1g) + Z(g_1, g) = Z(g_1, g_1) \pmod 2$ (since $Z(e, g) = 0$). If $Z(g_1, g_1) = 0$ one can verify that

$$Z_{g_1} \bar{Z}_{g_1} = \alpha^{-1}(g_1, g_1, g_1) \mathbb{1}, \tag{4.74}$$

while if $Z(g_1, g_1) = 1$ it holds that

$$Z_{g_1} \bar{Z}_{g_1} = \alpha^{-1}(g_1, g_1, g_1) P. \tag{4.75}$$

Since the super cocycle relation implies that $\alpha(g_1, g_1, g_1)^2 = (-1)^{Z(g_1, g_1)}$, these results are indeed compatible with the general theory of the Frobenius-Schur indicator discussed in section 4.3.

4.5.1 Group structure

We define the fusion tensors X_{g_2, g_1} associated to the fMPO group representation constructed from tensors (4.71) and (4.72) with components

$$\tag{4.76}$$

in the basis

$$\tag{4.77}$$

Note that the parity of this fusion tensor is $Z(g_1, h) + Z(g_2, g_1 h) + Z(g_2 g_1, h) = Z(g_2, g_1) \pmod 2$. At this point we would like to note that the parity of the internal fMPO indices has no physical value, we could as well interchange even with odd for the internal fMPO indices for any of the O_g . If we denote with $x(g) \in \{0, 1\}$ whether or not we have interchanged even and odd for the fMPO O_g , then the parity of the fusion tensors changes as $Z(g_2, g_1) \rightarrow Z(g_2, g_1) + x(g_2) + x(g_1) + x(g_2 g_1) \pmod 2$. So we see that the only invariant information associated to the fMPO is the second cohomology class $H^2(G, \mathbb{Z})$ represented by $Z(g_2, g_1)$. One can also check that PEPS constructed from different $Z(g_2, g_1)$ in the same cohomology class are equivalent in the following way: after taking the tensor product with product states such that the local physical super vector spaces are the same, there exists a strictly on-site unitary that maps one PEPS to the other and intertwines both left regular symmetry actions. Similarly to the bosonic

²This form can always be obtained by the coboundary rescaling $\alpha(g, h, k) \rightarrow \alpha'(g, h, k) = \alpha(g, h, k) \frac{\beta(g, h)\beta(g h, k)}{\beta(g, h k)\beta(h, k)}$ with $\beta(e, g) = \alpha^{-1}(e, g, g^{-1})$.

case, multiplying $X_{\mathfrak{g}_2, \mathfrak{g}_1}$ with the phase $\gamma(g_2, g_1)$ changes $\alpha(g_3, g_2, g_1)$ by a coboundary $\gamma(g_3, g_2)\gamma(g_3, g_2, g_1)\bar{\gamma}(g_2, g_1)\bar{\gamma}(g_3, g_2, g_1)$. This implies that only $\alpha(g_3, g_2, g_1)$ modulo coboundaries contains invariant information.

The super cocycle relation (4.70) implies that the fusion tensors defined above indeed satisfy the zipper condition:

$$(4.78)$$

Again applying the super cocycle relation shows that the F -move for these fusion tensors produces the super cocycle that we used to construct the PEPS:

$$(4.79)$$

This F -move is written down as an equation in the following way

$$\mathcal{C}(X_{\mathfrak{g}_3, \mathfrak{g}_2} \otimes_{\mathfrak{g}} X_{\mathfrak{g}_3 \mathfrak{g}_2, \mathfrak{g}_1}) = \alpha(g_3, g_2, g_1) \mathcal{C}(X_{\mathfrak{g}_2, \mathfrak{g}_1} \otimes_{\mathfrak{g}} X_{\mathfrak{g}_3, \mathfrak{g}_2 \mathfrak{g}_1}), \quad (4.80)$$

where \mathcal{C} represents the proper fermionic contraction as depicted in (4.79).

In the previous section we showed that the Frobenius-Schur indicator associated to an $\epsilon \equiv 0$ fMPO group representation is completely fixed by the supercocycle. The invariant algebraic data associated to the fMPO representation is therefore given by $Z(g_2, g_1)$ and $\alpha(g_3, g_2, g_1)$. Since the fMPO describes all possible anomalous symmetry actions on the boundary of the two-dimensional system, this data should directly classify the SPT phase of the short-range entangled bulk. Let us now ask the question of what happens to this data when we stack different SPT phases, i.e. when we take the graded tensor product of PEPS with the same global symmetry. It is clear that the stacked PEPS has a virtual symmetry given by the graded tensor product of the original fMPO representations. The fusion tensor of the graded tensor product of two fMPOs is also just the graded tensor product of the individual fusion tensors, which we denote by $X_{\mathfrak{g}_2, \mathfrak{g}_1}^1$ and $X_{\mathfrak{g}_2, \mathfrak{g}_1}^2$. Using the rules of fermionic contraction with super vector spaces we can now easily obtain the supercocycle for the stacked PEPS by evaluating the F -move for $X_{\mathfrak{g}_2, \mathfrak{g}_1}^1 \otimes_{\mathfrak{g}} X_{\mathfrak{g}_2, \mathfrak{g}_1}^2$:

$$\begin{aligned}
 & \mathcal{C} \left[\left(X_{\mathfrak{g}_3, \mathfrak{g}_2}^1 \otimes_{\mathfrak{g}} X_{\mathfrak{g}_3, \mathfrak{g}_2}^2 \right) \otimes_{\mathfrak{g}} \left(X_{\mathfrak{g}_3, \mathfrak{g}_2, \mathfrak{g}_1}^1 \otimes_{\mathfrak{g}} X_{\mathfrak{g}_3, \mathfrak{g}_2, \mathfrak{g}_1}^2 \right) \right] \\
 = & (-1)^{Z_1(g_3, g_2, g_1) Z_2(g_3, g_2)} \mathcal{C} \left[X_{\mathfrak{g}_3, \mathfrak{g}_2}^1 \otimes_{\mathfrak{g}} X_{\mathfrak{g}_3, \mathfrak{g}_2, \mathfrak{g}_1}^1 \otimes_{\mathfrak{g}} X_{\mathfrak{g}_3, \mathfrak{g}_2}^2 \otimes_{\mathfrak{g}} X_{\mathfrak{g}_3, \mathfrak{g}_2, \mathfrak{g}_1}^2 \right] \\
 = & (-1)^{Z_1(g_3, g_2, g_1) Z_2(g_3, g_2)} \alpha_1(g_3, g_2, g_1) \alpha_2(g_3, g_2, g_1) \\
 & \mathcal{C} \left[X_{\mathfrak{g}_2, \mathfrak{g}_1}^1 \otimes_{\mathfrak{g}} X_{\mathfrak{g}_3, \mathfrak{g}_2, \mathfrak{g}_1}^1 \otimes_{\mathfrak{g}} X_{\mathfrak{g}_2, \mathfrak{g}_1}^2 \otimes_{\mathfrak{g}} X_{\mathfrak{g}_3, \mathfrak{g}_2, \mathfrak{g}_1}^2 \right] \\
 = & (-1)^{Z_1(g_3, g_2, g_1) Z_2(g_3, g_2) + Z_1(g_3, g_2, g_1) Z_2(g_2, g_1)} \alpha_1(g_3, g_2, g_1) \alpha_2(g_3, g_2, g_1) \\
 & \mathcal{C} \left[\left(X_{\mathfrak{g}_2, \mathfrak{g}_1}^1 \otimes_{\mathfrak{g}} X_{\mathfrak{g}_2, \mathfrak{g}_1}^2 \right) \otimes_{\mathfrak{g}} \left(X_{\mathfrak{g}_3, \mathfrak{g}_2, \mathfrak{g}_1}^1 \otimes_{\mathfrak{g}} X_{\mathfrak{g}_3, \mathfrak{g}_2, \mathfrak{g}_1}^2 \right) \right]. \tag{4.81}
 \end{aligned}$$

The parity of $X_{\mathfrak{g}_2, \mathfrak{g}_1}^1 \otimes_{\mathfrak{g}} X_{\mathfrak{g}_2, \mathfrak{g}_1}^2$ is of course just given by $Z_1(g_2, g_1) + Z_2(g_2, g_1)$. We therefore find that the stacked SPT PEPS is described by the following algebraic data:

$$\begin{aligned}
 \tilde{\alpha}(g_3, g_2, g_1) &= (-1)^{Z_1(g_3, g_2, g_1) Z_2(g_3, g_2) + Z_1(g_3, g_2, g_1) Z_2(g_2, g_1)} \alpha_1(g_3, g_2, g_1) \alpha_2(g_3, g_2, g_1) \\
 \tilde{Z}(g_2, g_1) &= Z_1(g_2, g_1) + Z_2(g_2, g_1) \pmod{2}. \tag{4.82}
 \end{aligned}$$

This shows how the algebraic data changes under stacking and allows one to calculate the group structure of Gu-Wen SPT phases.

4.5.2 Projective transformation of symmetry defects

One of the characterizing physical properties of SPT phases is that symmetry defects can carry fractional quantum numbers. In this section we will discuss how the projective nature of defects in Gu-Wen phases is derived from the defining algebraic data $Z(g_2, g_2)$ and $\alpha(g_3, g_2, g_1)$.

π -flux defects

In section 4.4 we explained how the fixed-point PEPS obtained via the bootstrap method incorporate a lattice spin structure. Different spin structures can be obtained by choosing a closed path on the dual lattice and putting a parity matrix P on every virtual index that crosses this cut. It is important to note that internal fMPO indices crossing the path should also gain a parity matrix. In figure 4.2 we show a part of such a path and the associated parity matrices in the PEPS.

If we now choose an open path on the dual lattice and again insert parity matrices on links that cross the path we have created π -flux defects on the plaquettes where the path ends. Symmetry fMPOs on the virtual level of the PEPS that encircle one of these π -flux defects contain an even number of

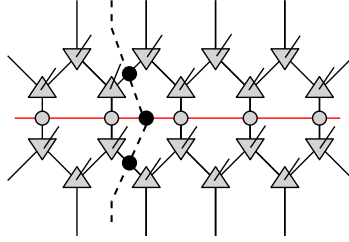


Figure 4.2: Section of a path on the dual lattice and the associated position of parity matrices (represented by the black dots) in the PEPS.

parity matrices on their internal indices. One can verify that group fMPOs O_g as constructed above satisfy

$$\tilde{O}_g \tilde{O}_h = (-1)^{Z(g,h)} \tilde{O}_{gh}, \quad (4.83)$$

where the tilde denotes the fact that the fMPOs contain an even number of parity matrices. This gives an explicit physical interpretation to $Z(g, h)$: it is the projective representation under which π -flux defects transform.

A convenient way to think about symmetry defects is the following: if we put the PEPS on a cylinder and we twist the boundary conditions along the periodic direction by the group element g , then there are symmetry defects at both ends of the cylinder. This boils down to simply placing a fMPO O_g on the virtual level going from one end of the cylinder to the other. Figure 4.3 contains a graphical representation of this situation. There is one subtlety if we apply this reasoning to π -flux defects. Let us consider the PEPS on the cylinder with periodic boundary conditions along the periodic direction. In this case a fMPO wrapping the non-contractible cycle will contain an even number of parity matrices on its internal indices. But as explained above, in this case the fMPOs form a projective representation. We can also define the PEPS with anti-periodic boundary conditions by choosing a path on the dual lattice extending from one end of the cylinder to the other and again inserting the appropriate parity matrices. Now the fMPOs wrapping the cylinder contain an odd number of parity matrices and form a non-projective representation. This shows that the PEPS with periodic boundary conditions should be interpreted as having a π -flux through the cylinder. The cylinder with anti-periodic boundary conditions contains no flux and can in principle be ‘capped off’ to a sphere. This is the tensor network analogue of the fact that the Neveu-Schwarz spin structure on the circle can be extended to the unique spin structure on a disc, while the Ramond spin structure does not have this property.

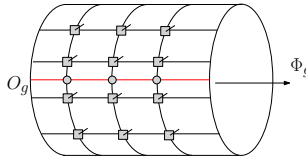


Figure 4.3: A PEPS on the cylinder with a flux Φ_g through the hole, or equivalently, with boundary conditions twisted by g along the periodic direction. The flux (or twisted boundary conditions) is realized by placing the fMPO O_g on the virtual level of the tensor network.

General defects

To study general symmetry defects we have to use a second type of fusion tensor, which in the basis

$$\begin{array}{c} \alpha \xrightarrow{g_2} \\ \gamma \xleftarrow{g_1} \end{array} \left[\begin{array}{c} \text{grey bar} \\ \text{grey bar} \end{array} \right] \begin{array}{c} \xrightarrow{g_2 g_1^{-1}} \\ \xleftarrow{\beta} \end{array} \leftrightarrow |\alpha\rangle\langle\beta| \langle\gamma| \quad , \quad (4.84)$$

has following components:

$$\begin{array}{c} g_2 h \\ h \\ g_1 \end{array} \left[\begin{array}{c} \text{grey bar} \\ \text{grey bar} \end{array} \right] \begin{array}{c} \xrightarrow{g_2 g_1^{-1}} \\ \xleftarrow{\beta} \end{array} = (-1)^{Z(g_1, h)} \alpha(g_2 g_1^{-1}, g_1, h) \quad . \quad (4.85)$$

This second type of fusion tensor can be obtained by reducing a right-handed and a left-handed fMPO tensor to a right-handed one. We now again consider the cylinder with boundary conditions twisted by g as in figure 4.3. We also impose anti-periodic boundary conditions such that there is no π -flux through the cylinder. One can check that the physical symmetry action of elements in \mathcal{Z}_g , the center of g , gets intertwined to an action on the left virtual indices and the right virtual indices. The action on the left virtual indices is given by the following fMPO:

A tedious, but straightforward calculation shows that this fMPO is a projective representation of \mathcal{Z}_g with 2-cocycle

$$\omega_g(h, k) = (-1)^{Z(h,k)(Z(hk,g)+Z(g,hk))} \frac{\alpha(h, g, k)}{\alpha(h, k, g)\alpha(g, h, k)} \quad (4.87)$$

For h, k and l commuting with g the supercocycle relation implies that this phase indeed satisfies the 2-cocycle relation:

$$\omega_g(h, k)\omega_g(hk, l) = \omega_g(h, kl)\omega_g(k, l). \quad (4.88)$$

The virtual symmetry action on the right boundary indices is of course also projective, but with 2-cocycle $\bar{\omega}_g(h, k)$. Equation (4.87) thus describes the fractionalization of symmetry defects in Gu-Wen SPT phases. It is a generalization of the slant product for bosonic SPT phases.

4.5.3 Modular transformations

Let us now consider the Gu-Wen tensor network on a torus. In this case we can twist the boundary conditions in both the x and y direction with group elements h and g , provided that $[g, h] = ghg^{-1}h^{-1} = e$, by putting fMPOs along the non-contractible cycles. These fMPOs labeled by h and g meet in one point, where they have to be connected using fusion tensors. There are many different possibilities to connect the fMPOs in this way, but using the pivotal properties of Gu-Wen fusion tensors discussed in appendix 4.C one can show that all these different choices only differ by a phase factor for the twisted wavefunction. In this section we find it convenient to work in the following basis for the twisted Gu-Wen states:



where opposite sides should be identified. This figure shows the position of the fMPOs O_h and O_g on the virtual level of the Gu-Wen tensor network on the torus and how they are connected using fusion tensors. S_x and S_y denote whether the boundary conditions are periodic or anti-periodic along the two non-contractible cycles of the torus, where $S = 0(1)$ means anti-periodic (periodic). Note that since all PEPS and fMPO tensors are even, the parity of the twisted state (4.89) is determined by the parity of the fusion tensors, which gives $Z(g, h) + Z(h, g) \bmod 2$.

We can now define the S transformation on these states as

$$(4.90)$$

Using the F move (4.79) and the pivotal properties (4.132) introduced in appendix 4.C the twisted state after the S transformation can be expressed back in the standard basis (4.89). If we denote the basis state (4.89) as $|(h, g); (S_x, S_y)\rangle$ then the S transformation takes following matrix form

$$S = \sum_{\substack{g,h \\ [g,h]=e}} \sum_{S_x, S_y} (-1)^{Z(g, g^{-1})S_x + (Z(g, h) + Z(h, g))S_y} \frac{\alpha(g^{-1}, h, g)}{\alpha(h, g^{-1}, g)\alpha(g^{-1}, g, h)} |(g^{-1}, h); (S_y, S_x)\rangle \langle (h, g); (S_x, S_y)|. \quad (4.91)$$

From the supercocycle relation it follows that the S matrix satisfies $S^4 = (-1)^{Z(g, h) + Z(h, g)} \mathbb{1}$, which is to be expected since S^4 represents a 2π rotation and $Z(g, h) + Z(h, g)$ is the fermion parity of the twisted state $|(h, g); (S_x, S_y)\rangle$.

We can now define the T transformation, corresponding to a Dehn twist on the twisted states:

$$(4.92)$$

The state after the T transformation can again be brought back into the standard basis (4.89) using F -moves and the pivotal properties of the fusion tensors. This gives following expression for the T matrix:

$$T = \sum_{\substack{g,h \\ [g,h]=e}} \sum_{S_x, S_y} (-1)^{Z(g, h)(S_y + Z(g, h) + Z(h, g))} \alpha(g, h, g) |(gh, g); (S_x + S_y, S_y)\rangle \langle (h, g); (S_x, S_y)|. \quad (4.93)$$

The S and T matrices obviously depend on the representative cocycles $Z(g, h)$ and $\alpha(g, h, k)$. However, under a coboundary transformation

$$\begin{aligned} Z(g, h) &\rightarrow Z(g, h) + x(g) + x(h) + x(gh) \text{ with } x(g) \in \{0, 1\} \\ \alpha(g, h, k) &\rightarrow \alpha(g, h, k) \frac{\gamma(g, h)\gamma(gh, k)}{\gamma(g, hk)\gamma(h, k)} \end{aligned} \quad (4.94)$$

the S matrix transforms as USU^\dagger , with U a diagonal unitary matrix. The T matrix does not have this property under coboundary transformations of $Z(g, h)$. This seems to imply that T is not an object containing universal information about the Gu-Wen phase. However, T^2 does have the desired property $T^2 \rightarrow UT^2U^\dagger$ under general coboundary transformations, implying that its eigenvalues are relevant invariants. This ambiguity has a physical meaning if we interpret the eigenvalues of T as $e^{i2\pi h}$, where h are the topological spins of the defects. Because the transparent particle in Gu-Wen phases is a fermion, the topological spins are only defined modulo $1/2$. This sign ambiguity in the eigenvalues of T can be avoided by looking at T^2 . As explained above, the coboundary transformation on $Z(g, h)$ can be interpreted as attaching a fermion to the virtual fMPO indices. Since g defects are connected via fMPOs O_g such a coboundary transformation indeed has the net effect of attaching fermions to the defects, changing the topological spin by $1/2$. The ambiguity in T also manifests itself in the relation $(ST)^3 = (-1)^{Z(g,h)}S^2$, which follows from the supercocycle relation. This shows that S and T only form a representation of $SL(2, \mathbb{Z})$ up to a minus sign which changes under coboundary transformations.

Finally, we want to point out that the S and T matrices for the gauged, topologically ordered PEPS can be obtained from those of the SPT phase [60, 200]. It was shown in Ref. [60] that the S and T matrices for the gauged theory are obtained by applying S and \mathcal{T} on the states

$$\frac{1}{|G|} \sum_{x \in G} U(x)^{\otimes L_x L_y} |(h, g); (S_x, S_y)\rangle, \quad (4.95)$$

where $U(x)$ is the on-site physical symmetry action and $L_x L_y$ is the size of the torus. If $k \in \mathcal{Z}_{h,g}$, the centralizer of both h and g , then the twisted states satisfy $U(k)^{\otimes L_x L_y} |(h, g); (S_x, S_y)\rangle = \epsilon_{h,g}^{S_x, S_y}(k) |(h, g); (S_x, S_y)\rangle$. Using the results of section 4.5.2 it follows that the one-dimensional representation $\epsilon_{h,g}^{S_x, S_y}(k)$ of $\mathcal{Z}_{h,g}$ is given by

$$\begin{aligned} & \epsilon_{h,g}^{S_x, S_y}(k) \\ &= (-1)^{(Z(h,k)+Z(k,h))S_y+(Z(g,k)+Z(k,g))S_x+(Z(g,h)+Z(h,g))(Z(g,k)+Z(k,g))} \frac{\omega_g(h, k)}{\omega_g(k, h)}. \end{aligned} \quad (4.96)$$

Since the states (4.95) are obtained by a projection on the symmetric subspace, only those states for which $\epsilon_{h,g}^{S_x, S_y}(k) = 1$ for all $k \in \mathcal{Z}_{h,g}$ are non-zero. Both S and \mathcal{T} commute with the global symmetry action $U(x)^{\otimes L_x L_y}$. For S , this is immediate, but for \mathcal{T} this follows from the results in [109]. From the commutativity of S, \mathcal{T} and $U(x)^{\otimes L_x L_y}$ one can easily infer the S and T matrices of the gauged theory from those of the Gu-Wen SPT. However, note that the S and T matrices obtained in this way are not expressed in the

basis that has a definite anyon flux through one of the holes of the torus. To compare the S and T matrices before and after gauging, note that the action of S and T on the states $\sum_{x \in G} \Gamma_{ij}^\mu(x) U(x)^{\otimes L_x L_y} |(h, g); (S_x, S_y)\rangle$, with $\Gamma^\mu(g)$ an irrep of G , is independent of μ, i and j . This shows that the S and T matrices of the SPT phase consist of multiple copies of the same block (up to diagonal unitary similarity transformations), and the gauging process selects only one of these identical blocks.

4.6 \mathbb{Z}_2 Majorana phases

In this section we consider the example of a fMPO representation of \mathbb{Z}_2 , where the non-trivial group element corresponds to an irreducible fMPO of the type $\epsilon = 1$. Concretely, we start from two fMPOs O_1^L and O_σ^L , satisfying

$$O_1^L O_1^L = O_1^L \quad O_1^L O_\sigma^L = O_\sigma^L O_1^L = O_\sigma^L \quad O_\sigma^L O_\sigma^L = O_1^L, \quad (4.97)$$

for every L . The matrix algebras spanned by the tensors of O_1^L and O_σ^L are of the type $\epsilon_1 = 0$ and $\epsilon_\sigma = 1$. Note that $N_{\sigma\sigma}^1 = 1$, which implies that we have defined O_σ^L with a global factor $1/\sqrt{2}$ as explained in section 4.3.

Without loss of generality we can take the parity of X_{11}^1 to be zero. With this convention we can solve the pentagon equation to get following the independent F -symbols:

$$\begin{aligned} [F_1^{111}]_{1,00}^{1,00} &= 1 \\ [F_\sigma^{11\sigma}]_{1,00}^{\sigma,00} &= [F_\sigma^{1\sigma 1}]_{\sigma,00}^{\sigma,00} = [F_\sigma^{\sigma 11}]_{\sigma,00}^{1,00} = 1 \\ [F_1^{1\sigma\sigma}]_{\sigma,00}^{1,00} &= [F_1^{\sigma 1\sigma}]_{\sigma,00}^{\sigma,00} = [F_1^{\sigma\sigma 1}]_{1,00}^{\sigma,00} = 1 \\ [F_\sigma^{\sigma\sigma\sigma}]_{1,00}^{1,00} &= (-1)^\rho \frac{1}{\sqrt{2}} \quad [F_\sigma^{\sigma\sigma\sigma}]_{1,11}^{1,00} = (-1)^{\eta+\rho} i \frac{1}{\sqrt{2}} \\ [F_\sigma^{\sigma\sigma\sigma}]_{1,00}^{1,11} &= (-1)^{\rho+1} \frac{1}{\sqrt{2}} \quad [F_\sigma^{\sigma\sigma\sigma}]_{1,11}^{1,11} = (-1)^{\eta+\rho} i \frac{1}{\sqrt{2}}, \end{aligned} \quad (4.98)$$

where $\rho \in \{0, 1\}$. Since μ and $\hat{\mu}$ as defined in the general formalism of fMPO super algebras are now one-dimensional (because $N_{ab}^c \in \{0, 1\}$) the row and column indices of the F -symbols consist only of the labels 1 and σ and the parities of the fusion tensors. The super pentagon equation also implies that $\zeta = \chi = 0$. So we have found four different solutions of the super pentagon equation for a \mathbb{Z}_2 fMPO representation with $\epsilon_\sigma = 1$, labeled by η and ρ . The set of F -symbols given above is not complete, one can obtain other ones by changing the parity of fusion tensors X_{ab}^c with $c = \sigma$ or $a = b = \sigma$ via suitable contractions with Y . However, these additional F -symbols are completely determined by the F -symbols given above and the relations (4.20), (4.21) and (4.22). We note that these F -symbols were first presented in [201].

Applying the general recipe of section 4.3.2 we find that the F -symbols need to be rescaled in the following way to obtain the \tilde{F} -symbols:

$$\begin{aligned} \tilde{F}_1^{111} &= F_1^{111} & \tilde{F}_\sigma^{11\sigma} &= \frac{1}{\sqrt{2}} F_\sigma^{11\sigma} & \tilde{F}_\sigma^{1\sigma 1} &= \frac{1}{2} F_\sigma^{1\sigma 1} & \tilde{F}_1^{1\sigma\sigma} &= \frac{1}{\sqrt{2}} F_1^{1\sigma\sigma} \\ \tilde{F}_\sigma^{\sigma 11} &= \frac{1}{\sqrt{2}} F_\sigma^{\sigma 11} & \tilde{F}_1^{\sigma\sigma 1} &= \frac{1}{\sqrt{2}} F_1^{\sigma\sigma 1} & \tilde{F}_1^{\sigma 1\sigma} &= \frac{1}{2} F_1^{\sigma 1\sigma} & \tilde{F}_\sigma^{\sigma\sigma\sigma} &= F_\sigma^{\sigma\sigma\sigma}. \end{aligned} \quad (4.99)$$

One can explicitly verify that these \tilde{F} -symbols satisfy the isometric properties (4.45) and (4.46). From the pivotal property (4.65) one finds that $d_1 = 1$ and $d_\sigma = 1/\sqrt{2}$. In figure 4.4 we explicitly give the non-zero tensor components of the fMPO O_σ , and in figure 4.5 we give the components of O_1 . We note that the tensor components of O_σ are of the form $B[\sigma]^{ij} = y^{|i|+|j|} \otimes C^{ij}$ in the basis $\sum_{ij\alpha\beta} B[\sigma]_{\alpha\beta}^{ij} |\alpha\rangle|i\rangle\langle j|\langle\beta|$. In Ref.[196] it was shown that this indeed corresponds to the normal form of $\epsilon = 1$ fMPOs.

Making use of the general expressions (4.52),(4.53) and (4.54),(4.55) one can construct the fixed-point PEPS corresponding to the $\{O_1, O_\sigma\}$ fMPO algebra³. The fixed-point PEPS construction might not be very insightful. However, some physical intuition can be gained by analyzing the PEPS tensors. Keeping in mind the fMPS expression for the Majorana chain [196] one can convince oneself that the PEPS wavefunction represents a superposition of all coverings of the honeycomb lattice with closed Majorana chains. In recent work an explicit commuting projector Hamiltonian stabilizing this type of ground state wave function was constructed [93]. It was pointed out that this system has the same topological properties as a $(p + ip) \times (p - ip)$ bilayer system where fermion parity in one of the layers is gauged. The corresponding phase of matter was first envisioned by starting from the Ising string-net and condensing the ψ anyon [201], which appears to be a general mechanism to obtain fermionic topological phases [90, 91, 203].

4.6.1 Spin structures and ground states on the torus

As explained in section 4.4, it is essential that every fMPO closed along a contractible loop has an odd number of parity matrices P inserted on its internal indices. In section 4.5 we explained that the number of parity matrices modulo two on fMPOs along non-contractible cycles is determined by the boundary conditions, or equivalently, by the spin structure. Here we will show that this leads to a non-trivial interplay between spin structure, ground state degeneracy and ground state parity for the topologically ordered fermionic PEPS constructed from the fMPO superalgebra $\{O_1^L, O_\sigma^L\}$ with $\epsilon_\sigma = 1$ via equations (4.53) and (4.55).

We start by showing that the fermionic PEPS on the torus with periodic boundary conditions in both directions (PP) evaluates to zero if no fMPO O_σ is inserted on the virtual level. To see this, first construct a tensor

³From private discussions we learned that this tensor network is found independently by different authors and will appear in Ref. [202]

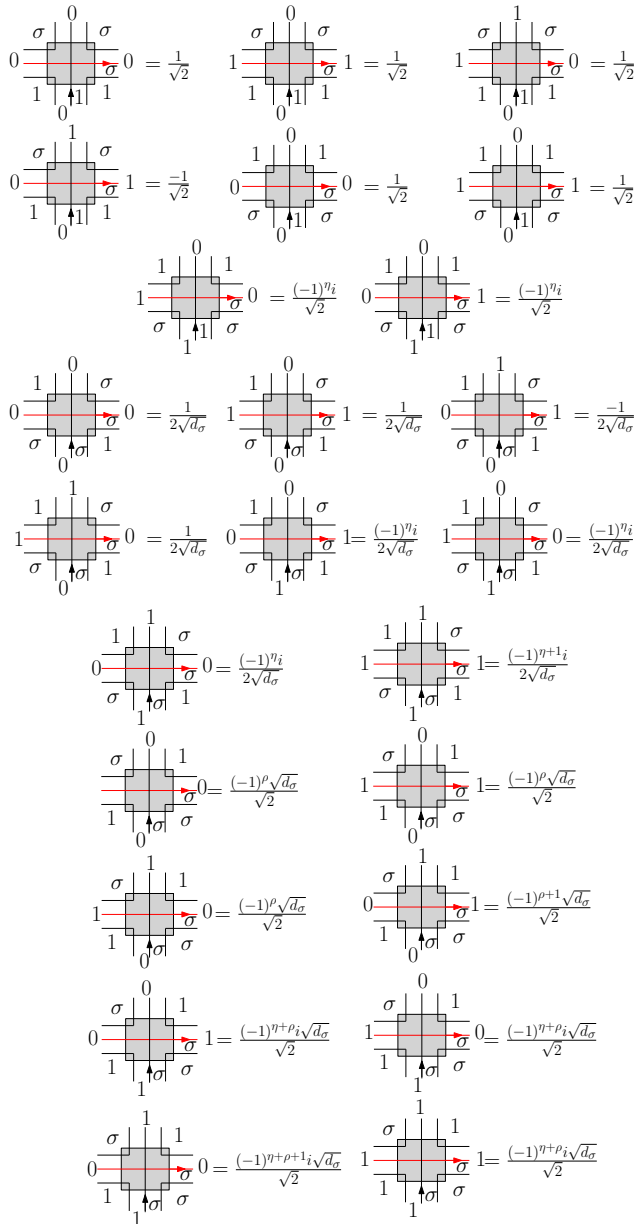


Figure 4.4: Non-zero tensor components of the fMPO O_σ in the basis (4.56) and with $d_\sigma = \frac{1}{\sqrt{2}}$. The outer most labels 0 and 1 denote the parity of the indices.

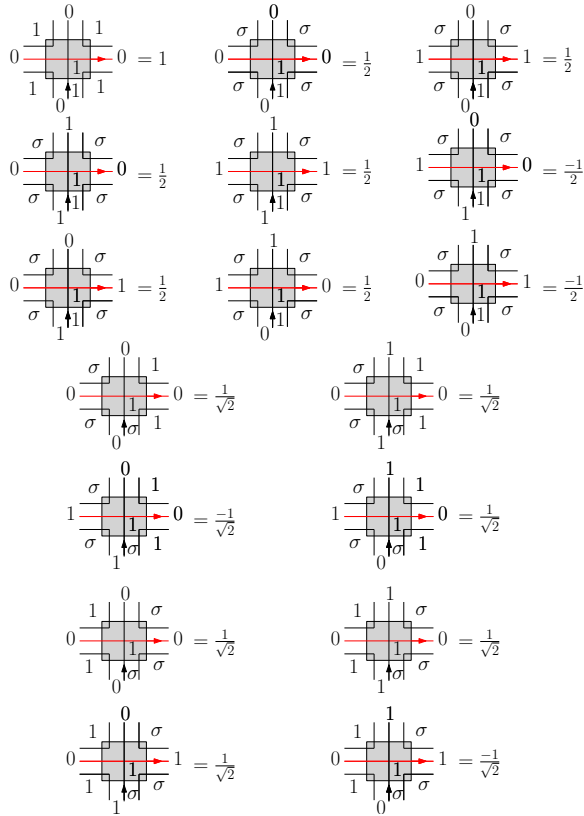
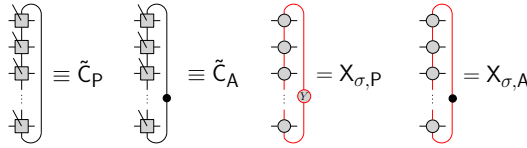


Figure 4.5: Non-zero tensor components of the fMPO O_1 in the basis (4.56). The outer most labels 0 and 1 denote the parity of the indices.


 Figure 4.6: Definition of the tensors \tilde{C}_P , \tilde{C}_A , $X_{\sigma,P}$ and $X_{\sigma,A}$.

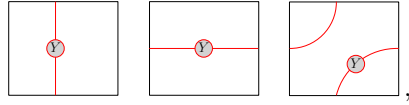
\tilde{C}_P by contracting all PEPS tensors that lie in the same column, where P denotes that we use periodic boundary conditions in the direction along the column. The ordering convention for the indices of \tilde{C}_P is as follows: first the virtual indices corresponding to the left hand side of the column, then the physical indices and lastly the virtual indices on the right hand side. The virtual indices are ordered such that contracting neighboring columns corresponds to matrix multiplication of the components of \tilde{C}_P . The procedure just described is of course just the fermionic version of standard reinterpretation of a PEPS on the cylinder as a matrix product state with tensors \tilde{C}_P . We will denote the fMPO $O_\sigma^{L_y}$ going along the periodic direction, with the external indices reordered in the same way as the virtual indices of \tilde{C} , as $X_{\sigma,P}$. It is crucial to note that $X_{\sigma,P}$ has odd parity while $X_{\sigma,A}$ is even. This is because $\epsilon_\sigma = 1$ and it was shown in Ref.[196] that such fMPOs have to be closed with Y on the internal indices under periodic boundary conditions in order to be non-zero. With anti-periodic boundary conditions $O_\sigma^{L_y}$ has to be closed without Y and is therefore even. Figure 4.6 gives a graphical representation of the tensors just defined.

Now we can easily show that the fermionic PEPS in the PP sector without any fMPO is zero. Its coefficients on a torus consisting of L_x columns are given by $\text{tr}(P^{\otimes L_y} \tilde{C}^{i_1} \tilde{C}^{i_2} \dots \tilde{C}^{i_{L_x}})$, where i_j represents the collection of all physical indices in the j th column and $P^{\otimes L_y}$, the tensor product of L_y parity matrices, is generated as a supertrace by the fermionic contraction (see Ref.[196] for more detail). In appendix 4.D we show that $X_{\sigma,P} X_{\sigma,P} = (-1)^{\eta_i} X_{1,P}$, which can now be used to show that

$$\begin{aligned}
 \text{tr}(P^{\otimes L_y} \tilde{C}^{i_1} \tilde{C}^{i_2} \dots \tilde{C}^{i_{L_x}}) &= (-1)^{\eta+1} \text{tr}(P^{\otimes L_y} \tilde{C}^{i_1} \tilde{C}^{i_2} \dots \tilde{C}^{i_{L_x}} X_{\sigma,P} X_{\sigma,P}) \\
 &= (-1)^{\eta_i} \text{tr}(P^{\otimes L_y} X_{\sigma,P} \tilde{C}^{i_1} \tilde{C}^{i_2} \dots \tilde{C}^{i_{L_x}} X_{\sigma,P}) \\
 &= (-1)^{\eta_i} \text{tr}(P^{\otimes L_y} \tilde{C}^{i_1} \tilde{C}^{i_2} \dots \tilde{C}^{i_{L_x}} X_{\sigma,P} X_{\sigma,P}) \\
 &= -\text{tr}(P^{\otimes L_y} \tilde{C}^{i_1} \tilde{C}^{i_2} \dots \tilde{C}^{i_{L_x}}), \tag{4.100}
 \end{aligned}$$

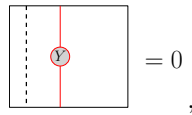
where the second equality follows from the fact that $X_{\sigma,P}$ is odd and the third equality follows from the pulling through property.

The non-zero states in the PP sector can be schematically represented as

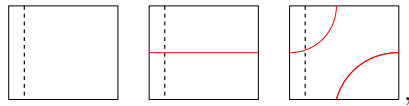

(4.101)

where the torus is depicted as a rectangle with opposite sides identified. The red line represents a fMPO X_σ on the virtual level of the PEPS wrapping a non-contractible cycle. The state on the left has coefficients $\text{tr}(X_{\sigma,P} \tilde{C}^{i_1} \tilde{C}^{i_2} \dots \tilde{C}^{i_{L_x}})$, where the fermionic contraction now does not generate a matrix $P^{\otimes L_y}$ because $X_{\sigma,P} \tilde{C}^{i_1} \tilde{C}^{i_2} \dots \tilde{C}^{i_{L_x}}$ has odd parity. For this reason we cannot conclude that this state is zero. Similar reasoning shows that the other two states in the PP sector may also be non-zero. Note that the three ground states in the PP sector all have odd fermion parity because of the matrix Y on the internal fMPO indices.

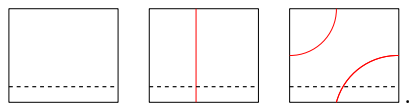
In the AP sector, with anti-periodic boundary conditions in the x -direction, one can show that the following state is zero:


(4.102)

where the dashed line represents the anti-periodic boundary conditions, i.e. along that line on the dual lattice we have inserted parity matrices P on the virtual indices. Note that the periodic boundary conditions in the y -direction imply that the fMPO O_σ^L is odd. The coefficients for this state are $\text{tr}(P^{\otimes L_y} X_{\sigma,P} \tilde{C}^{i_1} \tilde{C}^{i_2} \dots \tilde{C}^{i_{L_x}})$, where $P^{\otimes L_y}$ is now not generated by the fermionic contraction because $X_{\sigma,P}$ is odd but is inserted by hand because of the anti-periodic boundary conditions. This trace expression for the coefficients can easily be seen to be zero. The three non-zero states in the AP sector are


(4.103)

where both σ -fMPOs are even because they cross the dashed line an odd number of times. Note that the coefficients of the state in the AP sector without any fMPO are $\text{tr}(P^{\otimes L_y} \tilde{C}^{i_1} \tilde{C}^{i_2} P^{\otimes L_y} \dots \tilde{C}^{i_{L_x}})$, where one $P^{\otimes L_y}$ is generated by the supertrace of an even tensor and the second $P^{\otimes L_y}$ comes from the anti-periodic boundary conditions. Analogously, one can show that the three non-zero states in the PA sector are:


(4.104)

In the AA sector one can show that the following state is zero:

$$\begin{array}{|c|} \hline \text{Y} \\ \hline \end{array} = - \begin{array}{|c|} \hline \text{Y} \\ \hline \end{array} = 0, \tag{4.105}$$

where the fMPO is odd because it crosses a dashed line an even number of times. The state above is zero because the two graphical expressions given for it differ by a minus sign, as can easily be seen by using the pulling through property and the fact that Y is odd. The non-zero states in the AA sector are then given by

$$\begin{array}{|c|} \hline \\ \hline \end{array}, \begin{array}{|c|} \hline \text{---} \\ \hline \end{array}, \begin{array}{|c|} \hline \text{---} \\ \hline \end{array}. \tag{4.106}$$

So to conclude, we have found that the fermionic PEPS constructed from the fMPO algebra $\{O_1^L, O_\sigma^L\}$ with $\epsilon_\sigma = 1$ has three non-zero ground states in each spin structure sector. In the PP sector these states have odd parity, while in the AP, PA and AA sectors they have even parity. This agrees with the results of Ref. [93], where an explicit commuting projector Hamiltonian was constructed for the topological phases captured by the fermionic PEPS described in this section.

4.6.2 Symmetry-protected phases

Above we used the fMPO group representations $\{O_1^L, O_\sigma^L\}$ with $\epsilon_\sigma = 1$ to construct fermionic PEPS with non-trivial topological order. Here we will discuss applications of these fMPOs for \mathbb{Z}_2 symmetry-protected phases. In analogy to section 4.5, where we treated the case $\epsilon \equiv 0$, we construct the short-range entangled PEPS on the hexagonal lattice using the tensors

$$\begin{array}{c} \mu \quad b \quad d \quad c \quad \nu \\ \diagdown \quad \diagup \\ \kappa \\ \diagup \quad \diagdown \\ a \quad e \\ \uparrow \quad \downarrow \\ \lambda \quad f \end{array} = \left[\tilde{F}_e^{abc} \right]_{f,\lambda\kappa}^{d,\mu\nu} \frac{(d_a d_e)^{1/6}}{d^{1/3}} \frac{(d_c d_b)^{1/4}}{d^{1/4}} \tag{4.107}$$

for the A-sublattice and a similar modification of (4.55) for the B-sublattice. The resulting PEPS has a global \mathbb{Z}_2 symmetry, where the physical on-site symmetry action gets intertwined to a fMPO O_σ on the virtual indices, where O_σ is the same fMPO as before constructed from the tensor shown in figure 4.4.

The PEPS obtained via the tensors (4.107) describes a wave function where Majorana chains are bound to domain walls of the plaquette variables. An explicit commuting projector Hamiltonian with this type of ground state was constructed in [92]. A physical property of this SPT phase is that \mathbb{Z}_2

symmetry defects bind Majorana modes. In the tensor network language this can easily be seen by defining the PEPS on a cylinder with twisted boundary conditions along the non-contractible cycle. This is done by simply placing the fMPO O_σ along the cylinder on the virtual level, going from one end of the cylinder to the other. At the two boundaries of the cylinder this results in a symmetry defect. Because O_σ is of the type $\epsilon_\sigma = 1$, the resulting fMPS on the cylinder has a non-trivial center corresponding to Y acting on the internal fMPO index. One can use similar reasoning as in Ref. [196] to conclude that there will be Majorana modes at the ends of the cylinder.

Other immediate consequences of the results in Ref.[196] involve the entanglement spectrum and the physical systems that can realize this phase. First, the PEPS on a cylinder with periodic boundary conditions has at least a two-fold degeneracy in its entanglement spectrum for cuts wrapping the non-contractible cycle. This follows from the fact that the \mathbb{Z}_2 symmetry action \tilde{O}_σ on the boundary is odd and therefore anti-commutes with fermion parity. If we twist the boundary conditions with O_σ , then there will again be at least a two-fold degeneracy, both in the periodic and the anti-periodic sector. This degeneracy follows from the fact that $\epsilon_\sigma = 1$. By interpreting the PEPS on the cylinder with boundary conditions twisted by O_σ as a MPS and applying the results of Ref.[196] it follows that the \mathbb{Z}_2 Majorana SPT phases cannot occur in systems with (unbroken) particle number conservation.

In appendix 4.D we show that under periodic boundary conditions, the fMPOs \tilde{O}_σ satisfy $\tilde{O}_\sigma \tilde{O}_\sigma = (-1)^\eta \tilde{O}_1$. This gives a physical interpretation to the invariant η : it determines the projective representation of the global \mathbb{Z}_2 symmetry on π -flux defects. Note that since \tilde{O}_σ is odd, this projective representation is consistent with the fact that two π -flux defects fuse to the vacuum. The combined action on two π -flux defects is given by $\tilde{O}_\sigma \otimes_{\mathbb{g}} \tilde{O}_\sigma$, which satisfies

$$\begin{aligned} (\tilde{O}_\sigma \otimes_{\mathbb{g}} \tilde{O}_\sigma) (\tilde{O}_\sigma \otimes_{\mathbb{g}} \tilde{O}_\sigma) &= -\tilde{O}_\sigma \tilde{O}_\sigma \otimes_{\mathbb{g}} \tilde{O}_\sigma \tilde{O}_\sigma \\ &= -(-1)^\eta i (-1)^\eta i \tilde{O}_1 \otimes_{\mathbb{g}} \tilde{O}_1 = \tilde{O}_1 \otimes_{\mathbb{g}} \tilde{O}_1. \end{aligned} \tag{4.108}$$

This shows that the symmetry action on two π -flux defects is indeed non-projective.

For the fMPO O_σ we readily determine the Frobenius-Schur indicator as defined in the general theory of fMPO super algebras. We find that Z_σ as defined as in section 4.3 takes the following form:

$$\begin{aligned} \begin{array}{c} \sigma \\ \sigma \\ 0 \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \begin{array}{c} 1 \\ \sigma \\ \sigma \\ 0 \end{array} &= (-1)^\rho & \begin{array}{c} \sigma \\ \sigma \\ 1 \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \begin{array}{c} 1 \\ \sigma \\ \sigma \\ 1 \end{array} &= (-1)^{\eta+\rho} i \\ \begin{array}{c} 0 \\ \sigma \\ \sigma \\ 1 \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \begin{array}{c} \sigma \\ \sigma \\ 0 \\ 1 \end{array} &= 1 & \begin{array}{c} 0 \\ \sigma \\ 1 \\ \sigma \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \begin{array}{c} \sigma \\ \sigma \\ 1 \\ 1 \end{array} &= (-1)^\eta i \end{aligned} \tag{4.109}$$

Note that Z_σ is even. The first invariant associated to the Frobenius-Schur

indicator can now easily be obtained from

$$Z_\sigma \bar{Z}_\sigma = (-1)^\rho \mathbf{1}, \quad (4.110)$$

The second invariant determining the Frobenius-Schur indicator we get from

$$(Y Z_\sigma) (\bar{Y} \bar{Z}_\sigma) = (-1)^{\rho+\eta+1} iP. \quad (4.111)$$

From this we see that the value of the Frobenius-Schur indicator uniquely determines the F -symbols for the $\{O_1, O_\sigma\}$ group representation with $\epsilon_\sigma = 1$. The same holds for the case $\epsilon_\sigma = 0$, where the Frobenius-Schur indicator completely fixes one of the four supercohomology classes for \mathbb{Z}_2 . So in total we have eight different fermionic SPT phases with a global \mathbb{Z}_2 symmetry. In section 4.3 we also mentioned that the Frobenius-Schur indicator is isomorphic to \mathbb{Z}_8 , implying that the \mathbb{Z}_2 SPT phases form a \mathbb{Z}_8 group under stacking, agreeing with previous studies [204–207]. Since the Frobenius-Schur indicator has the same mathematical origin as the invariants associated to time-reversal or reflection invariant fMPS, we have thus connected the classification of two-dimensional unitary \mathbb{Z}_2 SPT phases to the classification of one-dimensional SPT phases with time-reversal or reflection symmetry. This is the tensor network manifestation of the Smith isomorphism, which relates the cobordism groups conjectured to describe both types of SPT phases [27].

4.7 Discussion and outlook

In this work we have studied the properties of fMPO super algebras. The resulting algebraic structure was used to construct explicit fermionic topological PEPS models, both for phases with intrinsic and symmetry-protected topological order. The fermionic string-nets and supercohomology phases were reproduced as a special ($\epsilon = 0$) subset of the general formalism.

The fixed-point fermionic PEPS models allow for a straightforward calculation of many interesting universal properties associated with the topological phases. We illustrated this for Gu-Wen SPT phases, where we determined the projective symmetry properties of defects and the modular matrices associated with symmetry-twisted states on the torus. Also for the \mathbb{Z}_2 Majorana phases, the PEPS construction enables us to relate the algebraic data classifying the different phases to physical properties of the system.

Starting from the tensor networks constructed here, there are many different directions to explore in future work. Perturbing the fixed-point models yields interesting PEPS to be studied numerically, which could give rise to new insights in e.g. entanglement properties and topological phase transitions. The SPT phases considered in this work only have discrete on-site unitary symmetries. However, we expect that fMPOs should also capture the phases associated with continuous, anti-unitary and/or spatial

symmetries. The global \mathbb{Z}_2 symmetry of fermionic PEPS corresponding to fermion parity can be gauged by applying the gauging map as introduced in [51]. This gives an explicit realization of the connection between fermionic topological phases and bosonic topological phases with an emergent fermion [90, 91, 201, 203]. For the fermionic PEPS with intrinsic topological order one would like to determine the anyons and their braiding properties as was done for spin systems [109, 162]. We refer to [202] for details on this construction. Once the anyons and their topological properties are understood, an interesting question is how they intertwine with a possible global symmetry in the system, which leads to the study of fermionic symmetry-enriched topological phases.

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4.A Fusion of fMPOs

In this appendix we provide further details about the fusion of fMPO tensors $B[a]$ and $B[b]$ into a tensor $B[c]$, and study the properties of the fusion tensors and the interplay with the fMPO types $\epsilon_a, \epsilon_b, \epsilon_c$ in full generality.

We use the same notation and conventions as in Section 4.3. Furthermore, we denote the virtual space of the fMPO tensor B_a as the super vector space $V_a \cong \mathbb{C}^{D_a^0|D_a^1}$ with $D_a = D_a^0 + D_a^1$ the total bond dimension, and D_a^0 (D_a^1) the dimension of the even (odd) part. Upon multiplying O_a and O_b , we obtain a new fMPO with tensor

$$B_{ab} = \sum_{\alpha, \alpha', i, k, \beta, \beta'} (B_{ab}^{ik})_{(\alpha, \alpha'), (\beta, \beta')} |\alpha\rangle |\alpha'\rangle |i\rangle \langle k| (\beta') |(\beta) \quad (4.112)$$

with

$$(B_{ab}^{ik})_{(\alpha, \alpha'), (\beta, \beta')} = \sum_j (-1)^{|\alpha'|(|i|+|j|)} (B_a^{ij})_{\alpha, \beta} (B_b^{jk})_{\alpha', \beta'}$$

$$= (-1)^{|\alpha'|(|\alpha|+|\beta|)} \sum_j (B_a^{ij})_{\alpha,\beta} (B_b^{jk})_{\alpha',\beta'}.$$

We can also write the right hand side of $O_a O_b = \sum_c N_{ab}^c O_c$ by taking a direct sum of N_{ab}^c copies of every tensor B_c , i.e. the tensor components would be equivalent to the matrices $\bigoplus_c \mathbb{1}_{N_{ab}^c} \otimes B_c^{ik}$.

As the trace expression for fMPOs with antiperiodic boundary conditions is (with the choice of ordering in B_{ab}) equivalent to that of a bosonic MPO/MPS (namely a product of matrices), we can use the fundamental theorem of MPS to show the existence of a gauge transform X_{ab} that brings the matrices B_{ab}^{ik} in a canonical form (block upper triangular) where the diagonal blocks can be equated with those of $\bigoplus_c \mathbb{1}_{N_{ab}^c} \otimes B_c^{ik}$. We furthermore assume that off diagonal blocks vanish, so that we obtain a strict equality

$$B_{ab}^{ik} X_{ab} = X_{ab} \bigoplus_c \mathbb{1}_{N_{ab}^c} \otimes B_c^{ik}. \quad (4.113)$$

This equation is referred to as the zipper condition in the main text. The gauge transformation X_{ab} is not unique, but any other gauge transformation \tilde{X}_{ab} that establishes the same relation is related to X_{ab} by an element in the center, i.e.

$$\tilde{X}_{ab} = X_{ab} \bigoplus_c \begin{cases} M_c \otimes \mathbb{1}_c, & \epsilon_c = 0 \\ M_c \otimes \mathbb{1}_c + M'_c \otimes Y_c, & \epsilon_c = 1 \end{cases}$$

with M_c and M'_c matrices acting on the N_{ab}^c -dimensional degeneracy space. Using $(-1)^{|i|+|j|} B_a^{ij} = P_a B_a^{ij} P_a$ with $P_a = P_a^{-1} = \mathbb{1}_{D_a^0} \oplus (-\mathbb{1}_{D_a^1})$ the parity matrices, we can construct a different $\tilde{X}_{ab} = (P_a \otimes P_b) X_{ab} (\bigoplus_c \mathbb{1}_{N_{ab}^c} \otimes P_c)$, from which we infer

$$(P_a \otimes P_b) X_{ab} = X_{ab} \bigoplus_c \begin{cases} M_c \otimes P_c, & \epsilon_c = 0 \\ M_c \otimes P_c + M'_c \otimes Y_c P_c, & \epsilon_c = 1 \end{cases}$$

Applying this relation twice leads to $M_c^2 = \mathbb{1}_c$ if $\epsilon_c = 0$, and to $M_c^2 + M_c'^2 = \mathbb{1}_c$ and $[M_c, M_c'] = 0$ if $\epsilon_c = 1$. In the first case $\epsilon_c = 0$, M_c is seen to have eigenvalues ± 1 and thus to act as a parity matrix in the degeneracy space V_{ab}^c . By an appropriate basis transform in this degeneracy space, it takes the standard form $(M_c)_{\mu,\nu} = (-1)^{|\mu|} \delta_{\mu,\nu}$ thus providing a definition of $|\mu|$. This clearly shows that V_{ab}^c is itself a \mathbb{Z}_2 graded vector space. For $\epsilon_c = 1$, a basis transform in the degeneracy space can be used to simultaneously diagonalize M_c and M'_c into $(M_c)_{\mu,\nu} = \cos(\theta_\mu) \delta_{\mu,\nu}$ and $(M'_c)_{\mu,\nu} = \sin(\theta_\mu) \delta_{\mu,\nu}$. However, a further transformation with $\bigoplus_\mu \cos(\theta_\mu/2) \mathbb{1}_c + \sin(\theta_\mu/2) Y_c$ results in $M_c = \mathbb{1}$, $M'_c = 0$.

Using this choice of basis, we now select the columns of X_{ab} and the rows of X_{ab}^{-1} corresponding to a single block c , which we denote as $X_{ab,\mu}^c$

and $X_{ab,\mu}^{c+}$ respectively. From these, we can build fermionic (splitting and) fusion tensors

$$X_{ab,\mu}^c = \sum_{\alpha,\beta,\gamma} (X_{ab,\mu}^c)_{(\alpha,\beta),\gamma} |\alpha\rangle |\beta\rangle \langle \gamma| \quad (4.114)$$

$$X_{ab,\mu}^{c+} = \sum_{\alpha,\beta,\gamma} (X_{ab,\mu}^{c+})_{\gamma,(\alpha,\beta)} |\gamma\rangle \langle \beta| \langle \alpha| \quad (4.115)$$

that satisfy the properties discussed in Section 4.3. Furthermore, when $\epsilon_c = 0$, the parity of the tensor $X_{ab,\mu}^c$ is given by $|\mu|$. When $\epsilon_c = 1$, we have ensured that the parity of $X_{ab,\mu}^c$ is even, but there exists an equivalent odd choice $\mathcal{C}(X_{ab,\mu}^c \otimes_{\mathfrak{g}} Y_c)$. Ultimately, this is a consequence of the fact that, at the level of the matrices, the Majarona type fMPOs have a further decomposition into a block diagonal form with two blocks, but which is protected by the \mathbb{Z}_2 grading (i.e. the fermion parity). For simplicity of notation below, we also denote the parity of the fusion tensor $X_{ab,\mu}^c$ as $|\mu|$ for the case $\epsilon_c = 1$, and of course have $|\mu| = 0$ since we restrict to even fusion tensors in that case.

Before moving on to the fusion of three fMPOs and the F -move, let us also discuss the influence of ϵ_a and ϵ_b . Note that there is a priori no relation between ϵ_a , ϵ_b and ϵ_c that we can deduce from the local fusion property of the fMPO tensors. As a global object, fMPOs with periodic boundary conditions have a total fermion parity that is equal to the fMPO type ϵ , and the latter therefore seems to follow the \mathbb{Z}_2 group structure of the former. This is however a global consequence of the properties we discuss below, and does not manifest itself when working with anti-periodic boundary conditions as arise on contractible loops in our topological fermionic PEPS.

If $\epsilon_a = 1$, we can define $\mathcal{C}(Y_a \otimes_{\mathfrak{g}} X_{ab,\mu}^c)$ as an equivalent tensor, but with opposite parity of $X_{ab,\mu}^c$. Considering the case $\epsilon_c = 0$, this implies the relation

$$\mathcal{C}(Y_a \otimes_{\mathfrak{g}} X_{ab,\mu}^c) = \sum_{\nu} (M_a)_{\nu,\mu} X_{ab,\mu}^c \quad (4.116)$$

where M_a is nonzero only if $|\mu| \neq |\nu|$. Applying this relation twice leads to $M_a^2 = -\mathbb{1}$, e.g. M_a acts as a Y matrix in the degeneracy space. This requires the degeneracy space V_{ab}^c to be even-dimensional with equal dimensions of even and odd parity. We can choose a suitable basis such that M_a takes a standard form and replace the labeling μ to $(\hat{\mu}, 0)$ and $(\hat{\mu}, 1)$ defined by

$$\mathcal{C}(Y_a \otimes_{\mathfrak{g}} X_{ab,(\hat{\mu},0)}^c) = X_{ab,(\hat{\mu},1)}^c, \quad \mathcal{C}(Y_a \otimes_{\mathfrak{g}} X_{ab,(\hat{\mu},1)}^c) = -X_{ab,(\hat{\mu},0)}^c. \quad (4.117)$$

An equivalent result holds when $\epsilon_b = 1$ (still assuming $\epsilon_c = 0$). However, if both $\epsilon_a = \epsilon_b = 1$, more care is required. As both Y_a and Y_b are odd tensors, their order of contraction matters (at the level of the matrices, contracting with Y_a and Y_b amounts to left multiplication of $X_{ab,\mu}^c$ with $Y_a \otimes \mathbb{1}_b$ and $P_a \otimes Y_b$ respectively). Hence, while the general relation with a generic M_a and M_b remains valid, we furthermore obtain $\{M_a, M_b\} = 0$ and only one of

the two matrices M_a and M_b can be brought into standard form. Choosing Eq. (4.117) to be still valid, we obtain for the contraction with Y_b the relation

$$\mathcal{C}(Y_b \otimes_{\mathfrak{g}} X_{ab,(\hat{\mu},0)}^c) = \sum_{\hat{\nu}} (\hat{M}_b)_{\hat{\nu},\hat{\mu}} X_{ab,(\hat{\nu},1)}^c = \sum_{\hat{\nu}} (\hat{M}_b)_{\hat{\nu},\hat{\mu}} \mathcal{C}(Y_a \otimes_{\mathfrak{g}} X_{ab,(\hat{\nu},0)}^c). \quad (4.118)$$

with $\hat{M}_b^2 = -1$ resulting from applying this relation twice. \hat{M}_b thus has eigenvalues $+i$ or $-i$ and can be diagonalized by a further basis transformation in the $\hat{\mu}$ space. Working in this basis, we have thus obtained

$$\mathcal{C}(Y_b \otimes_{\mathfrak{g}} X_{ab,\mu}^c) = (-1)^{\eta_{ab,\hat{\mu}}^c} i \mathcal{C}(Y_a \otimes_{\mathfrak{g}} X_{ab,\mu}^c). \quad (4.119)$$

If $\epsilon_a = \epsilon_c = 1$, the contraction of Y_a and $X_{ab,\mu}^c$ yields an odd tensor, so that we have the relation

$$\mathcal{C}(Y_a \otimes_{\mathfrak{g}} X_{ab,\mu}^c) = \sum_{\nu} (L_a)_{\nu,\mu} \mathcal{C}(X_{ab,\mu}^c \otimes_{\mathfrak{g}} Y_c) \quad (4.120)$$

and applying this relation twice learns that $L_a^2 = 1$. A proper choice of basis diagonalizes L_a and results in

$$\mathcal{C}(Y_a \otimes_{\mathfrak{g}} X_{ab,\mu}^c) = (-1)^{\xi_{ab,\mu}^c} \mathcal{C}(X_{ab,\mu}^c \otimes_{\mathfrak{g}} Y_c). \quad (4.121)$$

Similarly, if $\epsilon_b = \epsilon_c = 1$ we can choose a basis where

$$\mathcal{C}(Y_b \otimes_{\mathfrak{g}} X_{ab,\mu}^c) = (-1)^{\xi_{ab,\mu}^c} \mathcal{C}(X_{ab,\mu}^c \otimes_{\mathfrak{g}} Y_c). \quad (4.122)$$

However, if $\epsilon_a = \epsilon_b = \epsilon_c = 1$, we again obtain $\{L_a, L_b\} = 0$ and both matrices cannot be diagonalized simultaneously. This relation requires the degeneracy space to be even dimensional and L_a and L_b to have equally many $+1$ and -1 eigenvalues; e.g. the simplest representation could be $L_a = Z$ and $L_b = X$.

4.B Fixed-point fMPO representation

In this appendix we show that the fixed-point fMPOs constructed from the tensors (4.56), (4.57) form an explicit representation of the fMPO algebra whose \bar{F} -symbols were used to define the tensor components.

We define the fusion tensor $\check{X}_{ab,\mu}^c$ with internal ordering

$$\begin{array}{c} a \\ \beta \rightarrow \\ b \\ \alpha \rightarrow \end{array} \left[\begin{array}{c} \mu \\ c \end{array} \right] \gamma \leftrightarrow |\alpha\rangle|\beta\rangle\langle\gamma| \quad (4.123)$$

and components

$$= [\tilde{F}_e^{abi}]_{g,\lambda\kappa}^{c,\mu\nu} \quad (4.124)$$

One can now check that following tensor identity is equivalent to the super pentagon equation (4.24):

$$= \quad (4.125)$$

Combining this relation with the isometric property of the \tilde{F} -symbols implies that identities (4.14) and (4.15) hold, from which it follows that the fMPOs O_a constructed from tensors (4.56), (4.57) indeed satisfy the correct multiplication properties $O_a O_b = \sum_c N_{ab}^c O_c$. Note that also the stronger property (4.16) follows from (4.125) and unitarity. Taking the explicit expressions for the fusion tensors $\tilde{X}_{ab,\mu}^c$ it is straightforward to check that the F -move indeed produces the same \tilde{F} symbols as those defining all tensor components.

In this appendix we only considered right-handed fMPO tensors. However, similar to the bosonic case [109], all fMPOs consisting of an arbitrary number of right-handed and left-handed tensors form a representation of the fMPO algebra $O_a O_b = \sum_c N_{ab}^c O_c$ with the correct \tilde{F} -symbols.

4.C Pivotal properties of Gu-Wen fusion tensors

To study the pivotal properties of Gu-Wen fusion tensors we first introduce two new tensors. The first tensor has in the basis

$$\leftrightarrow |\mu\rangle|\nu\rangle \quad (4.126)$$

coefficients which take following form:

$$= \alpha(g_1^{-1}, g_1, h) (-1)^{Z(g_1^{-1}, g_1 h)} \quad (4.127)$$

The parity of its indices is given by $Z(g_1, h)$ and $Z(g_1^{-1}, g_1 h)$, implying that the total parity of this tensor is $Z(g_1^{-1}, g_1)$ (using that $Z(e, g) = 0$). The

second tensor is defined in the basis

$$\begin{array}{c} g_1^{-1} \\ \mu \rightarrow \triangleleft \end{array} \begin{array}{c} \rightarrow g_1 \\ \nu \end{array} \leftrightarrow |\mu\rangle\langle\nu| \quad (4.128)$$

and has coefficients given by

$$\begin{array}{c} g_1 h \\ \overline{g_1^{-1}} \leftarrow \triangleleft \end{array} \begin{array}{c} \rightarrow g_1 \\ h \end{array} = \alpha^{-1}(g_1^{-1}, g_1, h) \quad (4.129)$$

The parities of the indices are again $Z(g_1, h)$ and $Z(g_1^{-1}, g_1, h)$, such that the total parity is $Z(g_1^{-1}, g_1)$, similar to the previous tensor. One can verify that these tensors satisfy following relations

$$\begin{aligned} \begin{array}{c} g^{-1} \\ \mu \rightarrow \triangleleft \end{array} \begin{array}{c} \rightarrow g \\ \nu \end{array} &= \delta_{\mu,\nu} |\mu\rangle\langle\nu| & \begin{array}{c} g \\ \mu \rightarrow \triangleleft \end{array} \begin{array}{c} \rightarrow g^{-1} \\ \nu \end{array} &= \delta_{\mu,\nu} (-1)^{|\mu|} |\mu\rangle\langle\nu| \\ \begin{array}{c} g \\ \mu \rightarrow \triangleleft \end{array} \begin{array}{c} \rightarrow g^{-1} \\ \nu \end{array} &= \alpha(g, g^{-1}, g) \delta_{\mu,\nu} |\mu\rangle\langle\nu| \end{aligned} \quad (4.130)$$

where we, again without loss of generality, work with representative cocycles satisfying $\alpha(e, g, h) = 1$. Note that these tensors are very similar to the matrices Z_g as defined at the beginning of section 4.5. For details about the precise connection in the bosonic case we refer to [60, 109]. The reason for introducing these new tensors is that now we have following important tensor identity, relating right- and left-handed fMPO tensors:

$$\begin{array}{c} \uparrow g \\ \circ \end{array} \begin{array}{c} \rightarrow \\ \downarrow \end{array} = \begin{array}{c} \rightarrow g \\ \triangleleft \end{array} \begin{array}{c} \uparrow g^{-1} \\ \circ \end{array} \begin{array}{c} \rightarrow \\ \downarrow \end{array} \quad (4.131)$$

From (4.131) one can show that the fusion tensors should satisfy following relations:

$$\begin{aligned} \begin{array}{c} g_1^{-1} \\ \rightarrow \end{array} \begin{array}{c} \rightarrow g_1 \\ \bullet \end{array} &= \alpha(g_1, g_1^{-1}, g_0) \begin{array}{c} g_1^{-1} \\ \rightarrow \end{array} \begin{array}{c} \rightarrow g_0 \\ \bullet \end{array} \\ \begin{array}{c} g_1 g_0 \\ \rightarrow \end{array} \begin{array}{c} \rightarrow g_0 \\ \bullet \end{array} & \\ \begin{array}{c} g_1 g_0 \\ \rightarrow \end{array} \begin{array}{c} \rightarrow g_1 \\ \bullet \end{array} &= \alpha^{-1}(g_1, g_0, g_0^{-1}) \begin{array}{c} g_1 g_0 \\ \rightarrow \end{array} \begin{array}{c} \rightarrow g_1 \\ \bullet \end{array} \\ \begin{array}{c} g_1 g_0 \\ \rightarrow \end{array} \begin{array}{c} \rightarrow g_0^{-1} \\ \bullet \end{array} & \end{aligned} \quad (4.132)$$

Of course this can also be verified directly by taking the explicit expression (4.76),(4.77) for $X_{g,h}$. These expressions are of great value since they allow for a graphical calculation of many interesting properties.

4.D $\{\tilde{O}_1^L, \tilde{O}_\sigma^L\} \mathbb{Z}_2$ representation with periodic boundary conditions

In this appendix we derive the projective group action of \tilde{O}_σ , which is an fMPO constructed from the same tensor as O_σ , but with an even number of parity matrices on the internal indices. For concreteness, let us take \tilde{O}_σ to be

$$\tilde{O}_\sigma = \frac{1}{\sqrt{2}} \left(\text{Y} \text{---} \text{---} \text{---} \text{---} \text{---} \right) . \tag{4.133}$$

Of course, the length L of \tilde{O}_σ , which we took to be five here, and the specific even number of parity matrices and their positions on the internal fMPO indices is just an arbitrary choice and the result of this appendix does not depend on these choices. For example, as already explained in the main text, regardless of the length and specific even number of parity matrices, we always have to insert the odd matrix Y on the internal index for \tilde{O}_σ to be non-zero.

The product of two \tilde{O}_σ fMPOs can be represented as

$$\tilde{O}_\sigma \tilde{O}_\sigma = \frac{1}{2} \left(\text{Y} \text{---} \text{---} \text{---} \text{---} \text{---} \text{Y} \right) , \tag{4.134}$$

where the order of the Y matrices is determined by the order of multiplication of the fMPOs. Using properties (4.16) and (4.15) we obtain

$$\begin{aligned} \tilde{O}_\sigma \tilde{O}_\sigma &= \frac{1}{2} \left(\text{Y} \text{---} \text{---} \text{---} \text{---} \text{---} \text{Y} \right) \sigma \\ &+ \frac{1}{2} \left(\text{Y} \text{---} \text{---} \text{---} \text{---} \text{---} \text{Y} \right) \sigma , \end{aligned} \tag{4.135}$$

where we explicitly denote the parity of the fusion tensors. A few simple steps now lead to the desired result:

$$\begin{aligned} \tilde{O}_\sigma \tilde{O}_\sigma &= \frac{(-1)^{\eta_i}}{2} \left(\text{---} \text{---} \text{---} \text{---} \text{---} \right) \sigma \\ &+ \frac{(-1)^{\eta+1_i}}{2} \left(\text{---} \text{---} \text{---} \text{---} \text{---} \right) \sigma \\ &= \frac{(-1)^{\eta_i}}{2} \left(\text{---} \text{---} \text{---} \text{---} \text{---} \right) \\ &+ \frac{(-1)^{\eta_i}}{2} \left(\text{---} \text{---} \text{---} \text{---} \text{---} \right) \\ &= (-1)^{\eta_i} \left(\text{---} \text{---} \text{---} \text{---} \right) 1 . \end{aligned} \tag{4.136}$$

In the first line we used (4.20), in the second line we get the additional minus sign because the fusion tensor is odd and in the last line we again used (4.15).

Conclusions and outlook

In this dissertation we have studied how universal physical properties associated to topological phases of matter are encoded in the local structure of tensor network states. We have focussed on one- and two-dimensional systems consisting of either spins or fermions. For these systems a systematic mathematical language was developed that connects tensor networks and their local entanglement structure to physical properties of topological quantum many-body systems.

Although some steps towards a better understanding of topological tensor network states are made in this work, still a lot of progress is required. For fermionic PEPS, there are some loose ends that need to be tightened. For example, a general construction of fermionic tensor networks with Majorana symmetry fMPOs has to be developed in more detail, and also the construction of topological superselection sectors presented in chapter 3 for bosonic PEPS needs to be generalised. Apart from these two obvious open ends, there are many other questions one can ask about these topological phases that are not addressed in chapter 4, like for instance the stacking of general fermionic SPT PEPS. There is also another class of topological phases which was not considered in this dissertation: the so-called symmetry-enriched topological phases. We have discussed PEPS with a global symmetry and PEPS which exhibit topological excitations, but not tensor networks which have both properties simultaneously. It is known that there can be a non-trivial interplay between topological order and global symmetries. The tensor network manifestation of this phenomenon still needs to be worked out.

It should be possible to answer the questions above in the short-term future, using the insights presented in this dissertation. There are also open problems that I think will require more work and should therefore be seen as problems for the long-term future. On the theoretical side, one would of

course like to have a similar detailed understanding of topological tensor networks in three dimensions, which are far more relevant for real physical materials. In particular, interesting problems are the tensor network representation of loop-like anyons and beyond-cohomology SPT phases. In numerical applications one would like to study topological properties of a PEPS that is not in an obvious way related to some perturbation of an exactly known fixed-point PEPS. A major obstacle for the study of these tensor networks is that the virtual symmetries are not a priori known. For this reason, it would be very useful to find a general expression for MPOs forming an algebra. In other words, we would like to understand better the representation theory of these MPO algebras. Different representations will allow for the construction of new PEPS models, which might contain more parameters that can be optimised variationally in the study of a particular Hamiltonian. One would of course in the end like to combine the representation theory of MPO algebras with algorithms for fermionic tensor networks and in this way obtain competitive numerical data for systems where the sign problem prevents quantum Monte Carlo simulations.

The work presented in chapters 1 to 4 can serve as a starting point for these future directions. The theoretical framework developed in this dissertation connects entanglement, fusion categories, and topological phases beautifully but its true value should come from future applications. One of the main applications is for developing new algorithms to study topological phases. A better understanding of the theory underlying tensor networks can prove to be valuable for numerical simulations of quantum many-body systems. This was illustrated in Refs. [152, 208, 209], where the theory of matrix product operator algebras was used to simulate anyon condensation driven phase transitions. Other possible numerical applications are calculating entanglement spectra and developing general and user-friendly algorithms for fermionic tensor network states.

The field of tensor networks, and definitely its applications to topological phases, is relatively new so even the general philosophy behind the field has to be developed. This is in sharp contrast to well-established methods like effective field theory, where many tricks and applications are in the standard toolbox of condensed matter physicists. We hope that this dissertation can play a role in the development of tensor networks and can help to determine the strengths and weaknessess of the formalism, such that it can take its place amongst the more established methods.

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